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Mireille Bousquet-Mélou, Michèle Soria

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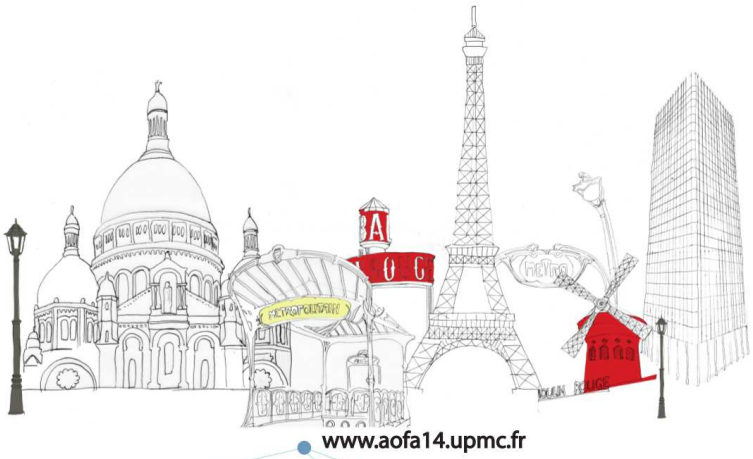
PROCEEDINGS



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- **DONALD KNUTH (Stanford, USA) : Flajolet lecture**
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- COLIN MCDIARMID (Oxford, England)
- CRISTOPHER MOORE (Santa Fe, USA)
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Discrete Mathematics and Theoretical Computer Science

Preface

The present volume collects the proceedings of Aofa'14, the 25th International Meeting on Probabilistic, Combinatorial, and Asymptotic Methods for the Analysis of Algorithms held at Université Pierre et Marie Curie, Paris, France, during June 16-20, 2014. The conference builds on the communities of the former series of conferences "Mathematics and Computer Science" and "Analysis of Algorithms", and aims at studying rigorously the combinatorial objects which appear in the analysis of data structures and algorithms, as well as the essential ubiquitous combinatorial structures. The program committee selected submissions covering this wide range of topics. These regular papers, that were presented in 30-minute talks, appear in the present volume. The conference included a poster session.

The conference also presented six invited plenary lectures. The "Flajolet lecture" was given by Donald Knuth (Stanford, USA) : Problems Philippe Would Have Liked, and the five invited talks were the following:

- Manuel Kauers (RISC-Linz, Austria):
  Analysis of summation algorithms
- Colin McDiarmid (Oxford, UK):
  Random graphs from a minor-closed class
- Christopher Moore (Santa Fe, USA):
  Les rendez-vous symétriques
- Marc Noy (Barcelona, Spain):
  Logical limit laws in combinatorics
- Gilles Schaeffer (École Polytechnique, France):
  Simple branched covers and planar maps: Cayley vs. Catalan

We thank the members of the steering and program committees for their involvement. We also thank the invited speakers, and the authors of the contributed papers. We express our gratitude to the members of the organization committee, for their invaluable help in making this meeting a great success. We are also grateful to the editor-in-chief of DMTCS-HAL Jens Gustedt for his help in the compilation of the proceedings.

Finally, our special thanks go to the sponsors of the conference for their contributions: UPMC, ANR Magnum, CPU, Alcatel-Lucent, LIP6, LIPN, LIAFA.

Mireille Bousquet-Mélou and Michèle Soria, Editors.

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Multivariate juggling probabilities

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Abstract. We consider refined versions of Markov chains related to juggling. We further generalize the construction to juggling with arbitrary heights as well as infinitely many balls, which are expressed more succinctly in terms of Markov chains on integer partitions. In all cases, we give explicit product formulas for the stationary probabilities and closed-form expressions for the normalization factor. We also refine and generalize enriched Markov chains on set partitions. Lastly, we prove that in one case, the stationary distribution is attained in finite time.

Keywords: Markov chain, Combinatorics, Juggling

1 Introduction

This is an extended abstract of [ABCN]. Although juggling as a human endeavour has been around since time immemorial, it is fairly recently that mathematicians have taken an active interest in exploring the field. Combinatorialists became interested in juggling towards the end of the last century after an article by [BEGW94]. Since then, their results have been q-ified by [ER96] and further refined in various ways by [Sta97, Sta02, CG07, CG08, BG10]. Further connections between juggling and mathematics appear for instance in algebraic geometry in [DM07, KLS13]. A mathematical history of juggling is given in the fascinating book by [Pol03]. [War05] gave exact combinatorial formulas for the stationary distribution of juggling models. More recently, a q-deformation of Warrington's original finite model was considered by [ELV], who also obtained exact expressions for the stationary distribution via an enriched chain formulated in terms of rook placements.

In this paper, we provide multivariate generalizations of all the models introduced in [War05], namely *juggling, add-drop juggling* and *annihilation juggling*. Furthermore, in the case of the juggling model with a conserved number of balls, we investigate the limiting case where balls can be thrown arbitrarily high. We also consider the limiting case where the number of balls tends to infinity. In all these cases, we obtain an exact formula for the stationary distribution. Our proofs were mainly obtained from two approaches. First, the general formulas can often be guessed, then proved straightforwardly by considering

†The authors are partially funded by ANR grants ANR-08-JCJC-0011 and ANR 12-JS02-001-01 and by the projet Émergences Combinatoire à Paris

the juggling process itself or its natural reformulation in terms of integer partitions. The other approach is Warrington's combinatorial approach consisting in introducing an enriched chain whose stationary distribution is simpler, and which yields the original chain by a projection or "lumping" procedure, see e.g. [LPW09].

The rest of the paper is organized as follows. In Section 2, we concentrate on the simplest version of our model, which we call the Multivariate Juggling Markov Chain (MJMC). The model is defined in Section 2.1, and we also discuss the uniqueness of the stationary distribution. The expression for the stationary distribution of the Markov chain is stated in Section 2.2. A combinatorial proof comes in Section 2.3 and involves set partitions with a prescribed number of elements and blocks. We then turn to extended models. Extensions to infinite state spaces are considered in Section 3 : in Section 3.1, we give an interesting reformulation in terms of integer partitions which will prove usefull. The case of a finite number of balls but *unbounded* heights (UMJMC) is discussed in Section 3.2, while the case of an *infinite* number of balls (IMJMC) is considered in Section 3.3. Extensions to a fluctuating number of balls (but with a finite state space) are considered in Section 4 : we provide the multivariate extension of the add-drop and the annihilation models introduced in [War05], in the respective Sections 4.1 and 4.2. We end with some remarks and questions for future study in Section 5.

Due to space restrictions, most proofs are omitted and we refer the reader to the long version of the paper [ABCN] for details.

2 The finite Multiparameter Juggling Markov Chain

2.1 Definition

In this section, we introduce our juggling model in the simplest setting, i.e. a Markov chain on a finite state space. Consider a person, called *Magnus* with no loss of generality, who is juggling with a fixed finite number ℓ of balls. Time is discretized in steps of one second and we assume that, at each second, Magnus is able to catch at most one ball, and then throws it back immediately. Besides this limitation Magnus juggles *perfectly*, i.e. in a such way that the ball will always return to him after some time. Magnus chooses how long it will take for the ball to return to him. We suppose for now that the number of seconds before the ball returns to Magnus is bounded by an integer h. Moreover Magnus must choose the successive launches in such a way that no two balls arrive to him at the same time. Thus, treating the balls as indisguishable, there are $\binom{h}{\ell}$ possible ball states. It is convenient to think of a state as a configuration of ℓ non overlapping particles on a one-dimensional lattice with h sites, where the i-th site (read from the left) is occupied if and only if a ball is scheduled to arrive i seconds in the future. We denote by $k = h - \ell$ the number of empty (unoccupied) sites.

In this language, the time evolution of a state is easy to describe: at each time step, all particles are moved one site to the left. If there is no particle on the first site, then nothing else has to be done. Otherwise the particle on the first site is *reinserted* at one of the $k + 1$ available (empty) sites on the lattice. This defines the transition graph of our model, illustrated on Figure 1 for $h = 3$, $l = 2$ and $k = 1$.

We now assume that Magnus juggles at random: each reinsertion is made at the i-th available site (read from the left) with probability x_{i-1}, independently of the past, so that our model is a Markov chain. Here, $x_0, \ldots, x_k$ are fixed nonnegative real numbers such that $x_0 + \cdots + x_k = 1$. This defines the *Multivariate Juggling Markov Chain* (MJMC).

We now provide a more formal mathematical definition of the MJMC. Following Warrington's notations, let St_h denote the set of words of length h on the alphabet $\{\bullet, \circ\}$, and let $\mathrm{St}_{h,k} \subset \mathrm{St}_h$ be the

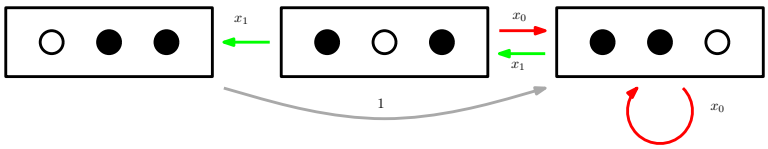

Fig. 1: The Markov chain with $h = 3$ and $k = 1$.

subset of such words containing exactly k occurrences of $\circ$. For $A \in \mathrm{St}_{h,k+1}$ and $i \in \{0, \dots, k\}$, we let $T_i(A) \in \mathrm{St}_{h,k}$ be the word obtained by replacing the $(i+1)$-th occurrence of $\circ$ in A by $\bullet$.

Definition 2.1 *Given h, k nonnegative integers such that $h \geq k$, and $x_0, \dots, x_k$ nonnegative real numbers such that $x_0 + \cdots + x_k = 1$, the* Multivariate Juggling Markov Chain *(MJMC) is the Markov chain on the state space $\mathrm{St}_{h,k}$ for which the transition probability from $A = a_1 a_2 \cdots a_h$ to B reads*

$$P_{A,B} = \begin{cases} 1 & \text{if } a_1 = \circ \text{ and } B = a_2 \cdots a_h \circ, \\ x_i & \text{if } a_1 = \bullet \text{ and } B = T_i(a_2 \cdots a_h \circ), \\ 0 & \text{otherwise.} \end{cases} \tag{2.1}$$

Proposition 2.2 *If $x_0 > 0$, then the MJMC has a unique closed communicating class, whose all states are aperiodic. If furthermore $x_k > 0$, then the MJMC is irreducible.*

Proof: Easy. Note that, when $x_0 = 0$, the chain may have several closed communicating classes (for instance, take $h = 4$, $k = 2$ and let $x_0 = x_1 = 0$). When $x_k = 0$, any state with a particle on site h is transient. □

2.2 Stationary distribution

From now on we assume $x_0 > 0$. By Proposition 2.2, the MJMC admits a unique stationary probability distribution. Our main result is an explicit form for it, given as follows.

Theorem 2.3 *The stationary probability distribution π of the MJMC is given by*

$$\pi(B) = \frac{1}{Z_{h,k}} \prod_{\substack{i \in \{1,\dots,h\} \\ b_i = \bullet}} y_{E_i(B)}, \tag{2.2}$$

where $B = b_1 \cdots b_h \in \mathrm{St}_{h,k}$, $E_i(B) = \#\{j < i | b_j = \circ\}$,

$$Z_{h,k} = h_\ell(y_0, y_1, \dots, y_k) \tag{2.3}$$

with h_ℓ the complete homogeneous symmetric polynomial of degree $\ell = h - k$, and where we introduce the shorthand notation

$$y_m = \sum_{j=m}^{k} x_j, \qquad m = 0, \dots, k. \tag{2.4}$$

We will prove in Section 2.3 that π is indeed a stationary distribution of the MJMC. The explicit expression (2.3) for the normalization factor is not difficult to check for instance by induction, by partitioning words in $\mathrm{St}_{h,k}$ according to their first letter. As specializations, we have in particular

$$\begin{aligned} &Z_{h,k}((1-q),(1-q)q,\dots,(1-q)q^{k-1},q^k) = \binom{h}{k}_q, \quad Z_{h,k}(1,1,\dots,1,1) = \left\{ {h+1 \atop k+1} \right\}, \\ &Z_{h,k}(q^k,q^{k-1},\dots,q,1) = \left\{ {h+1 \atop k+1} \right\}_q, \quad Z_{h,k}(1,q,\dots,q^{k-1},q^k) = q^{k(h-k)} \left\{ {h+1 \atop k+1} \right\}_{1/q}, \end{aligned} \tag{2.5}$$

where $\left\{ {\cdot \atop \cdot} \right\}$ denotes Stirling numbers of the second kind, $\left\{ {\cdot \atop \cdot} \right\}_q$ their q-analogues as defined in [Gou61] and $\binom{\cdot}{\cdot}_q$ q-binomial coefficients.

2.3 Enriched Markov chain on set partitions

The purpose of this Section is to prove by a combinatorial argument that the measure π over $\mathrm{St}_{h,k}$ defined in Theorem 2.3 is indeed a stationary measure of the MJMC. The main idea is to expand the product in the right hand side of (2.2) as a sum of monomials in the x_i's, and interpret each of these monomials as the stationary probability of an "enriched" state.

Let us introduce the shorthand notations $H = h+1$ and $K = k+1$. An *enriched state* is a partition of the set $\{1,2,\dots,H\}$ into K subsets called *blocks*. We denote by $\mathcal{S}(H,K)$ the set of enriched states. To each enriched state σ, we associate a word $\psi(\sigma) = a_1 \dots a_h$ by setting $a_i = \circ$ if i is a *block maximum* of σ, and $a_i = \bullet$ otherwise. Observe that ψ is a surjection from $\mathcal{S}(H,K)$ onto $\mathrm{St}_{h,k}$. See Figure 2 for an illustration.

We now define the enriched Markov chain on $\mathcal{S}(H,K)$. For an enriched state σ, we denote by $\sigma^{\downarrow}$ the partition of the set $\{1,\dots,h\}$ obtained by removing 1 from σ, and shifting all the remaining elements of all blocks down by 1. For $\tau \in \mathcal{S}(h,K)$ and $i \in \{0,\dots,k\}$, we denote by $I_i(\tau)$ the set partition of $\{1,\dots,H\}$ obtained by inserting H into the $(i+1)$-th block of τ, where the blocks are numbered by ascending order of their maxima. Note that $I_i(\tau) \in \mathcal{S}(H,K)$ and that the mapping $(\tau,i) \mapsto I_i(\tau)$ is injective.

Definition 2.4 *The* enriched chain *is the Markov chain on $\mathcal{S}(H,K)$ for which the transition probability from σ to τ is given by*

$$\tilde{P}_{\sigma,\tau} = \begin{cases} 1 & \text{if } \{1\} \in \sigma \text{ and } \tau = \sigma^{\downarrow} \cup \{H\}, \\ x_i & \text{if } \{1\} \notin \sigma \text{ and } \tau = I_i(\sigma^{\downarrow}) \text{ for some } i \in \{0,\dots,k\}, \\ 0 & \text{otherwise}. \end{cases} \tag{2.6}$$

The condition $x_0 + \dots + x_k = 1$ and the above remarks ensure that $\tilde{P}$ is indeed a (right) stochastic matrix.

Example 2.5 *For $H = 8$ and $K = 3$:*

- *the enriched state* $1\,|\,3\,5\,6\,|\,2\,4\,7\,8$ *jumps with probability* 1 *to* $2\,4\,5\,|\,1\,3\,6\,7\,|\,8$,
- *the enriched state* $3\,5\,|\,2\,6\,7\,|\,1\,4\,8$ *jumps with probability:* x_0 *to* $1\,5\,6\,|\,3\,7\,|\,2\,4\,8$, x_1 *to* $2\,4\,|\,3\,7\,|\,1\,5\,6\,8$, *and* x_2 *to* $2\,4\,|\,1\,5\,6\,|\,3\,7\,8$.

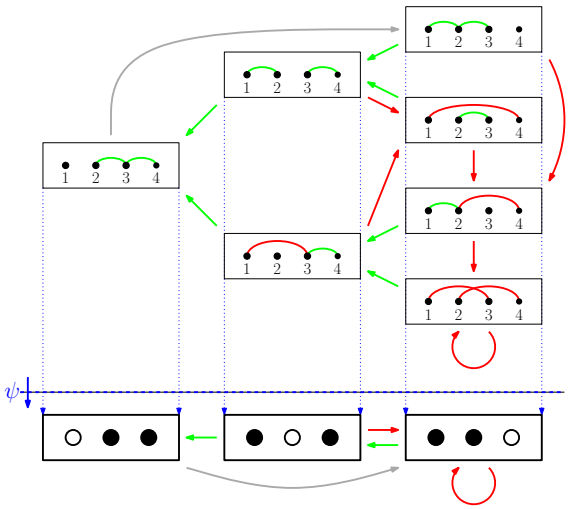

Fig. 2: Top: transition graph of the enriched chain for $H = 4$ and $K = 2$. Red, green and grey arrows represent transitions of respective probability x_0, x_1 and 1. Bottom: the projection onto the MJMC with $h = 3$ and $k = 1$.

Example 2.6 *For $H = 4$ and $K = 2$, the transition graph of the enriched chain is illustrated on Fig. 2.*

The existence and uniqueness of the stationary distribution of the enriched chain results from the following easy proposition.

Proposition 2.7 *For $x_0 > 0$, the enriched chain has a unique closed communicating class, whose all states are aperiodic. The chain is irreducible if and only if all x_i's are nonzero.*

It is not difficult to check that the surjection ψ introduced above defines a projection of the enriched chain onto the MJMC, compatible with the dynamics. More precisely, let Ψ be the rectangular matrix with rows indexed by elements of $\mathcal{S}(H, K)$ and columns indexed by elements of $\mathrm{St}_{h,k}$ in the obvious manner (namely a coefficient of Ψ is 1 if its column index is the image by ψ of its row index, and 0 otherwise), then it is straightforwardly checked that we have the "intertwining property" $\tilde{P}\Psi = \Psi P$, see Figure 2 for an illustration. The intertwining property immediately implies that the stationary measures π and $\tilde{\pi}$ of both chains are related by

$$\pi = \tilde{\pi}\Psi. \tag{2.7}$$

Our route to Theorem 2.3 is now clear. We want to find an explicit expression for $\tilde{\pi}$, then compute $\tilde{\pi}\Psi$. We first need to introduce some definitions and notations.

Definition 2.8 *Let σ be an enriched state and s, t two integers such that $1 \leq s < t \leq H$. We say that the pair (s, t) is an* arch *of σ if s and t belong to the same block β of σ, while no integer strictly between s and t belongs to β. For $1 \leq s < t \leq H$, we denote by $C_\sigma(s, t)$ the number of blocks containing at least one element in $\{s, s + 1, \ldots, t - 1, t\}$. When (s, t) is an arch, we say that these blocks are those* covered *by (s, t).*

Lemma 2.9 *For $\sigma \in \mathcal{S}(H,K)$, the monomial*

$$\tilde{w}(\sigma) = \prod_{(s,t) \text{ arch of } \sigma} x_{K-C_\sigma(s,t)} \tag{2.8}$$

defines an unnormalized stationary measure of the enriched chain.

Proof: See again Figure 2 for a proof by example: arches covering 1 or 2 blocks are represented in green or red respectively, and weighting them by respectively x_1 and x_0 indeed yields a stationary measure of the enriched chain. We refer the reader to [ABCN] for a formal proof. □

It is easily seen that there is one set partition in $\mathcal{S}(H,K)$ whose all arches cover K blocks, so that

$$Z_{h,k} = \sum_{\sigma \in \mathcal{S}(H,K)} \tilde{w}(\sigma) \tag{2.9}$$

is positive whenever $x_0 > 0$, and $\tilde{\pi} = \tilde{w}/Z_{h,k}$ is the stationary probability distribution of the enriched chain. For $B \in \mathrm{St}_{h,k}$, we set

$$w(B) = \sum_{\sigma \in \psi^{-1}(B)} \tilde{w}(\sigma), \tag{2.10}$$

that is $w = \tilde{w}\Psi$. Then, $\pi = w/Z_{h,k}$ is the stationary probability distribution of the MJMC. By considering the possible preimages of $B = b_1 \dots b_h \in \mathrm{St}_{h,k}$ by ψ, we find that

$$w(B) = \prod_{\substack{i \in \{1,\dots,h\} \\ b_i = \bullet}} \left(x_{E_i(B)} + \dots + x_k \right). \tag{2.11}$$

where $E_i(B) = \#\{j < i | b_j = \circ\}$ (see [ABCN] for details).

Example 2.10 *Returning again to the case $H = 4$, $K = 2$ (i.e. $h = 3$, $k = 1$) illustrated on Figure 2, we find*

$$w(\circ\bullet\bullet) = x_1^2, \qquad w(\bullet\circ\bullet) = (x_0+x_1)x_1 = x_1, \qquad w(\bullet\bullet\circ) = (x_0+x_1)^2 = 1. \tag{2.12}$$

This completes the proof that π defined by (2.2) is indeed the stationary distribution of the MJMC.

3 Extensions to infinite state spaces

In this section, we mention the possible extensions of the Multivariate Juggling Markov Chain to an infinite setting. This is most conveniently done by reformulating the MJMC in terms of integer partitions, which we do first. All the proofs are skipped, see [ABCN].

3.1 Reformulation of the MJMC in terms of integer partitions

There is a natural bijection between $\mathrm{St}_{h,k}$ and $\mathrm{Par}_{k,\ell}$ (with $\ell = h - k$), where $\mathrm{Par}_{k,\ell}$ is the set of integer partitions whose Young diagram fits within a $k \times \ell$ rectangle. Given A a state in $\mathrm{St}_{h,k}$, we denote by $s_1 < s_2 < \dots < s_{\ell-1} < s_\ell$ the positions of $\bullet$ in A, then the corresponding integer partition is $(s_\ell - \ell, s_{\ell-1} - (\ell-1), \dots, s_2 - 2, s_1 - 1)$. Remark that $s_i - i$ is equal to the number of $\circ$ appearing before the i-th $\bullet$ in A. We may reformulate the MJMC as follows.

Proposition 3.1 *For $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_\ell)$ and $\mu = (\mu_1, \mu_2, \ldots, \mu_\ell)$ two partitions in $\mathrm{Par}_{k,\ell}$, the transition probability from λ to μ reads*

$$P_{\lambda,\mu} = \begin{cases} 1 & \text{if } \lambda_\ell \neq 0 \text{ and } \mu = (\lambda_1 - 1, \lambda_2 - 1, \ldots, \lambda_\ell - 1), \\ x_i & \text{if } \lambda_\ell = 0 \text{ and there exists } j \in \{1, \ldots, \ell\} \text{ such that} \\ & \mu = (\lambda_1 - 1, \ldots, \lambda_{j-1} - 1, i, \lambda_j, \ldots, \lambda_{\ell-1}), \\ 0 & \text{otherwise.} \end{cases} \tag{3.1}$$

The stationary distribution of the MJMC thus takes a particularly simple form, namely Theorem 2.3 amounts to:

Theorem 3.2 *The stationary distribution π of the MJMC is given by*

$$\pi(\lambda) = \frac{1}{Z_{h,k}} \prod_{i=1}^{\ell} y_{\lambda_i} \tag{3.2}$$

where $\lambda = (\lambda_1, \ldots, \lambda_\ell)$ is an element of $\mathrm{Par}_{k,\ell}$ and where the y_m are as in (2.4)*.*

In [ABCN], we provide a direct proof of this statement without recourse to the enriched chain.

Example 3.3 *By specialization, we obtain the following interesting measures over $\mathrm{Par}_{k,\ell}$*

$$\pi(\lambda) = \begin{cases} \frac{1}{\left\{ {h+1 \atop k+1} \right\}} \prod_{i=1}^{\ell} (k + 1 - \lambda_i) & \text{for } x_i = \frac{1}{k+1}, \\ \frac{1}{q^{k\ell} \left\{ {h+1 \atop k+1} \right\}_{1/q}} \prod_{i=1}^{\ell} q^{\lambda_i} [k + 1 - \lambda_i]_q & \text{for } x_i = \frac{q^i}{[k+1]_q}, \\ \frac{1}{\binom{h}{k}_q} \prod_{i=1}^{\ell} q^{\lambda_i} & \text{for } x_i = (1-q)^{1-\delta_{i,k}} q^i \end{cases} \tag{3.3}$$

where the normalization factors follow from (3.1)*.*

3.2 Unbounded heights

As suggested in the conclusion of [War05], a first natural extension is to allow Magnus to throw balls arbitrarily high, or, in the integer partition model, to allow parts to be arbitrarily large. This corresponds to taking the limit $h \to \infty$ of the MJMC, keeping the number of balls ℓ fixed. We keep the MJMC prescription of choosing the i-th available site with probability x_{i-1}. We now have an infinite sequence $(x_i)_{i \geq 0}$ of nonnegative real numbers such that $\sum_{i=0}^{\infty} x_i = 1$. An immediate extension of Proposition 2.2 is that this *Unbounded Multivariate Juggling Markov Chain* (UMJMC) is irreducible and aperiodic whenever x_0 and infinitely many x_i's are nonzero.

Theorem 3.2 stills holds with few adaptations. Setting

$$y_m = \sum_{j=m}^{\infty} x_i, \tag{3.4}$$

we define a σ-finite measure w over the set of partitions with at most ℓ parts of unrestricted size via

$$w(\lambda) = \prod_{i=1}^{\ell} y_{\lambda_i}. \tag{3.5}$$

By the same lines as in the "direct" proof of Theorem 3.2, we find that w is an invariant measure of the UMJMC. Furthermore, it can be shown that this invariant measure is finite if and only if

$$\sum_{i=0}^{\infty} i x_i < \infty \tag{3.6}$$

in which case its total mass is given by the well-defined expression $Z^{(\ell)} = h_\ell(y_0, y_1, y_2, \ldots)$. By standard results on Markov chains, the UMJMC is positive recurrent if and only if (3.6) holds.

Example 3.4 *Fix $q \in (0,1)$ and pick $x_i = (1-q)q^i$. We recover the "JEP with memoryless height distribution" of parameter q considered in [LV12].*

3.3 Infinitely many balls

We now consider another limit which consists in having Magnus juggle with infinitely many balls ($\ell \to \infty$). In the partition model, this corresponds to removing the limitation on the number of parts. The transition probabilities are still defined as in Proposition 3.1, except that the case $\lambda_\ell \neq 0$ never occurs (since a partition always has a finite number of parts). This is the so-called *Infinite Multivariate Juggling Markov Chain* (IMJMC).

If $x_0 > 0$, then the IMJMC has a unique closed communicating class, whose all states are aperiodic. They are precisely the integer partitions whose parts are smaller than or equal to $\sup\{i : x_i > 0\}$. In particular, if infinitely many x_i's are nonzero, then the IMJMC is irreducible.

Again, we find that an invariant measure of the IMJMC is given by

$$w(\lambda) = \prod_{i=1}^{\infty} y_{\lambda_i} \tag{3.7}$$

with λ an arbitrary integer partition and y_m as in (3.4). Its total mass reads $Z = \prod_{m=1}^{\infty} 1/(1-y_m)$ and is finite (i.e. the IMJMC is positive recurrent) if and only if (3.6) holds.

Example 3.5 *Consider again the geometric case $x_i = (1-q)q^i$, $q \in [0,1)$. Then, the stationary distribution is nothing but the "q^{size}" measure over arbitrary integer partitions.*

4 Extensions with a fluctuating number of balls

We now mention, again without proofs, our results regarding extensions of the MJMC where the number of balls is not fixed but is allowed to fluctuate. These extensions are the natural multivariate generalizations of the so-called *add-drop* and *annihilation* models introduced in [War05, Section 4], to which we refer for motivations. Both models are defined on the same state space and have the same transition graph. The basic state space of the model will be $\mathrm{St}_h = \{\circ, \bullet\}^h$, with h a fixed nonnegative integer. It is here convenient to read a word from right to left, and for $A \in \mathrm{St}_h$ and i a nonnegative integer, we let $S_i(A)$ be the word obtained by replacing the i-th occurrence of $\circ$ in A by $\bullet$, upon reading the word *from the right* (if i is equal to 0 or larger than the number of occurrences of $\circ$ in A then we set $S_i(A) = A$ by convention). Note that $S_i(A) = T_{k-i}(A)$ for $A \in \mathrm{St}_{h,k}$ and $1 \leq i \leq k$, with T as in Section 2.1. The state space of the enriched model will be the set $\mathcal{S}(H)$ of all set partitions of $\{1, \ldots, H\}$, with $H = h+1$, and we recall the notations from Section 2.3: ψ is a surjection from $\mathcal{S}(H)$ onto St_h and $\sigma \mapsto \sigma^{\downarrow}$ is a mapping

from $\mathcal{S}(H)$ to $\mathcal{S}(h)$. For $\tau \in \mathcal{S}(h)$ and i a nonnegative integer, we let $J_i(\tau) \in \mathcal{S}(H)$ be the set partition obtained by inserting H into the i-th block of τ, now numbered by *decreasing* order of maxima (if i is equal to 0 or larger than the number of blocks of τ then we set $J_i(\tau) = \tau \cup \{H\}$ by convention). Note that $J_i(\tau) = I_{K-i}(\tau)$ for $\tau \in \mathcal{S}(h, K)$ and $1 \leq i \leq K$. Observe that we have the fundamental "intertwining" relation $\psi(J_i(\tau)) = S_i(\psi(\tau)\circ)$.

The basic transition graph is defined as follows: for any $A = a_1 a_2 \dots a_h \in \mathrm{St}_h$ and $i \geq 0$, we have an oriented edge from A to $S_i(a_2 \dots a_h \circ)$. See figure 3 for $h = 2$. Similarly, the enriched transition graph is obtained by connecting each $\sigma \in \mathcal{S}(H)$ to $J_i(\sigma^{\downarrow})$ for all $i \geq 0$. It is not difficult to check that both transition graphs are strongly connected.

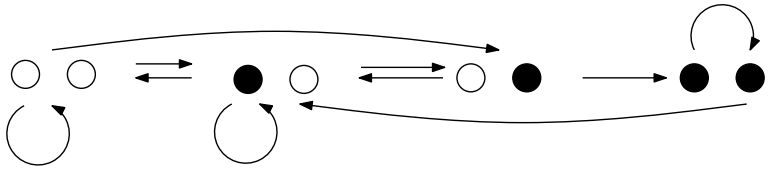

Fig. 3: The basic transition graph for $h = 2$

4.1 Add-drop juggling

Definition 4.1 *Given h a nonnegative integer and $z_0, z_1, \dots, z_h$ nonnegative real numbers, the (multivariate)* add-drop model *is the Markov chain on the state space St_h for which the transition probability from $A = a_1 a_2 \dots a_h$ to B reads*

$$P_{A,B} = \begin{cases} \dfrac{z_i}{z_0 + \cdots + z_k} & \text{if } B = S_i(a_2 \dots a_h \circ) \text{ for some } i \in \{0, \dots, k\}, \\ 0 & \text{otherwise,} \end{cases} \tag{4.1}$$

with k the number of occurrences of $\circ$ in $a_2 \dots a_h \circ$. The (multivariate) enriched add-drop model *is the Markov chain on the state space $\mathcal{S}(H)$ for which the transition probability from σ to τ is given by*

$$\tilde{P}_{\sigma,\tau} = \begin{cases} \dfrac{z_i}{z_0 + \cdots + z_k} & \text{if } \tau = J_i(\sigma^{\downarrow}) \text{ for some } i \in \{0, \dots, k\}, \\ 0 & \text{otherwise,} \end{cases} \tag{4.2}$$

with k the number of blocks of $\sigma^{\downarrow}$.

Warrington's add-drop model is recovered by taking $z_0 = \cdots = z_h = 1$. It is easily seen that, in general, the chain is aperiodic with a unique communicating class whenever $z_0 > 0$. Here is the multivariate generalization of [War05, Theorem 3, item 1]:

Theorem 4.2 *The stationary distribution of the add-drop model is given by*

$$\Pi(B) = \frac{z_0^k}{Z_h} \prod_{\substack{i=1 \\ b_i = \bullet}}^{h} \left(z_1 + \cdots + z_{\psi_i(B)+1} \right), \tag{4.3}$$

for $B = b_1 \dots b_h \in \mathrm{St}_{h,k}$, with $\psi_i(B) = \#\{j : i < j \leq h,\, b_j = \circ\}$ and

$$Z_h = \sum_{k=0}^{h} z_0^k h_{h-k}(z_1, z_1 + z_2, \dots, z_1 + z_2 + \dots + z_{k+1}), \tag{4.4}$$

where h_ℓ denotes again the complete homogeneous symmetric polynomial of degree ℓ.

It can be shown that the add-drop model is indeed the projection of the enriched chain, and furthermore that the enriched chain is aperiodic with a unique communicating class for $z_0 > 0$. Following the same line of arguments as in Section 2.3, proving Theorem 4.2 boils down to checking the simpler:

Lemma 4.3 *For $\sigma \in \mathcal{S}(H)$ with, say, K blocks and $C_\sigma(s,t)$ is in Definition 2.8, the monomial*

$$\tilde{W}(\sigma) = z_0^{K-1} \prod_{(s,t)\ arch\ of\ \sigma} z_{C_\sigma(s,t)}, \tag{4.5}$$

defines an unnormalized stationary distribution of the enriched chain.

4.2 Annihilation juggling

Definition 4.4 *Given h a nonnegative integer and $z_1, \dots, z_h, z_{h+1}$ nonnegative real numbers such that $z_1 + \dots + z_{h+1} = 1$, the (multivariate)* annihilation model *is the Markov chain on the state space St_h for which the transition probability from $A = a_1 a_2 \dots a_h$ to B reads*

$$P_{A,B} = \begin{cases} z_i & \text{if } B = S_i(a_2 \dots a_h \circ) \text{ for some } i \in \{1, \dots, k\}, \\ z_{k+1} + \dots + z_{h+1} & \text{if } B = a_2 \dots a_h \circ, \\ 0 & \text{otherwise,} \end{cases} \tag{4.6}$$

with k the number of occurrences of $\circ$ in $a_2 \dots a_h \circ$. Similarly, the (multivariate) enriched annihilation model *is the Markov chain on the state space $\mathcal{S}(H)$ (recall that $H = h + 1$) for which the transition probability from σ to τ is given by*

$$\tilde{P}_{\sigma,\tau} = \begin{cases} z_i & \text{if } \tau = J_i(\sigma^\downarrow) \text{ for some } i \in \{1, \dots, k\}, \\ z_{k+1} + \dots + z_H & \text{if } \tau = \sigma^\downarrow \cup \{H\}, \\ 0 & \text{otherwise,} \end{cases} \tag{4.7}$$

with k the number of blocks of $\sigma^\downarrow$.

Remark 4.5 *By our convention for defining $S_i(A)$ (resp. $J_i(\tau)$) when i is larger than the number of occurrences of $\circ$ in A (resp. the number of blocks of τ), we have the more compact expression $P_{A,B} = \sum z_i$ (resp. $\tilde{P}_{\sigma,\tau} = \sum z_i$) where the sum runs over all $i \in \{1, \dots, h+1\}$ such that $B = S_i(a_2 \dots a_h \circ)$ (resp. $\tau = J_i(\sigma^\downarrow)$).*

Warrington's annihilation model is recovered by taking $z_1 = \dots = z_{h+1} = 1/(h+1)$. Here is the multivariate generalization of [War05, Theorem 3, item 2]:

Theorem 4.6 *The stationary distribution of the annihilation model is given by*

$$\Pi(B) = \prod_{\substack{i=1 \\ b_i=\bullet}}^{h} \left(z_1 + \cdots + z_{\psi_i(B)+1}\right) \prod_{j=1}^{k} \left(z_{j+1} + \cdots + z_{h+1}\right), \tag{4.8}$$

for $B = b_1 \dots b_h \in St_{h,k}$, with $\psi_i(B) = \#\{j : i < j \leq h,\, b_j = \circ\}$ as before. Similarly, the stationary distribution of the enriched annihilation model is given by

$$\tilde{\Pi}(\sigma) = \prod_{(s,t) \text{ arch of } \sigma} z_{C_\sigma(s,t)} \prod_{i=1}^{K-1} (z_{i+1} + \cdots + z_H), \tag{4.9}$$

with $\sigma \in \mathcal{S}(H)$ and K its number of blocks. There is no normalization factor, as Π and $\tilde{\Pi}$ are already normalized for $z_1 + \cdots + z_{h+1} = 1$.

The annihilation has a remarkable property that departs it from the generic MJMC and add-drop model.

Theorem 4.7 *For any initial probability distribution η over $\mathrm{St}_{h,k}$ or $\tilde{\eta}$ over $\mathcal{S}(H)$, the distribution at time h is equal to the stationary distribution, namely*

$$\eta P^h = \Pi, \qquad \tilde{\eta}\tilde{P}^h = \tilde{\Pi}. \tag{4.10}$$

In particular, the only eigenvalues of P and $\tilde{P}$ are 1 (with multiplicity 1) and 0.

This result is stronger than a statement about mixing times since we reach the exact stationary state in finite time! See [ABCN] for a proof.

5 Conclusion and discussion

For the infinite setting, we prove that the UMJMC (for fixed ℓ) is positive recurrent if and only if $\sum_i i x_i < \infty$. When this condition does not hold, the chain may either be null recurrent or transient. For $\ell = 1$, the chain is null recurrent. Figuring out the situation for $\ell > 1$ is an intriguing open question.

Now that we gave some nice combinatorial interpretations of the stationary distribution of the MJMC, we would like to know if some special values of the x_i's could give some nice behaviors in a suitable limit, for example display some phase transitions or shock formations. Such phenomena were observed for instance in a related "juggling model with exclusion dynamics" introduced in [ABKM13].

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Anticipated rejection algorithms and the Darling–Mandelbrot distribution

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Abstract. We study in limit law the complexity of some anticipated rejection random sampling algorithms. We express this complexity in terms of a probabilistic process, the threshold sum process. We show that, under the right conditions, the complexity is linear and admits as a limit law a so-called Darling–Mandelbrot distribution, studied by Darling (1952) and Lew (1994). We also give an explicit form to the density of the Darling–Mandelbrot distribution and derive some of its analytic properties.

Keywords: Analysis of algorithms, random sampling, anticipated rejection, limit distribution, sum of i.i.d. random variables, Darling–Mandelbrot distribution

1 Introduction

This paper aims at answering the following algorithmic question: consider a program P that performs a random number of elementary operations and then terminates. Our goal is to have P performing n operations in one run. To do that, we run the program P until it reaches n operations; if it terminates before that, we simply restart it. The question is, how many elementary operations must we perform to reach this goal?

Algorithms of this type are abundant in the field of *random sampling*, where they are known as *anticipated rejection* algorithms. Given a class of discrete objects, a random sampling algorithm takes an integer n as input and outputs a random object of size n according to a specific (usually uniform) distribution. Given a random sampling algorithm for a class $\mathcal{A}$ and a subclass $\mathcal{B}$ of $\mathcal{A}$, an element of $\mathcal{B}$ can be sampled using a *rejection* algorithm: we repeatedly sample elements of $\mathcal{A}$ until we find one in $\mathcal{B}$. This algorithm can be improved when it is possible to know in advance, during the sampling procedure, that the drawn element is not going to be in $\mathcal{B}$: we can then prematurely reject the sample and start over, saving computing time. This scheme is called *anticipated rejection*. Assuming that sampling an element of $\mathcal{A}$ costs n elementary operations, this fits into the framework outlined above.

Such algorithms are found for example in [BPS94, BPS95,], sampling prefixes of Motzkin paths. Somewhat miraculously, these algorithms achieve an average linear time complexity, as, on average, the

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number of necessary trials is $\mathcal{O}(\sqrt{n})$ and each trial costs $\mathcal{O}(\sqrt{n})$. We show that this phenomenon is not isolated, but rather happens in a wider range of cases. Other algorithms of this family exist, sampling unary-binary trees [BBJ14,], Schröder prefixes [Bac14,], and constrained random walks.

In this paper, we study the full limit distribution of the complexity of these algorithms. This problem leads us to define a probabilistic process, the *threshold sum process*. Our main result is that, if the base distribution has a tail with exponent α in a certain range, this process admits a limit distribution depending only on α. This *universality* phenomenon is reminiscent of Lévy's well-known theory of α-stable distributions, which also deals with sums of independent random variables [GK68,].

Surprisingly, our limiting distribution has already been studied in relation to a different problem. It was first studied by Darling [Dar52,], then apparently by Mandelbrot in unpublished work, and by Lew [Lew94,], who named it the *Darling–Mandelbrot distribution*. This distribution has a parameter α, with $0 < \alpha < 1$; it is supported on $\mathbb{R}_+$ and is defined by its characteristic function:

$$\phi_\alpha(s) = \frac{(-is)^{-\alpha}}{-\alpha\gamma(-\alpha, -is)} = \left(1 - \sum_{n=1}^{\infty} \frac{\alpha}{n-\alpha} \frac{(is)^n}{n!}\right)^{-1}, \tag{1}$$

where in the first expression, $\gamma(\cdot,\cdot)$ denotes the lower incomplete gamma function[(i)]. The second expression allows to easily extract the moments of the distribution as rational functions of α. Lew showed that the distribution has an exponential tail; moreover, we show that its density is non-analytic at all integer points. Both properties contrast with the Lévy distributions, which have an analytic density and a heavy tail.

The paper is organized as follows. In Section 2, we define the threshold sum process and show that, under some conditions, its limit distribution is a Darling–Mandelbrot distribution. In Section 3, we give an explicit form for the Darling–Mandelbrot density and give analytic results expanding those of Lew. Finally, in Section 4, we use these results to analyse some anticipated rejection algorithms.

2 The threshold sum process

In the following, let $(X_i)_{i\geq 0}$ be a sequence of independent and identically distributed random variables with values in $\mathbb{N}$ or $\mathbb{R}_+$ and unbounded support. We denote by $F(x)$ the complementary cumulative distribution function of the X_i's:

$$F(x) = \mathbb{P}(X_i \geq x).$$

Let $t \geq 0$ and let $I(t)$ be the smallest index such that $X_{I(t)} \geq t$. Define the *threshold sum process* (TSP) Y_t as:

$$Y_t = X_0 + \cdots + X_{I(t)-1}.$$

The number t is called the *threshold*. This process resembles the classical sum of independent random variables, but the number of summands $I(t)$ is here a random variable depending on the real parameter t. Our main result on this process is the following.

Theorem 1 *Assume that, as x tends to infinity, $F(x)$ is equivalent to $c\,x^{-\alpha}$ for some $c > 0$ and $\alpha > 0$. Then, as t tends to infinity, the random variable Y_t satisfies:*

[(i)] Given the definition of the Gamma function, $\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}\mathrm{d}t$, the upper and lower incomplete versions are defined through the corresponding integrals on modified domains, $\Gamma(z,a) = \int_a^\infty \cdot$ and $\gamma(z,a) = \Gamma(z) - \Gamma(z,a) = \int_0^a \cdot$, respectively.

- *if $\alpha < 1$, then Y_t/t converges in distribution to the Darling–Mandelbrot law of parameter α;*
- *if $\alpha = 1$, then $Y_t/(t \log t)$ converges in distribution to the exponential law;*
- *if $\alpha > 1$, then Y_t/t^α converges in distribution to the exponential law times μ/c, where $\mu = \mathbb{E}(X_i)$.*

To us, the most interesting case is $\alpha < 1$, where the behavior of Y_t is strongly universal in that it only depends on the exponent α. Moreover, in contrast to Lévy's theory, the scaling factor is always t in that range. For $\alpha = 1$, the scaling factor is slightly higher; for $\alpha > 1$, the scaling factor is higher and we have a lesser form of universality, with the limit scaled by μ/c. Consequences of these facts to the analysis of algorithms are discussed in Section 4.

Proof: We prove this result using Lévy's Continuity Theorem, which states that a sequence of random variables tends in distribution to some limit if their characteristic functions converge pointwise to the characteristic function of the limit distribution.

Let $\psi_t(s) = \mathbb{E}(e^{isY_t/\tau})$ be the characteristic function of the random variable Y_t/τ, where τ is the scaling factor. The index $I(t)$ is geometrically distributed with parameter $F(t)$, which is the probability that $X_i \geq t$. The random variables $X_0, \ldots, X_{I(t)-1}$ are constrained to be less than t; let $\chi_t(s) = \mathbb{E}(e^{isX/t}|X < t)$ be the characteristic function of such a constrained variable. We have:

$$\psi_t(s) = \frac{F(t)}{1 - \big(1 - F(t)\big)\chi_t(s/\tau)}.$$

On the other hand, we have:

$$\chi_t(s) = \frac{1}{1 - F(t)} \sum_{n=0}^{\infty} M_{t,n} \frac{(is)^n}{n!}, \qquad \text{with} \qquad M_{t,n} = \int_0^t x^n dF(x).$$

We therefore have:

$$\psi_t(s) = \frac{F(t)}{1 - \displaystyle\sum_{n=0}^{\infty} \frac{M_{t,n}}{\tau^n} \frac{(is)^n}{n!}} = \frac{1}{1 - \displaystyle\sum_{n=1}^{\infty} \frac{M_{t,n}}{\tau^n F(t)} \frac{(is)^n}{n!}},$$

where the last simplification is due to the fact that $M_{t,0} = 1 - F(t)$.

Consider first the case where $\alpha < 1$. Using integration by parts, we find that the term $M_{t,n}$ satisfies as t tends to infinity:

$$M_{t,n} = -t^n F(t) + \int_0^t n x^{n-1} F(x) dx \sim \frac{\alpha}{n - \alpha}\, c\, t^{n-\alpha}.$$

Moreover, as F is nonincreasing, we have a bound $F(x) \leq c' x^{-\alpha}$ for some constant c'. This enables us to dominate $M_{t,n}$ by:

$$M_{t,n} \leq \frac{n}{n - \alpha} c' t^{n-\alpha}.$$

Picking $\tau = t$, a dominated convergence argument and the expression (1) therefore show that the characteristic function $\psi_t(s)$ tends to the characteristic function $\phi_\alpha(s)$ of the Darling–Mandelbrot distribution. We conclude using Lévy's theorem.

If $\alpha = 1$, we have $M_{t,1} \sim c \log t$ as t tends to infinity; if $\alpha > 1$, $M_{t,1}$ tends to the finite value μ. This means that the ratio $M_{t,1}/[\tau F(t)]$ tends to 1 with the respective values $\tau = t \log t$ and $\tau = \mu t^\alpha / c$. Moreover, in both cases, all the higher moments satisfy $M_{t,n} = \mathcal{O}(t^{n-1})$ and are negligible before $\tau^n F(t)$. This means that $\psi_t(s)$ satisfies:

$$\psi_t(s) \to \frac{1}{1 - is},$$

which is the characteristic function of the exponential distribution. □

3 The Darling–Mandelbrot density

This section is devoted to the computation and the derivation of properties of the density, denoted by g, of the Darling–Mandelbrot distribution. Lew [Lew94,] determined the behavior of g near 0 and infinity, namely:

$$g(x) = C_0 x^{\alpha-1} + \mathcal{O}(1), \qquad x \to 0^+; \tag{2}$$

$$g(x) = \frac{a_0}{\alpha} e^{-a_0(1+x)} + \mathcal{O}(e^{-a_1 x}), \qquad x \to \infty, \tag{3}$$

where C_0 is the constant:

$$C_0 = \frac{\sin \pi\alpha}{\pi} = \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)} \tag{4}$$

and where $-a_0$ is the real zero of the function $z^\alpha \gamma(-\alpha, z)$ and $a_1 > a_0$ (see the reference for details).

3.1 Explicit forms of the density

Theorem 2 *Let $0 < \alpha < 1$. The Darling–Mandelbrot density $g(x)$ is equal to:*

$$g(x) = \sum_{k=0}^{\infty} g_k(x), \tag{5}$$

where the function $g_k(x)$ is supported for $x > k$, analytic on its support, and has the two following equivalent definitions.

- *Let $a(x)$ and $b(x)$ be the functions, supported for $x > 0$ and $x > 1$ respectively, defined by:*

$$a(x) = C_0 x^{\alpha-1} \qquad \text{and} \qquad b(x) = -C_0 \frac{(x-1)^\alpha}{x},$$

where C_0 is defined by (4)*. Then $g_k(x)$ is equal to the convolution product:*

$$g_k(x) = a * \underbrace{b * \cdots * b}_{k \text{ times}}(x). \tag{6}$$

- *Let:*

$$\beta_k = \alpha + k(1+\alpha) \qquad \textit{and} \qquad C_k = \frac{1}{\Gamma(1-\alpha)\Gamma(-\alpha)^k\Gamma(\beta_k)}.$$

Then $g_k(x)$ has the power series representation[ii] *convergent for $k < x < k+1$ and analytically continuable for $x \geq k+1$:*

$$g_k(x) = C_k(x-k)^{\beta_k - 1} \sum_{n_1,\dots,n_k \geq 0} \frac{(1+\alpha)_{n_1} \cdots (1+\alpha)_{n_k}}{(\beta_k)_{n_1+\cdots+n_k}} (k-x)^{n_1+\cdots+n_k}, \tag{7}$$

where $(z)_n = \Gamma(z+n)/\Gamma(z)$ is the Pochhammer symbol for the rising factorial.

Again, we make some remarks before proving the theorem. First, since the summand $g_k(x)$ has support for $x > k$, the infinite sum in (5) is locally finite; moreover, since $b(x)$ is negative, the summands alternate in sign. In particular, if $x \leq 1$, we have $g(x) = g_0(x) = C_0 x^{\alpha-1}$. This shows that the error term in (2) is in fact zero. In the case $k = 1$, the sum in (7) takes the form of a hypergeometric function:

$$g_1(x) = C_1(x-1)^{2\alpha}\, {}_2F_1(1, 1+\alpha; 1+2\alpha; 1-x).$$

For $\alpha = 1/2$, this simplifies into:

$$g_1(x) = \frac{x^{-1/2} - 1}{\pi}.$$

Finally, the theorem enables us to find the singularities of the density $g(x)$. Since the leading term in the sum in (7) is 1, the function $g_k(x)$ has a singularity at k of the form:

$$g_k(x) = C_k(x-k)^{\beta_k - 1}\, \mathbf{1}_{x>k} + \mathcal{O}\big((x-k)^{\beta_k}\big).$$

Moreover, as the function $g_k(x)$ is analytic for $x > k$ and the sum (5) is locally finite, the density $g(x)$ is singular at all integer points and analytic otherwise, with the singularity at the point $x = k$ corresponding to the singularity of $g_k(x)$.

Plots of the density $g(x)$ are shown in Figure 1.

Proof of Theorem 2: Let us first prove the convolution product representation. From the identity (1) we find the Laplace transform of $g(x)$, that we denote by $G(z)$:

$$G(z) = \phi_\alpha(iz) = \frac{z^{-\alpha}}{-\alpha\gamma(-\alpha, z)}.$$

We transform this into:

$$G(z) = \frac{z^{-\alpha}}{-\alpha\big[\Gamma(-\alpha) - \Gamma(-\alpha, z)\big]} = \sum_{k\geq 0} A(z)B(z)^k,$$

where $\Gamma(\cdot,\cdot)$ is the upper incomplete gamma function and:

$$A(z) = \frac{z^{-\alpha}}{\Gamma(1-\alpha)} \qquad \text{and} \qquad B(z) = \frac{\Gamma(-\alpha, z)}{\Gamma(-\alpha)}$$

[ii] The sum in this expression can be seen as a special case of the Lauricella function $F_B^{(k)}$ where all variables are specialized to $-x$.

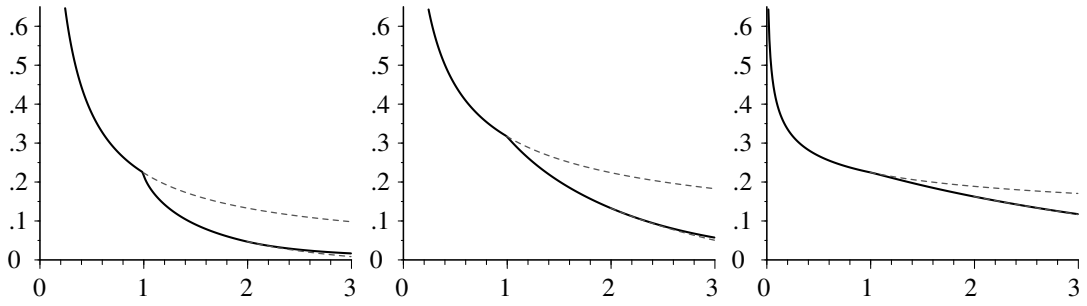

Fig. 1: Plots of the density $g(x)$ for $\alpha = 1/4$, $\alpha = 1/2$ and $\alpha = 3/4$ (from left to right). Dashed, the continuation of the partial sums $g_0 + \cdots + g_k$ beyond $x = k + 1$. The precision is far beyond line thickness (as easily obtained through the characterisation of the forthcoming Theorem 3).

(if z is large enough so that $|B(z)| < 1$; numerically, $\mathfrak{Re}(z) > 0.107878\ldots$ suffices, uniformly for all α).

Elementary integral computations show that the functions $a(x)$ and $b(x)$ defined in the theorem have Laplace transforms $A(z)$ and $B(z)$, respectively. Inverse Laplace transform thus yields (6). As the convolution product of analytic functions, the function $g_k(x)$ is analytic for $x > k$.

Let us now prove the power series representation. Let $1 < x < 2$. A Taylor expansion of the function $b(x)$ yields:

$$b(x) = C_0 \sum_{n\geq 0} (-1)^{n+1} (x-1)^{\alpha+n}.$$

Using the fact that the convolution product commutes with translations and expanding the equation (6), we find, for $k < x < k + 1$:

$$g_k(x) = C_0^{k+1} \sum_{n_1,\ldots,n_k\geq 0} (-1)^{k+n_1+\cdots+n_k} \left[x^{\alpha-1} * x^{\alpha+n_1} * \cdots * x^{\alpha+n_k}\right](x-k).$$

To lighten notation, set $n = n_1 + \cdots + n_k$. The convolution product transforms into:

$$g_k(x) = C_0^{k+1} \sum_{n_1,\ldots,n_k\geq 0} (-1)^{n+k} \frac{\Gamma(\alpha)\Gamma(1+\alpha+n_1)\cdots\Gamma(1+\alpha+n_k)}{\Gamma(\beta_k+n)} (x-k)^{\beta_k-1+n}.$$

The identity (7) follows by elementary operations on gamma functions. Finally, since $g_k(x)$ is analytic for $x > k$, its value for $x \geq k + 1$ can be found by analytic continuation. □

3.2 Differential equations satisfied by the density

In this section, we characterize the density g not explicitly, but implicitly as the solution of differential equations. Since g is singular at all integer points, all differential equations are understood to be satisfied only outside singular points.

Theorem 3 *The density $g(x)$ is the only continuous solution of the non-linear differential equation:*

$$-\frac{x}{\alpha} g'(x) - \frac{1-\alpha}{\alpha} g(x) = g * g(x-1), \tag{8}$$

with initial condition (2).

As the density g is positive, this result shows in particular that g is decreasing. In fact, it implies the stronger statement that $x^{1-\alpha}g(x)$ is nonincreasing. This answers a question of Lew, who suggested that $g(x)$ might show oscillations for small values of α.

Proof: Let us prove that g satisfies the equation. One way to proceed is by differentiating the Laplace transform $G(z)$. Another way, that we detail here, is to compare the threshold sum processes at thresholds t and $t(1+\varepsilon)$ and let ε tend to 0. There are two cases:

- if $X_{I(t)} \geq t(1+\varepsilon)$, then $Y_{t(1+\varepsilon)} = Y_t$. This occurs with probability $F(t(1+\varepsilon))/F(t) \sim 1-\varepsilon\alpha$;
- otherwise, at leading order in ε, we have $Y_{t(1+\varepsilon)} = Y_t + t + Y_t'$, where Y_t' is independent from and distributed like Y_t.

Dividing by t and remembering that Y_t/t tends to the law of density g, we get, as t tends to infinity:

$$\frac{1}{1+\varepsilon}g\left(\frac{x}{1+\varepsilon}\right) = (1-\varepsilon\alpha)g(x) + \varepsilon\alpha\, g * g(x-1) + \mathcal{O}(\varepsilon^2).$$

At first order in ε, we recover (8).

To show the uniqueness of the solution, we note that the right hand side of (8) depends only on the values of $g(y)$ for $y < x-1$; in particular, it is zero for $x < 1$. This enables us to solve iteratively the equation on the intervals $[k, k+1]$, treating the equation as an inhomogenous linear differential equation, with the initial value $f(k)$ found by continuity. This determines the solution uniquely. □

Our final result writes the density g as the solution of linear differential equations. Write $d_x = d/dx$ and let D_k and E_k be the differential operators:

$$D_k = (x-k)d_x + 1 - (k+1)\alpha; \qquad\qquad E_k = D_{k-1}\cdots D_0.$$

Theorem 4 *The operator E_k cancels the functions $g_0, \ldots, g_{k-1}$ defined in Theorem 2. In particular, it cancels the density g on the interval $[0, k]$.*

Proof: To prove the theorem, we need the following elementary facts about convolution products:

$$(u * v)' = u' * v; \qquad\qquad x(u * v) = (xu) * v + u * (xv).$$

We first prove by induction that, for $0 \leq \ell \leq k$, we have:

$$E_\ell \cdot g_k = \frac{k!}{(k-\ell)!}a_\ell * b^{*k-\ell} \qquad \text{where} \qquad a_\ell(x) = \frac{(x-\ell)^{(\ell+1)\alpha-1}}{\Gamma(1-\alpha)\Gamma(-\alpha)^\ell\Gamma\big((\ell+1)\alpha\big)}\mathbf{1}_{x>\ell}.$$

For $\ell = 0$, this is obvious as $a_0 = a$. Otherwise, assume that the identity is true and apply the operator D_ℓ to it. Using the above properties of convolution products, we have:

$$E_{\ell+1} \cdot g_k = \frac{k!}{(k-\ell)!}(D_\ell \cdot a_\ell) * b^{*k-\ell} + \frac{k!}{(k-\ell-1)!}a_\ell' * (xb) * b^{*k-\ell-1}.$$

Since D_ℓ annihilates a_ℓ, we conclude using the easily checked fact that $a_\ell' * (xb) = a_{\ell+1}$.

At $\ell = k$, we thus find $E_k \cdot g_k = k!a_k$. Since $D_k \cdot a_k = 0$, we have indeed $E_\ell \cdot g_k = 0$ for $\ell > k$. □

4 Applications

In this section, we apply our results to the analysis in limit law of random sampling algorithms. In all cases, this complexity is linked to a threshold sum process that falls within the conditions of Theorem 1. Among the three regimes in this theorem, the most favorable is the first one, with the scaling factor t meaning that the algorithm has linear complexity.

In the following, it will be convenient to consider the Darling–Mandelbrot distribution *shifted by one*, with characteristic function $e^{is}\phi_\alpha(s)$ (this coincides with Darling's initial definition). We denote by $\mathcal{D}(\alpha)$ this shifted distribution.

In some of the algorithms mentioned below, the limit law is not $\mathcal{D}(\alpha)$, but of the form $Y_1 + \cdots + Y_Z$, where the Y_i's are independent variables following the law $\mathcal{D}(\alpha)$ and $Z \geq 1$ is geometrically distributed with parameter p. Let $\mathcal{D}(\alpha, p)$ denote such a distribution and $e^{is}\phi_{\alpha,p}(s)$ be its characteristic function. We have:

$$\phi_{\alpha,p}(s) = \frac{p\,\phi_\alpha(s)}{1-(1-p)e^{is}\phi_\alpha(s)} = \left(1 - \sum_{n=1}^{\infty} \frac{\frac{1-p}{p}n + \alpha}{n-\alpha}\frac{(is)^n}{n!}\right)^{-1}. \tag{9}$$

4.1 Prefixes of Motzkin paths and directed animals

The simplest algorithm that fits in our framework is probably the one described in [BPS94,], which samples prefixes of Motzkin paths (i.e., lattice paths with steps in $\{\nearrow, \searrow, \rightarrow\}$ never stepping lower than their origin). Using a bijection of Penaud, they thus get a random sampling algorithm for directed animals. A generalization appears in [BPS94,], which deals with the case where there are several possible steps of each type (colored Motzkin prefixes).

The algorithm is very simple: the path is built by adding random steps one at a time. If, at any time, the path steps below the origin, the algorithm is started over from scratch. If the target size n is reached, the path is output. To our knowledge, this is the best known algorithm for exactly sampling such structures, with the exception of the special case in which there is no $\rightarrow$ step (i.e., *prefixes of Dyck paths*).[(iii)]

Proposition 5 *Assume the number of possible $\nearrow$ and $\searrow$ steps is the same. Let Y_n be the number of steps drawn by the algorithm to sample a path of length n. As n tends to infinity, the random variable Y_n/n tends in distribution to the law $\mathcal{D}\left(\frac{1}{2}\right)$.*

In particular, we recover estimates of the expected value and variance given by Barcucci et al., namely:

$$\mathbb{E}(Y_n) \sim 2n; \qquad \mathbb{V}(Y_n) \sim \frac{4}{3}n^2.$$

Proof: Let k be the total number of available steps. If there are as much different $\nearrow$ and $\searrow$ steps, the number m_n of Motzkin prefixes of length n satisfies $m_n \sim ck^n n^{-1/2}$, where c is a constant.

Let X be the random variable counting the number of steps before a random path goes below the origin. We have $X > n$ if and only if the first n steps form a Motzkin prefix, which happens with probability $m_n/k^n \sim cn^{-1/2}$.

The random variable Y_n consists of two parts: the cost of the unsuccessful trials, which follows a threshold sum process with base distribution X and threshold n, and the cost of the final successful trial, which is n. By Theorem 1, the quotient Y_n/n thus tends to the shifted law $\mathcal{D}\left(\frac{1}{2}\right)$. □

[(iii)] To sample these, a better (in fact, optimal) algorithm consists in using the algorithm of [BBJ14,] to sample a pointed binary plane tree and using classical bijections to get a Dyck prefix.

4.2 Prefixes of Schröder paths

A variant of the previous algorithm, sampling prefixes of Schröder paths, is found in [Bac14,], in relation to directed animals on the king's lattice. A Schröder path has the same constraints as a Motzkin path and takes steps in $\{\nearrow, \searrow, \longrightarrow\}$ (where $\longrightarrow$ has length 2).

The algorithm is similar to the one above, but the steps $\nearrow, \searrow, \longrightarrow$ are taken with respective probabilities ρ, ρ, ρ^2 with $\rho = \sqrt{2}-1$. There is another difference: when sampling for a target size n, it is possible to jump from $n-1$ to $n+1$ by generating a $\longrightarrow$. In this case, we must discard the path and start over. As the following result shows, this modifies slightly the limit behavior of the complexity while keeping it linear.

Proposition 6 *Let Y_n be the total length of the steps drawn by the algorithm to sample a Schröder prefix of length n. The random variable Y_n/n tends in distribution to the law $\mathcal{D}\big(\frac{1}{2}, \frac{2+\sqrt{2}}{4}\big)$.*

From (9), we get the expected value and variance of Y_n:

$$\mathbb{E}(Y_n) \sim \big(8-4\sqrt{2}\big)n; \qquad \mathbb{V}(Y_n) \sim \frac{16}{3}\big(16-11\sqrt{2}\big)n^2.$$

Proof: Let s_n be the number of Schröder prefixes of length n and p_n be the probability to reach one of them. As we have $s_n \sim c\rho^{-n}n^{-1/2}$, we have $p_n \sim cn^{-1/2}$, where c is a constant.

Let X be the random variable counting the length of the path sampled before it goes below the origin. The event $X \geq n$ can occur in two ways: either we sample a Schröder prefix of length n or a prefix of length $n-1$ followed by a $\longrightarrow$; the probability of this is $p_n + \rho^2 p_{n-1} \sim (1+\rho^2)cn^{-1/2}$. In the same way as for Proposition 5, the time necessary to reach this tends in distribution to $\mathcal{D}\big(\frac{1}{2}\big)$.

Finally, out of the two above possibilities, we are interested only in the case where we draw a Schröder prefix of length n. This happens with probability $p_n/(p_n + \rho^2 p_{n-1}) \to 1/(1+\rho^2) = (2+\sqrt{2})/4$. The number of times the size n is reached is geometrically distributed, hence the result. □

4.3 Unary-binary trees

Another recent anticipated rejection algorithm appears in [BBJ14,], sampling unary-binary plane trees. The algorithm works by letting a tree grow from size 1 to n using a *grafting* process akin to Rémy's algorithm for binary trees. This process may fail, however, in which case the algorithm is restarted. For our analysis, we use the following two facts: first, the probability of sampling a tree of size n satisfies $p_n \sim cn^{-1/2}$, with c a constant; second, at each step, the tree grows by 1 or 2 nodes with respective probabilities $2/3$ and $1/3$. If this takes the size of the tree from $n-1$ to $n+1$, the algorithm is restarted.

Proposition 7 *Let Y_n be the number of nodes of the trees built by the algorithm to sample a tree with n nodes. The random variable Y_n/n tends in distribution to the law $\mathcal{D}\big(\frac{1}{2}, \frac{3}{4}\big)$.*

Again, we deduce the expected value and variance from (9):

$$\mathbb{E}(Y_n) \sim \frac{8}{3}n; \qquad \mathbb{V}(Y_n) \sim \frac{32}{9}n^2.$$

Proof: The proof is identical to the one of Proposition 6. The form of the probability p_n shows that the time necessary to reach size n is, normalized by n, distributed like $\mathcal{D}\big(\frac{1}{2}\big)$. Knowing we have reached at least n nodes, the probability to hit exactly n is $p_n/(p_n + 1/3p_{n-1}) \to 3/4$. This concludes the proof. □

4.4 Random walks in conical domains

In this section, we study models of constrained random walks. The complexity of the anticipated rejection algorithm is governed by the survival probability of the model, that is, the probability of a random walk of length t to satisfy the constraints.

The first case is random walks in $\mathbb{Z}^2$ constrained to remain in a wedge of angle θ. As explained in [Red01, Section 7.2], the survival probability satisfies in this case $F(t) \sim ct^{-\pi/(2\theta)}$, so that $2\theta\alpha = \pi$ (this result is actually due to Sommerfeld). This gives an exponent α ranging from $1/4$ (for excluding just a half-line) to arbitrarily large (for a narrow wedge); however, arbitrarily small values of α can be found by considering values of θ greater than 2π, by taking into account the winding number of the walk. In particular, we find:

- for $\theta > \pi/2$, the algorithm has linear average complexity and limit law $\mathcal{D}\big(\frac{\pi}{2\theta}\big)$.
- for $\theta = \pi/2$, the algorithm has average complexity $n \log n$ and exponential limit law;
- for $\theta < \pi/2$, the algorithm has average complexity $\mathcal{O}\big(n^{\frac{\pi}{2\theta}}\big)$ and an exponential limit law.

For specific values of θ, these walks can be realized as *walks in the quarter plane* with some prescribed steps [BM10,]. For instance, Gessel's walks, with steps $\{\swarrow, \leftarrow, \nearrow, \rightarrow\}$, correspond to walks in the square lattice in a wedge of angle $3\pi/4$. The variant of Kreweras' walks with steps $\{\downarrow, \swarrow, \leftarrow, \uparrow, \nearrow, \rightarrow\}$ correspond to walks in the triangular lattice in a wedge of angle $2\pi/3$. The anticipated rejection algorithm thus has linear complexity in both cases, with respective limit laws $\mathcal{D}\big(\frac{2}{3}\big)$ and $\mathcal{D}\big(\frac{3}{4}\big)$.

A more complicated case is random walks in $\mathbb{Z}^3$ constrained in a cone defined by $\theta < \theta_{\max}$ (in spherical coordinates). In this case, the survival probability is $F(t) \sim ct^{-\nu/2}$, where ν is the smallest positive number such that $P_\nu(\cos\theta_{\max}) = 0$, where P_ν is the Legendre function [Red01, Section 7.3]. This allows for the exponent $\alpha = \nu/2$ to be any positive number. In particular, since $P_2(x) = (3x^2-1)/2$, an exponent $\alpha < 1$, and thus a linear-time algorithm, is achieved for $\theta_{\max} > \arccos(1/\sqrt{3})$.

In fact, generic cones in generic dimensions can also be handled in this way; see [DWar,] for full details[(iv)]. Let Ω be a cone of $\mathbb{R}^d$ and let $\Omega_0 = \Omega \cap \mathbb{S}^{d-1}$. The survival probability in the cone Ω satisfies:

$$F(t) \sim ct^{-\nu/2},$$

where ν is the smallest positive number such that there exists a function $h_\nu(\theta)$ on the unit sphere vanishing at the border of Ω_0 and satisfying:

$$\Delta_S h_\nu(\theta) = -\lambda h_\nu(\theta), \qquad \lambda = \nu(\nu + d - 2),$$

where Δ_S is the spherical Laplace operator.

Thus, we are again in the conditions of Theorem 1, with $\alpha = \nu/2$. The exponent ν is, however, difficult to compute in general.

4.5 More complex random walk problems

In the previous section we considered random walks on a lattice that shall avoid some "wall" prescribed deterministically. Here we consider a more complex problem in which the growing structure produces the

[(iv)] We thank M. Bousquet-Mélou and K. Rashel for having suggested us this reference.

walls dynamically. Say that two paths on a graph *intersect* if they share some vertex. We have two classes of problems: (P1) a walk ω of length n, starting at a neighbour of the origin, such that there exists some infinite walk connecting the origin to infinity and not intersecting ω. (P2) for $k \geq 2$, k-tuples of walks $(\omega_1, \ldots, \omega_k)$, of length n, starting from nearby vertices (e.g., aligned along a line), that shall not intersect each other.

For undirected random walks, the simplest lattice is $\mathbb{Z}^D$, i.e. with the $2D$ possible steps $\{s^\alpha\} = \{(0, 0, \ldots, \pm 1, \ldots, 0)\}$ uniformly chosen. The correspective for directed random walks is $\mathbb{N} \times \mathbb{Z}^{D-1}$, i.e. with the $2(D-1)$ possible steps $\{s^\alpha\} = \{(1, 0, \ldots, \pm 1, \ldots, 0)\}$ uniformly chosen. More generally, we may consider unbiased isotropic (undirected) random walks i.e., walks that can perform steps $s^\alpha \in \mathbb{Z}^D$ with weight w_α, such that $\sum_\alpha w_\alpha s_i^\alpha = 0$ for all $i = 1, \ldots, D$ and $\sum_\alpha w_\alpha s_i^\alpha s_j^\alpha = C\delta_{ij}$. In the directed variant we have $s_1^\alpha = 1$ for all steps α, and all other compatible constraints are left as are.

The associated exponents, when non-trivial (i.e., for D sufficiently small), are in general hard to evaluate. For directed walks in $D = 2$, (P1) is trivial, and (P2) is called *vicious walkers*. Things become easier, and well-known works on the relation with classical ensembles of random matrices give $\alpha = k(k-1)/4$, thus we have no problems in the interesting range $0 < \alpha < 1$, except for $k = 2$, which, on $\mathbb{N} \times \mathbb{Z}$, reduces to prefixes of Dyck paths through a simple bijection [(v)].

For undirected walks in $D = 2$, conformal invariance, and even better the connection with the exactly solvable analysis on random planar graphs via KPZ relation ([KPZ88]), lead to conjectures which are well-verified numerically and widely believed (see [Dup98] and references therein). We have $\alpha = \frac{1}{24}(4k^2 - 1)$, in a unified formula for (P1) (using $k = 1$) and for (P2).[(vi)] Thus we have two new problems in the interesting range: problem (P1), following the law $\mathcal{D}(\frac{1}{8})$, and problem (P2) with $k = 2$, following the law $\mathcal{D}(\frac{5}{8})$.

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[(v)] It is worth noting that, still on $\mathbb{N} \times \mathbb{Z}$, and at generic k, in the variant in which the endpoints are prescribed, exact enumeration formulas allow for an optimal algorithm, involving no anticipated rejection (see [Bon02, Chapt. 4]). We thank the anonymous referee for pointing us towards this reference.

[(vi)] Incidentally, note that also in the directed case the formula for $\alpha(k)$ matches with the trivial value $\alpha = 0$ for problem (P1).

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Some reflections on directed lattice paths.

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Abstract. This article analyzes *directed lattice paths*, when a boundary reflecting or absorbing condition is added to the classical models. The lattice paths are characterized by two time-independent sets of rules (also called steps) which have a privileged direction of increase and are therefore essentially one-dimensional objects. Depending on the spatial coordinate, one of the two sets of rules applies, namely one for altitude 0 and one for altitude bigger than 0. The abscissa $y = 0$ thus acts as a border which either absorbs or reflects steps. The absorption model corresponds to the model analyzed by Banderier and Flajolet ("Analytic combinatorics of directed lattice paths"), while the reflecting model leads to a more complicated situation. We show how the generating functions are then modified: the kernel method strikes again but here it unfortunately does not give a nice product formula. This makes the analysis more challenging, and, in the case of Łukasiewicz walks, we give the asymptotics for the number of excursions, arches and meanders. Limit laws for the number of returns to 0 of excursions are given. We also compute the limit laws of the final altitude of meanders. The full analytic situation is more complicated than the Banderier–Flajolet model (partly because new "critical compositions" appear, forcing us to introduce new key quantities, like the drift at 0), and we quantify to what extent the global drift, and the drift at 0 play a rôle in the "universal" behavior of such walks.

Keywords: Lattice Path; Analytic Combinatorics; Singularity Analysis; Limit Laws; Space Inhomogenous Walk; Kernel method

1 Introduction

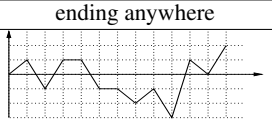
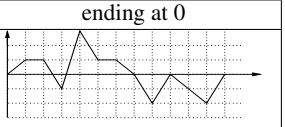
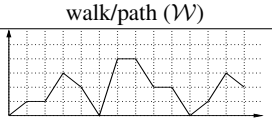
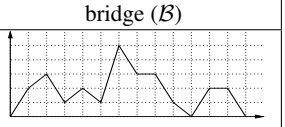
In Brownian motion theory, many possible boundary conditions for a Brownian-like process have been considered (e.g. absorption, killed Brownian motion, reflected Brownian motion... see [Fel54]). Solving a stochastic differential equation with a reflecting boundary condition is known as the Skorokhod problem (see [Sko62]). Such models appear e.g. in queueing theory (see [Kin62]). In this article, we want to investigate properties of a discrete equivalent of such models, namely directed lattice paths in $\mathbb{Z}^2$, having a reflecting boundary at $y = 0$.

If one considers lattice paths which are "killed" or "absorbed" at $y = 0$, then this is equivalent to the model analyzed in [BF02]. In what follows, we want to compare the basic properties (exact enumeration, asymptotics, limit laws) of these two discrete models (absorption versus reflection). In particular, we will consider the Łukasiewicz paths (defined hereafter), which are present in numerous fields like algebra, analysis of algorithms, combinatorics, language theory, probability theory and biology. This broad applicability is due to a bijection with simple families of trees, see e.g. [MM78]. The enumerative and analytic properties of such lattice paths were considered in [BG06] where limit laws for the area beneath

Łukasiewicz paths are derived, and also in [BIP11] where they are used to model polymers in chemistry, or e.g. in [BN10], which tackles the problem of enumeration and asymptotics of such walks of bounded height.

Our key tools will be the kernel method and analytic combinatorics (see [FS09]). However, as we will see, the situation is more complicated in the case of a reflecting boundary: first, bad luck, one does not have a nice product formula for the generating function anymore (unlike the absorption model), second, the drift still plays a key rôle, but also does a "second" drift at 0, and last but not least, several simultaneous singular behaviors can happen. We first begin with a few definitions:

Definition 1.1: A *step set* $\mathcal{S} \subset \mathbb{Z}^2$, is a finite set of vectors $\{(a_1, b_1), \ldots, (a_m, b_m)\}$. An n-step *lattice path* or *walk* is a sequence of vectors $v = (v_1, \ldots, v_n)$, such that v_j is in $\mathcal{S}$. Geometrically, it is a set of points $\omega = (\omega_0, \omega_1, \ldots, \omega_n)$ where $\omega_i \in \mathbb{Z}^2, \omega_0 = (0, 0)$ and $\omega_i - \omega_{i-1} = v_i$ for $i = 1, \ldots, n$. The elements of $\mathcal{S}$ are called *steps* or *jumps*. The *length* $|\omega|$ of a lattice path is its number n of jumps. $\Diamond$

	ending anywhere	ending at 0
unconstrained (on $\mathbb{Z}$)	 walk/path ($\mathcal{W}$)	 bridge ($\mathcal{B}$)
constrained (on $\mathbb{N}$)	 meander ($\mathcal{M}$)	 excursion ($\mathcal{E}$)

Tab. 1: The four types of paths: walks, bridges, meanders and excursions.

We restrict our attention to *directed paths* which are defined by the fact that for $(a, b) \in \mathcal{S}$ one must have $a > 0$. However, we will focus only on the subclass of *simple paths*, where every element in the step set $\mathcal{S}$ is of the form $(1, b)$. In other words, these walks constantly move one step to the right, thus they are essentially unidimensional objects. We introduce the abbreviation $\mathcal{S} = \{b_1, \ldots, b_n\}$ in this case. A *Łukasiewicz path* is a simple path where its associated step set $\mathcal{S}$ is a subset of $\{-1, 0, 1, \ldots\}$ and $-1 \in \mathcal{S}$.

Definition 1.2: For a given step set $\mathcal{S} = \{s_1, \ldots, s_m\}$, we define the respective *system of weights* as $\{w_1, \ldots, w_m\}$ with $w_j > 0$ the associated weight to step s_j for $j = 1, \ldots, m$. The *weight of a path* is defined as the product of the weights of its individual steps. $\Diamond$

This article mainly builds on the work done in [BF02]. Therein, the class of directed lattice paths in $\mathbb{Z}^2$ (under the absorption model) was investigated thoroughly by means of analytic combinatorics (see [FS09]). First, in Section 2, the reflection-absorption model and the general framework are introduced. The needed bivariate generating function is defined and the governing functional equation is derived and solved: here the "kernel method" plays the most significant rôle in order to obtain the generating function (as typical for many combinatorial objects which are recursively defined with a "catalytic parameter", see [BMJ06]). In Section 3, we turn our attention to Łukasiewicz paths, and the asymptotic number of excursions is given. In Section 4, the limit laws for the number of returns to zero of excursions are derived. In Section 5, we establish the asymptotics of meanders. Section 6 gives the asymptotics for the expected final altitude of meanders.

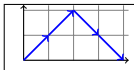
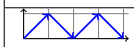
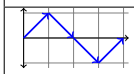
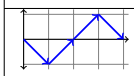
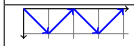
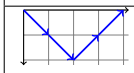
2 Generating functions

Let us consider directed walks on $\mathbb{N}^2$, with a weighted step set $\mathcal{S}$, starting at the origin, confined to the upper half plane, and which have another weighted step set $\mathcal{S}_0$ on the boundary $y = 0$. All such walks are called *meanders*, and the meanders ending on the abscissa are called *excursions*.

This walk model is thus encoded by two *characteristic polynomials*: $P(u)$ and $P_0(u)$ are Laurent polynomials describing the allowed jumps when the walk is at altitude $k > 0$ or $k = 0$, respectively. We fix $c, d, c_0, d_0 \in \mathbb{N}$ and introduce the following notations:

$$P(u) = \sum_{i=-c}^{d} p_i u^i, \qquad P_0(u) = \sum_{i=-c_0}^{d_0} p_{0,i} u^i, \qquad P_0^{\geq}(u) = \sum_{i=0}^{d_0} p_{0,i} u^i.$$

In order to exclude trivial cases we require $p_c, p_d \neq 0$. These weights are probabilities, which means $p_i, p_{0,i} \geq 0$ and $P(1) = P_0(1) = 1$. These step polynomials characterize the *reflection-absorption model*: depending of the chosen weights, the boundary behaves like a reflecting or an absorbing wall. We talk about a *reflection model* if $P_0^{\geq}(u) = P_0(u)$, while we talk about an *absorption model* if $P_0^{\geq}(u) \neq P_0(u)$.

Dyck path	bridges, uniform model	absolute value of bridges	excursions, reflection model	excursions, absorption model
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$ [(i)]	$\frac{1}{2}$
	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{1}{2}$
	$\frac{1}{6}$	0	0	0
	$\frac{1}{6}$	0	0	0
	$\frac{1}{6}$	0	0	0
	$\frac{1}{6}$	0	0	0

Tab. 2: Different constraints on the boundary $y = 0$ lead to different probabilistic models. We give the probabilities of Dyck paths of length 4 in the uniform, absolute value, reflection, and absorption model. From this table, one can already see one paradox associated to the reflection model: one may think that the "reflection" will make the walk go far away. However, this is in part counterbalanced by the fact that 0 has a "heavier" weight in this model (no loss of mass here, contrary to the absorption model). Accordingly, there will be some interplay between the boundary, the drift of the walk and the drift at 0. We quantify this in our next sections.

[(i)] Note that the absolute value and the reflection model are in general not equivalent if the jumps (with their weights) are not symmetric: Let $P(u) = pu + qu^{-1}$ and $P_0(u) = p_0 u + q_0 u^{-1}$, then the probability of this first path (which is $1/3$ when $p = q = 1/2$ and $p_0 = 1$) is $1/(1 + q_0/q + p_0/p)$ in the absolute value model, while it is $p/(1 + p)$ in the reflection model.

We define the generating function for our meanders to be

$$F(z,u) := \sum_{n,k\geq 0} F_{n,k} u^k z^n = \sum_{n\geq 0} f_n(u) z^n = \sum_{k\geq 0} F_k(z) u^k,$$

where the polynomials $f_n(u)$ describe the possible positions after n steps, and where $F_k(z)$ are the generating functions of walks starting at 0 and ending at altitude k.

Theorem 2.1 (Generating function for meanders and excursions) *The bivariate generating function of meanders (where z marks size and u marks final altitude) in the reflection-absorption model is algebraic:*

$$F(z,u) = \frac{1 - z\sum_{k=0}^{c-1} r_k(u) F_k(z)}{1 - zP(u)}, \tag{1}$$

where r_k is a Laurent polynomial given by $r_k(u) = \sum_{j=-c}^{-k-1} p_j u^{j+k}$ for $k > 0$ and $r_0(u) = P(u) - P_0^{\geq}(u)$. Furthermore, the F_k's are algebraic functions belonging to $\mathbb{Q}(u_1, \ldots, u_c, p_{-c}, \ldots, p_d, p_0^0, \ldots, p_d^0, z)$, where the u_i's are the roots of the equation $1 - zP(u) = 0$, such that $\lim_{z\to 0} u_i(z) = 0$. The F_k's can be made explicit, e.g. the generating function for excursions is

$$F_0(z) = \frac{\sum_{\ell=1}^{c} (-1)^{\ell+1} u_\ell^{c-1} V(\ell)}{\sum_{\ell=1}^{c} (-1)^{\ell+1} u_\ell^{c-1} \left(1 - zP_0^{\geq}(u_\ell)\right) V(\ell)}, \tag{2}$$

where $V(\ell) = \prod_{\substack{1\leq m<n\leq c \\ m\neq\ell,\ n\neq\ell}} (u_m - u_n)$.

Proof (Sketch): It is straightforward to derive a recurrence relation, by a step-by-step approach:

$$f_0(u) = 1, \qquad f_{n+1}(u) = \{u^{\geq 0}\}\left[P(u)\{u^{>0}\}f_n(u) + P_0(u)\{u^0\}f_n(u)\right], \tag{3}$$

where $\{u^{>0}\}$ extracts all the monomials of positive degree in u. This recurrence leads to the following functional equation

$$F(z,u) = 1 + zP(u)F(z,u) - z\{u^{<0}\}P(u)F(z,u) - zF_0(z)\left(\{u^{\geq 0}\}P_0(u) - \{u^{\geq 0}\}P(u)\right), \tag{4}$$

$$F(z,u)(1 - zP(u)) = 1 - z\left(P(u) - P_0^{\geq}(u)\right)F_0(z) - z\sum_{k=1}^{c-1} r_k(u)F_k(z). \tag{5}$$

The main tool for solving the functional equation is the *kernel method*, which consists of binding z and u in such a way that the left hand side vanishes. From the theory of Newton–Puiseux expansions, we know that the kernel equation $1 - zP(u) = 0$ has $c + d$ distinct solutions, with c of them being called "small branches", as they map 0 to 0 and are in modulus smaller than the other d "large branches" which grow to infinity while approaching 0. We call the small branches $u_1, \ldots, u_c$.

Inserting the c small branches into (5), we get a linear system of c equations in c unknowns $F_0, \ldots, F_{c-1}$:

$$\begin{cases} u_1^c - z\sum_{k=0}^{c-1} u_1^c r_k(u_1) F_k(z) &= 0, \\ \qquad\qquad \vdots & \\ u_c^c - z\sum_{k=0}^{c-1} u_c^c r_k(u_c) F_k(z) &= 0. \end{cases}$$

The system is non-singular, as can be proven via the local behavior of the u_i's (and therefore of the $r_k(u_j)$'s) for $z \sim 0$. Using Cramer's formula on this matrix does not give (directly) a nice formula ; it is better to use first column subtraction for the r_k's in the corresponding determinants, and then expanding with respect to the $r_0(u_i)$ column leads to a nicer formula for each F_i via Vandermonde-like formulæ. □

Let us recall that the generating functions $\widetilde{E}(z)$ of the excursions in the absorption model of Banderier–Flajolet (i.e. when $P_0(u) = P(u)$) is given by $\widetilde{E}(z) = (-1)^{c+1}(\prod u_i(z))/(zp_{-c})$, see [BF02, Equation (20)]. It is interesting to compare this simple formula with the more cumbersome formula that one gets for the generating functions $E(z)$ of the excursions in our reflection-absorption model (coming from a rewriting of (2)):

$$E(z) := F_0(z) = \frac{\widetilde{E}(z)}{1 - z\widetilde{E}(z)\sum_{i=1}^{c} r_0(u_i)u_i^{c-1}/V(i)}\,. \tag{6}$$

In one sense, this formula quantifies to what extent the border "perturbs" the former $\widetilde{E}(z)$ to lead to our new $E(z)$. We now investigate the analytic counterparts of this perturbation.

3 Asymptotics of excursions

From now on, we are going to work with *aperiodic Łukasiewicz paths*. By these, we understand paths with one jump of size 1 down and finitely but arbitrarily many jumps up. Aperiodic means that there is no $p > 1$ and there exists no polynomial $H(u)$ s.t. $P(u) = u^{-1}H(u^p)$. Thus, the step polynomial is given as

$$P(u) = p_{-1}u^{-1} + p_0 + p_1u + \ldots + p_du^d,$$

with $p_{-1} + \ldots + p_d = 1$ and $p_i \in [0, 1]$. Since $c = 1$, the linear system derived from (5) transforms into

$$1 + z\left(P_0^{\geq}(u_1) - P(u_1)\right)F_0(z) = 0.$$

We use the kernel equation $1 - zP(u_1) = 0$ to derive the generating function of excursions:

$$E(z) := \sum e_n z^n := F_0(z) = \frac{1}{1 - zP_0^{\geq}(u_1(z))}. \tag{7}$$

This nice formula has a natural combinatorial interpretation as $\mathrm{Seq}\left(zP_0^{\geq}\left(\widetilde{E}(z)p_{-1}z\right)\right)$, i.e. an excursion (in the reflection model) is a sequence of arches (i.e. an excursion touching 0 just at its two ends), and each arch begins with a positive jump $+k$, which has to be compensated by k excursions (well, shifted excursions: from altitude j to altitude j, for j from 1 to k, thus not touching 0, and thus in bijection with excursions, counted by $\widetilde{E}(z)$ and defined above formula (6)) followed each by a -1 jump.

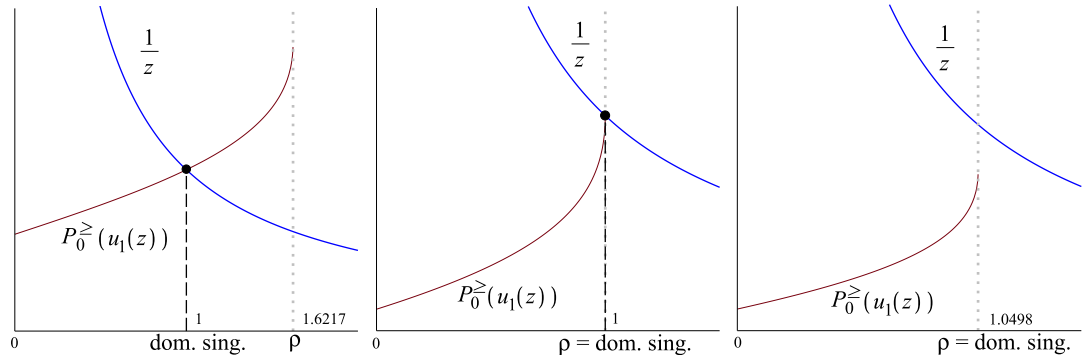
In [BF02, Equation (42)], it was shown that the principal branch $u_1(z)$ possesses the following asymptotic expansion for $z \to \rho^-$, where ρ is the structural radius defined as $\rho = \frac{1}{P(\tau)}$ and $\tau > 0$ is the unique root of $P'(\tau) = 0$ (note that P is a convex function):

$$u_1(z) = \tau - \sqrt{2\frac{P(\tau)}{P''(\tau)}}\sqrt{1 - z/\rho} + \mathcal{O}(1 - z/\rho), \qquad \text{for } z \to \rho^-. \tag{8}$$

As this expansion will appear repeatedly in the sequel, we define $C := \sqrt{2\frac{P(\tau)}{P''(\tau)}}$. The singularities of (7) depend on the roots of the denominator and on the singular behavior of $u_1(z)$, that is why we need the following lemma:

Lemma 3.1 (Singularity of the denominator) *Let $u_1(z)$ be the unique small branch of the kernel equation $1 - zP(u) = 0$. Then the equation $1 - zP_0^{\geq}(u_1(z)) = 0$ has at most one solution in $z \in (0, \rho]$, which we denote by ρ_1.*

Proof: The functions $u_1(z)$ and $P_0^{\geq}(u)$ are increasing on $[0, \rho)$ (see [BF02]). Figure 1 shows the three possible configurations. The naming convention is adopted from its use in functional composition schemes in [FS09, Chapter VI.9]. □



(a) supercritical case (b) critical case (c) subcritical case

Fig. 1: Different singular behaviors of the generating function for the number of excursions. The increasing function represents $P_0^{\geq}(u_1(z))$ where the decreasing function is $1/z$. The dotted line is at abscissa ρ and the dashed line marks the dominant singularity. The latter is either located at the intersection or at ρ.

Theorem 3.2 (Asymptotics of excursions) *Let τ be the structural constant determined by $P'(\tau) = 0$, $\tau > 0$, let $\rho = 1/P(\tau)$ be the structural radius and ρ_1 defined as in Lemma 3.1. Define the constants $\alpha = (P_0^{\geq}(u_1(z)))'\Big|_{z=\rho_1}$, $\gamma = \frac{1}{\alpha\rho_1^2+1}$, and $\kappa = C\rho(P_0^{\geq})'(\tau)$. The excursions in the reflection-absorption model possess the following asymptotic expansion:*

$$E(z) = \begin{cases} \gamma(1 - z/\rho_1)^{-1} + \mathcal{O}(1), & \text{supercritical case: } P(\tau) < P_0^{\geq}(\tau), \\ \frac{1}{\kappa}(1 - z/\rho)^{-1/2} + \mathcal{O}(1), & \text{critical case: } P(\tau) = P_0^{\geq}(\tau), \\ E(\rho) - E(\rho)^2\kappa(1 - z/\rho)^{1/2} + \mathcal{O}(1 - z/\rho), & \text{subcritical case: } P(\tau) > P_0^{\geq}(\tau). \end{cases} \quad (9)$$

Proof (Sketch): We investigate $E(z)$ by means of singularity analysis. Therefore, three different cases are distinguished as the dominant singularity depends on the singular behavior (as illustrated by Figure 1). Then, the analysis of the corresponding Puiseux expansion yields the result. □

4 Limit laws for the number of returns to zero

An *arch* is defined as an excursion of size > 0 whose only contact with the x-axis is at its end points. We denote the set of arches by $\mathcal{A}$. Every excursion (set $\mathcal{E}$) consists of a sequence of arches, i.e. $\mathcal{E} = \mathrm{SEQ}(\mathcal{A})$.

The symbolic method (see e.g. [FS09]) directly provides the functional equation

$$E(z) = \frac{1}{1 - A(z)}, \tag{10}$$

which is easily solved to give the generating function for arches $A(z) = 1 - \frac{1}{E(z)}$.

Proposition 4.1 (Asymptotics of arches) *For a Łukasiewicz walk, the number of arches satisfies*

$$[z^n]A(z) \underset{n\to\infty}{\sim} \frac{\kappa}{2\sqrt{\pi n^3}}, \qquad \textit{where } \kappa = C\rho(P_0^{\geq})'(\tau). \tag{11}$$

Proof (Sketch): Define $\lambda := \frac{P_0^{\geq}(\tau)}{P(\tau)} = \frac{\rho}{\rho_0^{\geq}}$, then by (7) we get for $z \to \rho-$ that $A(z) = zP_0^{\geq}(u_1(z)) = \lambda - \kappa\sqrt{1 - z/\rho} + \mathcal{O}(1 - z/\rho)$. □

A *return to zero* is a vertex of a path of altitude 0 whose abscissa is positive, i.e. the number of returns to zero is the number of times the abscissa is touched again after leaving the origin. In order to count the number of returns to zero of excursions of fixed size n, we can reverse the construction above for the generating function of arches. The generating function for excursions with exactly k returns to zero is equal to $A(z)^k$. As stated in [BF02], for any fixed k, this function also has a singularity of the square root type and is amenable to singularity analysis. Hence, we are able to derive the probability $\mathbb{P}_{n,k}$ that a random excursion of size n has exactly k returns to zero for any fixed k:

$$\mathbb{P}_{n,k} := \mathbb{P}[\text{size} = n,\ \#\text{ returns to zero} = k] = \frac{[z^n]A(z)^k}{[z^n]E(z)}. \tag{12}$$

Let X_n be the random variable for the number of arches among all excursions of size n. Note that X_n also represents the returns to zero of a random excursion of size n.

Theorem 4.2 (Limit laws for returns to zero) *Additionally to the previously used constants α, γ and κ, we define $\alpha_2 = (P_0^{\geq}(u_1(z)))''\Big|_{z=\rho_1}$. The number X_n of returns to zero of a random excursion of size n admits a limit distribution:*

1. *In the supercritical case, i.e. $P(\tau) < P_0^{\geq}(\tau)$,*

$$\frac{X_n - \mu n}{\sigma\sqrt{n}}, \qquad \mu = \gamma, \qquad \sigma = \alpha_2(\rho_1\gamma)^3 - \gamma + \gamma^2(\rho_1 + 2) - 2\gamma^3,$$

   converges in law to a Gaussian variable $N(0, 1)$.

2. *In the critical case, i.e. $P(\tau) = P_0^{\geq}(\tau)$, the normalized random variable $\frac{\kappa}{\sqrt{2\pi}}(X_n - 1)$, converges in law to a Rayleigh distribution defined by the density $xe^{-x^2/2}$.*

3. *In the subcritical case, i.e. $P(\tau) > P_0^{\geq}(\tau)$, the limit distribution of $X_n - 1$ is a discrete limit law, namely the negative binomial distribution $\mathrm{NegBin}(2, \lambda)$, with $\lambda = \rho/\rho_0^{\geq}$:*

$$\mathbb{P}(X_n - 1 = k) \sim (k + 1)\lambda^k(1 - \lambda)^2\,.$$

5 Asymptotics of meanders

A *meander* is the natural generalization of an excursion, as it is defined as a directed walk confined to the upper half plane. We want to investigate the number of meanders or equivalently the ratio of meanders among all walks. This is a way to measure the effect of removing the constraint of ending on the x-axis.

Theorem 5.1 (Asymptotics of meanders) *Consider Łukasiewicz walks in the absorption model. The asymptotic behavior of the ratio of meanders of size n is given in Table 3.*

$[z^n]M(z) \sim$	$\delta < 0$	$\delta = 0$	$\delta > 0$
Supercritical	$\frac{\rho_1 \gamma}{E(1)(\rho_1 - 1)} \rho_1^{-n}$	—	$1 - (1 - P_0^{\geq}(1))E(1)$
Critical	$\frac{\rho}{E(1)\kappa(\rho-1)} \frac{\rho^{-n}}{\sqrt{\pi n}}$	—	
Subcritical	$\frac{E(\rho)^2}{E(1)} \frac{\kappa\rho}{2(\rho-1)} \frac{\rho^{-n}}{\sqrt{\pi n^3}}$	$\frac{E(1)\kappa}{\sqrt{\pi n}}$	

Tab. 3: Asymptotic ratio of meanders in the absorption model ($P_0^{\geq}(1) < 1$) with the structural constant $\tau > 0$, $P'(\tau) = 0$, the structural radius $\rho = 1/P(\tau)$ and the drift $\delta = P'(1)$. The constant ρ_1 is defined in Lemma 3.1, whereas γ and κ are given in Theorem 3.2. The two missing cases for $\delta = 0$ are not possible in the absorption model.

Proof (Sketch): From (5), we get the bivariate generating function for meanders as

$$F(z,u) = \frac{1 - z\left(P(u) - P_0^{\geq}(u)\right)E(z)}{1 - zP(u)}. \tag{13}$$

Hence, the generating function $M(z)$ for meanders is given by substituting $u = 1$ in (13):

$$M(z) := F(z,1) = \frac{1}{1-z} - \left(1 - P_0^{\geq}(1)\right)\frac{zE(z)}{1-z}. \tag{14}$$

An elementary simplification of the last factor gives

$$[z^n]M(z) = 1 - \left(1 - P_0^{\geq}(1)\right)\left([z^n]\frac{E(z)}{1-z} - [z^n]E(z)\right). \tag{15}$$

The asymptotics of the last term are known from Section 3. For the function $\frac{E(z)}{1-z}$, we use (9) and elementary singularity analysis, like [FS09, Fig. VI.5]. The result follows by distinguishing all different cases. □

Remark 5.2: Formula (14) possesses a combinatorial interpretation: a walk can only be absorbed after hitting the x-boundary, and at this place the walk is thus an excursion. Let e_n be the probability that a random walk of length n is an excursion. A walk survives with probability $P_0^{\geq}(1)$ and is killed with probability $(1 - P_0^{\geq}(1))$. The probability m_{n+1} describing the number of meanders of length $n+1$ among all walks of length $n+1$ is given by all surviving walks of smaller length: $m_{n+1} = 1 - \left(1 - P_0^{\geq}(1)\right)\sum_{k=0}^{n} e_k$.

6 Final altitude of meanders

The *final altitude* of a path is defined as the ordinate of its endpoint.

Let X_n be the random variable associated to the final altitude of all meanders of length n. It satisfies

$$\mathbb{P}[X_n = k] = \frac{[z^n u^k]F(z,u)}{[z^n]F(z,1)}\,, \tag{16}$$

where $F(z,u)$ is the bivariate generating function for meanders from (13).

Theorem 6.1 (Final altitude of meanders) *Consider the model of Łukasiewicz walks. Let τ be the structural constant determined by $P'(\tau) = 0$, $\tau > 0$, $\delta = P'(1)$ be the drift and $\delta_0^{\geq} = (P_0^{\geq})'(1)$ be the drift at 0. The limit laws and the asymptotics of the expected final altitude of meanders for the reflection model are given in Table 4 and the ones for the absorption model are given in Table 5.*

	$\delta < 0$	$\delta = 0$	$\delta > 0$
Limit law	Discrete	Rayleigh	Gaussian
Supercritical	$\mathbb{E}[X_n] \sim \dfrac{\delta_0^{\geq} P''(1) + \delta {P_0^{\geq}}''(1)}{2\delta(\delta - \delta_0^{\geq})}$	—	$\mathbb{E}[X_n] \sim \delta n$
Critical	—	$\mathbb{E}[X_n] \sim \sqrt{\dfrac{2P''(1)n}{\pi}}$	
Subcritical	—	—	

Tab. 4: Asymptotics of $\mathbb{E}[X_n]$ in the reflection model (i.e. $P_0^{\geq}(1) = 1$). The unfilled cases are not occurring under this model.

	$\delta < 0$	$\delta = 0$	$\delta > 0$
Limit law	Discrete	Rayleigh	Gaussian
Supercritical	$\mathbb{E}[X_n] \sim \left(1 - \dfrac{1}{\rho_1}\right) \dfrac{E(1)F_u(\rho_1,1)}{E(\rho_1)}$	—	$\mathbb{E}[X_n] \sim \delta n$
Critical	$\mathbb{E}[X_n] \sim \kappa \left(1 - \dfrac{1}{\rho}\right) \dfrac{E(1)F_u(\rho,1)}{E(\rho)}$	—	
Subcritical	$\mathbb{E}[X_n] \sim r \left(1 - \dfrac{1}{\rho}\right) \dfrac{E(1)}{E(\rho)}$	$\mathbb{E}[X_n] \sim \sqrt{\dfrac{P''(1)\pi n}{2}}$	

Tab. 5: Asymptotics of $\mathbb{E}[X_n]$ in the absorption model ($P_0^{\geq}(1) < 1$). The unfilled cases are not occurring under this model. We denote by $F_u(\rho,1)$ the limit $z \to \rho$ and $u \to 1$ of the derivative of $F(z,u)$ with respect to u. Note that in $\frac{F_u(\rho,1)}{E(\rho)}$ the singularities at $z = \rho$ cancel and the limit exists. Furthermore, we have $r = F_u(\rho,1) - \frac{\delta\rho}{(1-\rho)^2}$.

Proof (Sketch): Definition (16) leads to the following formula for the expected value:

$$\mathbb{E}[X_n] = \frac{[z^n]\ \frac{\partial}{\partial u}F(z,u)\big|_{u=1}}{[z^n]F(z,1)}. \tag{17}$$

Differentiating the Formula (13) for $F(z,u)$ with respect to u yields

$$\frac{\partial}{\partial u}F(z,u)\bigg|_{u=1} = (P_0^{\geq})'(1)\frac{zE(z)}{1-z} + P'(1)\left(P_0^{\geq}(1) - P_0^{\geq}(u_1(z)\right)\frac{z^2E(z)}{(1-z)^2}. \tag{18}$$

As a next step, we evaluate the $[z^n]$-operator term by term. Firstly, note that the quotient $\frac{E(z)}{(1-z)^\beta}$ appears twice with $\beta = 1$ and $\beta = 2$. We use [FS09, Theorem VI.12], which gives the asymptotics for two generating functions with different radii of convergence, and previous results for E like Theorem 3.2. Secondly, the following lemma gives the behavior of the composition $P_0^{\geq}(u_1(z))$:

Lemma 6.2 (A Puiseux behavior lemma) *Let $P_0^{\geq}$ be the non-negative part of P_0, and u_1 be the small branch of the kernel equation in the Łukasiewicz case. Then*

$$P_0^{\geq}(u_1(z)) = \begin{cases} P_0^{\geq}(u_1(1)) - \alpha(1-z) + \frac{\alpha_2}{2}(1-z)^2 + o((1-z)^2), & \text{for } \rho > 1, \\ P_0^{\geq}(1) - \kappa\sqrt{1-z} + \mathcal{O}(1-z), & \text{for } \rho = 1, \end{cases}$$

with $\alpha = \left(P_0^{\geq} \circ u_1\right)'(1) = -(P_0^{\geq})'(u_1(1))/P'(u_1(1))$ and $\alpha_2 = \left(P_0^{\geq} \circ u_1\right)''(1)$.

The computations of the asymptotics of the expected value are then finalized by considering that the denominator of (17) is either 1 in the reflection model or its asymptotics is given by Theorem 5.1 in the absorption model.

We now turn to the derivation of the underlying limit laws. Let u be a fixed positive real number in $(0,1)$. Then the dominant singularity of $F(z,u)$ is either $z = \rho$, the singularity of $E(z)$, or $z = 1/P(u)$, the singularity of the denominator (compare (13)). Which one is the dominant one? This depends on the value of the drift δ:

- If the drift is negative then, the dominant singularity is found at $z = \rho$ and by the "continuity theorem of discrete laws", Theorem IX.1 from [FS09], this leads to a discrete limit law.
- If the drift is zero then, the dominant singularity is at $z = \rho = 1/P(1) = 1$ and by the application of the "semi-large powers theorem" (see [BFSS01]), this leads to a Rayleigh limit law, see also [DS97].
- If the drift is positive then, in the needed environment of $u = 1$, the dominant singularity is found at $z = 1/P(u)$ (this is due to $\rho > 1$ in this case) and by the application of the "quasi-powers theorem" (Theorem IX.8 from [FS09]), this leads to a Gaussian limit law.

The special rôle of the drift and an intuition of the underlying limit laws can be obtained by considering the influence of the drift on the expected number of meanders in Theorem 5.1. □

7 Conclusion

In this article, we investigated the generating functions of lattice paths on $\mathbb{N}$ with an absorbing or reflecting border at 0. To sum it up, our analysis of this reflection-absorption model can be divided into three parts. Firstly, we determined the general formula for the generating function by means of the kernel method. Secondly, we focused on Łukasiewicz walks (i.e. the family of lattice paths in bijection with trees), and derived asymptotic results on the number of meanders and excursions, by means of singularity analysis and transfer theorems from analytic combinatorics. Thirdly, we investigated the limit laws for the returns to zero and the final altitude by utilizing schemes on generating functions which yield the convergence of the underlying distributions. Therein, we applied the "continuity theorem of discrete laws" [FS09, Theorem IX.1], the "quasi-powers theorem" [FS09, Theorem IX.8], and the "semi-large powers theorem" [BFSS01]. Numerical values confirm our results (see figure below).

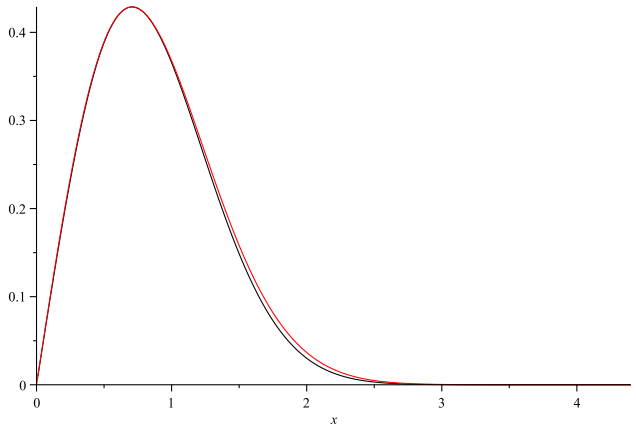


Fig. 2: In Theorem 4.2, we proved that the number of returns to 0 follows asymptotically a Rayleigh limit law (in the critical case of the reflection model). Our figure shows a perfect fit between the plot of the theoretical Rayleigh density (in black) and the plot of the empirical distribution (in red) for Motzkin paths of length $n = 2000$. The tiny discrepancy around $x = 2$ is completely coherent with the error term, i.e. the speed of convergence, in $\mathcal{O}(1/\sqrt{n})$.

The situation is more tricky than what happens for the classical "absorption model" of lattice paths considered in [BF02]: one has to pay a price for introducing a more general model, as different cases (subcritical, critical and supercritical) have then to be distinguished and additional structural constants like $\delta_0^{\geq}$ (the drift at 0) play a key rôle. Putting it all together, there arose 9 different cases for each model. Interestingly though, elementary considerations implied that some of these were impossible in the specific models (compare Table 4 and Table 5 where non-existing cases are marked by a hyphen). In the full version of this work, we give all details of the proofs omitted here (we say a word on matters of periodicity, and we extend the results to excursions, meanders, walks, bridges, arches, beyond the Łukasiewicz case, i.e. when the correspondence with trees do not hold anymore). In another work in preparation, we give the asymptotics for some other harder parameters (area, height).

Acknowledgements

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On the distance-profile of random rooted plane graphs

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Abstract. We study the distance-profile of the random rooted plane graph G_n with n edges (by a plane graph we mean a planar map with no loops nor multiple edges). Our main result is that the profile and radius of G_n (with respect to the root-vertex), rescaled by $(2n)^{1/4}$, converge to explicit distributions related to the Brownian snake. A crucial ingredient of our proof is a bijection we have recently introduced between rooted outer-triangular plane graphs and rooted eulerian triangulations, combined with ingredients from Chassaing and Schaeffer (2004), Bousquet-Mélou and Schaeffer (2000), and Addario-Berry and Albenque (2013). Our convergence result for plane graphs implies similar convergence results for random rooted loopless and general maps.

Keywords: Planar maps, bijections, ISE, Brownian snake, distance-profile

1 Introduction

A *planar map* is a connected planar graph embedded in the plane considered up to deformation. Planar maps can be considered as metric spaces by defining the *distance* between vertices as the minimal number of edges of the paths joining them. The study of the metric properties of random planar maps has been a very active subject of research for the past decade. The first key results were obtained in the seminal paper [CS04], focusing on the class of *rooted* quadrangulations (a map is rooted by marking a directed edge having the outer face on its left, the origin of the root is called the *root-vertex*). It was shown there that typical distances in a uniformly random rooted quadrangulation Q_n with n vertices are of order $n^{1/4}$ (in contrast with the typical distances of order $n^{1/2}$ for random plane trees), and that the distance-profile (the collection of distances of the n vertices from the root-vertex) converges in law to an explicit distribution related to the *ISE* (the *integrated superBrownian excursion* is the occupation measure of the Brownian snake introduced in [Ald93]). This result was then generalized to other classes of random maps, in particular to random rooted maps with n vertices and Boltzmann weights on the faces in [MM07, MW08].

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In this article, we prove this type of result on the profile for rooted simple maps, that is, maps without loops nor multiple edges, which are classically called *plane graphs*. We also show that it implies the same type of result for the class of loopless maps, and for the class of all maps. We now give a few definitions in view of stating our main result. For a rooted planar map $G = (V, E)$ with n edges, the *distance* $d(e)$ of an edge $e \in E$ (with respect to the root) is the length of a shortest path of G starting at (an extremity of) e and ending at the root-vertex, the *distance-profile* of G is the n-set $\{d(e)\}_{e\in E}$ (note that we consider a distance-profile at edges, not at vertices). Let us now give some terminology for the type of convergence results to be obtained. We denote by $\mathcal{M}_1$ the set of probability measures on $\mathbf{R}$, endowed with the *weak topology* (that is, the topology given by the convergence in law). For $\mu \in \mathcal{M}_1$, we denote by $F_\mu(x)$ the cumulative function of μ, $\inf(\mu) := \inf\{x : \ F_\mu(x) > 0\}$ and $\sup(\mu) := \sup\{x : \ F_\mu(x) < 1\}$, and define the *width* of μ as $\sup(\mu) - \inf(\mu)$. We also define the *nonnegative shift* of μ as the probability measure (with support in $\mathbf{R}_+$) whose cumulative function is $x \mapsto F_\mu(x + \inf(\mu))$.

Definition 1 *We denote by $\mu_{\rm ISE}$ a random variable with ISE law (as defined in [Ald93]), and by $\mu_{\rm ISE}^{\rm shift}$ its non-negative shift; these are random variables taking values in $\mathcal{M}_1$. A sequence $\mu^{(n)}$ of random variables taking values in $\mathcal{M}_1$ is said to satisfy the* ISE limit property *if the following properties hold:*

- *$\mu^{(n)}$ converges in law to $\mu_{\rm ISE}^{\rm shift}$ (for the weak topology on $\mathcal{M}_1$).*
- *$\sup(\mu^{(n)})$ converges in law to $\sup(\mu_{\rm ISE}^{\rm shift})$ (i.e., the width of $\mu_{\rm ISE}$).*

For $\mu \in \mathcal{M}_1$, we denote by $X(\mu)$ a real random variable with distribution given by μ. It is easy to see that if a sequence $\mu^{(n)}$ of random variables taking values in $\mathcal{M}_1$ converges in law to μ, then $X(\mu^{(n)})$ converges in law to $X(\mu)$. It is known that $X(\mu_{\rm ISE}^{\rm shift})$ is distributed as $\sup(\mu_{\rm ISE})$ (whose cumulative function has an explicit expression, see [BFG03]). Hence, if $\mu^{(n)}$ has the ISE limit property, then $X(\mu^{(n)})$ converges in law to $\sup(\mu_{\rm ISE})$.

For an n-set $\mathbf{x} = \{x_1, \dots, x_n\}$ of nonnegative values, and for $a > 0$, define $\mu_a(\mathbf{x})$ as the probability measure

$$\mu_a(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i/(an)^{1/4}},$$

where δ_x denotes the Dirac measure at x. Our main result is the following:

Theorem 2 *For $n \geq 1$, let π_n be the distance-profile of the uniformly random rooted plane graph with n edges. Then $\mu_2(\pi_n)$ satisfies the ISE limit property.*

Relation with other work and perspectives. Although we focus here on the convergence of the profile of random maps, much stronger results have now been proved for several classes of maps. More precisely, for a given class $\mathcal{C}$ of maps, one can consider the uniformly random map C_n of size n as a random metric space. It is then natural to study the limit of the random metric space C_n (rescaled by $n^{1/4}$) in the Gromov Hausdorff topology. In a series of groundbreaking papers, this type of convergence was proved to hold for triangulations and $2p$-angulations in [Le 07, Le 13] and independently for quadrangulations in [Mie13]. The limit is a (continuous) random metric space called the *Brownian map*, which has almost surely spherical topology. Combining the techniques of [Le 13] with some new ingredients, the same result was proved for simple triangulations and simple quadrangulations in [ABA13], for general maps in [BJM13], and for bipartite maps in [Abr13]. Work in progress gives us good hope to obtain this type of convergence result for plane graphs (simple planar maps) as well. We mention that much less is known

on the distance profile of *unembedded* planar graphs, the most precise result known at the moment, shown by [CFGN10], is that the diameter is $n^{1/4+o(1)}$ in probability.

We close this section by recalling a useful classical result. For μ and ν two elements of $\mathcal{M}_1$, the *linear Wasserstein distance* between μ and ν is defined as

$$W_1(\mu,\nu) = \int_{\mathbf{R}} |F_\mu(x) - F_\nu(x)| \mathrm{d}x,$$

which endows $\mathcal{M}_1$ with a metric structure. Another characterization of $W_1(\mu,\nu)$ is to be the infimum of $\mathbf{E}(|X-Y|)$ over all couplings (X,Y) where the law of X is μ and the law of Y is ν. It is known that if a sequence $\mu^{(n)}$ of elements of $\mathcal{M}_1$ converges to μ for the metric W_1, then $\mu^{(n)}$ also converges to μ for the weak topology on $\mathcal{M}_1$. Hence the following claim:

Claim 3 *Let $\mu^{(n)}$ and $\nu^{(n)}$ be two sequences of random variables in $\mathcal{M}_1$ (i.e., each variable is a random probability measure), living in the same probability space. Assume that $\mu^{(n)}$ satisfies the ISE limit property and that, for each fixed $\epsilon > 0$, $P(W_1(\mu^{(n)},\nu^{(n)}) \geq \epsilon)$ converges to 0 and $P(|\sup(\mu^{(n)}) - \sup(\nu^{(n)})| \geq \epsilon)$ converges to 0. Then $\nu^{(n)}$ satisfies the ISE limit property.*

2 Bijection between outer-triangular plane graphs and eulerian triangulations, and transfer of canonical paths

In this section we recall a bijection established in [BCF14] between outer-triangular plane graphs and eulerian triangulations, and establish a crucial property for canonical paths.

A rooted plane graph C is said to be *outer-triangular* if its outer face (that is, the root face, drawn as the infinite face in the planar representation of C) has degree 3. Given an outer-triangular plane graph G, a 3-*orientation with buds* of G is an orientation of the inner edges of G (outer edges are left unoriented), with additional outgoing half-edges at inner vertices, called *buds*, such that each inner (resp. outer) vertex has outdegree 3 (resp. 0), and each inner face of degree $d+3$ has d incident buds [(i)]. It is shown in [BF12] that each rooted outer-triangular plane graph G admits a unique 3-orientation with buds, called the *canonical 3-orientation*, satisfying the following properties:

- *Outer-accessibility*: there is a directed path from any inner vertex to a vertex of the outer face.
- *Minimality*: There is no clockwise circuit.
- *Local property at buds*: the first edge following each bud in clockwise order must be outgoing [(ii)].

Figure 1.(a) shows such an outer-triangular plane graph endowed with its canonical 3-orientation.

A *rooted eulerian triangulation* is a rooted planar map (which may have multiple edges) where each face has degree 3 and each vertex has even degree. Hence faces can be properly bicolored (in light or dark) such that each light (resp. dark) face is adjacent only to dark (resp. light) faces. By convention (since there are exactly two possible colorings), the root face is dark.

As shown in [BCF14], there exists a bijection between these two families of maps. We just recall here how to obtain a rooted eulerian triangulation from a rooted outer-triangular plane graph. Let C be an outer-triangular plane graph endowed with its canonical 3-orientation with buds. The bijection illustrated

[(i)] When G is a maximal plane graph, 3-orientations have no bud, and correspond to the well-known Schnyder structures, introduced in [Sch89].

[(ii)] This condition implies that an inner vertex has no more than 2 buds.

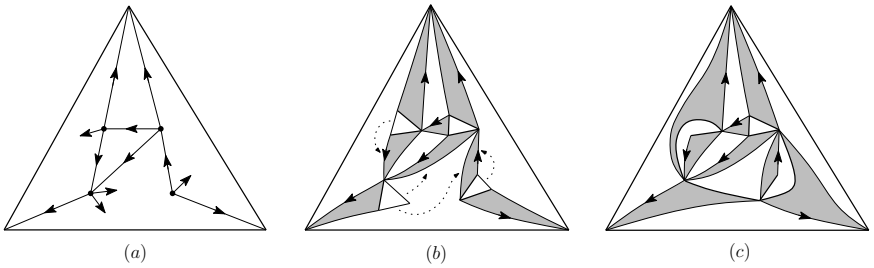
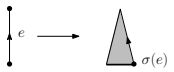


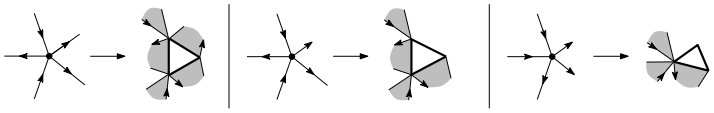
Fig. 1: (a) An outer-triangular plane graph endowed with its canonical 3-orientation with buds, (b) after inflation and (c) after merging, the resulting eulerian triangulation endowed with its canonical 1-orientation.

in Figure 1 has two steps: *inflation*, then *merging*. First, inner edges and inner vertices will be inflated in the following way:

- Each inner edge becomes a dark triangle as indicated below.



- Each inner vertex becomes a light triangle whose edges correspond to the outgoing half-edges (including buds). The cases with 0,1 or 2 buds are illustrated below.



After inflation, former inner faces of degree $d+3$ ($d \geq 0$) have now degree $2d+3$ (the d incident buds have turned into edges). Considering edges coming from buds as opening parentheses, and remaining edges as closing parentheses, one can form a clockwise parenthesis system leaving 3 edges unmatched. Hence, after merging the matched edges, the 3 unmatched edges form a light triangle. This ensures that each face of the resulting map is a triangle; see Figure 1. Moreover, the edges created by the inflation are incident to a dark and a light face, except for edges coming from buds, which are incident to two light faces. After merging, these edges are necessarily incident to a dark face as well. Therefore the triangulation is properly bicolored and is an eulerian triangulation (the outer face, which is left unchanged, is colored dark).

Let C be an outer-triangular rooted plane graph. For each inner edge e, we define its *canonical path* $P(e)$ to be the directed path in the canonical 3-orientation of C starting at e and following the rightmost (with respect to the previous edge on the path) outgoing edge until reaching a vertex of the outer face ($P(e)$ exist because the canonical 3-orientation is minimal and outer-accessible). Let G be a rooted eulerian triangulation. A 1-*orientation* of G is an orientation of some inner edges (outer edges are left unoriented), such that each dark inner face has one directed edge, which is counterclockwise, and each inner (resp. outer) vertex has outdegree 1 (resp. 0). As shown in [BMS00], G has a unique 1-orientation, called its *canonical 1-orientation*, which satisfies *outer-accessibility*; see Figure 1(c). The oriented edges

form a spanning forest of 3 trees (one rooted at each of the outer vertices), and accordingly each vertex has a *canonical (oriented) path* reaching an outer vertex.

For each inner edge e of an outer-triangular rooted plane graph C, we denote by $\sigma(e)$ the inner vertex in the associated rooted eulerian triangulation G which is the origin of e after inflating e into a dark triangle.

Proposition 4 *Let C be an outer-triangular rooted plane graph and G be the associated eulerian triangulation. The mapping σ gives a bijection between the edges of C and the inner vertices of G. Moreover the canonical path of an edge e of C has the same length as the canonical path of the vertex $\sigma(e)$ of G.*

Proof: The canonical 3-orientation of C gives a partial orientation Ω of G. It is not hard to see that Ω is a 1-orientation, therefore σ gives a bijection between the edges of C and the inner vertices of G. Moreover all the canonical paths of C are directed paths in the orientation Ω (that is, they are preserved by the inflation process), thus Ω is outer-accessible. Thus Ω is the canonical 1-orientation of G, and the canonical path of e becomes the canonical path of $\sigma(e)$. This completes the proof. □

Remark 5 *Beside the bijection between outer-triangular plane graphs and eulerian triangulations, we will also use the following mapping from rooted outer-triangular plane graphs to rooted simple triangulations. Given a rooted outer-triangular plane graph C endowed with its canonical 3-orientation, every inner face of degree $d+3$ contains d buds. We consider the triangulation T obtained from C by triangulating each inner face by completing the buds into complete edges and gluing these edges in counterclockwise order around each inner face; see Figure 2. The 3-orientation of C gives a 3-orientation of T (which implies that T is simple) and we contend that it is the* canonical *3-orientation of T. This follows easily from the fact that the canonical paths of C are canonical paths in T (because of the* local property at buds*) and therefore no clockwise cycle exists.*

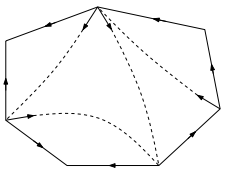


Fig. 2: Generic situation in a face of degree 7 with its 4 incident buds, and its canonical triangulation (dashed lines).

3 The profile of random rooted eulerian triangulations

3.1 Profile with respect to the root-vertex

Let T be a rooted eulerian triangulation with $n+1$ vertices, let V be the vertex-set and let v_0 be the root-vertex. Recall that the faces of T are properly bicolored with the outer face being dark. A path P from a vertex v to a vertex v' is called *admissible* if each traversed edge of P has a dark face on its left. Let $\ell(v)$ be the length of a shortest admissible path from v to v_0. The n-set $\{\ell(v)\}_{v\in V\setminus v_0}$ is called the *root-vertex profile* of T.

Proposition 6 *Let π_n be the root-vertex profile of a uniformly random rooted eulerian triangulation with $n+1$ vertices. Then $\mu_2(\pi_n)$ satisfies the ISE limit property.*

Proof: It is shown in [BFG04] that random rooted eulerian triangulations with $n+1$ vertices are in bijection with so-called *very well-labelled trees* with n nodes, i.e., rooted plane trees with n nodes, each node having a positive label such that adjacent node labels differ by 1 in absolute value, and the root is at a node of label 1. In addition the root-vertex profile of the eulerian triangulation corresponds to the n-set of labels of the corresponding tree. Hence π_n is distributed as the n-set of labels of the random very well-labelled tree with n nodes. The results in [Le 06] imply [(iii)] that $\mu_2(\pi_n)$ satisfies the ISE limit property. □

Remark 7 *Alternatively one could prove Proposition 6 by recycling the combinatorial arguments from Sections 4.4 and 4.5 in [CS04]. This would require a detour via a model of "blossoming trees" (actually the one used in [BMS00]) in order to drop the condition that the labels are positive.*

3.2 Profile with respect to the outer face

Let T be a rooted eulerian triangulation, and let V be its set of inner vertices. For $v \in V$, we denote by $\tilde{d}(v)$ the length of the canonical path of v. The set $\{\tilde{d}(v)\}_{v\in V}$ is called the *root-face profile* of T. Then it is proved in [BMS00] that $\tilde{d}(v)$ is the length of a shortest admissible path from v to (a vertex of) the root-face. Hence $\ell(v) - 2 \leq \tilde{d}(v) \leq \ell(v)$. Thus Proposition 6 immediately gives (via Claim 3) the following result.

Proposition 8 *Let π_n be the root-face profile of a uniformly random rooted eulerian triangulation with n inner vertices. Then $\mu_2(\pi_n)$ satisfies the ISE limit property.*

4 The profile of random rooted plane graphs

4.1 Profile of random rooted outer-triangular plane graphs

Let G be a rooted outer-triangular plane graph, and let E_i be its set of inner edges. For $e \in E_i$ we denote by $\tilde{d}(e)$ the length of the canonical path of e, and by $d(e)$ the length of a shortest path starting at (an extremity of) e and ending at (a vertex of) the root-face. The set $\{\tilde{d}(e)\}_{e\in E_i}$ is called the *canonical path profile* of G, and the set $\{d(e)\}_{e\in E_i}$ is called the *distance-profile at inner edges* of G. By Proposition 4 the canonical path profile of G coincides with the root-face profile of the rooted eulerian triangulation associated with G by the bijection of Section 2. Thus Proposition 8 gives:

Proposition 9 *Let π_n be the canonical path profile of a uniformly random rooted outer-triangular plane graph with $n+3$ edges. Then $\mu_2(\pi_n)$ satisfies the ISE limit property.*

We will now prove that with high probability the canonical path profile is close to the distance-profile using the following (non-random) result from [ABA13].

Lemma 10 ([ABA13]) *There exist positive constants k_1, k_2 such that the following holds. Let G be a rooted simple triangulation, let e be an inner edge of G, let P be the canonical path of e (for the canonical 3-orientation of G), and let Q be another path in G from the origin of e to the root-face. If the length d of P is greater than the length d' of Q, then there exists a cycle C contained in $P \cup Q$ of length a most $k_1 d'/(d-d'))$ such that each of the two parts of G resulting from cutting along C contains a (consecutive) subpath of Q of length at least $k_2(d-d')$.*

[(iii)] See in particular Theorem 8.2 where the methodology is applied to the very close model where adjacent node labels differ by at most 1 in absolute value.

This implies the following (non-random) statement for rooted outer-triangular plane graphs, where the *diameter* $\mathrm{Diam}(G)$ of a graph G is the maximal distance between pairs of vertices.

Lemma 11 *The statement of Lemma 10 also holds if one replaces "simple triangulation" by "outer triangular plane graph". Consequently, for any $\Delta > 0$, if G is a rooted outer-triangular plane graph, and e is an inner edge such that $d(e) \leq \tilde{d}(e) - \Delta$, then G has a cycle C of length at most $k_1 d(e)/\Delta$ such that the two parts G_ℓ, G_r resulting from cutting along C each have diameter at least $k_2\Delta$.*

Proof: Let G be a rooted outer triangular plane graph. We consider its canonical 3-orientation with buds. As explained in Remark 5, there is a canonical way to complete the buds of G into complete edges so as to triangulate each inner face of G and obtain a simple triangulation $\hat{G}$ endowed with its canonical 3-orientation. Moreover, for any inner edge e of G, the canonical path of e is the same in G as in $\hat{G}$. This proves the first statement. The second statement is a simple consequence obtained by considering the canonical path P of an edge e of G and a geodesic path Q. In this case G has a cycle C of length at most $k_1 d(e)/(\tilde{d}(e) - d(e))) \leq k_1 d(e)/\Delta$ such that the two parts G_ℓ, G_r resulting from cutting along C each have a subpath of Q of length at least $k_2(\tilde{d}(e) - d(e)) \geq k_2\Delta$. Since a subpath of a geodesic path is geodesic, we conclude that each of G_ℓ, G_r has diameter at least $k_2\Delta$. □

Definition 12 *A sequence X_n of real random variables is said to have the* uniform exponential decay property *if there exist constants $a, b > 0$ such that for all n, $P(X_n \geq x) \leq a \exp(-b\, x))$.*

Lemma 13 *Let H_n be the uniformly random rooted outer-triangular plane graph with $n+3$ edges. Then $\mathrm{Diam}(H_n)/n^{1/4}$ satisfies the uniform exponential decay property.*

Proof: The property is inherited from eulerian triangulations. Precisely, let π_n denote the root-vertex profile of the uniformly random rooted eulerian triangulation. The calculations done in Section 6.2 of [CS04] for well-labeled trees (which correspond to rooted quadrangulations) can be adapted verbatim to very well-labelled trees (which correspond to rooted eulerian triangulations) in order to show that $\sup(\mu_2(\pi_n))$ has the uniform exponential decay property. Hence, if π'_n denotes the root-face profile of the uniformly random rooted eulerian triangulation with n vertices, then $\sup(\mu_2(\pi'_n))$ has the uniform exponential decay property. This is in turn transferred (bijectively) to $\sup(\mu_2(\pi''_n))$, where π''_n is the canonical path profile of H_n. Since $d(e) \leq \tilde{d}(e)$, the property is also satisfied by $\sup(\mu_2(\pi'''_n))$, where $\pi'''_n = \{d(e)\}_{e \in E_i}$ is the distance-profile at inner edges of H_n. Since $\mathrm{Diam}(H_n) \leq 2 \cdot \max_{e \in E_i}(d(e)) + 2$, we conclude that $\mathrm{Diam}(H_n)/n^{1/4}$ satisfies the uniform exponential decay property. □

For $n \geq 0$ we denote by $\mathcal{M}_n$ the set of rooted plane graphs with n edges, and $\mathcal{C}_n$ the subset of outer-triangular plane graphs in $\mathcal{M}_n$. It was shown in [BCF14] that

$$|\mathcal{C}_n| = 3 \cdot 2^{n-1} \frac{(2n)!}{n!(n+2)!} = O(8^n n^{-5/2}). \tag{1}$$

Observe that there is an injective map ϕ from $\mathcal{M}_n$ to $\mathcal{C}_{n+2}$ as shown in the figure below.

Thus $|\mathcal{M}_n| \leq |\mathcal{C}_{n+2}| = O(8^n n^{-5/2})$. Moreover $\mathrm{Diam}(\phi(G)) - \mathrm{Diam}(G) \in \{0,1\}$. Thus (observing that $\frac{|\mathcal{M}_n|}{|\mathcal{C}_{n+2}|} \geq \frac{|\mathcal{C}_n|}{|\mathcal{C}_{n+2}|}$ is bounded away from 0) Lemma 13 implies the following.

Corollary 14 *Let G_n be the uniformly random rooted plane graph with n edges. Then $\mathrm{Diam}(G_n)/n^{1/4}$ satisfies the uniform exponential decay property. Therefore there exist constants $a, b > 0$ such that for all $n \geq 0$ and $x > 0$ the number of elements in $\mathcal{M}$ of diameter at least $xn^{1/4}$ is at most $a8^n n^{-5/2} \exp(-bx)$.*

Lemma 15 *Let $\epsilon > 0$ and let G_n be the random rooted outer-triangular plane graph with $n+3$ edges. Let $\mathcal{E}_{n,\epsilon}$ be the event that G_n has an inner edge e for which $d(e) \leq \tilde{d}(e) - \epsilon n^{1/4}$. Then $\lim_{n\to\infty} P(\mathcal{E}_{n,\epsilon}) = 0$.*

Proof: We first show the statement for the event $\mathcal{E}_{n,\epsilon,A} = \mathcal{E}_{n,\epsilon} \cap \{\mathrm{Diam}(G_n) \leq An^{1/4}\}$, where A is an arbitrary fixed positive constant. Let U_n be the set of rooted outer-triangular plane graphs with n edges of diameter at most $An^{1/4}$ having an inner edge e for which $d(e) \leq \tilde{d}(e) - \epsilon n^{1/4}$. By (1), it suffices to show that $|U_n| = o(8^n n^{-5/2})$. By Lemma 11 (applied to $\Delta = \epsilon n^{1/4}$), any map in U_n has a cycle of length $c \leq k_1 d(e)/\epsilon n^{1/4} \leq k_1 A/\epsilon$ separating two maps of diameter at least $k_2 \epsilon n^{1/4}$. We now fix a positive integer c, and denote by V_n^c the set of pairs (G, C) where G is a rooted outer-triangular plane graph with n edges and C is a cycle of G of length c such that the two parts of G obtained by cutting along C each have diameter at least $k_2 \epsilon n^{1/4}$. It suffices to prove that $|V_n^c| = o(8^n n^{-5/2})$. Let $w_{i,n}$ be the number of maps in $\mathcal{M}_i$ of diameter at least $k_2 \epsilon n^{1/4}$. By Corollary 14 there are constants $a, b' > 0$ such that $w_{i,n} \leq a8^i i^{-5/2} \exp(-b'(n/i)^{1/4})$. Decomposing pairs $(G, C) \in V_n^c$ into two maps gives

$$|V_n^c| \leq \sum_{i+j=n+c} 2n \cdot w_{i,n} w_{j,n}$$

where the factor $2n$ accounts for choosing the position of the root edge of G. Let S be the above sum restricted to $\{i > n/(\log(n)^8)\} \cap \{j > n/(\log(n)^8)\}$ and S' the sum of the other terms. Since $w_{i,n} \leq a8^i i^{-5/2}$,

$$S \leq (n+c) \cdot 2n \cdot a^2 8^{n+c} (n/\log(n)^8)^{-5} = o(8^n n^{-5/2}).$$

And since $w_{i,n} \leq a8^i \exp(-b'(n/i)^{1/4})$,

$$S' \leq 2n/(\log(n)^8) \cdot 2n \cdot a^2 8^{n+c} \exp(-b'(\log(n))^2) = o(8^n n^{-5/2}).$$

Hence $|V_n^c| = o(8^n n^{-5/2})$ and this completes the proof that for any $A > 0$, $\lim_{n\to\infty} P(\mathcal{E}_{n,\epsilon,A}) = 0$. Thus for all $A > 0$,

$$\lim_{n\to\infty} P(\mathcal{E}_{n,\epsilon}) \leq \lim_{n\to\infty} (P(\mathcal{E}_{n,\epsilon,A}) + P(\mathrm{Diam}(G_n) > An^{1/4})) \leq \sup_n P(\mathrm{Diam}(G_n) > An^{1/4})).$$

And since by Lemma 13, $\lim_{A\to\infty} \sup_n P(\mathrm{Diam}(G_n) > An^{1/4})) = 0$, we get $\lim_{n\to\infty} P(\mathcal{E}_{n,\epsilon}) = 0$. □

Remark 16 *A result similar to Lemma 15 is given in [ABA13] for random rooted simple triangulations. However, we could not deduce Lemma 15 from that result and instead had to start from Lemma 10 above.*

We can now prove the main result of this section.

Proposition 17 *Let π_n be the distance-profile at inner edges of a uniformly random rooted outer-triangular plane graph with $n+3$ edges. Then $\mu_2(\pi_n)$ satisfies the ISE limit property.*

Proof: Let G_n be the uniform random rooted outer-triangular plane graph with n inner edges, and let E_i be the set of inner edges. We consider the n-sets $\mathbf{d} = \{d_e\}_{e\in E_i}$ and $\tilde{\mathbf{d}} = \{\tilde{d}(e)\}_{e\in E_i}$. When $\mathcal{E}_{n,\epsilon}$ does not hold, then $W_1(\mu_2(\mathbf{d}), \mu_2(\tilde{\mathbf{d}})) \leq \epsilon/2^{1/4}$, and $|\sup(\mu_2(\mathbf{d})) - \sup(\mu_2(\tilde{\mathbf{d}}))| \leq \epsilon/2^{1/4}$. Hence, the result follows from Proposition 9 and Lemma 15, using Claim 3. □

4.2 Profile of random rooted plane graphs

We now transfer our result for outer-triangular plane graphs to general plane graphs. For this we exploit an easy decomposition (already described in [BCF14]) of rooted plane graphs in terms of rooted outer-triangular plane graphs. Let $\mathcal{M}$ be the family of rooted plane graphs, and let $\mathcal{C}$ be the family of rooted outer-triangular plane graphs. Let p be the rooted plane graph with two edges meeting at a point, which is the root-vertex, and let $\mathcal{D} = \mathcal{C} \cup \{p\}$. For an element of $\mathcal{D}$, the *right-edge* is the edge following the root-edge in counterclockwise order around the root-face. It is shown in [BCF14] that each graph $\gamma \in \mathcal{M}$ is uniquely obtained from a sequence $\gamma_1, \ldots, \gamma_k$ of elements of $\mathcal{D}$ where the following operations are performed:

(i) for $i \in [1..k-1]$, merge the right-edge of γ_i with the root-edge of γ_{i+1} (identifying the root-vertices),

(ii) delete the right-edge of γ_k.

In the decomposition, γ_i (if it exists, i.e., if $i \leq k$) is called the ith component. This decomposition also ensures that the generating functions $M(z)$ of $\mathcal{M}$ and $C(z)$ of $\mathcal{C}$ (according to the number of edges) are related by

$$M(z) = \sum_{k\geq 1}(z + C(z)/z)^k = \frac{D(z)}{1 - D(z)}, \text{ where } D(z) := z + C(z)/z.$$

Let G_n be the random rooted plane graph with n edges, and for $i, j \geq 1$, let $\mathcal{E}_n^{(i,j)}$ be the event that, in the decomposition $\gamma_1, \ldots, \gamma_k$ of G_n, the ith component γ_i exists (i.e., $i \leq k$) and has $n - j + 1$ edges. And let $\pi_n^{(i,j)}$ be the probability that $\mathcal{E}_n^{(i,j)}$ occurs.

Lemma 18 *For any $i, j \geq 1$, there exists a non-negative constant $\pi^{(i,j)}$ such that $\pi_n^{(i,j)}$ converges to $\pi^{(i,j)}$. In addition $\sum_{i,j} \pi^{(i,j)} = 1$.*

Proof: Let m_n be the number of rooted plane graphs with n edges, $m_n^{(i,j)}$ the number of rooted plane graphs with n edges for which $\mathcal{E}_n^{(i,j)}$ occurs (note that $\pi_n^{(i,j)} = m_n^{(i,j)}/m_n$), and d_n be the number of elements of $\mathcal{D}$ with n edges. From $C(z) = \sum_{n\geq 1} \frac{3\cdot 2^{n-1}(2n)!}{n!(n+2)!} z^{n+2} = \frac{z^2(-1+12z+\sqrt{1-8z})}{(1+\sqrt{1-8z})^2}$. one finds that $D(z)$ and $M(z)$ have the following singular expansion at $z = 1/8$, with the notation $Z = \sqrt{1-8z}$ and with $d := 5/32$ and $e = 1/4$:

$$D(z) = d + eZ^3 - 9Z^2/32 + O(Z^4), \quad M(z) = \frac{d}{1-d} + \frac{e}{(1-d)^2}Z^3 - 32Z^2/81 + O(Z^4).$$

Now, let $M^{(i,j)}(z) = \sum_n m_n^{(i,j)} z^n$. It is easy to see that $M^{(i,j)}(z) = a^{(i,j)} z^j D(z)$, where $a^{(i,j)} = [z^j]\frac{D(z)^{i-1}}{1-D(z)}$ counts the number of possibilities for the components γ_s for $s \neq i$. Hence $M^{(i,j)}(z)$ has

a singular expansion of the form $M^{(i,j)}(z) = d^{(i,j)} + e^{(i,j)}Z^{3/2} + g^{(i,j)}Z^2 + O(Z^4)$, with $e^{(i,j)} = a^{(i,j)} \cdot e \cdot 8^{-j}$. By classical transfer lemmas of singularity analysis in [FS09],

$$m_n \sim \frac{1}{\sqrt{\pi}} \frac{e}{(1-d)^2} 8^n n^{-5/2}, \;\; m_n^{(i,j)} \sim \frac{1}{\sqrt{\pi}} a^{(i,j)} \cdot e \cdot 8^{-j} \cdot 8^n n^{-5/2}.$$

Hence $\pi_n^{(i,j)} = m_n^{(i,j)}/m_n$ converges to $\pi^{(i,j)} := (1-d)^2 8^{-j} [z^j] \frac{D(z)^{i-1}}{1-D(z)}$. We have for each $i \geq 1$, $\sum_j \pi^{(i,j)} = (1-d)^2 \cdot D(1/8)^{i-1}/(1-D(1/8)) = (1-d)^2 \cdot d^{i-1}/(1-d)$, hence $\sum_{i,j} \pi^{(i,j)} = 1$. □

Lemma 19 *For $i, j \geq 1$ fixed, let $\pi_n^{(i,j)}$ be the profile of the random rooted plane graph $G_n^{(i,j)}$ with n edges conditioned on $\mathcal{E}_n^{(i,j)}$. Then $\mu_2(\pi_n^{(i,j)})$ satisfies the ISE limit property.*

Proof: Let E be the set of edges of $G_n^{(i,j)}$ and let E_i be the set of inner edges of γ_i. Let $\mathbf{d} = \{d_e\}_{e \in E}$ be the n-set of distances of the edges of $G_n^{(i,j)}$ from the root-vertex, and let $\mathbf{d}' = \{d_e\}_{e \in E_i}$ be the $(n-j-2)$-set of distances of inner edges of γ_i from the root-vertex of γ_i (which is also the root-vertex of $G_n^{(i,j)}$). It is easy to see that there exists a constant $A > 0$ (depending only on i and j) such that, for any rooted plane graph with n edges and satisfying $\mathcal{E}_n^{(i,j)}$,

$$W_1(\mu_2(\mathbf{d}), \mu_2(\mathbf{d}')) \leq A \cdot \frac{\mathrm{Diam}(\gamma_i)}{n}.$$

Since γ_i is a uniformly random rooted outer-triangular plane graph with $n-j+1$ edges, Lemma 13 ensures that $\mathrm{Diam}(\gamma_i)/n^{1/4}$ satisfies the uniform exponential decay property, hence

$$P(W_1(\mu_2(\mathbf{d}), \mu_2(\mathbf{d}')) \geq A/\sqrt{n}) = O(\exp(-\Omega(n^{1/4}))).$$

Similarly

$$P(|\sup(\mu_2(\mathbf{d})) - \sup(\mu_2(\mathbf{d}'))| \geq A/\sqrt{n}) = O(\exp(-\Omega(n^{1/4}))).$$

Since $\mu_2(\mathbf{d}')$ satisfies the ISE limit property according to Proposition 17, we conclude from Claim 3 that $\mu_2(\mathbf{d})$ also satisfies the ISE limit property. □

Proof of Theorem 2. Let $\eta > 0$. Let k be the smallest value such that $\sum_{i \leq k, j \leq k} \pi^{(i,j)} > 1 - \eta$, and let $\mathcal{E}_{n,\eta}$ be the event that $\mathcal{E}_n^{(i,j)}$ holds for some $i \leq k$ and $j \leq k$. By Lemma 19, conditioned on $\mathcal{E}_{n,\eta}$, the random rooted plane graph with n edges satisfies the ISE limit property. Note that, as $n \to \infty$ the probability that $\mathcal{E}_{n,\eta}$ holds converges to $c_\eta := \sum_{i \leq k, j \leq k} \pi^{(i,j)}$ (because for n large enough two events $\mathcal{E}_n^{(i,j)}$ and $\mathcal{E}_n^{(i',j')}$ do not intersect), hence for n large enough, the probability that $\mathcal{E}_{n,\eta}$ holds is at least $1 - \eta$. Taking η arbitrarily small, we conclude that G_n satisfies the ISE limit property. □

We define the *radius* $r(G)$ of a planar map G as the largest possible distance of a vertex of G from the root-vertex.

Proposition 20 *Let R_n be the radius of the random rooted plane graph G_n with n edges. Then $R_n/(2n)^{1/4}$ converges in law to the width of μ_{ISE}, and the convergence also holds for the moments.*

Proof: The convergence in law follows from Theorem 2. The convergence of the moments then follows from the uniform exponential decay property of $R_n/(2n)^{1/4}$ which is given by Corollary 14. □

5 The profile of random rooted loopless and general maps

It is known that any loopless map decomposes along multiple edges into a tree of components of two types: simple maps and multi-edges, see e.g. [Fus07, Sec2.1] for a description of the decomposition in the quadrangulated case. In addition, denoting by L_n the uniformly random rooted loopless map of size n, it has been shown in [GW99, BFSS01] that, when n gets large, the (decomposition-) tree of L_n has almost surely a unique "giant component" S, which is a uniformly random simple map whose size is concentrated around $2n/3$, and the second largest component has size $O(n^{2/3+\delta})$ for any $\delta > 0$. Hence L_n can be seen as a random simple map S of size $\sim 2n/3$ whose edges are possibly substituted by "small" random rooted loopless maps. Based on this, it can be deduced from Theorem 2 that $\mu_{4/3}(\pi(L_n))$ satisfies the ISE limit property ($\pi(M)$ denotes the distance-profile of a map M). The scaling constant $4/3$ that appears here can be thought of as $2 \cdot (2/3)$, indeed it combines the effects of the scaling constant 2 applied to the giant simple map S, and of the fact that the size of S is asymptotically $2/3$ of the size of L_n.

Similarly, any general map decomposes along loops into a tree of components that are loopless maps (the edges of the tree corresponding to the loops of the map). Again, denoting by M_n the random rooted map with n edges, it has been shown in [GW99, BFSS01] that when n gets large, the (decomposition-) tree of M_n has almost surely a unique "giant component" L, which is a uniformly random loopless map whose size is concentrated around $2n/3$, and the second largest component has size $O(n^{2/3+\delta})$ for any $\delta > 0$. Based on this, it can be shown that $\mu_{8/9}(\pi(M_n))$ satisfies the ISE limit property. We recover here a known result, which alternatively follows from the study by [CS04] of the profile of random rooted quadrangulations, combined with the recent profile-preserving bijection in [AB13] between quadrangulations and maps.

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Efficiently Navigating a Random Delaunay Triangulation

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Abstract. Planar graph navigation is an important problem with significant implications to both point location in geometric data structures and routing in networks. Whilst many algorithms have been proposed, very little theoretical analysis is available for the properties of the paths generated or the computational resources required to generate them. In this work, we propose and analyse a new planar navigation algorithm for the Delaunay triangulation. We then demonstrate a number of strong theoretical guarantees for the algorithm when it is applied to a random set of points in a convex region.

Keywords: Routing, Point Location, Randomised Analysis, Delaunay Triangulation

1 Introduction

Given a planar embedding of a graph $G = (V, E)$, a source node $z \in V$ and a destination point $q \in \mathbb{R}^2$, we consider the *planar graph navigation* problem of finding a route in G from z to the nearest neighbour of q in V. In particular, we assume that any vertex $v \in V$ may access its coordinates in $\mathbb{R}^2$ with a constant time query. The importance of this problem is twofold. On the one hand, finding a short path between two nodes in a network is currently a very active area of research in the context of routing in networks [1, 19, 22]. On the other, the problem of locating a face containing a point in a convex subdivision (point location) is an important sub-routine in many algorithms manipulating geometric data structures [10, 11, 17, 20]. A number of algorithms have been proposed within each of these fields, many of which are in fact equivalent. It seems the majority of the literature in these areas is concerned with the existence of algorithms which always succeed under different types of constraints, such as the *competitiveness* of the algorithm, or the class of network. Apart from worst-case bounds, very little is known concerning the properties of the path lengths and running times for these algorithms under random distribution hypotheses for the input vertices. We aim to bridge the gap between these two fields by giving and analysing an algorithm that is provably efficient within both of these contexts when the underlying graph is the Delaunay triangulation. More precisely, we show that even for the worst possible

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pair of source and destination chosen from a uniformly random input, our algorithm remains efficient in an asymptotic sense. To the best of our knowledge, our results provide the first analysis for a *localised*[(i)] routing algorithm on a randomly generated planar graph. In addition, we take particular care when dealing with boundary effects that occur when the routing algorithm approaches the edge of the domain, achieving bounds that remain asymptotically the same irrespective of where in the process the input points are chosen from. Finally, we believe our results help provide convincing evidence that similar asymptotic results should hold for other localised routing algorithms such as *greedy routing* (which we define in Section 1.2).

In this extended abstract we will outline the main ingredients towards the theorems given in Section 1.3, and give a proof that the number of vertices accessed by the algorithm is proportional to the length of the walk, for a fixed source and destination that are sufficiently far apart. For the full technical details, we refer the reader to [8].

1.1 Definitions

In the following, we define the *competitiveness* of an algorithm to be the worst case ratio between the length of the path generated by the algorithm and the Euclidean distance between the source and the destination. Thus competitiveness may depend on the class of graphs one allows, but not the pair of source and destination. Let $\mathbf{N}_d(v)$ denote the set of neighbours of v within d hops of v. We shall sometimes refer to the d'th neighbourhood of a set X, to denote the set of all sites that can be accessed from a site in X with fewer than d hops. We call an algorithm *c-memoryless* if at each step in the navigation, it only has access to the destination q, the current vertex v and $\mathbf{N}_c(v)$. Some authors use the term *online* to refer to an algorithm that only has access to q, the current vertex v, $\mathbf{N}_1(v)$ and $O(1)$ words of memory which may be used to store information about the history of the navigation. Finally, an algorithm may be either deterministic or randomised. We define a randomised algorithm to be an algorithm that has access to a random oracle at each step.

1.2 Previous results

Graph Navigation for Point location. The problem of point location is most often studied in the context of triangulations and the algorithms are referred to as *walking algorithms* [11]. A walking algorithm may work by following edges or by following incidences between neighbouring faces, which is equivalent to a navigation in the dual graph. There are three main algorithms that have received attention in the literature: *straight walk*, which is a walk that visits all triangles crossed by the line segment zq; *greedy vertex walk*, which always chooses the vertex in $\mathbf{N}_1(v)$ which is closest to q and *visibility walk* which walks to an adjacent triangle if and only if it shares the same half-space as q relative to the shared edge. It is known that these algorithms always terminate if the underlying triangulation is Delaunay [11].

The aim is generally to analyse the expected number of steps that the algorithm requires to reach the destination under a given distribution hypothesis. Such an analysis has only been provided by Devroye et al. [13] who succeeded in showing that straight walk reaches the destination after $O(\|zq\|\sqrt{n})$ steps in expectation, for n random points in the unit square.[(ii)] The analysis in this case is facilitated since it is possible to compute the probability that a triangle is part of the walk without looking at the other vertices.

[(i)] We call a routing algorithm *localised* if it eventually 'forgets' where it came from in a technical sense that we define in Section 1.3.

[(ii)] Zhu also provides a tentative $O\left(\sqrt{n \log n}\right)$ bound for visibility walk [23]. This is a proof by induction for "a random edge at distance d". It considers the next edge in the walk and applies an induction hypothesis to try and bound the progress. Unfortunately, the new edge cannot be considered as random: each edge that is visited has been chosen by the algorithm and the edges do not all

Straight walk is online, but not memoryless since at every step the algorithm must know the location of the source point, z. It is also rarely used in practice since it is usually outperformed empirically by one of the remaining two algorithms, *visibility walk* or *greedy vertex* walk, which are both 1-memoryless [11]. The complex dependence between the steps of the algorithm in these cases makes the analysis difficult, and it remains an important open question to provide an analysis for either of these two algorithms.

Graph Navigation for Routing. In the context of packet routing in a network, each vertex represents a node which knows its approximate location and can communicate with a selected set of neighbouring nodes. One example is in wireless networks where a node communicates with all devices within its communication range. In such cases, it is often convenient for the nodes to agree on a communication protocol such that the graph of directly communicating nodes is planar, since this can make routing more efficient. Delaunay triangulations have been used in this context due to their ability to act as spanners (the length of shortest paths in the graph, seen as curves in $\mathbb{R}^2$, do not exceed the Euclidean distance by more than a constant factor), and methods exist to locally construct the full Delaunay triangulation, given some conditions on the point distribution [16, 18, 21].

Commonly referenced algorithms in this field are: *greedy routing*, which is the same algorithm as *greedy vertex walk*, given in the context of point location; *compass routing* which is similar to greedy, except that instead of choosing the point in $\mathbf{N}_1(v)$ minimising the distance to q, it chooses the point in $x \in \mathbf{N}_1(v)$ minimising the angle $\angle q, v, x$, and also *face routing* which is a generalisation of straight walk that can be applied to any planar graph. In this context, overall computation time is usually considered less important than trying to construct algorithms that find short paths in a given network topology under certain memory constraints. We give a brief overview of results relating to this work.

Bose et al. [7] demonstrated that it is not possible to construct a deterministic online algorithm that finds a path with constant competitiveness in an *arbitrary* triangulation. They also demonstrated by counter example that neither greedy routing, nor compass routing is $O(1)$-competitive on the Delaunay triangulation [5]. Bose and Morin [6] went on to show that there does, however, exist an online c-competitive algorithm that works on any graph satisfying a property they refer to as the 'diamond property', which is satisfied by Delaunay triangulations. They show this by providing an algorithm which is essentially a modified version of the straight walk. Bose and Morin also show that there is no algorithm that is competitive for the Delaunay triangulation under the link length (the link length is the number of edges visited by the algorithm) [7].

In terms of time analysis, it appears the only relevant results are those by Chen et al. [9], who show that no memoryless routing algorithm is asymptotically better than a random walk when the underlying graph is an arbitrary convex subdivision.

Navigation in the Plane. We briefly remark that for the related problem of navigation in the plane, several probabilistic results exist; for example [2] and [3]. In this context, the input is a set of vertices in the plane along with an oracle that can compute the next step given the current step and the destination in $O(1)$ time. Although the steps are also dependent in these cases, the case of Delaunay triangulations we treat here is more delicate because of the geometry of the region of dependence implied by the Delaunay property.

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have the same probability to be chosen at each step in the walk. Restarting the walk from a given edge is not possible either (as done in [12]), since the knowledge that an edge is a Delaunay edge influences the local point distribution.

1.3 Contributions

In this paper we give a new deterministic planar graph navigation algorithm which we call *cone walk* that succeeds on any Delaunay triangulation and produces a path which is 3.7-competitive. We briefly underline the fact that our algorithm has been designed for theoretical demonstration, and we do not claim that it would be faster in a practical sense than, for example, *greedy routing* or *face routing*. On the other hand, direct comparisons would perhaps be unfair, since *greedy routing* is not $O(1)$-competitive on the Delunay triangulation [5] whereas we prove that cone walk is; and *face routing* is not memoryless in any sense (since it must always remember the initial vertex), whilst cone walk is localised in the sense given by Theorem 1. In the theorems that follow, we characterise the asymptotic properties of the cone walk algorithm applied to a random input.

Let $\mathcal{D}$ be a smooth convex domain of the plane with area 1, and write $\mathcal{D}_n = \sqrt{n}\mathcal{D}$ for its scaling to area n. For $x, y \in \mathcal{D}$, let $\|xy\|$ denote the Euclidean distance between x and y. Under the hypothesis that the input is the Delaunay triangulation of n points uniformly distributed in a convex domain of unit area, we prove that, for any $\varepsilon > 0$, our algorithm is $O(\log^{3+\varepsilon} n)$-memoryless with probability tending to one. In the case of cone walk, this is equivalent to bounding the number of neighbourhoods that might be accessed during a step, which we deal with in the following theorem.

Theorem 1 *Let $\mathbf{X}_n := \{X_1, X_2, \dots, X_n\}$ be a collection of n independent uniformly random points in $\mathcal{D}_n$. For $z \in \mathbf{X}_n$ and $q \in \mathcal{D}_n$, let $M(z, q)$ be the maximum number of neighbourhoods needed to compute any step of the walk. Then, for every $\varepsilon > 0$,*

$$\mathbb{P}\Big(\exists z \in \mathbf{X}_n,\, q \in \mathcal{D}_n : M(z, q) > \log^{3+\varepsilon} n\Big) \leq \frac{1}{n}. \tag{1}$$

In particular, as $n \to \infty$, $\mathbb{E}[\sup_{z\in\mathbf{X}_n, q\in\mathcal{D}_n} M(z, q)] = O(\log^{3+\varepsilon} n)$, for every $\varepsilon > 0$.

Also with probability close to one, we show that the path length, the number of edges and the number of vertices accessed are $O(\,\|zq\| + \log^6 n\,)$ for any pair of points in the domain. We formalise these properties in the following theorem.

Theorem 2 *Let $\mathbf{X}_n := \{X_1, X_2, \dots, X_n\}$ be a collection of n independent uniformly random points in $\mathcal{D}_n$. Let $\Gamma(z, q)$ denote either the Euclidean length of the path generated by the cone walk from $z \in \mathbf{X}_n$ to $q \in \mathcal{D}_n$, its number of edges, or the number of vertices accessed by the algorithm when generating it. Then there exist constants $C_{\Gamma,\mathcal{D}}$ depending only on Γ and on the shape of $\mathcal{D}$ such that, for all n large enough,*

$$\mathbb{P}\left(\exists z \in \mathbf{X}_n,\, q \in \mathcal{D}_n \;:\; \Gamma(z, q) > C_{\Gamma,\mathcal{D}} \cdot \|zq\| + 4\Big(1 + \sqrt{\|zq\|}\Big)\log^6 n\right) \leq \frac{1}{n}. \tag{2}$$

In particular, as $n \to \infty$,

$$\mathbb{E}\left[\sup_{z\in\mathbf{X}_n,\, q\in\mathcal{D}_n} \Gamma(z, q)\right] = O(\sqrt{n}\,). \tag{3}$$

Finally, we bound the computational complexity of the algorithm, $T(z, q)$.

Theorem 3 *Let $\mathbf{X}_n := \{X_1, X_2, \dots, X_n\}$ be a collection of n independent uniformly random points in $\mathcal{D}_n$. Then in the RAM model of computation, there exists a constant C depending only on the shape of $\mathcal{D}$*

and the particular implementation of the algorithm such that for all n large enough,

$$\mathbb{P}\left(\exists z \in \mathbf{X}_n,\, q \in \mathcal{D}_n \;:\; T(z,q) > C \cdot \|zq\| \log\log n + \left(1 + \sqrt{\|zq\|}\right) \log^6 n\right) \leq \frac{1}{n}. \tag{4}$$

In particular, as $n \to \infty$,

$$\mathbb{E}\left[\sup_{z \in \mathbf{X}_n,\, q \in \mathcal{D}_n} T(z,q)\right] = O(\sqrt{n} \log\log n\,). \tag{5}$$

Remark 1 *We conjecture that the factor of* $\log\log(n)$ *in Theorem 3 can be removed. However, we were unable to demonstrate this due to the complex dependancy structure between the steps.*

Remark 2 *The choice of the initial vertex is never discussed. However, previous results show that choosing this point carefully can result in an expected asymptotic speed up for any graph navigation algorithm [20].*

2 The Cone Walk Algorithm

Consider the finite set of sites in general position, $\mathbf{X} \subset \mathbb{R}^2$ contained within a compact convex domain $\mathcal{D} \subset \mathbb{R}^2$. Let $\mathrm{DT}(\mathbf{X})$ be the Delaunay triangulation of $\mathbf{X}$, which is the graph in which three sites $x, y, z \in \mathbf{X}$ form a triangle if and only if the disc with x, y and z on its boundary does not contain any site in $\mathbf{X}$. Given two points $z, q \in \mathbb{R}^2$ and a number $r \in \mathbb{R}$ we define $\mathrm{Disc}(z,q,r)$ to be the closed disc whose diameter spans z and the point at a distance $2r$ from z on the ray zq. Finally, we define $\mathrm{Cone}(z,q,r)$ to be the sub-region of $\mathrm{Disc}(z,q,r)$ contained within a closed cone of apex z, axis zq and half angle $\frac{\pi}{8}$ (see Figure 2).

Given a site $z \in \mathbf{X}$ and a destination point $q \in \mathcal{D}$, we define one *step* of the cone walk algorithm by growing the region $\mathrm{Cone}(z,q,r)$ anchored at z from $r = 0$ until the first point $z' \in \mathbf{X}$ is found such that the region is non-empty. Once z' has been determined, we refer to it as the *stopper*. We call the region $\mathrm{Cone}(z,q,r)$ for the given r a *search cone*, and we call the associated disc $\mathrm{Disc}(z,q,r)$ the *search disc* (see Figure 2). The point z' is then selected as the anchor of a new search cone $\mathrm{Cone}(z',q,\cdot)$ and the next step of the walk begins. See Figure 1 for an example run of the algorithm.

To find the stopper using only neighbour incidences in the Delaunay triangulation, we need only access vertices in a well-defined local neighbourhood of the search disc. Define the points $\mathbf{X} \cap \mathrm{Disc}(z,q,r) \setminus \{z, z'\}$ to be the *intermediate vertices*. The algorithm finds the stopper at each step by gradually growing a disc anchored at z in the direction of the destination, adding the neighbours of all vertices in $\mathbf{X}$ intersected along the way. This is achieved in practice by maintaining a series of candidate vertices initialised to the neighbours of z and selecting amongst them the vertex defining the smallest search disc at each iteration. Each time we find a new vertex intersecting this disc, we check to see if it is contained within $\mathrm{Cone}(z,q,\infty)$. If it is, this point is the next stopper and this step is finished. Otherwise the point must be an intermediate vertex and we add its neighbours to the list of candidate vertices. This procedure works because the intermediate vertex defining the next largest disc is always a neighbour of one of the intermediate vertices that we have already visited during the current step.

We terminate the algorithm when the destination q is contained within the current search disc for a given step. At this point we know that one of the points contained within $\mathrm{Disc}(z,q,r)$ is a Delaunay neighbour of q in $\mathrm{DT}(\mathbf{X} \cup \{q\})$. We can further compute the triangle of $\mathrm{DT}(\mathbf{X})$ containing the query

point q (point location) or find the nearest neighbour of q in $\mathrm{DT}(\mathbf{X})$ by simulating the insertion of the point q into $\mathrm{DT}(\mathbf{X})$ and performing an exhaustive search on the neighbours of q in $\mathrm{DT}(\mathbf{X} \cup \{q\})$.

We will distinguish between the *visited* vertices, which we take to be the set of all sites contained within the search discs for each step, and the *accessed* vertices, which we define to be the visited vertices along with their 1-hop neighbourhood. This distinction will be important, since the sequence of steps in the walk depends only on the vertices visited, but the cone walk algorithm must access the set of 'vertices accessed' in order to compute the sequence of steps efficiently using only local information.

The pseudo-code below gives a detailed algorithmic description of the CONE-WALK algorithm. We take as input some $z \in \mathbf{X}$, $q \in \mathcal{D}$ and return a Delaunay neighbour of q in $\mathrm{DT}(\mathbf{X} \cup \{q\})$. Recalling that $\mathbf{N}_1(v)$ refers to the Delaunay neighbours of $v \in \mathrm{DT}(\mathbf{X})$ and additionally defining NEXT-VERTEX(S, z, q) to be the procedure that returns the vertex in S with the smallest r such that $\mathrm{Disc}(z, q, r)$ touches a vertex in S and IN-CONE(z, q, y) to be `true` when $y \in \mathrm{Cone}(z, q, \infty)$.

```
CONE-WALK(z, q)
 1  Substeps = {z}
 2  Candidates = N_1(z)
 3  while true
 4      y = NEXT-VERTEX(Candidates ∪ {q}, z, q)
 5      if IN-CONE(z, q, y)
 6          if y = q
 7              // Destination reached.
 8              return NEXT-VERTEX(Substeps, q, z)
 9          // y is a stopper
10          z = y
11          Substeps = {z}
12          Candidates = N_1(z)
13      else
14          // y is an intermediate vertex.
15          Substeps = Substeps ∪ {y}
16          Candidates = Candidates ∪ N_1(y) \ Substeps
```

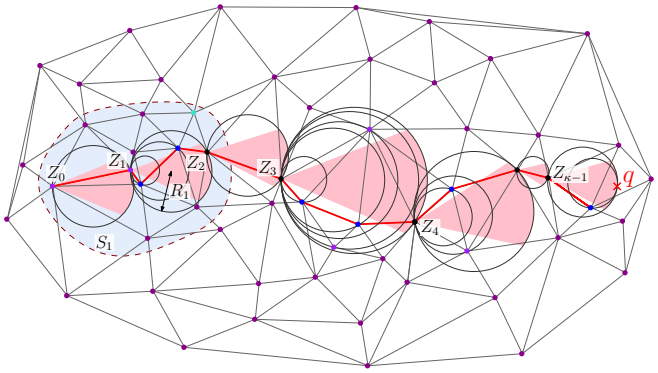

Fig. 1: An example of cone walk.

We note that the order in which the vertices are discovered during the walk does not necessarily define a path in $\mathrm{DT}(\mathbf{X})$. If we only wish to find a point of the triangulation that is close to the destination (for example, in point location), this is not a problem. However, in the case of routing, a path in the triangulation is required to provide a route for data packets. To this end, we provide two options that we shall refer to as SIMPLE-PATH and COMPETITIVE-PATH. SIMPLE-PATH is a simple heuristic that can quickly generate a path that is provably short on average. We conjecture that SIMPLE-PATH is indeed competitive, however we were unable to prove this. COMPETITIVE-PATH is slightly more complex from an implementation point of view, however we show that for any possible input the algorithm will always generate a path of constant competitiveness whilst still maintaining the same asymptotic behaviour as SIMPLE-PATH.

3 Asymptotic Analysis for Cone Walk

We now focus on the asymptotic properties of cone walk applied to points drawn from a randomly generated input. We will derive all of our results using a spatial Poisson process, since it has useful independence properties that are not available when one simply samples n random points in a fixed region. The theorems in Section 1.3 then follow by 'de-poissonising' (details given in [8]). Let $\mathbf{\Phi}_n$ be a planar Pois-

son process contained within $\mathcal{D}_n$, with intensity measure given by the standard two-dimensional Lebesgue measure λ. We have the following properties, for A, B Borel subsets of $\mathcal{D}_n$.

1. $\mathbb{E}\,|A \cap \mathbf{\Phi}_n| = \lambda(A)$, so in particular $\mathbb{E}\,|\mathbf{\Phi}_n| = n$;
2. if $A \cap B = \varnothing$ then $\mathbb{P}(|A \cap \mathbf{\Phi}_n| = k \mid |B \cap \mathbf{\Phi}_n| = t) = \mathbb{P}(|A \cap \mathbf{\Phi}_n| = k)$;
3. $\mathbb{P}(|A \cap \mathbf{\Phi}_n| = \varnothing) = \exp(-\lambda(A))$;
4. for all $k > e^2 \cdot \lambda(A)$ we have $\mathbb{P}(|A \cap \mathbf{\Phi}_n| \geq k) \leq \exp(-k)$.

In this extended abstract, we limit ourselves to studying the number of vertices that may be accessed by the walk for a fixed pair of randomly chosen start and destination points, since we believe this is one of the key properties of the cone walk algorithm. The results given here may then be extended to bound the number of steps accessed for any run of the algorithm by showing that it is possible to generate a 'small enough' sample containing every possible instance of cone walk on $\mathbf{\Phi}_n \times \mathcal{D}_n$ with high probability. This proof is quite technical, and we omit it here. In the following, we shall denote the sequence of stoppers visited by the walk process between fixed z and q as $(Z_i)_{i>0}$ (taking $Z_0 := z$), and the sequence of radii of the discs $(R_i)_{i>0}$. We also write $D_i := \mathrm{Disc}(Z_i, q, R_i)$, the i'th disc and let $W := \cup_{i>0} D_i$.

3.1 The number of sites accessed

Let $K := |\mathbf{\Phi}_n \cap W|$ be the number of *visited* vertices for an instance of cone walk. Recall that if we now wish to count the number of vertices that would be *accessed* by the cone walk algorithm to compute this walk, we will need to take K and add the number of vertices of $\mathbf{\Phi}_n$ that are within the 1-hop neighbourhood of the *visited* vertices. The difficulty in bounding this quantity comes from the fact that the vertices outside of the walk discs may be visited multiple times, introducing complex dependency relationships and making the analysis more subtle.

We begin by noting that any vertex outside of W is accessed by the cone walk algorithm exactly once for each edge leaving that vertex and crossing the boundary of W. We call the union of all such edges for every accessed vertex the *crossing edges*. To give a bound on the number of accessed vertices, we now require Proposition 4 given below. Its proof follows from the fact that, given some conditions, the contents of the cones (and discs) for each step behave as independent and identically distributed random variables. These technical details are dealt with in [8]. In the following, let ω_n be a sequence satisfying $\omega_n \geq \log n$.

Proposition 4 *Let K be the number of vertices visited by cone walk starting from a given site z with $L = \|zq\|$. Then, for $c_1 > 0$ a constant defined in [8] and for all n large enough,*

$$\mathbb{P}\left(K \geq c_1 L + \sqrt{L}\,\omega_n^4 + \omega_n^3\right) \leq 7 \exp\left(-\omega_n^{3/2}\right). \tag{6}$$

The following proposition now bounds the number of vertices accessed.

Proposition 5 *Let $A = A(z, q)$ be the number of sites in $\mathbf{\Phi}_n$ accessed by the cone walk algorithm (with multiplicity) when walking towards q from z, and $L = \|zq\|$. Then there exists a constant $c_2 > 0$ such that (for n sufficiently large)*

$$\mathbb{P}\left(A(z, q) > c_2\, L + 4\left(\sqrt{L} + 1\right)\omega_n^6\right) \leq 3 \exp\left(-\omega_n^{5/4}\right). \tag{7}$$

Proof: In order to bound the number of such edges, we adapt the concept of the *border point* introduced by Bose and Devroye [4] to bound the stabbing number of a random Delaunay triangulation. For $B \subseteq \mathcal{D}_n$ and a point $x \in \mathcal{D}_n$, let $\|xB\| := \inf\{\|xy\| : y \in B\}$ denote the distance from x to B.

We consider the walk from z to q in $\mathcal{D}_n$, letting

$$W = \bigcup_{i=1}^{\kappa} D_i \qquad \text{and} \qquad W^{\odot} := b(\mathbf{w}, 2\max\{\|zq\|, \omega_n^5\}), \tag{8}$$

where $\mathbf{w}$ denotes the centroid of the segment zq and we recall that $b(\mathbf{x}, r)$ denotes the closed ball centred at $\mathbf{x}$ of radius r. Then, for $x \in W^{\odot}$, let C be the disc centered at x and with radius $\min\{\|xW\|, \|x\partial W^{\odot}\|\}$ (where ∂A is used to denote the boundary of A). Partition the disc C into eight cone-shaped sectors (such that one of the separation lines is vertical, say) truncated to a radius of $\sqrt{3}/2$ times that of the outer disc (see Figure 3). We now say that x is a *border point* if one of the eight cones does not contain any points in $\mathbf{\Phi}_n$. If $x \in W^{\odot}$ is not a border point then there is no Delaunay edge between x and a point lying outside C, since a circle trough x and $y \notin C \subset W^{\odot} \setminus W$ must entirely enclose at least one sector of C (see dotted circle in Figure 3). Thus if x has a Delaunay edge with extremity in W, then x must be a border point.

The connection between border points and the number of crossing edges can be made via Euler's relation, since it follows that a crossing edge is an edge of the (planar) subgraph of $\mathrm{DT}(\mathbf{\Phi})$ induced by the points which either lie inside W, are border points, or lie outside of $W^{\odot}$ and have a neighbour in W. Let B_W denote of set of border points, E_W the collection of crossing edges, and Y_W the collection of points lying outside of $W^{\odot}$ and having a Delaunay neighbor within W. Then

$$A(z,q) \leq |E_W| \leq 3(|W \cap \mathbf{\Phi}| + |B_W| + |Y_W|). \tag{9}$$

Proposition 4 bounds $|W \cap \mathbf{\Phi}|$, as this is exactly the set of *visited vertices*. Lemmas 6 and 7 bounding $|B_W|$ and $|Y_W|$ complete the proof. □

Lemma 6 *For all n large enough, we have*

$$\mathbb{P}\Big(|Y_W| \geq 10\max\{L, \omega_n^5\}\Big) \leq 2\exp\left(-\omega_n^{5/4}\right). \tag{10}$$

Proof: Heuristically, our proof will follow from the fact that, with high probability, a Delaunay edge away from the boundary of the domain is not long enough to span the distance between a point within the walk, and a point outside of $W^{\odot}$. Unfortunately our proof is complicated by points on the walk which are very close to the boundary of the domain, since in this case, those points might have 'bad' edges which are long enough to escape $W^{\odot}$. To deal with this, we will take all points in the walk that are close to the border, and imagine that every Delaunay edge touching one of these points is such a 'bad' edge. The total number of these edges will be bounded by the maximum degree.

To begin, we give the first case. Consider an arbitrary point $x \in W \cap \mathbf{\Phi}$ that is at least ω_n^{-3} away from the boundary of $\mathcal{D}_n$. Suppose this point has a neighbour outside of $W^{\odot}$, then its circumcircle implicitly overlaps an unconditioned region of $\mathcal{D}_n$ with area at least $c\,\omega_n^{-3}\,\omega_n^5 = c\,\omega_n^2$ (for $c > 0$ a constant depending on the shape of the domain). The probability that this happens for x is thus at most $\exp\left(-\omega_n^2\right)$. Now note that there are at most $2n$ points in $\mathbf{\Phi}$ with probability bounded by $\exp\left(-\omega_n^2\right)$

and at most $4n^2$ edges between points of $x \in W \cap \mathbf{\Phi}$ and $x \in \{W^{\odot}\}^c \cap \mathbf{\Phi}$. By the union bound, the probability that any such edge exists is at most

$$(4n^2)\exp\left(-c\omega_n^2\right) + \exp\left(-\omega \right) \tag{11}$$

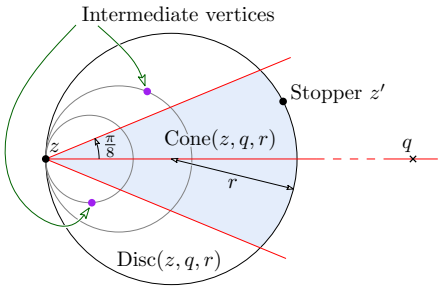

Fig. 2: One step of the cone-walk algorithm.

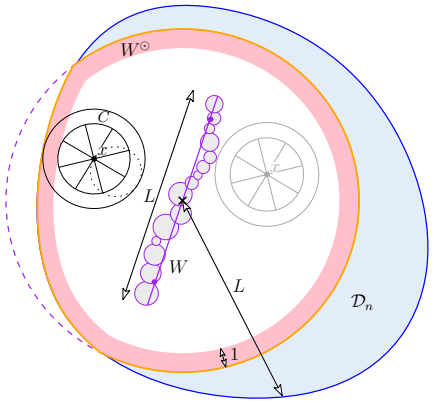

Fig. 3: For the proof of Proposition 5.

For the second case, we count the number of points within ω_n^{-3} of the boundary of the domain. Using standard arguments, we have that there are no more than $10\max\{L,\omega_n^5\}\cdot\omega_n^{-3}$ such points, with probability at least $\exp\left(-\omega_n^2\right)$. Each of these has at most $\Delta_{\mathbf{\Phi}}$ edges that could exit $W^{\odot}$, where $\Delta_{\mathbf{\Phi}}$ is the maximum degree of any vertex in $\mathrm{DT}(\mathbf{\Phi})$, which is bounded in Proposition 30 of [8]. Thus, the number of such bad edges is at most $10\max\{L,\omega_n^5\}\omega_n^{-3}\cdot\omega_n^3$ with probability at least $\exp(-\omega_n^2)+\exp(-\omega_n^{5/4})$ □

Lemma 7 *For all n large enough, and universal constant $C>0$,*

$$\mathbb{P}\Big(|B_W| \geq C\max\{L,\omega_n^7\}\Big) \leq 2\exp\left(-\omega_n^{3/2}\right). \tag{12}$$

Proof: Since $|B_W|$ is a sum of indicator random variables, it can be bounded using (a version of) Chernoff–Hoeffding's method. The only slight annoyance is that the indicators $\mathbf{1}_{\{x\in B_W\}}, x\in\mathbf{\Phi}_n\cap W^{\odot}$ are not independent. Note however that $\mathbf{1}_{\{x\in B_W\}}$ and $\mathbf{1}_{\{y\in B_W\}}$ are only dependent if the discs used to define membership to B_W for x and y intersect. There is a priori no bound on the radius of these discs, and so we shall first discard the points $x\in\mathbf{\Phi}_n$ lying far away from $\partial W^{\odot}$ and W. More precisely, let $B_W^{\star}$ denote the set of border points lying within distance ω_n of either W or $\partial W^{\odot}$, and $B_W^{\bullet}=B_W\setminus B_W^{\star}$. We now bound $|B_W^{\bullet}|$ by noting that the probability that there exists an empty circle of radius greater than $c\cdot\omega_n$ (for any $c>0$) in $\mathcal{D}_n$ is at most $\exp(-\omega_n^{3/2})$; and that each cone in the border point construction implicitly contains an empty circle (this is formally dealt with in Lemma 10 in [8]). Thus for sufficiently large n,

$$\mathbb{P}\big(|B_W^{\bullet}|\neq 0\big) \leq \exp\left(-\omega_n^{3/2}\right). \tag{13}$$

Bounding $|B_W^{\star}|$ is now easy since the amount of dependence in the family $\mathbf{1}_{\{x\in B_W\}}, x\in\mathbf{\Phi}_n\setminus W$ is controlled and we can use the inequality by Janson [14, 15]. We start by bounding the expected value

$\mathbb{E}\,|B^\star_W|$. Note that for a single point $x \in \mathbf{\Phi}_n$, by definition the disc used to define whether x is a border point does not intersect W and stays entirely within $\mathcal{D}_n$, so

$$\begin{aligned}\mathbb{P}_x(x \in B^\star_W) = \mathbb{P}(x \in B^\star_W) &\leq 24\exp\Big(-\frac{\pi}{32}\min\{\|xW\|, \|x\partial W^{\odot}\|\}^2\Big)\\ &\leq 24\exp\Big(-\frac{\pi}{32}\|xW\|^2\Big) + 24\exp\Big(-\frac{\pi}{32}\|x\partial W^{\odot}\|^2\Big) \qquad (14)\end{aligned}$$

and $\mathbf{\Phi}_n$ is unconditioned in $\mathcal{D}\setminus W$. Partition $\mathcal{D}\setminus W$ into disjoint sets as follows:

$$\mathcal{D}\setminus W = \bigcup_{i=0}^{\infty} U_i \qquad (15)$$

where $U_i := \{x \in \mathcal{D} \,:\, i \leq \|xW\| < i{+}1\}$. Similarly, the sets $U'_i := \{x \in W^{\odot} : i \leq \|x\partial W^{\odot}\| < i{+}1\}$ form a similar partition for $W^{\odot}$. Using (14) above, we may apply the Slivnyak-Mecke formula to get

$$\begin{aligned}\mathbb{E}|B^\star_W| &= \mathbb{E}\left[\sum_{x\in\mathbf{\Phi}_n} \mathbf{1}_{\{x\in W^{\odot}\setminus W\}}\,\mathbf{1}_{\{x\in B^\star_W\}}\right] &(16)\\ &= \int_{W^{\odot}\setminus W} \mathbb{P}_x(x \in B^\star_W)\,\lambda(dx) &(17)\\ &\leq \sum_{i=0}^{\infty}\int_{U_i} 24\exp\big(-\pi i^2/32\big)\;\lambda(dx) + \sum_{i=0}^{\infty}\int_{U'_i} 24\exp\big(-\pi i^2/32\big)\;\lambda(dx) &(18)\\ &= 24\sum_{i=0}^{\infty}(\lambda(U_i)+\lambda(U'_i))\;\exp\big(-\pi i^2/32\big)\,. &(19)\end{aligned}$$

We may now bound $\lambda(U_i)$ and $\lambda(U'_i)$ as follows. Recall that W is a union of discs $W = \cup_i D_i$. We clearly have that

$$U_i \subseteq \bigcup_{j=0}^{\kappa-1}\big\{x\in\mathcal{D} \,:\, i \leq \|xD_j\| < i+1\big\}. \qquad (20)$$

Note that

$$\begin{aligned}\lambda\big(\big\{x\in\mathcal{D} \,:\, i \leq \|xD_j\| < i+1\big\}\big) &\leq \pi((R_j+i+1)^2 - (R_j+i)^2) &(21)\\ &= \pi(2(R_j+i)+1). &(22)\end{aligned}$$

So, assuming there are κ steps in the walk we get

$$\lambda(U_i) \;\leq\; \sum_{j=0}^{\kappa-1}\pi(2(R_j+i)+1) \;=\; 2\pi\sum_{j=0}^{\kappa-1} R_j + \pi(i+1)\kappa. \qquad (23)$$

Regarding $\lambda(U'_i)$, note first that $W^{\odot}$ is convex for it is the intersection of two convex regions. It follows that its perimeter is bounded by $4\pi\max\{\|zq\|,\omega_n\}$, so that $\lambda(U'_i) \leq 4\pi\max\{\|zq\|,\omega_n\}$ for every $i \geq 0$.

It now follows easily that there exist universal constants C, C' such that

$$\mathbb{E}\,|B^\star_W| = \mathbb{E}\,\mathbb{E}\big[|B^\star_W| \;\big|\; R_i, i \geq 0\big] \leq C\,\mathbb{E}\left[\sum_{j=0}^{\kappa-1} R_j + \kappa + \max\{\|zq\|, \omega_n\}\right] \leq C' \max\{\|zq\|, \omega_n^6\}. \tag{24}$$

For the concentration, we use the fact that if $\|xW\|, \|x\partial W^\odot\| \leq \omega_n$ then the chromatic number χ of the dependence graph of the family $\mathbf{1}_{\{x \in B^\star_W\}}$ is bounded by the maximum number of points of $\mathbf{\Phi}_n$ contained in a disc of radius $2\omega_n$. Let $\mathrm{Po}(\lambda)$ denote a Poisson distributed random variable of rate λ. We have

$$\begin{aligned}
\mathbb{P}(\chi \geq 8\pi\omega_n^2) &\leq \mathbb{P}(\exists x \in \mathcal{D} : \mathbf{\Phi}_n \cap b(x, 2\omega_n)) && (25)\\
&\leq \mathbb{E}\left[\sum_{x \in \mathbf{\Phi}_n} \mathbb{P}_x(|b(x, 2\omega_n) \cap \mathbf{\Phi}_n| \geq 8\pi\omega_n^2)\right] && (26)\\
&\leq \mathbb{E}\left[\sum_{x \in \mathbf{\Phi}_n} \mathbb{P}(\mathrm{Po}(4\pi\omega_n^2) \geq 8\pi\omega_n^2)\right] && (27)\\
&\leq \exp\left(-\omega_n^2\right), && (28)
\end{aligned}$$

for all n large enough. Let

$$W^\partial := \big\{x \in W^\odot \;\big|\; \max\{\|xW\|, \|x\partial W^\odot\|\} \leq \omega_n\big\}.$$

Following Equation (21) and by the convexity of $W^\odot$, there exists a universal constant C'' such that

$$\mathbb{P}\Big(|\mathbf{\Phi}_n \cap W^\partial| \geq C'' \max\{L, \omega_n^5\} \cdot \omega_n^2\Big) \leq \exp\left(-\omega_n^2\right).$$

We thus obtain for $t > 0$ and by Theorem 3.2 of [14],

$$\begin{aligned}
\mathbb{P}(|B^\star_W| \geq \mathbb{E}\,|B^\star_W| + t) &\leq \mathbb{E}\left[\exp\left(-\frac{2t^2}{\chi \cdot |\mathbf{\Phi}_n \cap W^\odot|}\right)\right] && (29)\\
&\leq \exp\left(-\frac{t^2}{8\pi\, C'' \max\{L, \omega_n^5\} \cdot \omega_n^5}\right) + \mathbb{P}(\chi \geq 8\pi\omega_n^2) + \mathbb{P}(|\mathbf{\Phi}_n \cap W^\partial| > C'' \max\{L, \omega_n^5\} \cdot \omega_n^4) && (30)\\
&\leq \exp\left(-\frac{t^2}{8\pi\, C'' \max\{L, \omega_n^5\} \cdot \omega_n^4}\right) + 2\exp\left(-\omega_n^2\right). && (31)
\end{aligned}$$

And the claimed result follows for n sufficiently large by choosing $t := C''\left(L + \omega_n^6\right)$. □

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Free Energy Rates for a Class of Very Noisy Optimization Problems

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Abstract. We study a class of stochastic optimization problems for which the cardinality of the set of feasible solutions (called also configurations) m and the size of every feasible solution N satisfy $\log m = o(N)$. Assuming the data to be random, e.g., weights of a graph, edges in spanning tree problem, elements of matrices in assignment problem, etc. fluctuate due to measurements, we adopt the maximum entropy framework by weighting solutions with a Boltzmann distribution where the inverse computational temperature β controls the cost resolution of the solution space. Large fluctuations of the costs due to high input randomness correspond to a low cost resolution β. For such a high noise level in the instances implying low β, we estimate the free energy in the asymptotic limit. This quantity plays a significant role in many applications, including algorithm analysis, robust optimization and so on. In particular, we prove that the free energy exhibits a phase transition in the second order term.

Keywords: Combinatorial optimization, Boltzmann distribution, free energy, partition function

1 Introduction

We consider a class of stochastic optimization problems that can be formulated as follows: Let n be an integer (e.g., number of vertices in a graph, size of a matrix, number of keys in a digital tree, etc.), and $\mathcal{S}_n$ a set of objects (e.g., set of vertices, elements of a matrix, keys, etc). The data X denote a set of random variables which enter into the definition of an instance (e.g., weights of edges in a weighted graph). One often is interested in asymptotic behavior of the optimal values $R_{\max}(\mathcal{S}_n, X)$ or $R_{\min}(\mathcal{S}_n, X)$ defined as

$$R_{\max}(\mathcal{S}_n, X) = \max_{c\in\mathcal{C}_n}\Big\{ \sum_{i\in\mathcal{S}_n(c)} w_i(c, X)\Big\}\,, \quad R_{\min}(\mathcal{S}_n, X) = \min_{c\in\mathcal{C}_n}\Big\{ \sum_{i\in\mathcal{S}_n(c)} w_i(c, X)\Big\}\,, \tag{1}$$

where $\mathcal{C}_n$ is a set of all feasible solutions, $\mathcal{S}_n(c)$ is a set of objects from $\mathcal{S}_n$ belonging to the c-th feasible solution (e.g., set of edges belonging to a spanning tree), and $w_i(c, X)$ is the weight assigned to the i-th object in the c-th feasible solution. Throughout this work, we assume that the weight distribution only depends on the data X but it is invariant on the feasible solution c, if $\mathcal{S}_n(c)$ is given. By this assumption,

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the data and, consequently, the weights will not change during optimization and we can adopt the notation $w_i(X) := w_i(c, X)$.

Combinatorial optimization problems arise in many areas of science and engineering. Among others we mention here: the assignment problem [15], the quadratic assignment problem [7, 9], computation of the minimum spanning tree, the minimum weighted k-clique problem [15], geometric location problems, and so forth. Often, the data entering the problem specification are random and sets of solutions have to be considered as equally likely given the stochastic instance. We analyze this class of random problems in a probabilistic framework which assumes that the weights $w_i(X)$ are Borel functions of X, s.t. $w_i(X)$ are i.i.d. with some distribution $F(\cdot)$. We also assume that the cardinality of the feasible set is m (i.e., $|\mathcal{C}_n| = m$) and the cardinality of $\mathcal{S}_n(c)$ is N for every $c \in \mathcal{C}_n$. Throughout this paper we shall demand that $\log m = o(N)$.

We study these optimization problems in the maximum entropy framework. Therefore, we consider the Boltzmann distribution over all configurations. This distribution is parametrized by $\beta = 1/T$ which is the inverse computational temperature T. More precisely, defining the objective function $R(c, X) = \sum_{i \in \mathcal{S}_n(c)} w_i(X)$, the Boltzmann distribution $p_\beta(c|X)$ of $c \in \mathcal{C}_n$ is

$$p_\beta(c|X) = \frac{1}{Z(\beta, X)} \exp(-\beta R(c, X)) \text{ with partition function } Z(\beta, X) = \sum_{c \in \mathcal{C}} \exp(-\beta R(c, X)) . \quad (2)$$

It is quite revealing to study optimization problems in the maximum entropy framework through the Boltzmann distribution. For high temperature when $\beta \to 0$, this distribution selects all configurations uniformly. On the other hand, when $\beta \to \infty$ the Boltzmann distribution concentrates on the set of optimal solutions with costs $R_{\max}$. Intermediate values of β define an appropriate resolution of the solution space such that the fluctuations in the input are not overfitted by the optimization algorithm.

$Z(\beta, X)$ can also be used to characterize some thermodynamic limits such as entropy and free energy rates [8, 13]. In this paper, we focus on the free energy rates for high temperature when $\beta \to 0$. This high computational temperature limit is most interesting when the instances of optimization problems are affected by strong fluctuations which only support estimation of low cost resolution results.

The *free energy* is related to $\mathbb{E}_X[\log Z(\beta, X)]$ while the free energy *rate* is the *normalized* version of the free energy. The normalization matters! Usually, one defines the free energy rate as

$$\gamma(\beta) = \lim_{n \to \infty} \frac{\mathbb{E}_X[\log Z(\beta, X)]}{\log |\mathcal{C}_n|}. \quad (3)$$

However, such a limit may not exist or it may be trivial. The latter refers to the case where either $\log m = \log |\mathcal{C}_n|$ or $N = |\mathcal{S}_n|$ dominates, that is, $\log m \neq \Theta(N)$. In [14] the case $\log m \gg O(N)$ was analyzed, while here we focus on a class of optimization problems with $\log m = o(N)$ (e.g., the quadratic assignment problem [7, 9, 10] in which $N = n^2$ and $m = n!$). For this class of optimization problems, Szpankowski [10] proved that any solution is asymptotically optimal with high probability.

Furthermore, the free energy rate plays an important role in the novel verification approach for cost functions and algorithms proposed recently in [1]. Namely, optimization of $R(c, X')$ and $R(c, X'')$ under the two sample set scenario with *noisy* instances X', X'' requires to be robust w.r.t. noise. A framework of robust optimization has been developed in [1, 2] by using information theoretic arguments (see also [3]). Stable recovery of solution sets under two noisy inputs requires to optimize the resolution of the

solution space w.r.t. β by

$$\beta^\star \in \arg\max_{\beta\in\mathbb{R}_+} \mathcal{I}_\beta = \arg\max_{\beta\in\mathbb{R}_+} \mathbb{E}_{X',X''} \log\Big(|\mathcal{C}_n| \sum_{c\in\mathcal{C}_n} p_\beta(c|X')p_\beta(c|X'')\Big) \tag{4}$$

and then considering the solutions sampled from the Gibbs measure $p_{\beta^\star}(c|X')$ taken at the optimal $\beta^\star$. $\mathcal{I}_\beta$ can be interpreted as a generalization capacity for cost functions or algorithms. Maximizing $\mathcal{I}_\beta$ requires to understand how $\mathbb{E}_X \log Z(\beta, X)$ behaves as a function of β.

For the mentioned framework, it is crucial to understand the asymptotics of the terms in the above equation. In the present paper, we establish such asymptotics for certain temperature regimes. We shall argue that for the case $\log m = o(N)$, the proper normalization requires $\beta = \Theta(\sqrt{\log m/N}) \to 0$. In this *"high temperature"* regime we will be able to determine the free energy rate. In fact, we shall prove that the second order term of the free energy rate exhibits a phase transition. We illustrate our findings on the quadratic assignment problem.

2 Main Results and Their Consequences

In this section, we formally introduce the problem, and present our main findings. We aim at understanding the asymptotic behavior of the expectation of logarithm of partition function defined in (2), that is,

$$Z(\beta, X) = \sum_{c\in\mathcal{C}} \exp(-\beta R(c, X)) \tag{5}$$

where $\mathcal{C} := \mathcal{C}_n$ of cardinality $m := |\mathcal{C}_n|$ is the set of configurations or feasible solutions of the objective function $R(c, X) = \sum_{i\in\mathcal{S}_n(c)} w_i(X)$.

Since the weights $w_i(X)$ are Borel functions of X, they are random variables. We assume them to be i.i.d. realizations of a random variable $W(X)$ with the probability distribution F that does not depend on i. Furthermore, we postulate that the moment generating function $\mathbb{E}_X[\exp(tW(X))] < \infty$ exists for some $t > 0$. In particular, we denote

$$\mu = \mathbb{E}_X[W(X)], \quad \text{and} \quad \sigma^2 = \mathbb{V}_X[W(X)], \tag{6}$$

where $\mathbb{V}_X[W(X)] := \mathbb{E}_X[(W(X) - \mathbb{E}_X[W(X)])^2]$ denotes the variance. To simplify our analysis, we actually shall investigate the centralized weights $\overline{W}(X) := W(X) - \mu$ and denote by $\widehat{G}(\beta)$, where $\beta > 0$, the moment generating function of $(-\overline{W}(X))$, that is

$$\widehat{G}(\beta) = \mathbb{E}_X[\exp(\beta(-\overline{W}(X)))] < \infty. \tag{7}$$

Our goal is to estimate $\mathbb{E}_X[\log Z(\beta, X)]$ which can be upper bounded by Jensen's inequality as

$$\mathbb{E}_X[\log Z(\beta, X)] \le \log \mathbb{E}_X[Z(\beta, X)]. \tag{8}$$

Remark. In the following, we will omit X as an argument of $Z(\beta, X)$ and $R(c, X)$ for the sake of simplicity. (The expectation $\mathbb{E}[.]$, the variance $\mathbb{V}[.]$ and other probabilistic operations are still meant to be taken with respect to the randomness of X).

We need to evaluate $\mathbb{E}[Z(\beta)]$, so we proceed as follows

$$\mathbb{E}[Z(\beta)] = \mathbb{E}\Big[\sum_{c\in\mathcal{C}} \exp(-\beta R(c))\Big] = \exp(-\beta N\mu)\mathbb{E}\Big[\sum_{c\in\mathcal{C}} \exp\big(-\beta(R(c) - N\mu)\big)\Big]$$
$$= \exp(-\beta N\mu) m \widehat{G}^N(\beta). \tag{9}$$

Thus

$$\log \mathbb{E}[Z(\beta)] = -\beta N\mu + \log m + N \log \widehat{G}(\beta) \tag{10}$$

since the r.v.s W_i are i.i.d.

From the above relation (10) one must conclude that in order to get a nontrivial limit of $\log \mathbb{E}[Z(\beta)]/\log m$ we need to choose the limit $\beta \to 0$. Under this assumption, we can expand $\widehat{G}(\beta)$ in the Taylor series to obtain

$$\widehat{G}(\beta) = 1 + \frac{1}{2}\beta^2\sigma^2 + O(\beta^3). \tag{11}$$

We find as long as $\beta \to 0$

$$\log \mathbb{E}[Z(\beta)] = -\beta N\mu + \log m + N \log \widehat{G}(\beta) = -\beta N\mu + \log m + N \log\Big(1 + \frac{1}{2}\beta^2\sigma^2 + O(\beta^3)\Big)$$
$$= -\beta N\mu + \log m + \frac{1}{2}N\beta^2\sigma^2(1 + O(\beta)). \tag{12}$$

This suggests that the right choice for β is

$$\beta = \widehat{\beta}\sqrt{\frac{\log m}{N}} \tag{13}$$

for some constant $\widehat{\beta}$. Thus we arrive at

$$\frac{\log \mathbb{E}[Z(\beta)] + \beta N\mu}{\log m} = 1 + \frac{1}{2}\widehat{\beta}^2\sigma^2(1 + O(\beta)). \tag{14}$$

In terms of $\mathbb{E}[\log Z(\beta)]$ we find

$$\frac{\mathbb{E}[\log Z(\beta)] + \widehat{\beta}\mu\sqrt{N\log m}}{\log m} \le 1 + \frac{1}{2}\widehat{\beta}^2\sigma^2\left(1 + O\left(\sqrt{\frac{\log m}{N}}\right)\right). \tag{15}$$

But there is a surprise! Let us denote

$$\phi(\beta) = \mathbb{E}[\log Z(\beta)] + \beta N\mu =: \mathbb{E}[\log \widehat{Z}(\beta)] \tag{16}$$

where $\widehat{Z}(\beta) = \sum_{c\in\mathcal{C}} \exp(\beta \overline{R}(c))$ with $\overline{R}(c) = -\sum_{i\in\mathcal{S}(c)} \overline{W}_i$. It is easy to observe that

$$\beta \max_{c\in\mathcal{C}} \overline{R}(c) \le \log \widehat{Z}(\beta). \tag{17}$$

Using the upper bound obtained in (15) we find

$$\frac{\mathbb{E}[\max_{c\in\mathcal{C}} \overline{R}(c)]}{\log m} \le \sqrt{\frac{N}{\log m}}\left(\widehat{\beta}^{-1} + \frac{1}{2}\widehat{\beta}\sigma^2\right). \tag{18}$$

Choosing $\widehat{\beta}^* = \sqrt{2}/\sigma$ that minimizes the right-hand side of (18) we arrive at

$$\mathbb{E}[\max_{c\in\mathcal{C}} \overline{R}(c)] \leq \sqrt{2\sigma^2 N \log m} \tag{19}$$

Now proceeding as in Talagrand [13, Proposition 1.1.3] we obtain

$$\phi'(\beta) \leq \mathbb{E}[\max_{c\in\mathcal{C}} \overline{R}(c)]. \tag{20}$$

But for $\beta > \beta^* := \widehat{\beta}^* \sqrt{\log m/N}$,

$$\phi(\beta) \leq \phi(\beta^*) + \phi'(\beta^*)(\beta - \beta^*), \tag{21}$$

since $\phi(\beta)$ is known to be convex. Applying the upper bound for $\phi'(\beta)$ yields

$$\mathbb{E}[\log \widehat{Z}(\beta)] \leq \widehat{\beta}\sigma\sqrt{2}\log m \tag{22}$$

and the second upper bound in Theorem 1.

It is now worth proving that the lower bounds for $\mathbb{E}[\log \widehat{Z}(\beta)]$ are asymptotically the same as (15),(22). For that, we will follow the techniques used in Talagrand [13, Proposition 1.1.5, pp. 11–12].

For the following, note that since the weights are i.i.d., then $\overline{R}(c) \xrightarrow{d} \mathcal{N}(0, N\sigma^2)$, where $\mathcal{N}$ represents normal distribution. Let Y be the cardinality of the solution subset for which the centered negative cost function (see above) $\overline{R}(c)$ is large enough:

$$Y := \operatorname{card}\{c\colon \overline{R}(c) \geq s\log m\} \quad \text{for some} \quad s \geq 0. \tag{23}$$

It is obvious that

$$\mathbb{E}[Y] = ma, \quad \text{where} \quad a := \mathbb{P}(\overline{R}(c) \geq s\log m). \tag{24}$$

It is quite straightforward then to prove that

$$\mathbb{E}[Y^2] = ma + m(m-1)a, \quad \text{thus} \quad \mathbb{V}[Y] = ma - ma^2 \leq ma. \tag{25}$$

Let A denote an event $\{Y \leq ma/2\}$. Now by Markov inequality (second transition in the following chain)

$$\mathbb{P}(A) \leq \mathbb{P}\big((Y - \mathbb{E}[Y])^2 \geq m^2a^2/4\big) \leq 4\mathbb{V}[Y]/(m^2a^2) \leq 4/(ma). \tag{26}$$

Next, we derive lower bounds for $\mathbb{E}[\log Z(\beta)]$ on the events A and $\Omega \setminus A$. For the latter, we have:

$$\widehat{Z}(\beta) = \sum_{c\in\mathcal{C}} \exp(\beta\overline{R}(c)) \geq \sum_{c\in\mathcal{C}} \exp(\beta s\log m) \geq \frac{m}{2} a \exp(\beta s \log m), \tag{27}$$

thus

$$\mathbb{E}[\mathbb{1}_{\Omega\setminus A} \log \widehat{Z}(\beta)] \geq (1 - 4/(ma))(\log m - \log 2 + \log a + \beta s \log m). \tag{28}$$

For event A, we derive the lower bound in the following way. Choosing an arbitrary solution c_0, we notice that $Z(\beta) \geq \exp(\beta\overline{R}(c_0))$ and thus

$$\mathbb{E}[\mathbb{1}_A \log \widehat{Z}(\beta)] \geq -\beta\mathbb{E}[-\mathbb{1}_A \overline{R}(c)] \geq -\beta\mathbb{E}[|\overline{R}(c)|] \geq -L\sigma\beta\sqrt{N}, \tag{29}$$

where L is some constant coming from expectation of half-normal distribution, which is the thermodynamic limit distribution for $|\overline{R}(c)|$. Here we use the fact that $|\overline{R}(c)|$ converges in distribution to a half-normal (due to CLT), and then we determine that, due to the dominated convergence theorem and uniform integrability of $|\overline{R}(c)|$ [6, Ch. XVI.7], the expectation value of $|\overline{R}(c)|$ also converges to the one of half-normal.

Combining (28) and (29), we obtain

$$\mathbb{E}[\log \widehat{Z}(\beta)] \geq \Big(1 - \frac{4}{ma}\Big)(\log m - \log 2 + \log a + \beta s \log m) - L\sigma\beta\sqrt{N}. \tag{30}$$

From the properties of centered Gaussian, which is the thermodynamic limiting distribution of $\overline{R}(c)$, we get the following bound on a (small terms correspond to large deviation bounds):

$$(1+o(1))\frac{\sigma\sqrt{N}}{Ls\log m}\exp\Big(-\frac{s^2\log^2 m}{2\sigma^2 N}\Big) \leq a \leq (1+o(1))\exp\Big(-\frac{s^2\log^2 m}{2\sigma^2 N}\Big), \tag{31}$$

which means that in the thermodynamic limit ($n \to \infty$) holds true $ma \to \infty$, thus (30) turns into (we also normalize by $\log m$ here)

$$\frac{\mathbb{E}[\log \widehat{Z}(\beta)]}{\log m} \geq 1 - s^2\frac{\log m}{2\sigma^2 N} + \beta s - \frac{L\sigma\beta\sqrt{N}}{\log m} + \log\left(\frac{\sigma\sqrt{N}}{Ls\log m}\right)/\log m + o(1) \tag{32}$$

Now for the regime $\beta \leq \widehat{\beta}^*\sqrt{\log m/N}$ we choose $s := \beta\frac{\sigma^2 N}{\log m} = \widehat{\beta}\sigma^2\sqrt{N/\log m}$, which yields a lower bound

$$\frac{\mathbb{E}[\log \widehat{Z}(\beta)]}{\log m} \geq 1 + \frac{\widehat{\beta}^2\sigma^2}{2} + O\Big(\frac{1}{\log m}\Big) + O\Big(\frac{\log\log m}{\log m}\Big) + o(1), \tag{33}$$

and for regime $\beta \geq \widehat{\beta}^*\sqrt{\log m/N}$ we choose $s = \sqrt{2\sigma^2 N/\log m}$, which yields a lower bound

$$\frac{\mathbb{E}[\log \widehat{Z}(\beta)]}{\log m} \geq \widehat{\beta}\sqrt{2}\sigma + O\Big(\frac{1}{\log m}\Big) + O\Big(\frac{\log\log m}{\log m}\Big) + o(1). \tag{34}$$

Additional terms $O(\cdot)$ are small in the thermodynamic limit, so we obtain the requested asymptotical lower bounds.

In passing, one should observe that the bounds (both lower and upper) are distinctively different for two different regimes. Thus the normalized free energy rate exhibits a phase transition at the second order term.

In summary, we have just proved the following finding.

Theorem 1 *Consider a class of combinatorial optimization problems in which the cardinality of feasible solutions m and the size of feasible solution N are related as $\log m = o(N)$. Assume that weights W_i are i.i.d. distributed with mean μ and variance σ^2 and moment generating function of $(-W_i)$ is finite. Define*

$$\beta = \widehat{\beta}\sqrt{\log m/N}. \tag{35}$$

Then the function $Z(\beta)$ satisfies

$$\lim_{n\to\infty} \frac{\mathbb{E}[\log Z(\beta)] + \widehat{\beta}\mu\sqrt{N\log m}}{\log m} = \begin{cases} 1 + \dfrac{\widehat{\beta}^2\sigma^2}{2}, & \widehat{\beta} < \dfrac{\sqrt{2}}{\sigma}, \\ \widehat{\beta}\sigma\sqrt{2}, & \widehat{\beta} \geq \dfrac{\sqrt{2}}{\sigma}. \end{cases} \tag{36}$$

In other words, the free energy rate $\gamma(\beta) = \lim_{n\to\infty} \mathbb{E}[\log Z(\beta)]/\log m$ becomes

$$\gamma(\beta) = -\widehat{\beta}\mu\sqrt{\frac{N}{\log m}} + O(1) \tag{37}$$

with a phase transition at the second order term.

Remarks: First, the reader should note that the critical inverse temperature $\widehat{\beta}^* = \sqrt{2}/\sigma$ relates the low β limit to the high noise regime of optimization problems (see also Derrida's random energy model [5]). Second, it may be useful to provide an heuristic argument behind Theorem 1. Let $Z(\beta) = \exp(-\beta N\mu)\widehat{Z}(\beta)$ where (note the minus sign which we put into $\widehat{R}(c)$ for convenience)

$$\widehat{Z}(\beta) = \sum_{c\in\mathcal{C}} \exp\left(-\beta\sqrt{N}\frac{\sum_{i\in\mathcal{S}(c)} W_i - N\mu}{\sqrt{N}}\right) = \sum_{c\in\mathcal{C}} \exp\big(\beta\sqrt{N}\cdot\widehat{R}(c)\big). \tag{38}$$

Since W_i are i.i.d. we conclude that $\widehat{R}(c)\xrightarrow{d}\mathcal{N}(0,\sigma^2)$, where $\mathcal{N}(0,\sigma^2)$ represents the normal distribution with mean zero and variance σ^2. We now consider two regimes of β. In the first regime, we re-compute $\mathbb{E}[\widehat{Z}(\beta)]$ by noting that its main contribution comes from one large $\widehat{R}(c)$. Indeed, note that

$$\mathbb{E}\big[\exp\big(\beta\sqrt{N}\widehat{R}(c)\big)\big] \sim \frac{1}{\sqrt{2\pi\sigma}}\int \exp\left(\beta\sqrt{N}t - \frac{t^2}{2\sigma^2}\right)dt. \tag{39}$$

But the above integral achieves at $t_0 = \beta\sigma^2\sqrt{N}$ its maximum value (by the saddle point method)

$$\mathbb{E}[\exp(\beta\sqrt{N}\widehat{R}(c))] \sim \exp\left(\frac{\beta^2 N\sigma^2}{2}\right). \tag{40}$$

Most of $\mathbb{E}[\widehat{Z}(\beta)]$ comes from this one large $\widehat{R}(c)$. But its probability is bounded by

$$\mathbb{P}\Big(\bigcup_{c\in\mathcal{C}} \widehat{R}(c) > t_0\Big) \leq \exp\left(\log m - \frac{\beta^2 N\sigma^2}{2}\right) \tag{41}$$

which is very small for

$$\beta > \widehat{\beta}^*\sqrt{\log m/N}, \quad \widehat{\beta}^* = \sqrt{2}/\sigma. \tag{42}$$

Thus for $\widehat{\beta} < \widehat{\beta}^*$ we recover the first upper bound in (36).

To find the second bound, we we postulate for $\beta > \sqrt{2\log m/(N\sigma^2)}$ that

$$\widehat{Z}(\beta) \sim \exp\big(\beta\sqrt{N}\max_{c\in\mathcal{C}}\widehat{R}(c)\big) \text{ so that } \log\widehat{Z}(\beta) \sim \beta\sqrt{N}\max_{c\in\mathcal{C}}\widehat{R}(c). \tag{43}$$

But

$$\mathbb{P}\left(\max_{c\in\mathcal{C}}\widehat{R}(c) > t\right) \le \exp\left(\log m - \frac{t^2}{2\sigma^2}\right). \tag{44}$$

Therefore, with high probability we can assume that

$$\max_{c\in\mathcal{C}}\widehat{R}(c) \sim \sqrt{2\sigma^2 \log m}. \tag{45}$$

Combining it with the above lead to the second bound in (36).

In many applications (see [1, 2]) one needs more refined information about $\log Z(\beta)$. In particular, we must know whether $\log Z(\beta)$ is concentrated around $\mathbb{E}[\log Z(\beta)]$. In other words, whether

$$\log Z(\beta)/\mathbb{E}[\log Z(\beta)] \xrightarrow{\mathbb{P}} 1 \tag{46}$$

where $\xrightarrow{\mathbb{P}}$ represents convergence in probability.

To address this question, we first estimate the variance of $Z(\beta)$ or, preferably, of $\log Z(\beta)$. The next lemma gives us a precise evaluation of the variance $\mathbb{V}[Z(\beta)] = \mathbb{E}[(Z(\beta) - \mathbb{E}[Z(\beta)])^2]$.

Lemma 1 *For any $\beta > 0$ we have*

$$\mathbb{V}[Z(\beta)] = (\mathbb{E}[Z(\beta)])^2\left(\mathbb{E}_D\left(\frac{G(2\beta)}{(G(\beta))^2}\right)^D - 1\right) \tag{47}$$

where D is a random variable denoting the cardinality of the overlap $\mathcal{S}(c)\cap\mathcal{S}(c')$ for two distinct (chosen uniformly at random) feasible solutions $c, c' \in \mathcal{C}$. Here, $G(\beta)$ is the moment generating function of the negative weights $(-W)$.

To illustrate an application of the above lemma and the behavior of the overlap D we discuss below the quadratic assignment problem [7, 9].

Example 1. *Quadratic Assignment Problem*
In the Quadratic Assignment Problem (further referred to as QAP), we consider two $n \times n$ matrices, namely the weight matrix V and the distance matrix H. The solution space is the set of all the n-element permutations S_n. The objective function island

$$R_{\text{QAP}}(\pi) = \sum_{i,j=1}^{n} V(i,j)\cdot H(\pi(i),\pi(j)), \quad \pi \in S_n.$$

Thus, in our notation, $\mathcal{C} = S_n$, $N = n^2$ and $m = n!$.

As introduced above, D is a random variable denoting the overlap of two arbitrary feasible solutions. We claim that $\mathbb{E}_D[D] = O(1)$.

Indeed, let π, π' be two random permutations and Y_{ij} be an indicator random variable of the event

$$\text{ovr}(i,j) = \{V(i,j)\cdot H(\pi(i),\pi(j)) = V(i,j)\cdot H(\pi'(i),\pi'(j))\},$$

thus

$$\mathbb{E}_D[D] = \mathbb{E}_D\Big[\sum_{i,j=1}^{n} Y_{ij}\Big] = \sum_{i,j=1}^{n}\mathbb{E}_D[Y_{ij}] = \sum_{i,j=1}^{n}\mathbb{P}(\text{ovr}(i,j)).$$

Now note that for each i, j the event $\mathrm{ovr}(i, j)$ occurs, if and only if $\pi(i) = \pi'(i)$ and $\pi(j) = \pi'(j)$. Thus $\mathbb{P}(\mathrm{ovr}(i, j)) = 1/n(n-1)$ and

$$\mathbb{E}_D[D] = \sum_{i,j=1}^{n} \mathbb{P}(\mathrm{ovr}(i,j)) = n^2 \frac{1}{n(n-1)} = O(1), \tag{48}$$

which proves $\mathbb{E}_D[D] = O(1)$.

Now, we are ready to formulate our second main finding.

Theorem 2 *If $\beta\mathbb{E}_D[D] \to 0$, then*

$$Z(\beta)/\mathbb{E}[Z(\beta)] \xrightarrow{\mathbb{P}} 1. \tag{49}$$

More precisely,

$$\mathbb{P}(|Z(\beta) - \mathbb{E}[Z(\beta)]| \geq \epsilon\mathbb{E}[Z(\beta)]) \leq \frac{\mathbb{V}[Z(\beta)]}{\epsilon^2(\mathbb{E}[Z(\beta)])^2} = O(\beta^2\mathbb{E}_D[D]) \to 0. \tag{50}$$

Proof: Put $G(\beta) = \mathbb{E}[\exp(\beta(-W))]$, where W is a random variable with expectation μ and variance σ^2. The Taylor expansion of $G(\beta)$ around 0 is

$$G(\beta) = 1 - \beta\mu + \frac{\beta^2\mathbb{E}[W^2]}{2} + O(\beta^3). \tag{51}$$

Thus,

$$\begin{aligned}\left(\frac{G(2\beta)}{(G(\beta))^2}\right)^D &= \left(\frac{1 - 2\beta\mu + 2\beta^2\mathbb{E}[W^2] + O(\beta^3)}{[1 - \beta\mu + \beta^2\mathbb{E}[W^2]/2 + O(\beta^3)]^2}\right)^D = \left(\frac{1 - 2\beta\mu + 2\beta^2\mathbb{E}[W^2] + O(\beta^3)}{1 - 2\beta\mu + (\mu^2 + \mathbb{E}[W^2])\beta^2 + O(\beta^3)}\right)^D \\ &= (1 + (\mathbb{E}[W^2] - \mu^2)\beta^2 + O(\beta^3))^D = 1 + D\sigma^2\beta^2 + O(\beta^3)\end{aligned} \tag{52}$$

leading to

$$\mathbb{E}_D\left(\frac{G(2\beta)}{(G(\beta))^2}\right)^D = 1 + \sigma^2\beta^2\mathbb{E}_D[D] + O(\beta^3). \tag{53}$$

From the above, we obtain the β-asymptotics of $\mathbb{V}[Z(\beta)]$:

$$\mathbb{V}[Z(\beta)] = (\mathbb{E}[Z(\beta)])^2\left(\mathbb{E}_D\left(\frac{G(2\beta)}{(G(\beta))^2}\right)^D - 1\right) = (\mathbb{E}[Z(\beta)])^2(\sigma^2\beta^2\mathbb{E}_D[D] + O(\beta^3)), \tag{54}$$

and the theorem is proved. □

The last theorem implies that

$$\log Z(\beta) - \mathbb{E}[\log Z(\beta)] \xrightarrow{\mathbb{P}} 0. \tag{55}$$

But we would like to establish a stronger statement, say

$$\log Z(\beta) - \log \mathbb{E}[Z(\beta)] \xrightarrow{\mathbb{P}} 0 \tag{56}$$

or even $\log Z(\beta)/\mathbb{E}[\log Z(\beta)] \xrightarrow{\mathbb{P}} 1$. The following considerations should imply this. Observe that by expanding $\log Z(\beta)$ in the Taylor series around $\mathbb{E}[Z(\beta)]$ we have

$$\log Z(\beta) = \log \mathbb{E}[Z(\beta)] + \frac{Z(\beta) - \mathbb{E}[Z(\beta)]}{\mathbb{E}[Z(\beta)]} - \frac{1}{2}\frac{(Z(\beta) - \mathbb{E}[Z(\beta)])^2}{(\mathbb{E}[Z(\beta)])^2} + \sum_{k=3}^{\infty} \frac{(-1)^{k+1}}{k!} \frac{(Z(\beta) - \mathbb{E}[Z(\beta)])^k}{(\mathbb{E}[Z(\beta)])^k}.$$

Taking the expectation, we obtain

$$\mathbb{E}[\log Z(\beta)] = \log \mathbb{E}[Z(\beta)] - \frac{1}{2}\frac{\mathbb{V}[Z(\beta)]}{(\mathbb{E}[Z(\beta)])^2} + \sum_{k=3}^{\infty} \frac{(-1)^{k+1}}{k!} \frac{\mathbb{E}[(Z(\beta) - \mathbb{E}[Z(\beta)])^k]}{(\mathbb{E}[Z(\beta)])^k}. \tag{57}$$

Now we apply Theorem 2 in a stronger form. From the proof of Lemma 1 presented in the next section, we actually can conclude a stronger form of (50), namely, for any $k \geq 2$

$$\mathbb{P}\big(|(Z(\beta) - \mathbb{E}[Z(\beta)])^k| \geq \epsilon(\mathbb{E}[Z(\beta)])^k\big) \leq \frac{\mathbb{E}[(Z(\beta) - \mathbb{E}[Z(\beta)])^k]}{\epsilon(\mathbb{E}[Z(\beta)])^k} = O(\beta^2 \mathbb{E}_D[D_2(k)]) \tag{58}$$

where $D_2(k)$ is a random variable representing the cardinality of the joint pairwise overlaps $\bigcup_{s<t}\big(\mathcal{S}(c_s) \cap \mathcal{S}(c_k)\big)$ among k selected configurations $c_1, \ldots, c_k \in \mathcal{C}$. In many combinatorial optimization problems $E[D_2(k)]$ is constant or grows very slowly (e.g., in the quadratic assignment problem $E[D_2(k)] = O(1)$). Then (56) will follow.

3 Proof of Lemma 1

We prove now Lemma 1. Let

$$Z(\beta) = \exp(-\beta N \mu) \sum_{c \in \mathcal{C}} T(c), \quad T(c) = \exp\Big(\beta\Big(-\sum_{i \in \mathcal{S}(c)} \overline{W}_i\Big)\Big). \tag{59}$$

Now define $\widehat{Z}(\beta) = \sum_{c \in \mathcal{C}} T(c)$. To compute $\mathbb{V}[\widehat{Z}(\beta)]$, we proceed as follows

$$\mathbb{E}[(\widehat{Z}(\beta))^2] = \mathbb{E}\Big[\sum_{c \in \mathcal{C}} T(c) \cdot \sum_{c' \in C} T(c')\Big] = \sum_{c, c' \in \mathcal{C}} \mathbb{E} \exp\Big(-\beta\Big(\sum_{i \in \mathcal{S}(c)} \overline{W}_i + \beta \sum_{j \in \mathcal{S}(c')} \overline{W}_j\Big)\Big). \tag{60}$$

Now let the solutions c and c' have an overlap $\mathcal{S}(c, c') := \mathcal{S}(c) \cap \mathcal{S}(c')$ of cardinality $d = d(c, c') := |\mathcal{S}(c, c')|$ (which we will call a *summand overlap*). We also define the symmetric difference $\overline{\mathcal{S}}(c, c') := \mathcal{S}(c) \triangle \mathcal{S}(c')$ and continue the chain of equalities:

$$\mathbb{E}[(\widehat{Z}(\beta))^2] = \sum_{c, c' \in \mathcal{C}} \mathbb{E} \exp\Big(-\beta\Big(2 \sum_{i \in \mathcal{S}(c, c')} \overline{W}_i + \sum_{j \in \overline{\mathcal{S}}(c, c')} \overline{W}_j\Big)\Big). \tag{61}$$

Here the sets of $\mathcal{S}(c,c')$ and $\bar{\mathcal{S}}(c,c')$ are independent, allowing us to decompose the expectation into the product:

$$\begin{aligned}\mathbb{E}[(\widehat{Z}(\beta))^2] &= \sum_{c,c'\in\mathcal{C}} \mathbb{E}\exp\Big(-\beta\Big(2\sum_{i\in\mathcal{S}(c,c')}\overline{W}_i\Big)\Big)\cdot\mathbb{E}\exp\Big(-\beta\Big(\sum_{j\in\bar{\mathcal{S}}(c,c')}\overline{W}_j\Big)\Big)\\ &= \sum_{c,c'\in\mathcal{C}} (\widehat{G}(2\beta))^d(\widehat{G}(\beta))^{2(N-d)} = (\widehat{G}(\beta))^{2N}\sum_{c,c'\in\mathcal{C}}\left(\frac{\widehat{G}(2\beta)}{(\widehat{G}(\beta))^2}\right)^d. \qquad (62)\end{aligned}$$

Now assume that the probability of the two solutions c and c', chosen uniformly at random, to have a d-element overlap is $P_{\text{ovr}}(d)$ and rewrite the above as follows:

$$\begin{aligned}\mathbb{E}[(\widehat{Z}(\beta))^2] &= (\widehat{G}(\beta))^{2N}\sum_{d=0}^{N} m^2 P_{\text{ovr}}(d)\left(\frac{\widehat{G}(2\beta)}{(\widehat{G}(\beta))^2}\right)^d = m^2(\widehat{G}(\beta))^{2N}\sum_{d=0}^{N} P_{\text{ovr}}(d)\left(\frac{\widehat{G}(2\beta)}{(\widehat{G}(\beta))^2}\right)^d\\ &= (\mathbb{E}[\widehat{Z}(\beta)])^2\sum_{d=0}^{N} P_{\text{ovr}}(d)\left(\frac{\widehat{G}(2\beta)}{(\widehat{G}(\beta))^2}\right)^d. \qquad (63)\end{aligned}$$

We conclude that

$$\mathbb{V}[\widehat{Z}(\beta)] = \mathbb{E}[(\widehat{Z}(\beta))^2] - (\mathbb{E}[\widehat{Z}(\beta)])^2 = (\mathbb{E}[\widehat{Z}(\beta)])^2\left(\mathbb{E}_D\left(\frac{\widehat{G}(2\beta)}{(\widehat{G}(\beta))^2}\right)^D - 1\right),$$

where D is a random variable denoting the summand overlap in two randomly chosen solutions. Recalling that $Z(\beta) = \exp(-\beta N\mu)\widehat{Z}(\beta)$ and, as well, $G(\beta) = \exp(-\beta\mu)\widehat{G}(\beta)$, we obtain the version without hats:

$$\mathbb{V}[Z(\beta)] = \mathbb{E}[(Z(\beta))^2] - (\mathbb{E}[Z(\beta)])^2 = (\mathbb{E}[Z(\beta)])^2\left(\mathbb{E}_D\left(\frac{G(2\beta)}{(G(\beta))^2}\right)^D - 1\right).$$

This proves Lemma 1.

4 Conclusion and Outlook

This paper discusses the low β asymptotics of the free energy for a class of optimization functions that show a bounded growth of the configuration space w.r.t. the solution complexity. In the concrete example of the quadratic assignment problem, the configuration space is the symmetric group with $n!$ configurations and assignment solutions of complexity n^2 for $n \times n$ matrices. Theorem 1 establishes a proportionality between the critical temperature and the noise level in the optimization problem. Consequently, the low β limit is justified for very noisy optimization problems as they arise in a variety of modern high throughput experimental designs, especially in the life sciences. There, the precision of the individual experiments is traded off against the number of experiments that can be performed. This situation appears to us being prevalent in many *big data* scenarios today.

In addition, we like to emphasize that free energies evaluated on two different data instances determine a model validation criterion for cost functions and algorithms. The results of theorem 1 will enable us to determine the optimal resolution of optimization problems and the optimal precision of algorithms in the high noise limit.

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Limit Laws for the Number of Groups formed by Social Animals under the Extra Clustering Model

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Abstract. We provide a complete description of the limiting behaviour of the number X_n of groups that are formed by social animals when the number n of animals tends to infinity. The analysis is based on a random model by Durand, Blum and François, where it is assumed that groups are formed more likely by animals which are genetically related. The random variable X_n can be described by a stochastic recurrence equation that is very similar to equations that occur in the stochastic analysis of divide-and-conquer algorithms although it does not fall into already known cases. In particular, we obtain (in the most interesting) "neutral model" a curious central limit theorem, where the normalizing factor is $\sqrt{\mathrm{Var}(X_n)/2}$. In the non-neutral (or extra clustering) cases the results are completely different. We obtain either a mixture of a discrete and a continuous limit law or just a discrete limit law.

Keywords: Animal group patterns, number of groups, limit laws, Riccati differential equation, Whittaker functions, singularity perturbation analysis, method of moments.

1 Introduction and Results

An important problem in biology is to understand animal group patterns of social animals like wolves, lions, springboks, deers, gazelles, elephants, etc. For this purpose, many models have been proposed such as fusion/fissions models, models based on kin-selection and game-theoretic models; see Durand, Blum and François [7] for a thorough discussion and references.

In [7], the authors proposed a new model which is based on the reasonable assumption that groups are formed more likely by animals which are genetically related. They used a phylogenetic tree as decision criteria for genetic relatedness. The groups then are all the maximal *clades* of the tree, where the clade of a given external node (which corresponds to an animal) in the phylogenetic tree is the set of all external

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nodes (animals) belonging to the tree rooted at the parent of the given external node (what we call here *clade* was called *minimal clade* in Blum and François [3] and Chang and Fuchs [5]).

We describe the model of [7] now in more details. Let n be the number of animals. We consider a random phylogenetic tree of size n which is a rooted, ordered, binary tree with n external nodes (and consequently, $n-1$ internal nodes). As random model, we consider the Yule-Harding model which can be described as follows: start with the root of the tree which has two external nodes as children; choose one external node uniformly at random and replace it by a cherry (an internal node with two external nodes); recursively repeat this procedure until a tree with n external nodes is constructed. Note that alternatively, this random model can be also described by a coalescence process starting from the n external nodes; see [5] for more details. Finally, the binary search tree model from computer science is also equivalent to this model; see Blum, François and Janson [4].

As mentioned above, the decision of genetic relatedness will be based on the random phylogenetic tree of size n (this was called the *neutral model* in [7]). Let X_n denote the number of maximal clades of the tree, or in other words, the number of groups formed by the n animals. Then, X_n can be computed recursively as follows

$$X_n \stackrel{d}{=} \begin{cases} 1, & \text{if } I_n = 1 \text{ or } I_n = n-1; \\ X_{I_n} + X^*_{n-I_n}, & \text{otherwise,} \end{cases} \qquad (n \geq 3), \tag{1}$$

where the initial condition is given by $X_2 = 1$, X_n^* is an independent copy of X_n and I_n is the size of the left subtree of the random phylogenetic tree which has a uniform distribution on $\{1, \ldots, n-1\}$.

Distributional recurrences of the above type have been investigated in many recent studies, since similar recurrences hold for shape parameters in binary search trees and performance characteristics of the quicksort algorithm; see Hwang and Neininger [14] for a very general framework. Note, however, that the framework from [14] does not apply to the current situation as will become clear from the results below.

Mean and higher moments of X_n are easy to derive by either directly considering recurrences arising from the recursive definition (1) and similar ideas as in [14] or by using generating functions and singularity analysis; see Chapter VI in Flajolet and Sedgewick [13]. Durand and François in [8] used the latter tools in order to obtain the following result for the mean: they proved that, as $n \to \infty$,

$$\mathbb{E}(X_n) \sim \frac{1-e^{-2}}{4} n. \tag{2}$$

Using an extension of their argument, one can also derive higher moments. For the variance, one obtains that, as $n \to \infty$,

$$\mathrm{Var}(X_n) \sim \frac{(1-e^{-2})^2}{4} n \log n \tag{3}$$

and for all higher central moments that

$$\mathbb{E}\left(X_n - \mathbb{E}(X_n)\right)^k \sim (-1)^k \frac{2k}{k-2} \left(\frac{1-e^{-2}}{4}\right)^k n^{k-1}, \qquad (k \geq 3). \tag{4}$$

Note that from this, the limiting distribution of X_n (centralized and normalized) cannot be identified with the method of moments.

In order to find the limiting distribution of X_n, we will use bivariate generating functions and singularity perturbation analysis. Our first main result is the following (surprising) central limit theorem.

Theorem 1 *For the number of groups X_n under the neutral model, we have*

$$\frac{X_n - \mathbb{E}(X_n)}{\sqrt{\mathrm{Var}(X_n)/2}} \xrightarrow{d} N(0,1),$$

where $N(0,1)$ denotes the standard normal distribution and $\xrightarrow{d}$ denotes convergence in distribution.

Remark 1 *We point out the curious normalization (half the variance). The same phenomenon was observed by Janson and Kersting [15] for the total length of external branches in the Kingman's coalescent.*

Remark 2 *A similar situation as the one above was faced by Drmota, Iksanov, Möhle and Rösler in [9], where they analyzed the number of cuts needed to isolate the root of a random recursive tree, a sequence of random variables for which the limiting distribution also cannot be found from its asymptotic moments; see Panholzer [16]. In fact, we will prove Theorem 1 with a similar approach as in [9].*

The above neutral model was extended in [7] to the *extra clustering model* in order to test whether genetic relatedness is really the main driving force behind the group formation process (as seems not to be the case for social animals with many predators such as deers, gazelles and springboks; see Figure 3 in [7]). We recall the definition from [7].

Let $0 \le p \le 1$ be a fixed probability. Then, the number of groups (which with a slight abuse of notation, we will again denote by X_n) is given as follows: $X_2 = 1$ and

$$X_n \stackrel{d}{=} \begin{cases} 1, & \text{with probability } p; \\ \text{neutral model (1)}, & \text{with probability } 1-p, \end{cases} \qquad (n \ge 3). \tag{5}$$

Note that $p = 0$ is the above neutral model. For the other values of p, we will extend our above analysis. (Note that the authors of [7] again did not provide any result beyond the mean.)

Theorem 2 *(a) Let $0 < p < 1/2$. Then, we have*

$$\frac{X_n}{n^{1-2p}} \xrightarrow{d} X,$$

where the law of X is the sum of a discrete distribution of measure $p/(1-p)$ that is concentrated at zero and a continuous distribution on $[0,\infty)$ with density

$$f(x) = \frac{4(1-2p)^3}{1-p}\frac{1}{2\pi i}\int_{\mathcal{H}} t^{-2p} e^{-\delta(p)t^{1-2p}x - t}\,dt = \frac{4(1-2p)^3}{1-p}\sum_{k\ge 0}\frac{(-\delta(p))^k}{k!\Gamma(2(k+1)p-k)}x^k, \tag{6}$$

where $\mathcal{H}$ is the Hankel contour (starting in the upper half plane and winding around 0 counterclockwise) and

$$\delta(p) = \frac{(1-2p)^2 W_{p,(1-2p)/2}(-2(1-p))}{4^{p-1}(1-p)^{2p} M_{p,(1-2p)/2}(-2(1-p))},$$

where $M_{\kappa,\mu}(z)$ and $W_{\kappa,\mu}(z)$ are the Whittaker M and Whittaker W function (see, e.g., Chapter 6 in Beals and Wong [1] for a precise definition of these functions).

We also have convergence of all moments, where the moments of X are given by $\mathbb{E}(X^k) = d_k/\Gamma(k(1-2p)+1)$ and d_k is given by

$$d_1 =: c(p) = \frac{1}{e^{2(1-p)}} \int_0^1 (1-t)^{-2p} e^{2(1-p)t}(1-(1-p)t^2)\mathrm{d}t$$

and for $k \geq 2$,

$$d_k = \frac{2(1-p)}{(k-1)(1-2p)} \sum_{j=0}^{k-2} \binom{k-1}{j} d_{k-1-j} d_{j+1}.$$

(b) Let $1/2 \leq p \leq 1$ Then, we have

$$X_n \xrightarrow{d} X,$$

where X is a discrete random variable with probability generating function

$$\mathbb{E}\left(u^X\right) = \frac{1-\sqrt{1-4p(1-p)u}}{2(1-p)}.$$

In particular, for $1/2 < p \leq 1$, we also have convergence of moments, where the moments are given by $\mathbb{E}(X^k) = e_k$ and e_k is given by $e_1 = p/(2p-1)$ and for $k \geq 2$,

$$e_k = \frac{2(1-p)}{2p-1} \sum_{j=0}^{k-2} \binom{k-1}{j} e_{k-1-j} e_{j+1} + \frac{p}{2p-1}.$$

In the case $p = 1/2$, we only have weak convergence. More precisely, the moments of X are infinite and the moments of X_n are given by

$$\mathbb{E}(X_n^k) \sim \frac{k! J_{2k-1}}{(2k-1)! 2^{2k-1}} \log^{2k-1} n,$$

where J_{2k-1} are the tangent numbers (or Euler numbers of odd index)

Remark 3 *In the cases $0 < p < 1/2$ and $1/2 < p \leq 1$, we have convergence of moments and the result can be proved by the method of moments (see below).*

For $p = 1/2$, we use a variant of the method of proof of Theorem 1. In fact, this method can also be applied to the cases $0 < p < 1/2$ and $1/2 < p \leq 1$ to give an alternative proof of our result in these cases. For the first range such an approach gives in addition that the moment generating function of X has the integral representation

$$\mathbb{E}\left(e^{yX}\right) = \frac{1}{2\pi i} \int_{\mathcal{H}} \Phi(y,t) e^{-t} \mathrm{d}t,$$

where $\mathcal{H}$ is the Hankel contour and

$$\Phi(y,t) = \frac{4(1-2p)^2 - ypm(p)4^p(1-p)^{2p-1}t^{2p-1}}{4(1-2p)^2 t - ym(p)4^p(1-p)^{2p}t^{2p}}$$

with determination of the powers in t chosen such that the branch cut is at $[0,\infty)$ and the constant $m(p)$ is given by $m(p) = M_{p,(1-2p)/2}(-2(1-p))/W_{p,(1-2p)/2}(-2(1-p))$.

It is now an exercise to check that this is precisely the moment generating function of the probability measure that is the sum of a discrete distribution of measure $p/(1-p)$ concentrated at zero and a continuous distribution on $[0,\infty)$ with density (6).

We conclude the introduction with a short sketch of the paper. In the next section, we consider the neutral model and derive asymptotic expansions of moments of X_n. Moreover, a strong law of large numbers will be stated as well. In Section 3, we will sketch the proof of Theorem 1. In Section 4, we will prove the moment convergence part of Theorem 2, part (a). More details and the proofs of the remaining claims of Theorem 2 are postponed to the journal version of this paper.

2 Moments and Strong Law of Large Numbers - Neutral Model

In this section, we will re-prove (2) and prove (3). Moment pumping can then be used to obtain (4); for the latter method which was frequently used in the analysis of algorithms see, e.g., Chern, Fuchs and Hwang [6] and Fill and Kapur [11] and references therein.

Now, in order to prove (2) and (3), first observe that (1) yields

$$\mathbb{E}(e^{yX_n}) = \frac{2}{n-1}e^y + \frac{1}{n-1}\sum_{j=2}^{n-2}\mathbb{E}(e^{yX_j})\mathbb{E}(e^{yX_{n-j}}), \qquad (n \geq 3)$$

with initial condition $\mathbb{E}(e^{yX_2}) = e^y$. Next, set

$$X(y,z) = \sum_{n\geq 2}\mathbb{E}(e^{yX_n})z^n.$$

Then, by a standard computation

$$z\frac{\partial}{\partial z}X(y,z) = X(y,z) + X^2(y,z) + e^y z^2 + \frac{2e^y z^3}{1-z} \tag{7}$$

with initial condition $X(y,0) = 0$.

From (7), we obtain differential equations for the generating functions of moments of X_n by differentiation. For instance, if we set

$$E(z) = \sum_{n\geq 2}\mathbb{E}(X_n)z^n \qquad \text{and} \qquad S(z) = \sum_{n\geq 2}\mathbb{E}(X_n^2)z^n,$$

we obtain that

$$E'(z) = \left(\frac{1}{z} + \frac{2z}{1-z}\right)E(z) + \frac{z(1+z)}{1-z}, \tag{8}$$

$$S'(z) = \left(\frac{1}{z} + \frac{2z}{1-z}\right)S(z) + \frac{2}{z}E(z)^2 + \frac{z(1+z)}{1-z} \tag{9}$$

with $E(0) = S(0) = 0$. Note that both of these differential equations (as well as the corresponding differential equations for higher moments) have all the same form.

In order to solve them, we need the following lemma.

Lemma 1 *Let $f(z)$ be a function analytic at $z = 0$ with*

$$f'(z) = \left(\frac{1}{z} + \frac{2z}{1-z}\right) f(z) + g(z),$$

where $f(0) = 0$. Then,

$$f(z) = \frac{z}{(1-z)^2 e^{2z}} \int_0^z \frac{(1-t)^2 e^{2t}}{t} g(t) \mathrm{d}t.$$

Now, for the mean, applying the above lemma to (8), we obtain that

$$E(z) = \frac{(-1 + e^{2z} + 2ze^{2z} - 2z^2 e^{2z})z}{(1-z)^2 4e^{2z}}.$$

From this, by a standard application of singularity analysis, we obtain that

$$\mathbb{E}(X_n) = \frac{1 - e^{-2}}{4} n + \mathcal{O}(1).$$

Next, for the second moment, by another application of Lemma 1, we have

$$S(z) = \frac{z}{(1-z)^2 e^{2z}} \int_0^z \left(\frac{2(1-t)^2 e^{2t}}{t^2} E(t)^2 + (1-t)^2 e^{2t} \right) \mathrm{d}t.$$

Plugging into this the above expression for $E(t)$ and using Maple yields the following singularity expansion for the integrand, as $t \to 1$,

$$\frac{2(1-t)^2 e^{2t}}{t^2} E(t)^2 + (1-t)^2 e^{2t} \sim \frac{(e^2-1)^2}{8e^2} \frac{1}{(1-t)^2} + \frac{(e^2-1)^2}{4e^2} \frac{1}{1-t}.$$

Then, by the closure properties of singularity analysis from Fill, Flajolet and Kapur [10], we obtain that, as $z \to 1$,

$$S(z) \sim \frac{(1-e^{-2})^2}{8} \frac{1}{(1-z)^3} + \frac{(1-e^{-2})^2}{4} \frac{1}{(1-z)^2} \log\left(\frac{1}{1-z}\right).$$

Hence, by singularity analysis

$$\mathbb{E}(X_n^2) \sim \frac{(1-e^{-2})^2}{16} n^2 + \frac{(1-e^{-2})^2}{4} n \log n.$$

This and the above expansion for the mean yields (3).

From these results for mean and variance, we deduce the following strong law of large numbers for X_n, where the sequence is now constructed on the same probability space via the tree evolution process underlying the Yule-Harding model.

Theorem 3 *We have, as $n \to \infty$,*

$$P\left(\lim_{n\to\infty} \left| \frac{X_n}{\mathbb{E}(X_n)} - 1 \right| = 0 \right) = 1.$$

Finally, for the central moments, we set

$$\bar{X}(y,z) = X(y, ze^{-ya}),$$

where $a = (1-e^{-2})/4$. Then, (7) becomes

$$z\frac{\partial}{\partial z}\bar{X}(y,z) = \bar{X}(y,z) + \bar{X}^2(y,z) + e^{y(1-2a)}z^2 + \frac{2e^{y(1-3a)}z^3}{1-ze^{-ya}}.$$

From this, by using similar arguments as before and moment pumping, one obtains (4).

3 Sketch of Proof of Theorem 1

In the previous section, we saw that the limiting distribution of X_n cannot be obtained from the method of moments. To solve this problem, we will work directly with the bivariate generating function $X(y,z)$ which satisfies the Riccati differential equation (7). Note that Flajolet, Gourdon and Martinez in [12] proposed a theory for deriving limit laws for bivariate generating functions satisfying Riccati differential equations. However, their theory does not apply to the present situation due to singularities in differential equations (see (11) below). Therefore, we have to devise another approach.

We start by solving (7). First set

$$\tilde{X}(y,z) = \frac{X(y,z)}{z}.$$

Then,

$$\frac{\partial}{\partial z}\tilde{X}(y,z) = \tilde{X}^2(y,z) + e^y\frac{1+z}{1-z}.$$

Next, set

$$\tilde{X}(y,z) = -\frac{V'(y,z)}{V(y,z)}, \tag{10}$$

where here and subsequently differentiation is always with respect to z. For $V(y,z)$, we obtain that

$$V''(y,z) + e^y\frac{1+z}{1-z}V(y,z) = 0. \tag{11}$$

This differential equation is a variant of Whittaker's differential equation (see [1]) and has the following solution

$$V(y,z) = \mathrm{M}_{-e^{y/2},1/2}\left(2e^{y/2}(z-1)\right) + c(y)\mathrm{W}_{-e^{y/2},1/2}\left(2e^{y/2}(z-1)\right),$$

where $\mathrm{M}_{\kappa,\mu}(z)$ and $\mathrm{W}_{\kappa,\mu}(z)$ are the Whittaker M and Whittaker W function and

$$c(y) = -\frac{\left(e^{y/2}-1\right)\mathrm{M}_{-e^{y/2}+1,1/2}\left(-2e^{y/2}\right)}{\mathrm{W}_{-e^{y/2}+1,1/2}\left(-2e^{y/2}\right)}.$$

Whittaker functions are well-studied objects and a lot of (asymptotic) properties are known; see [1]. Using these properties, we obtain the following lemma.

Lemma 2 *Let $|y| < \eta$ and*

$$\Delta = \{z \in \mathbb{C} \,:\, |z| < 1 + \delta, \arg(1-z) \neq \pi\},$$

where $\eta, \delta > 0$. Then, $V(y,z)$ is analytic in Δ and satisfies

$$V(y,z) = 2(z-1) + 2ay + 4ay(z-1)\log(z-1) + \mathcal{O}(\max\{y(z-1), (z-1)^2\}), \tag{12}$$
$$V'(y,z) = 2 + 4ay\log(z-1) + \mathcal{O}(\max\{y, z-1\}), \tag{13}$$

where $a = (1-e^{-2})/4$.

Next, we need information about the zeros of $V(y,z)$ for small y.

Lemma 3 *For η, δ sufficiently small, $V(y,z)$ has only one (simple) zero $z_0(y)$ in z which satisfies, as $y \to 0$,*

$$z_0(y) = 1 - ay + 2a^2y^2\log y + \mathcal{O}(y^2).$$

From the last two lemmas and (10), we see that $X(y,z)$ has a logarithmic singularity at $z = 1$ and a polar singularity at $z = z_0(y)$ for y small (note that both singularities coalesce as $y \to 0$). The main property for the proof of Theorem 1 is the following proposition.

Proposition 1 *Let $y = it/(2a\sqrt{n\log n})$. Then,*

$$\mathbb{E}(e^{yX_n}) = z_0(y)^{-n} + \mathcal{O}\left(\frac{(\log n)^3}{n}\right).$$

Before proving it, we show how to use it to complete the proof of Theorem 1. As in the proposition, we set $y = it/(2a\sqrt{n\log n})$. Then, as $n \to \infty$,

$$z_0(y) = 1 - \frac{it}{2\sqrt{n\log n}} + \frac{t^2}{4n} + \mathcal{O}\left(\frac{\log\log n}{n\log n}\right).$$

Plugging this into the proposition above, we obtain that

$$\mathbb{E}(e^{yX_n}) = \exp\left(\frac{it\sqrt{n}}{2\sqrt{\log n}} - \frac{t^2}{4}\right)\left(1 + \mathcal{O}\left(\frac{\log\log n}{\log n}\right)\right)$$

which gives the claimed result.

Hence it remains to prove Proposition 1.

Proof: We again assume that $y = it/(2a\sqrt{n\log n})$ for some real number t. Then, by Cauchy integration, we have

$$\begin{aligned}\mathbb{E}(e^{yX_n}) &= [z^n]\, X(y,z) = -[z^{n-1}]\frac{V'(y,z)}{V(y,z)} \\ &= -\frac{1}{2\pi i}\int_\gamma \frac{V'(y,z)}{V(y,z)}\frac{dz}{z^n} \\ &= z_0(y)^{-n} - \frac{1}{2\pi i}\int_{\gamma'} \frac{V'(y,z)}{V(y,z)}\frac{dz}{z^n},\end{aligned}$$

where γ is a small positively oriented cycle around zero of radius < 1 and $\gamma' = \gamma'_1 \cup \gamma'_2$ with

$$\gamma'_1 = \{z = 1 + v/n : v \in \mathcal{H}_n\},$$

where $\mathcal{H}_n$ denotes the *major part* of a Hankel contour

$$\mathcal{H}_n = \{v \in \mathbb{C} : |v| = 1,\ \Re(v) \le 0\} \cup \{v \in \mathbb{C} : 0 \le \Re(v) \le (\log n)^2,\ \Im(v) = \pm 1\}$$

and γ'_2 completes the contour with an almost-cycle of radius $R = |1 + ((\log n)^2 + i)/n|$, so that we have to add the residue

$$\operatorname{Res}\left(\frac{V'(y,z)}{V(y,z)} z^{-n}, z = z_0(y)\right) = z_0(y)^{-n}.$$

By (12) and (13), it follows that, for $z \in \gamma'_1$,

$$\frac{V'(y,z)}{V(y,z)} = \frac{2\sqrt{n \log n}}{it} + \mathcal{O}\left((\log n)^3\right).$$

Hence, we obtain that

$$\begin{aligned}
-\frac{1}{2\pi i}\int_{\gamma'_1} \frac{V'(y,z)}{V(y,z)} \frac{dz}{z^n} &= -\frac{1}{2\pi i}\int_{\mathcal{H}_n} \left(\frac{2\sqrt{n\log n}}{it} + \mathcal{O}\left((\log n)^3\right)\right) e^{-v} \left(1 + \mathcal{O}\left(\frac{(\log n)^4}{n}\right)\right) \frac{dv}{n} \\
&= \frac{1}{\pi}\frac{\sqrt{n\log n}}{nt}\int_{\mathcal{H}_n} e^{-v}\, dv + \mathcal{O}\left(\frac{(\log n)^3}{n}\right) \\
&= \mathcal{O}\left(\sqrt{\frac{\log n}{n}} e^{-(\log n)^2}\right) + \mathcal{O}\left(\frac{(\log n)^3}{n}\right) \\
&= \mathcal{O}\left(\frac{(\log n)^3}{n}\right).
\end{aligned}$$

Finally, suppose that $|z| = R = |1 + ((\log n)^2 + i)/n|$. Here, we can use (12) and (13) and the property $z_0(y) = 1 + \mathcal{O}(1/\sqrt{n \log n})$ to deduce that

$$\frac{V'(y,z)}{V(y,z)} = \mathcal{O}\left(\frac{n}{(\log n)^2}\right).$$

Consequently,

$$-\frac{1}{2\pi i}\int_{\gamma'_2} \frac{V'(y,z)}{V(y,z)} \frac{dz}{z^n} = \mathcal{O}\left(\frac{n}{(\log n)^2} R^{-n}\right) = \mathcal{O}\left(\frac{1}{n}\right).$$

This completes the proof of Proposition 1. □

4 Extra Clustering Model

Here, we consider the extra clustering model and give a proof of the moment convergence part of Theorem 2, part (a). We will use the method of moments. First, observe that by (5) the bivariate generating function

$$X(y,z) = \sum_{n \ge 2} \mathbb{E}(e^{yX_n}) z^n$$

satisfies the Riccati differential equation

$$z\frac{\partial}{\partial z}X(y,z) = X(y,z) + (1-p)X(y,z)^2 + e^y\frac{z^2(1-(1-p)z^2)}{(1-z)^2} \tag{14}$$

with $X(y,0) = 0$.

Set

$$E^{[k]}(z) = \frac{\partial^k}{\partial z^k}X(y,z)\Big|_{y=0}.$$

Then, by differentiation, we obtain that

$$\frac{\mathrm{d}}{\mathrm{d}z}E^{[k]}(z) = \left(\frac{1}{z} + \frac{2(1-p)z}{1-z}\right)E^{[k]}(z) + \frac{2(1-p)}{z}\sum_{j=0}^{k-2}\binom{k-1}{j}E^{[k-1-j]}(z)E^{[j+1]}(z) + \frac{z(1-(1-p)z^2)}{(1-z)^2}$$

with $E^{[k]}(0) = 0$. Again, all these differential equations have the same shape and we have the following extension of Lemma 1.

Lemma 4 *Let $f(z)$ be a function analytic at $z = 0$ with*

$$f'(z) = \left(\frac{1}{z} + \frac{2(1-p)z}{1-z}\right)f(z) + g(z),$$

where $f(0) = 0$. Then,

$$f(z) = \frac{z}{(1-z)^{2(1-p)}e^{2(1-p)z}}\int_0^z \frac{(1-t)^{2(1-p)}e^{2(1-p)t}}{t}g(t)\mathrm{d}t.$$

Using this and moment pumping, we obtain the following result.

Proposition 2 *Let $p < 1/2$. Then, as $n \to \infty$,*

$$\mathbb{E}(X_n^k) \sim \frac{d_k}{\Gamma(k(1-2p)+1)}n^{k(1-2p)},$$

where d_k is the sequence from Theorem 2, part (a).

Proof: We use induction to show that, as $z \to 1$,

$$E^{[k]}(z) \sim \frac{d_k}{(1-z)^{k(1-2p)+1}}.$$

The claimed result follows then by singularity analysis.

First, start with $k = 1$ and set $E(z) = E^{[1]}(z)$. Then, from Lemma 4,

$$E(z) = \frac{z}{(1-z)^{2(1-p)}e^{2(1-p)z}}\int_0^z (1-t)^{-2p}e^{2(1-p)t}\left(1-(1-p)t^2\right)\mathrm{d}t.$$

Observe that the integrand satisfies, as $t \to 1$,

$$(1-t)^{-2p} e^{2(1-p)t}(1-(1-p)t^2) \sim p e^{2(1-p)}(1-t)^{-2p}.$$

Thus, from the closure properties of singularity analysis, as $z \to \infty$,

$$E(z) \sim \frac{c(p)}{(1-z)^{2(1-p)}}$$

which is the claimed result for $k = 1$.

Now, for the general case, assume that claim holds for all k' with $k' < k$. In order to prove it for k, we again use Lemma 4 which now gives an integral representation for $E^{[k]}(z)$ with integrand

$$\frac{2(1-p)(1-t)^{2(1-p)}e^{2(1-p)t}}{t^2} \sum_{j=0}^{k-2} \binom{k-1}{j} E^{[k-1-j]}(z) E^{[j+1]}(z) + (1-t)^{-2p} e^{2(1-p)t}(1-(1-p)t^2)$$

$$\sim (k-1)(1-2p) d_k e^{2(1-p)} \cdot \frac{1}{(1-t)^{(k-1)(1-2p)+1}},$$

as $t \to 1$, where the last asymptotics follows from the induction hypothesis. Now, another application of the closure properties of singularity analysis yields the claimed result. □

Proof of moment convergence in Theorem 2, part (a): By Theorem 30.1 in Billingsley [2], it suffices to show that

$$\sum_{k \geq 1} \frac{d_k z^k}{\Gamma(k(1-2p)+1)k!}$$

has a positive radius of convergence. This clearly follows from the estimate

$$d_k \leq A^k k! k^{k(1-2p)}$$

for a suitable large A which can be proved by induction by using the recurrence satisfied by d_k. □

Similarly, one can prove the moment convergence part of Theorem 2, part (b) for $1/2 < p \leq 1$. As for $p = 1/2$, by using moment pumping, one obtains the following result.

Proposition 3 *Let $p = 1/2$. Then, as $n \to \infty$,*

$$\mathbb{E}(X_n^k) \sim \frac{k! J_{2k-1}}{(2k-1)! 2^{2k-1}} \log^{2k-1} n,$$

where J_{2k-1} are the tangent numbers (or Euler numbers of odd index).

Thus, as for $p = 0$, the limit law again cannot be characterized via the moments. However, working directly with the Riccati differential equation (14) whose solution can again be expressed in terms of the Whittaker functions one obtains a proof for the case $p = 1/2$ (all other parts of Theorem 2 can also be proved via such a bivariate approach). Details are postponed to the journal version of this paper.

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An Asymptotic Analysis of Unlabeled k-Trees

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Abstract. In this paper we solve the *asymptotic counting problem* for unlabeled k-trees. By applying a proper singularity analysis of generating functions we show that the numbers U_n of unlabeled k-trees of size n are asymptotically given by $U_n \sim c_k n^{-5/2} \rho_k^{-n}$, where $c_k > 0$ and $\rho_k > 0$ denotes the radius of convergence of the generating function $U(z) = \sum_{n \geq 0} U_n z^n$. Furthermore we prove that the number of *leaves* and more generally the number of *nodes* of given degree satisfy a central limit theorem with mean value and variance that are asymptotically linear in the number of hedra where a hedron is a $(k+1)$-clique in a k-tree.

Keywords: k-tree, k-coding tree, generating function, singularity analysis, degree distribution, central limit theorem

1 Introduction

A k-tree is – in some sense – a generalization of a tree and can be defined recursively: a k-tree is either a complete graph on k vertices or a graph obtained from a smaller k-tree by adjoining a new vertex together with k edges connecting it to a k-clique of the smaller k-tree. In particular, a 1-tree is a usual tree.

The notion of a k-tree originates from the parameter *tree-width* $\mathrm{tw}(G)$ of a graph G, which is the minimum width among all possible tree decompositions of G, or equivalently, $\mathrm{tw}(G)$ is the minimum k such that G is a subgraph of a k-tree. The concept of tree-width is of central importance to the analysis of graphs with forbidden minors from Robertson and Seymour [20] and received more algorithmic attention due to the general complexity result of Courcelle saying that monadic second-order logic graph properties are decidable in linear time for graphs with bounded tree-width [3, 4]. It seems that many NP-hard problems on graphs of bounded tree-width can be solved in polynomial time [13]. A k-tree, as a bounded tree-width graph, is exactly the maximal graph with a fixed tree-width k such that no more edges can be added without increasing its tree width.

Labeled k-trees have been already counted by Beineke, Pippert, Moon and Foata [2, 18, 9] four decades ago. They showed that the number B_n of k-trees having n labeled vertices is $B_n = \binom{n}{k}(k(n-k)+1)^{n-k-2}$. Instead the counting problem of unlabeled k-trees is much more difficult. Only the case of 2-trees was already solved by Harary and Palmer [15, 16] and Fowler *et al* [10] by using the dissimilarity characteristic theorem. The general case was a long-standing open problem and was solved just recently

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by Gainer-Dewar [11]. Subsequently both Gessel and Gainer-Dewar [12] simplified the generating function approach for unlabeled k-trees by coloring the vertices of a k-tree in $(k+1)$ colors such that adjacent vertices have different colors. This breaks the symmetry of k-trees and avoids the use of compatible cyclic orientation of each $(k+1)$-clique in a k-tree.

The purpose of this paper is to provide a first asymptotic analysis of k-trees. First we will solve the *asymptotic counting problem* and show (see Theorem 1) that the numbers U_n of unlabeled k-trees of size n are asymptotically given by

$$U_n \sim c_k n^{-5/2} \rho_k^{-n},$$

where $c_k > 0$ and $\rho_k > 0$ denotes the radius of convergence of the generating function $U(z) = \sum_{n\geq 0} U_n z^n$. This is in complete accordance with Otter's result for trees [19], Labelle's *et al.* result for unlabeled 2-trees [17], and also with the corresponding results for labeled k-trees.

Second we provide a first structural analysis of unlabeled k-trees. We prove that the number of *leaves* and more generally the number of *nodes* of given degree satisfy a central limit theorem with mean value and variance that are asymptotically linear in the number of hedra (Theorems 2 and 3) where a hedron is a $(k+1)$-clique in a k-tree. This is also a natural generalization of corresponding results for (unlabeled) trees, see [6].

Actually we expect that unlabeled k-trees have many asymptotic properties in common with trees. For example, it is very likely that k-trees scaled by $1/\sqrt{n}$ converge weakly to the so-called *continuum random tree* as it holds for unlabeled trees (see [1, 14]). In this case it would follow that the diameter D_n scaled by $1/\sqrt{n}$ has a limiting distribution etc.

However, there are other parameters of interest – like the maximum degree – that cannot characterized by a continuum tree property. Anyway, as in the case of trees (see [5]) we expect that the maximum degree of k-trees should be concentrated at $c \log n$ (for a proper constant $c > 0$). We plan to work on these (and related) questions in a follow-up paper.

The plan of the paper is as follows. In Section 2 we recall the combinatorial background from [12], in particular a system of equations for generating functions. This system is then used to solve the asymptotic counting problem in Section 3. Finally the number of leaves and the number of nodes of given degree are discussed in Sections 4 and 5.

2 Combinatorics of Unlabeled k-Trees

Here we shall use the terminology introduced in [11, 12] to state the system of equations for the generating functions. Let $g \in \mathfrak{S}_m$ be a permutation of $\{1, 2, \cdots, m\}$ that has ℓ_i cycles of size i, $1 \leq i \leq k$, in its cyclic decomposition. Then its cycle type $\lambda = (1^{\ell_1}\, 2^{\ell_2} \cdots k^{\ell_k})$ is a partition of m where $m = \ell_1 + 2\ell_2 + \cdots + k\ell_k$. (In what follows we will denote by $\lambda \vdash m$ that λ is a partition of m.) Furthermore we set $z_\lambda = 1^{\ell_1}\ell_1! 2^{\ell_2}\ell_2! \cdots k^{\ell_k}\ell_k!$ and note that $\frac{m!}{z_\lambda}$ is the number of permutations in $\mathfrak{S}_m$ of cycle type λ.

A hedron is a $(k+1)$-clique in a k-tree and a front is a k-clique in a k-tree. According to the inductive construction of a k-tree, the number of vertices in a k-tree having n hedra is $k+1+(n-1) = n+k$. A colored hedron-labeled k-tree is a k-tree that has each vertex colored from the set $\{1', 2', \cdots, (k+1)'\}$ so that any two adjacent vertices are colored differently, and each hedron is labeled with a distinct number from $\{1, 2, \cdots, n\}$. The only automorphism that preserves hedra and colors of a colored hedron-labeled k-tree is the identity automorphism, for which we can ignore the colors of vertices. We now introduce k-coding trees. A k-coding tree has labeled black vertices and colored vertices. Each edge connects

a labeled black vertex with a colored vertex from colors $\{1, 2, \cdots, k+1\}$. To construct a k-coding tree from a colored hedron-labeled k-tree, we color each front of a hedron with a distinct color from $\{1, 2, \cdots, k+1\}$. The corresponding k-coding tree has each black vertex labeled with i representing each hedron of the k-tree with label i and each j-colored vertex representing each front of the k-tree with color j. We connect a black vertex with a colored vertex if and only if the corresponding hedron contains the corresponding front. As a result, a colored hedron-labeled k-tree is bijective to a k-coding tree. Under the action of $\mathfrak{S}_n$ and $\mathfrak{S}_{k+1}$, the orbits of colored hedron-labeled k-tree, which are unlabeled k-trees are bijective to the orbits of unlabeled k-coding trees under the action $\mathfrak{S}_{k+1}$. See Figure 1 for an example. In [12] the following system of equations was set up that determines the generating function $U(z)$ for

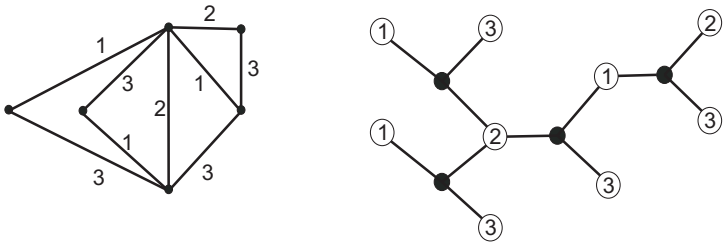

Fig. 1: The bijection between an unlabeled colored 2-tree (left) and an unlabeled 2-coding tree (right).

unlabeled k-trees by

$$U(z) = B(z) + C(z) - E(z),$$

where

$$B(z) = \sum_{\lambda \vdash k+1} \frac{B_\lambda(z)}{z_\lambda} \quad (1) \qquad B_\lambda(z) = z \prod_i C_{\lambda^i}(z^i) \quad (4)$$

$$C(z) = \sum_{\mu \vdash k} \frac{C_\mu(z)}{z_\mu} \quad (2) \qquad \bar{B}_\mu(z) = z \prod_i C_{\mu^i}(z^i) \quad (5)$$

$$E(z) = \sum_{\mu \vdash k} \frac{\bar{B}_\mu(z) C_\mu(z)}{z_\mu} \quad (3) \qquad C_\mu(z) = \exp\left[\sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}(z^m)}{m}\right]. \quad (6)$$

Here $B(z)$ is the generating function for color-orbits of black-rooted unlabeled k-coding trees, $C(z)$ is the generating function for color-orbits of colored-rooted unlabeled k-coding trees and $E(z)$ is the generating function for color-orbits of unlabeled k-coding trees rooted at an edge. We call an unlabeled k-coding tree an j-reduced black-rooted tree if it is a black-rooted tree with all the neighbors of the root are colored by $\{1, 2, \cdots, j-1, j+1 \cdots, k+1\}$. $\bar{B}(z)$ is the generating function for j-reduced black-rooted tree. For any $\pi \in \mathfrak{S}_{k+1}$, $B_\lambda(z)$ is the generating function for black-rooted tree that are fixed by π where π has cycle type λ. For any $\sigma \in \mathfrak{S}_k$, $\bar{B}_\mu(z)$ (resp. $C_\mu(z)$) is the generating function for j-reduced black-rooted tree (resp. colored-rooted tree) that are fixed by σ where σ has cycle type μ. Here $\bar{B}_\mu(z) = \bar{B}_\lambda(z)$, $C_\mu(z) = C_\lambda(z)$ if λ is obtained from μ by adding a part 1. $C_{\lambda^i}(z)$ is the generating function for color-rooted trees that are fixed by π^i and λ^i denotes the cycle type of permutation π^i where $\pi \in \mathfrak{S}_{k+1}$ has cycle type λ and i is a part of λ. Finally, the above products over i range over all parts i

of λ or μ, respectively, that is, if i is contained m times in λ then it appears m times in the product. For simplicity, we write $B_\lambda(z) = B_{1^{\ell_1}\,2^{\ell_2}\,\dots\,k^{\ell_k}}(z)$, $\bar{B}_\lambda(z) = \bar{B}_{1^{\ell_1}\,2^{\ell_2}\,\dots\,k^{\ell_k}}(z)$, $C_\lambda(z) = C_{1^{\ell_1}\,2^{\ell_2}\,\dots\,k^{\ell_k}}(z)$ and $z_\lambda = z_{1^{\ell_1}\,2^{\ell_2}\,\dots\,k^{\ell_k}}$ if $\lambda = (1^{\ell_1}\,2^{\ell_2}\,\cdots\,k^{\ell_k})$.

3 Asymptotics of unlabeled k-trees

Let $U_n = [z^n]U(z)$ denote the number of unlabeled k-trees having n hedra. Then we have the following asymptotic property.

Theorem 1 *The numbers of unlabeled k-trees are asymptotically given by*

$$U_n = \frac{1}{k!}\frac{(k\rho_k)^{-\frac{1}{k}}}{\sqrt{2\pi k^2}}\left[\frac{\rho_k m'(\rho_k)}{m(\rho_k)}\right]^{3/2} n^{-5/2}\rho_k^{-n}(1+O(n^{-1})). \tag{7}$$

where $m(z) = z\exp\left[k\sum_{m=2}^{\infty}\bar{B}_{1^k}(z^m)/m\right]$, $\bar{B}_{1^k}(z) = m(z)e^{k\bar{B}_{1^k}(z)}$ and ρ_k is the unique real positive solution of $m(z) = (ek)^{-1}$.

Proof: For $\mu = (1^k)$, from eq. (5) and (6), we have

$$\bar{B}_{1^k}(z) = z\exp\left[k\sum_{m=1}^{\infty}\frac{\bar{B}_{1^k}(z^m)}{m}\right] = \exp(k\bar{B}_{1^k}(z))\cdot z\cdot\exp\left[k\sum_{m=2}^{\infty}\frac{\bar{B}_{1^k}(z^m)}{m}\right]. \tag{8}$$

Setting

$$m(z) = z\exp\left[k\sum_{m=2}^{\infty}\frac{\bar{B}_{1^k}(z^m)}{m}\right], \tag{9}$$

and $\bar{B}_{1^k}(z) = T(m(z))$ for some power series $T(z)$ we thus obtain $T(z) = z\exp(kT(z))$. Hence, if $W(z)$ denotes the classical tree function that is given by $W(z) = z\exp(W(z))$ it follows that $T(z) = \frac{1}{k}W(kz)$. It is very well known that $W(z)$ has radius of convergence $\rho = 1/e$, that it has a singular expansion of the form

$$W(z) = 1 - \sqrt{2}(1-ez)^{1/2} + \frac{2}{3}(1-ez) + \cdots$$

around $z = 1/e$ and that $W(z)$ can be analytically continued to a region of the form $\{z\in\mathbb{C} : |z| < 1/e+\eta\}\setminus[1/e,\infty)$ for some $\eta > 0$. In particular it follows that $T(z)$ has corresponding properties, of course its radius of convergence equals $1/(ke)$. Actually, in what follows we will only need that $T(z)$ is analytic in a so-called Δ-domain

$$\Delta_\alpha(M,\phi) = \{z \mid |z| < M, z\neq\alpha, |\arg(z-\alpha)| > \phi\}$$

where $0 < \phi < \frac{\pi}{2}$. (Analyticity in Δ-domains is used to *transfer* the singular expansion of the generating function into an asymptotic expansion for the coefficients, see Chapter VI.3 of [8].) In our case we know that $T(z)$ is analytic in $\Delta_{1/(ke)}(1/(ke)+\eta,\phi)$.

Let ρ_k be the unique dominant singularity of $\bar{B}_{1^k}(z)$, then we shall show $(4k)^{-1} \le \rho_k \le (ek)^{-1}$. Since $[z^n]\bar{B}_{1^k}(z) > 0$, $[z^n]T(z) > 0$ and $\bar{B}_{1^k}(z) = T(m(z))$ where $m(z) = z+\cdots$ has non-negative

coefficients, we have $[z^n]\bar{B}_{1^k}(z) \geq [z^n]T(z)$ which indicates the radius of convergence for $\bar{B}_{1^k}(z)$ is at most that for $T(z)$ which is $(ek)^{-1}$. On the other hand, the radius of convergence for $\bar{B}_{1^k}(z)$ is at least that for $M(z)$ where $M(z) = z(1 - kM(z))^{-1}$ and accordingly $\rho_k \geq (4k)^{-1}$.

Within the next step we shall prove that the dominant singularity $z = \rho_k$ of $\bar{B}_{1^k}(z)$ is of square root type, too. Since $m(z)$ has radius of convergence $\sqrt{\rho_k} > \rho_k$ it follows that it is analytic at $z = \rho_k$. More precisely the singular expansion of $\bar{B}_{1^k}(z)$ close to $z = \rho_k$ comes from composing the singular expansion of $T(z)$ at $1/(ek)$ with the analytic expansion of $m(z)$ at ρ_k. In this context we also observe that $m(\rho_k) = (ek)^{-1}$ and $m'(\rho_k) > 1$. According to this we get the local expansion

$$\begin{aligned}\bar{B}_{1^k}(z) &= \frac{1}{k} - \frac{\sqrt{2}}{k}\left[1 - \frac{m(z)}{m(\rho_k)}\right]^{1/2} + \frac{2}{3k}\left[1 - \frac{m(z)}{m(\rho_k)}\right] + \sum_{i\geq 3}(-1)^i m_i \left[1 - \frac{m(z)}{m(\rho_k)}\right]^{i/2} \\ &= \frac{1}{k} - \frac{\sqrt{2}}{k}\left[\frac{(\rho_k - z)m'(\rho_k)}{m(\rho_k)}\right]^{1/2} + \frac{2}{3k}\left[\frac{(\rho_k - z)m'(\rho_k)}{m(\rho_k)}\right] + O(\rho_k - z)^{3/2}.\end{aligned}$$

Henceforth $C_{1^k}(z) = z^{-1/k}\bar{B}_{1^k}(z)^{1/k}$ has $z = \rho_k$ as dominant singularity of square root type, too, and a local expansion of the form

$$C_{1^k}(z) = (k\rho_k)^{-1/k} + a(\rho_k - z)^{1/2} + b(\rho_k - z) + c(\rho_k - z)^{3/2} + O(\rho_k - z)^2 \tag{10}$$

where a, b are given by

$$a = -\frac{\sqrt{2}(k\rho_k)^{(k-1)/k}}{k^2\rho_k}\left[\frac{m'(\rho_k)}{m(\rho_k)}\right]^{1/2}, \quad b = \frac{3-k}{3k^3}\frac{(k\rho_k)^{(k-1)/k}}{\rho_k}\left[\frac{m'(\rho_k)}{m(\rho_k)}\right].$$

Actually the functions $\bar{B}_{1^k}(z) = \bar{B}_{1^{k+1}}(z)$, $C_{1^k}(z) = C_{1^{k+1}}(z)$, and $B_{1^{k+1}}(z)$ have the same radius of convergence ρ_k (which is a square-root singularity).

Furthermore we observe that for any $k \geq 2$ and $\mu \neq (1^k)$, $\bar{B}_\mu(z)$ and $C_\mu(z)$ are analytic at $z = \rho_k$. Let τ_μ be the unique dominant singularity of $\bar{B}_\mu(z)$ for $\mu \neq (1^k)$. Since the number of black-rooted trees that are fixed by permutation of type $\mu \neq (1^k)$ is less than or equal to those fixed by identity permutation, i.e., $[z^n]\bar{B}_\mu(z) \leq [z^n]\bar{B}_{1^k}(z)$ it follows that $\tau_\mu \geq \rho_k$. Therefore it remains to prove $\tau_\mu \neq \rho_k$. If μ has exactly j parts of size 1, where $0 < j < k$, then we have

$$\bar{B}_\mu(z) = zC_\mu(z)^j \prod_{i\neq 1} C_{\mu^i}(z^i) \text{ and } C_\mu(z) = \exp(\bar{B}_\mu(z))\exp\left[\sum_{m=2}^{\infty}\frac{\bar{B}_{\mu^m}(z^m)}{m}\right] \tag{11}$$

which lead to

$$\bar{B}_\mu(z) = z\prod_{i\neq 1} C_{\mu^i}(z^i)\exp(j\bar{B}_\mu(z))\exp\left[j\sum_{m=2}^{\infty}\frac{\bar{B}_{\mu^m}(z^m)}{m}\right]. \tag{12}$$

By setting $\bar{B}_\mu(z) = y$, it follows that $(\rho_\mu, \bar{B}_\mu(\rho_\mu))$ is the unique solution of

$$\begin{aligned}M(z,y) &= z\prod_{i\neq 1} C_{\mu^i}(z^i)\exp(jy)\exp\left[j\sum_{m=2}^{\infty}\frac{\bar{B}_{\mu^m}(z^m)}{m}\right] = y \\ M_y(z,y) &= jz\prod_{i\neq 1} C_{\mu^i}(z^i)\exp(jy)\exp\left[j\sum_{m=2}^{\infty}\frac{\bar{B}_{\mu^m}(z^m)}{m}\right] = 1,\end{aligned}$$

and consequently $\bar{B}_\mu(\tau_\mu) = 1/j$. Recall that $\bar{B}_{1^k}(\rho_k) = 1/k$, thus, we have $k\bar{B}_{1^k}(\rho_k) = j\bar{B}_\mu(\tau_\mu) = 1$. If $\tau_\mu = \rho_k$, then $k\bar{B}_{1^k}(\rho_k) > j\bar{B}_\mu(\rho_k) = 1$, which contradicts the relation $k\bar{B}_{1^k}(\rho_k) = 1$. Therefore we can conclude that $\rho_k < \tau_\mu$ and from eq. (11), eq. (12), $C_\mu(z)$ also has dominant singularity τ_μ. In the case μ has no part of size 1, then $\bar{B}_\mu(z)$ is a product of $C_{\mu^i}(z^i)$ where $i \geq 2$ and μ^i has part of size 1. Consequently we have $\tau_\mu > \min\{\tau_{\mu^i} : i \in \mu\} > \rho_k$. Now we can conclude for any $k \geq 2$ and $\mu \neq (1^k)$, $\rho_k < \tau_\mu$, namely $\bar{B}_\mu(z)$ and $C_\mu(z)$ are analytic at $z = \rho_k$.

Summing up, since $B_{1^{k+1}}(z) = zC_{1^k}(z)^{k+1}$ has a square-root singularity at $z = \rho_k$ and B_λ for any $\lambda \neq (1^{k+1})$ is analytic at ρ_k, the dominant term in the singular expansion of $U(z)$ comes from

$$\frac{B_{1^{k+1}}(z)}{z_{1^{k+1}}} + \frac{C_{1^k}(z)}{z_{1^k}} - \frac{C_{1^k}(z)\bar{B}_{1^k}(z)}{z_{1^k}} \quad = \quad \frac{-kzC_{1^k}(z)^{k+1}}{(k+1)!} + \frac{C_{1^k}(z)}{k!}.$$

All the other terms are all analytic at $z = \rho_k$. Together with the singular expansion of $C_{1^k}(z)$ shown in eq. (10), we can calculate the constant for the term $(\rho_k - z)^{1/2}$ in the singular expansion of $U(z)$, which is $\frac{-k\rho_k}{(k+1)!}\binom{k+1}{1}\frac{a}{k\rho_k} + \frac{a}{k!} = 0$. Similarly the constant for the term $(\rho_k - z)^{3/2}$ in the singular expansion of $U(z)$ is

$$\frac{-k\rho_k}{(k-1)!}a(b(k\rho_k)^{-\frac{1}{k}} + \frac{k-1}{3!}a^2)(k\rho_k)^{-\frac{k-2}{k}} = \frac{2\sqrt{2}}{k!}\frac{(k\rho_k)^{-\frac{1}{k}}}{3k^2}\left[\frac{m'(\rho_k)}{m(\rho_k)}\right]^{3/2}$$

which is positive. Now we have derived the singular expansion of $U(z)$ at $z = \rho_k$:

$$U(z) = U(\rho_k) + \frac{2\sqrt{2}}{k!}\frac{(k\rho_k)^{-\frac{1}{k}}}{3k^2}\left[\frac{(\rho_k - z)m'(\rho_k)}{m(\rho_k)}\right]^{3/2} + c_1(\rho_k - z) + c_2(\rho_k - z)^2 + O(\rho_k - z)^{5/2}. \quad (13)$$

By applying the transfer theorem ([8, Theorem VI.3] or [5, Corollary 2.15]), we get eq. (7) and the proof is complete. □

It is worthwhile to mention that the coefficients for the asymptotics of $[z^n]\bar{B}_{1^k}(z)$, $[z^n]C_{1^k}(z)$ and $[z^n]U(z)$ are determined by $m(z)$ and ρ_k where the value of ρ_k can be computed by following Otter's work on 1-trees [19]. More precisely, let $T_n = [z^n]\bar{B}_{1^k}(z)$ and $m_n = [z^n]m(z)$. Then by taking the derivative of eq. (8), eq. (9) and equating the coefficients, we get the recurrences for T_n and m_n, namely

$$T_n \quad = \quad \frac{k}{n-1}\sum_{i=1}^{n-1} T_{n-i}\sum_{m|i} mT_m \quad \text{for } n > 1 \text{ and } T_1 = 1.$$

$$m_n \quad = \quad \frac{k}{n-1}\sum_{i=2}^{n-1} m_{n-i}\sum_{m|i, m\neq i} mT_m \quad \text{for } n > 2 \text{ and } m_1 = 1, m_2 = 0.$$

From these two recurrences we can compute the exact value of m_n. Then the value of ρ_k is obtained by solving numerically the equation $m(z) = 1/(ek)$. The series $m(z)$ can be estimated by its first 20 terms in its expansion at $z = 0$ since the resulting error term is extremely small. For $k = 2$, ρ_2 is already computed in [10] and turns out to be approximately 0.177.

4 Leaves of unlabeled k-trees

As we have explained in Section 2 unlabeled k-trees are bijective to the orbits of unlabeled k-coding tree under the action $\mathfrak{S}_{k+1}$. We call a black node a *leaf* if only one of its colored neighbor connects with other black nodes. It is obvious that this notion corresponds to the only meaningful notion of a *leaf* of a k-tree.

In the sequel we shall weight each black node by z and each leaf by w. Let $U(z,w)$ be the generating function for unlabeled color-orbits of unlabeled k-coding trees, then we have:

Theorem 2 *Let X_n be the random variable associated with the number of leaves of k-coding trees, that is $\mathbb{P}(X_n = r) = \frac{[z^n w^r]U(z,w)}{[z^n]U(z,1)}$. Then there exists positive constants μ and σ^2 such that $\mathbb{E}(X_n) = \mu\, n + O(1)$ and $\mathbb{V}ar(X_n) = \sigma^2\, n + O(1)$. Furthermore X_n satisfies a central limit theorem of type*

$$\frac{X_n - \mathbb{E}(X_n)}{\sqrt{\mathbb{V}ar(X_n)}} \longrightarrow N(0,1).$$

Proof: Let $B(z,w)$ be the generating function for color-orbits of black-rooted trees, let $C(z,w)$ be the generating function for color-orbits of color-rooted trees and let $E(z,w)$ be the generating function for color-orbits of k-coding trees rooted at an edge, then according to the dissymmetry theorem and Cauchy-Frobenius theorem, we have $U(z,w) = B(z,w) + C(z,w) - E(z,w)$ where

$$\begin{aligned}
B(z,w) &= \sum_{\lambda\vdash k+1} \frac{B_\lambda(z,w)}{z_\lambda},\ C(z,w) = \sum_{\mu\vdash k} \frac{C_\mu(z,w)}{z_\mu},\ B_\lambda(z,w) = z\prod_i C_{\lambda^i}(z^i,w^i) + z(w-1)\\
E(z,w) &= \sum_{\mu\vdash k} \frac{(\bar{B}_\mu(z,w) - zw + z)C_\mu(z,w) + z(w-1)}{z_\mu}\\
\bar{B}_\mu(z,w) &= z\prod_i C_{\mu^i}(z^i,w^i) + z(w-1) \qquad (14)\\
C_\mu(z,w) &= \exp\left[\sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}(z^m,w^m)}{m}\right]. \qquad (15)
\end{aligned}$$

For $\mu = (1^k)$, from eq. (14) and (15), we obtain

$$\bar{B}_{1^k}(z,w) = z\exp\left[k\sum_{m=1}^{\infty} \frac{\bar{B}_{1^k}(z^m,w^m)}{m}\right] + z(w-1). \qquad (16)$$

We first show for $\mu \neq (1^k)$ and $m \geq 2$, $\bar{B}_\mu(z,w)$ and $\bar{B}_{1^k}(z^m,w^m)$ are analytic if (z,w) is close to $(\rho_k, 1)$. For sufficiently small $\epsilon > 0$, we consider $|w| \leq \frac{\rho_k}{\rho_k+\epsilon}$ and $|z| \leq \rho_k + \epsilon$, then for $m \geq 2$,

$$\begin{aligned}
|\bar{B}_\mu(z,w)| &\leq \bar{B}_\mu(|zw|,1) \leq \bar{B}_\mu(\rho_k,1) \leq K\rho_k,\\
|\bar{B}_{1^k}(z^m,w^m)| &\leq \bar{B}_{1^k}(|zw|^m,1) \leq \bar{B}_{1^k}(\rho_k^m,1) \leq M\rho_k^m.
\end{aligned}$$

The last inequality holds because $\bar{B}_\mu(z,1)$ and $\bar{B}_{1^k}(z,1)$ are convex for $z \in [0,\rho_k]$ and $z \in [0,\rho_k^2]$, respectively. Now we set

$$F(y,z,w) = z\exp\left[ky + k\sum_{m=2}^{\infty} \frac{\bar{B}_{1^k}(z^m,w^m)}{m}\right] + z(w-1)$$

which is analytic for (y,z,w) around $(0,0,0)$ and we have $F(y,0,w)\equiv 0$, $F(0,z,w)\not\equiv 0$. Furthermore, the coefficients of $F(y,z,w)$ are all non-negative. Since $\bar{B}_{1^k}(z,w)$ is the unique solution of $F(y,z,w)=y$ it can be expressed as

$$\bar{B}_{1^k}(z,w)=\alpha(z,w)-\beta(z,w)\left[1-\frac{z}{\rho_k(w)}\right]^{1/2},$$

where $\alpha(z,w),\beta(z,w),\rho_k(w)$ are analytic for $|w-1|\le\epsilon$, $|z-\rho_k(w)|<\varepsilon$, $\arg(z-\rho_k(w))|>\phi$ (for some $\phi\in(0,\pi/2)$) and ϵ,ε are sufficiently small. Furthermore, $\beta(\rho_k(w),w)\neq 0$ and $\bar{B}_{1^k}(\rho_k(w),w)=\alpha(\rho_k(w),w)=k^{-1}+(w-1)\rho_k(w)$. Since $\bar{B}_{1^k}(z,w)=zC_{1^k}(z,w)^k+z(w-1)$, $C_{1^k}(z,w)$ has a corresponding representation

$$C_{1^k}(z,w)=a(z,w)+b(z,w)\left[1-\frac{z}{\rho_k(w)}\right]^{1/2} \tag{17}$$

where $a(z,w),b(z,w)$ are analytic functions around $(z,w)=(\rho_k,1)$, $b(\rho_k(w),w)\neq 0$, $C_{1^k}(\rho_k(w),w)=a(\rho_k(w),w)=(k\rho_k(w))^{-1/k}$. Analogous to $\bar{B}_{1^k}(z,w)$, for $m\ge 2$ and $\mu\neq(1^k)$, $C_\mu(z,w)$ and $C_{1^k}(z^m,w^m)$ are analytic if (z,w) is close to $(\rho_k,1)$. Consequently for $|w-1|\le\epsilon$, $|z-\rho_k(w)|<\varepsilon$, $\arg(z-\rho_k(w))|>\phi$ and ϵ,ε are sufficiently small, $U(z,w)$ has the expansion

$$U(z,w)=-\frac{kz}{(k+1)!}C_{1^k}(z,w)^{k+1}+\frac{1}{k!}C_{1^k}(z,w)+H_1(z,w)$$

where $H_1(z,w)$ is an analytic function around $(z,w)=(\rho_k,1)$. By substituting $C_{1^k}(z,w)$ by its singular expansion in eq. (17), $U(z,w)$ can be expanded locally around $z=\rho_k(w)$, i.e.,

$$U(z,w)=g(z,w)+\left[-\frac{za^k(z,w)}{(k-1)!}+\frac{1}{k!}+O(\rho_k(w)-z)\right]b(z,w)\left[1-\frac{z}{\rho_k(w)}\right]^{1/2},$$

Since $-\rho_k(w)\frac{a^k(\rho_k(w),w)}{(k-1)!}+\frac{1}{k!}=0$, together with the fact $a(z,w)=a(\rho_k(w),w)+O(\rho_k(w)-z)$ and $b(\rho_k(w),w)\neq 0$, we can conclude

$$U(z,w)=g(z,w)+f(z,w)\left[1-\frac{z}{\rho_k(w)}\right]^{3/2} \tag{18}$$

where $f(\rho_k,1)\neq 0$ from Section 3 and therefore $f(\rho_k(w),w)\neq 0$. By applying [5, Theorem 2.25] to eq. (18), there is a central limit theorem for $(X_n-\mathbb{E}(X_n))/\sqrt{n}$. More precisely there exist μ and σ^2 with $\mathbb{E}(X_n)=\mu\,n+O(1)$ and $\mathbb{V}\mathrm{ar}(X_n)=\sigma^2\,n+O(1)$ where $\mu=-\rho_k'(1)/\rho_k(1)$ and $\sigma^2=-\rho_k''(1)/\rho_k(1)+\mu+\mu^2$. By applying Lemma 4 of [7] it actually follows that $\sigma^2>0$ and X_n satisfies a central limit theorem as stated. □

5 The degree distribution of unlabeled k-trees

We again refer to the unlabeled k-coding trees and consider here the degree distribution. Clearly every black node in the k-coding tree has degree $k+1$. So we concentrate on the degree distribution of colored

nodes. First of all we change the statistics slightly by measuring the size according to the number of colored nodes. Formally the variable x (instead of z) takes care of the number of colored nodes. Now let $U(x)$ be the generating function for unlabeled color-orbits of unlabeled k-coding trees, let $B(x)$ be the generating function for color-orbits of black-rooted trees, let $C(x)$ be the generating function for color-orbits of color-rooted trees and let $E(x)$ be the generating function for color-orbits of unlabeled k-coding trees rooted at an edge, then we have similarly to the above: $U(x) = B(x) + C(x) - E(x)$ where

$$\begin{aligned} B(x) &= \sum_{\lambda\vdash k+1} \frac{B_\lambda(x)}{z_\lambda} & B_\lambda(x) &= \prod_i C_{\lambda^i}(x^i) \\ C(x) &= \sum_{\mu\vdash k} \frac{C_\mu(x)}{z_\mu} & \bar{B}_\mu(x) &= \prod_i C_{\mu^i}(x^i) \\ E(x) &= \sum_{\mu\vdash k} \frac{\bar{B}_\mu(x) C_\mu(x)}{z_\mu} & C_\mu(x) &= x\exp\left[\sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}(x^m)}{m}\right]. \end{aligned}$$

In completely the same way as in Section 3, we can find the singular expansion of $U(x)$ given by

$$U(x) = U(\gamma_k) + \bar{c}_1(\gamma_k - x) + r(\gamma_k - x)^{3/2} + \bar{c}_2(\gamma_k - x)^2 + O((\gamma_k - x)^{5/2})$$

for some positive constant r and some constants $\bar{c}_1, \bar{c}_2$. Furthermore $\bar{B}_{1^k}(\gamma_k) = 1/k$, and it follows that $\rho_k = \gamma_k$.

Now we give each colored node of degree d_i with weight u_i. Let $\mathbf{u} = (u_1, \cdots, u_M)$, $\mathbf{m} = (m_1, \cdots, m_M)$ where $m_i \geq 0$ and $\mathbf{d} = (d_1, \cdots, d_M)$ where $d_i > 0$, then the coefficient of $x^n \mathbf{u}^{\mathbf{m}}$ in the generating function $U^{(\mathbf{d})}(x, \mathbf{u})$ is the number of of unlabeled k-trees that there are m_i colored nodes out of n total colored nodes having degree d_i. Then we have

Theorem 3 *Let $Y_{n,\mathbf{d}} = (Y^{(1)}_{n,d_1}, \cdots, Y^{(M)}_{n,d_M})$ be the random vector of the number of colored nodes in an unlabeled k-tree that have degrees $(d_1, \cdots, d_M)$, that is, $\mathbb{P}(Y_{n,\mathbf{d}} = \mathbf{m}) = \frac{[x^n \mathbf{u}^{\mathbf{m}}] U^{(\mathbf{d})}(x,\mathbf{u})}{[x^n] U^{(\mathbf{d})}(x,\mathbf{1})}$. Then there exists an M-dimensional vector μ and an $M \times M$ positive semidefinite matrix Σ such that $\mathbb{E}(Y_{n,\mathbf{d}}) = \mu\, n + O(1)$ and $\mathbb{C}\mathrm{ov}(Y_{n,\mathbf{d}}) = \Sigma\, n + O(1)$. Furthermore $Y_{n,\mathbf{d}}$ satisfies a central limit theorem of the form*

$$\frac{Y_{n,\mathbf{d}} - \mathbb{E}(Y_{n,\mathbf{d}})}{\sqrt{n}} \longrightarrow N(0, \Sigma).$$

Proof: Let $C^{(\mathbf{d})}(x, \mathbf{u})$ be the generating function for color-orbits of colored-rooted trees that has each colored node of degree d_i weighted by u_i. Let $P^{(\mathbf{d})}(x, \mathbf{u})$ be the generating function for the trees whose root is only connected with the root of a color-orbit of colored node-rooted tree, so that $C^{(\mathbf{d})}(x, \mathbf{1}) = P^{(\mathbf{d})}(x, \mathbf{1})$. Let $B^{(\mathbf{d})}(x, \mathbf{u})$ be the generating function for color-orbits of black-rooted trees that has each node of degree d_i weighted by u_i. $E^{(\mathbf{d})}(x, \mathbf{u})$ be the generating function for color-orbits of unlabeled k-coding trees rooted at an edge that has each node of degree d_i weighted by u_i. Here we introduce $P^{(\mathbf{d})}(x, \mathbf{u})$ to distinguish the case that the colored root has degree d_i for some $1 \leq i \leq M$. Let $Z(\mathfrak{S}_p, \bar{B}^{(\mathbf{d})}_\mu(x, \mathbf{u}))$ represent the generating function for $\mathfrak{S}_p$-orbits of objects counted by $\bar{B}^{(\mathbf{d})}_\mu(x, \mathbf{u})$:

$$Z(\mathfrak{S}_p, \bar{B}^{(\mathbf{d})}_\mu(x, \mathbf{u})) = Z(\mathfrak{S}_p, \bar{B}^{(\mathbf{d})}_\mu(x, \mathbf{u}), \bar{B}^{(\mathbf{d})}_{\mu^2}(x^2, \mathbf{u}^2), \cdots, \bar{B}^{(\mathbf{d})}_{\mu^p}(x^p, \mathbf{u}^p))$$

$$= \sum_{\lambda\vdash p} \frac{1}{z_\lambda} \bar{B}_\mu^{(\mathbf{d})}(x,\mathbf{u})^{\lambda_1} \bar{B}_{\mu^2}^{(\mathbf{d})}(x^2,\mathbf{u}^2)^{\lambda_2} \cdots \bar{B}_{\mu^p}^{(\mathbf{d})}(x^p,\mathbf{u}^p)^{\lambda_p}$$

where $\lambda = (1^{\lambda_1} \cdots p^{\lambda_p})$. Then the generating function $U(x,\mathbf{u})$ for unlabeled k-trees with colored nodes of degree $\mathbf{d}$ is given by $U^{(\mathbf{d})}(x,\mathbf{u}) = B^{(\mathbf{d})}(x,\mathbf{u}) + C^{(\mathbf{d})}(x,\mathbf{u}) - E^{(\mathbf{d})}(x,\mathbf{u})$ where

$$B^{(\mathbf{d})}(x,\mathbf{u}) = \sum_{\lambda\vdash k+1} \frac{B_\lambda^{(\mathbf{d})}(x,\mathbf{u})}{z_\lambda},\ C^{(\mathbf{d})}(x,\mathbf{u}) = \sum_{\mu\vdash k} \frac{C_\mu^{(\mathbf{d})}(x,\mathbf{u})}{z_\mu},\ B_\lambda^{(\mathbf{d})}(x,\mathbf{u}) = \prod_i P_{\lambda^i}^{(\mathbf{d})}(x^i,\mathbf{u}^i)$$

$$E^{(\mathbf{d})}(x,\mathbf{u}) = \sum_{\mu\vdash k} \frac{\bar{B}_\mu^{(\mathbf{d})}(x,\mathbf{u}) P_\mu^{(\mathbf{d})}(x,\mathbf{u})}{z_\mu},\ \bar{B}_\mu^{(\mathbf{d})}(x,\mathbf{u}) = \prod_i P_{\mu^i}^{(\mathbf{d})}(x^i,\mathbf{u}^i)$$

$$C_\mu^{(\mathbf{d})}(x,\mathbf{u}) = x\exp\left[\sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}^{(\mathbf{d})}(x^m,\mathbf{u}^m)}{m}\right] + \sum_{j=1}^{M} x(u_j-1) Z(\mathfrak{S}_{d_j}, \bar{B}_\mu^{(\mathbf{d})}(x,\mathbf{u})) \tag{19}$$

$$P_\mu^{(\mathbf{d})}(x,\mathbf{u}) = x\exp\left[\sum_{m=1}^{\infty} \frac{\bar{B}_{\mu^m}^{(\mathbf{d})}(x^m,\mathbf{u}^m)}{m}\right] + \sum_{j=1}^{M} x(u_j-1) Z(\mathfrak{S}_{d_j-1}, \bar{B}_\mu^{(\mathbf{d})}(x,\mathbf{u})). \tag{20}$$

The dominant singularity for $\bar{B}_{1^k}(x,\mathbf{1})$ is ρ_k. As before, for $\mu \neq (1^k)$, $\bar{B}_\mu(x,\mathbf{u})$ and for $m \geq 2$, $\bar{B}_{1^k}(x^m,\mathbf{u}^m)$ are analytic if $(x,\mathbf{u})$ is close to $(\rho_k,\mathbf{1})$. Next we consider

$$\begin{aligned} S(x,y,\mathbf{u}) &= \left(xe^y \exp\left(\sum_{m=2}^{\infty} \frac{\bar{B}_{1^k}^{(\mathbf{d})}(x^m,\mathbf{u}^m)}{m} \right) \right. \\ &+ \left. \sum_{j=1}^{M} x(u_j-1) Z(\mathfrak{S}_{d_j-1}, y, \bar{B}_{1^k}^{(\mathbf{d})}(x^2,\mathbf{u}^2), \cdots, \bar{B}_{1^k}^{(\mathbf{d})}(x^{d_j-1},\mathbf{u}^{d_j-1})) \right)^k. \end{aligned}$$

Since $S(0,y,\mathbf{u}) \equiv 0$, $S(x,0,\mathbf{u}) \not\equiv 0$ and all coefficients of $S(x,y,\mathbf{1})$ are real and positive, then $y(x,\mathbf{u}) = \bar{B}_{1^k}^{(\mathbf{d})}(x,\mathbf{u})$ is the unique solution of the functional equation $S(x,y,\mathbf{u}) = y$. Furthermore, $(x,y) = (\rho_k, 1/k)$ is the only solution of $S(x,y,\mathbf{1}) = 0$ and $S_y(x,y,\mathbf{1}) = 1$ with $S_x(\rho_k, 1/k, \mathbf{1}) \neq 0$, $S_{yy}(\rho_k, 1/k, \mathbf{1}) \neq 0$. Consequently, $\bar{B}_{1^k}^{(\mathbf{d})}(x,\mathbf{u})$ can be represented as

$$\bar{B}_{1^k}^{(\mathbf{d})}(x,\mathbf{u}) = g(x,\mathbf{u}) - h(x,\mathbf{u}) \left[1 - \frac{x}{\rho_k(\mathbf{u})}\right]^{1/2} \tag{21}$$

which holds locally around $(x,\mathbf{u}) = (\rho_k,\mathbf{1})$ and $h(\rho_k(\mathbf{u}),\mathbf{u}) \neq 0$. In view of $\bar{B}_{1^k}^{(\mathbf{d})}(x,\mathbf{u}) = P_{1^k}^{(\mathbf{d})}(x,\mathbf{u})^k$, $P_{1^k}^{(\mathbf{d})}(x,\mathbf{u})$ also has expansion of square root type, i.e.,

$$P_{1^k}^{(\mathbf{d})}(x,\mathbf{u}) = s(x,\mathbf{u}) - t(x,\mathbf{u}) \left[1 - \frac{x}{\rho_k(\mathbf{u})}\right]^{1/2} \tag{22}$$

where $t(\rho_k(\mathbf{u}),\mathbf{u}) \neq 0$. From eq. (19) and eq. (20), we have

$$C_\mu^{(\mathbf{d})}(x,\mathbf{u}) = P_\mu^{(\mathbf{d})}(x,\mathbf{u}) + \sum_{j=1}^{M} x(u_j-1) \left[Z(\mathfrak{S}_{d_j}, \bar{B}_\mu^{(\mathbf{d})}(x,\mathbf{u})) - Z(\mathfrak{S}_{d_j-1}, \bar{B}_\mu^{(\mathbf{d})}(x,\mathbf{u})) \right]$$

based on which we shall next compute the dominant term in the singular expansion of $U(x, \mathbf{u})$. For simplicity we will omit variables $(x, \mathbf{u})$ and degree $\mathbf{d}$.

$$\begin{aligned} U(x,\mathbf{u}) &= \frac{P_{1^k}^{k+1}}{(k+1)!} + \frac{C_{1^k}}{k!} - \frac{P_{1^k}^{k+1}}{k!} + M_1 = \frac{P_{1^k}^{k+1}}{(k+1)!} + \frac{1}{k!}(1 - P_{1^k}^k)P_{1^k} + \frac{1}{k!}(C_{1^k} - P_{1^k}) + M_1 \\ &= -\frac{kP_{1^k}^{k+1}}{(k+1)!} + \frac{P_{1^k}}{k!} + \frac{1}{k!}\sum_{j=1}^{M} x(u_j - 1)\left[Z(\mathfrak{S}_{d_j}, \bar{B}_{1^k}) - Z(\mathfrak{S}_{d_j-1}, \bar{B}_{1^k})\right] + M_1, \end{aligned}$$

where M_1 is an analytic function around $(x, \mathbf{u}) = (\rho_k, \mathbf{1})$. It is now convenient to write $U(x, \mathbf{u}) = f(x, \mathbf{u}) + \bar{h}(x, \mathbf{u})\left[1 - \frac{x}{\rho_k(\mathbf{u})}\right]^{1/2}$. Then by substituting P_{1^k}, $\bar{B}_{1^k}$ with its representation in eq. (22) and eq. (21), we obtain

$$\bar{h}(x,\mathbf{u}) = \frac{s^k\, t}{(k-1)!} - \frac{t}{k!} + \frac{h}{k!}\sum_{j=1}^{M} x(u_j - 1)\left[Z'(\mathfrak{S}_{d_j-1}, g, X_2, \cdots, X_{d_j-1}) - Z'(\mathfrak{S}_{d_j}, g, X_2, \cdots, X_{d_j})\right]$$

where X_i are analytic functions around $(x, \mathbf{u}) = (\rho_k, \mathbf{1})$ and Z' is the derivative w.r.t. the first variable of $Z(\mathfrak{S}_k, x_1, \cdots, x_k)$, namely $Z'(\mathfrak{S}_k, x_1, \cdots, x_k) = Z(\mathfrak{S}_{k-1}, x_1, \cdots, x_{k-1})$. Furthermore, by replacing s, t by $g = s^k$ and $h = ks^{k-1}t$, we can further simplify $\bar{h}(x, \mathbf{u})$, that is

$$\bar{h}(x,\mathbf{u}) = \frac{h}{k!}\frac{g - \frac{1}{k}}{g^{1-\frac{1}{k}}} + \frac{h}{k!}\sum_{j=1}^{M} x(u_j - 1)\left[Z'(\mathfrak{S}_{d_j-1}, g, X_2, \cdots, X_{d_j-1}) - Z'(\mathfrak{S}_{d_j}, g, X_2, \cdots, X_{d_j})\right].$$

Now we use the fact that $y = g(\rho_k(\mathbf{u}), \mathbf{u})$ and $x = \rho_k(\mathbf{u})$ is the solution of $S(x, y, \mathbf{u}) = y$ and $S_y(x, y, \mathbf{u}) = 1$, which yields

$$\begin{aligned} g(\rho_k(\mathbf{u}),\mathbf{u}) &= \frac{1}{k} + g(\rho_k(\mathbf{u}),\mathbf{u})^{\frac{k-1}{k}} \\ &\times \sum_{j=1}^{M} x(u_j - 1)\left[Z(\mathfrak{S}_{d_j-1}, g, X_2, \cdots, X_{d_j-1}) - Z'(\mathfrak{S}_{d_j-1}, g, X_2, \cdots, X_{d_j-1})\right] \end{aligned}$$

and consequently $h(\rho_k(\mathbf{u}), \mathbf{u}) \equiv 0$ and $U(x, \mathbf{u})$ has a local expansion around $(x, \mathbf{u}) = (\rho_k, \mathbf{1})$ of the form

$$U(x,\mathbf{u}) = w(x,\mathbf{u}) + r(x,\mathbf{u})\left[1 - \frac{x}{\rho_k(\mathbf{u})}\right]^{3/2}. \tag{23}$$

where $r(\rho_k(\mathbf{u}), \mathbf{u}) \neq 0$ since $r(\rho_k, \mathbf{1}) = r \neq 0$ and w, r are analytic function around $(x, \mathbf{u}) = (\rho_k, \mathbf{1})$. Thus a central limit theorem follows. More precisely by setting $A(\mathbf{u}) = \log \rho_k(\mathbf{1}) - \log \rho_k(\mathbf{u})$, $\mu = (A_{u_j}(\mathbf{1}))_{1\le j\le M}$ and $\Sigma = (A_{u_i u_j}(\mathbf{1}) + \delta_{i,j} A_{u_j}(\mathbf{1}))_{1\le j\le M}$ then $\mathbb{E}(Y_{n,\mathbf{d}}) = \mu\, n + O(1)$ and $\mathbb{C}\mathrm{ov}(Y_{n,\mathbf{d}}) = \Sigma\, n + O(1)$.

□

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On the Average Performance of Fixed Partial Match Queries in Random Relaxed K-d Trees

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Abstract. We obtain an explicit formula for the expected cost of a fixed partial match query in a random relaxed K-d tree, that is, the expected cost for a query of the form

$$q = (q_0, q_1, \ldots, q_{K-1})$$

with $0 < s < K$ specified coordinates with values $z_0, \ldots, z_{s-1} \in (0, 1)$. This is a generalization of previous results in the literature for $s = 1$. Qualitatively similar results hold for standard K-d trees and we conjecture that this also holds for other multidimensional tree structures such as quadtrees and K-d tries.

Keywords: Partial match, K-d trees, multidimensional data structures, associative queries

1 Introduction

Consider a collection F of n multidimensional records, each record endowed with a K-dimensional key $\mathbf{x} = (x_0, \ldots, x_{K-1})$, with coordinate x_i drawn from a totally ordered domain $\mathcal{D}_i$. In a *partial match query* in F, we are given the query $\mathbf{q} = (q_0, \ldots, q_{K-1})$ with $q_i \in \mathcal{D}_i$ or $q_i = *$ (don't care symbol), and the goal is to retrieve those records in F that match the query, that is, the records[(i)] in F with key $\mathbf{x}$ such that $x_i = q_i$ whenever $q_i \neq *$.

Partial match is an associative query of independent interest (see, for instance [FP86, DECM98, Nei00, DJZC00, MPP01, CH06] and references therein), but its importance derives from the fact that the performance of many other associative queries, such as orthogonal range queries and nearest neighbor queries [CDZC01, DM02], or the selection by rank along a given coordinate [DJM12], is intimately related to the performance of partial matches.

There are several multidimensional data structures that support efficiently partial match queries (at least, on average). In this work, we will focus on the analysis of partial match queries in *relaxed K-d trees* (see [DECM98] for details), but most of the steps and ideas involved in our analysis should carry on for other multidimensional data structures such as standard K-d trees, quadtrees, K-d tries, etc. For general background on associative queries and multidimensional data structures we refer the reader to the book of Samet [Sam06] and the papers already cited.

[(i)] From now on, we will identify records with their K-dimensional keys.

Let us recall that a K-d tree t of size $n \geq 0$ is a binary search tree that is either empty ($n = 0$) or it stores a set of ($n > 0$) K-dimensional records in such a way that its root stores a record with key $\hat{\mathbf{x}}$ and a discriminant i, $0 \leq i < K$, and the remaining $n-1$ records are stored in the left and right subtrees of t, say t_L and t_R. Both t_L and t_R are K-d trees and, for any key $\mathbf{x} \in t_L$, it holds that $x_i \leq \hat{x}_i$, whereas for any key $\mathbf{x}' \in t_R$ we have $\hat{x}_i < x'_i$. The way of assigning discriminants to each node depends on the class of K-d tree, in relaxed K-d trees the discriminants are assigned uniformly at random while in standard K-d trees discriminants are assigned cyclically, nodes at level i discriminate with respect to the coordinate $i \mod K$.

As usual in the literature, we measure the cost of a partial match query as the number of visited nodes in the tree, and we assume that every coordinate of the n records of the collection is independently and uniformly drawn from $[0, 1]$ and every record inserted into an initially empty K-d tree. A tree built this way is called a *random* (K-dimensional) tree.

The vast majority of the literature on the analysis of partial match considers *random partial match queries*, that is, queries in which the specified coordinates are drawn from the same distribution as the data coordinates. Under this model, the cost of the partial match will depend on the *query pattern*, that is, which coordinates are specified and which are not. For a query $\mathbf{q}$, we define its pattern $\mathbf{w}(\mathbf{q}) = (w_0, w_1, \ldots, w_{K-1})$ with $w_i = *$ if $q_i = *$ and $w_i = S$ otherwise. Here and for the rest of the paper, s denotes the number of specified coordinates in the query (that is, the number of Ss in the query pattern). The expected cost $\bar{P}_{n,\mathbf{w}}$ of a random partial match with query pattern $\mathbf{w}$ is

$$\bar{P}_{n,\mathbf{w}} = \beta_{\mathbf{w}} n^{\alpha} + o(n^{\alpha}), \tag{1}$$

where the exponent α depends on the particular type of multidimensional data structure used and it also depends on the ratio $\rho = s/K$ [DECM98, MPP01].

In the case of relaxed K-d trees, the query pattern is irrelevant (since discriminants are random and independently chosen for each node), and thus the constant factor $\beta_{\mathbf{w}} := \beta(\rho)$ only depends on the ratio ρ, not on the query pattern. Furthermore, $\alpha := \alpha(\rho)$ is the positive solution of

$$1 - 2\rho\frac{1}{\alpha+2} - 2(1-\rho)\frac{1}{\alpha+1} = 0, \tag{2}$$

that is,

$$\alpha := \alpha(\rho) = \frac{1}{2}\left(\sqrt{9-8\rho} - 1\right), \tag{3}$$

and

$$\beta := \beta(\rho) = \frac{\Gamma(2\alpha+1)}{(1-\rho)(1+\alpha)\alpha^3\Gamma^3(\alpha)}. \tag{4}$$

It hasn't been until very recently that the performance of partial matches with fixed queries has been investigated. The cost of a partial match with exactly one specified coordinate is analyzed in depth in the papers [CJ11, BNS12] for the case of 2-dimensional quadtrees; in [DJM12] the analysis is carried out for the expected value of a partial match with one specified coordinate in relaxed and standard K-d trees.

In [DJM12], it is shown that the expected cost $P_{n,r}$ of a partial match in a random relaxed K-d tree of size n where the query specifies only one coordinate q_i such that exactly r records satisfy $x_i < q_i$ (and thus $n - r$ records satisfy $x_i > q_i$) is

$$P_{n,r} = \nu_{1,K}\sqrt{\left(\frac{r}{n}\right)^{\alpha}\left(1-\frac{r}{n}\right)^{\alpha}}\, n^{\alpha} + o(n^{\alpha}) = \nu_{1,K}\sqrt{r^{\alpha}(n-r)^{\alpha}} + o(n^{\alpha}). \tag{5}$$

In the asymptotic estimate above the constant $\nu_{1,K}$ only depends on $\rho := 1/K$ and $\alpha := \alpha(1/K)$:

$$\nu_{1,K} = \frac{\Gamma(2\alpha+1)}{(1-\rho)(\alpha+1)\alpha^3\Gamma^3(\alpha)} \frac{\Gamma(\alpha+2)}{\Gamma^2(\alpha/2+1)}.$$

In this work, we generalize the previous results to the case of s specified coordinates, $0 < s < K$. From now on, the s specified values in the query, from left to right, will be denoted z_0, z_1, ..., z_{s-1}. Let us observe that while (5) is expressed in terms of ranks, this generalization is expressed in terms of the query values, but the results are equivalent given the relation $r_i = z_i \cdot n + o(n)$.

Theorem 1 *For a query of the form $\mathbf{q} = (z_0, z_1, \ldots, z_{s-1}, *, \ldots, *)$, with $0 < z_i < 1$, and all queries resulting from a permutation of the coordinates of $\mathbf{q}$ (whether specified or not), the expected cost $P_{n,\mathbf{q}}$ of the partial match in a random relaxed K-d tree of size n is*

$$P_{n,\mathbf{q}} = \nu_{s,K} \left(\prod_{i=0}^{s-1} z_i(1-z_i) \right)^{\alpha/2} n^\alpha + o(n^\alpha),$$

where $\rho = s/K$, $\alpha = \alpha(\rho)$ is given in (3) *and $\nu_{s,K}$ is: $\nu_{s,K} = \frac{\Gamma(2\alpha+1)}{(1-\rho)(\alpha+1)\alpha^3\Gamma^3(\alpha)} \frac{\Gamma^s(\alpha+2)}{\Gamma^{2s}(\alpha/2+1)}$.*

The rest of this extended abstract is organized as follows. In Section 2 we give the analytic details of the theorem above. In Section 3 we present some results of the simulations that we have conducted. Despite the asymptotic nature of our result, the experiments show that it already gives reasonable predictions for moderate values of n. We finish with some conclusions and directions for future work in Section 4.

2 Analysis

Given a query $\mathbf{q}$ and a collection F, we call $\mathbf{r} = \mathbf{r}(\mathbf{q}) = (r_0, \ldots, r_{K-1})$ its *rank vector*, with $r_i = *$ if $q_i = *$, otherwise r_i is the number of records $\mathbf{x}$ in F such that $x_i < q_i$. Let $\mathcal{P}_{n,\mathbf{q}}$ and $\mathcal{P}_{n,\mathbf{r}}$ be the cost of a partial match in a random relaxed K-d tree of size n with query $\mathbf{q}$ and rank vector of the query $\mathbf{r}$ respectively and let $P_{n,\mathbf{q}} = \mathbb{E}\{\mathcal{P}_{n,\mathbf{q}}\}$ and $P_{n,\mathbf{r}} = \mathbb{E}\{\mathcal{P}_{n,\mathbf{r}}\}$ be their expected values.

Because of the symmetry of relaxed K-d trees, for a query with s specified coordinates, we can safely assume that the query pattern is $\mathbf{w} = (S, S, \ldots, S, *, \ldots, *)$ and thus the rank vector is of the form $\mathbf{r} = (r_0, r_1, \ldots, r_{s-1}, *, \ldots, *)$—we will simply write $\mathbf{r} = (r_0, \ldots, r_{s-1})$ from now on. Moreover, for any i and j, the expected cost of the partial match with rank vector $\mathbf{r} = (r_0, \ldots, r_{s-1})$ is the same as with rank vector $\mathbf{r}' = (r_0, \ldots, r_{i-1}, r_j, r_{i+1}, \ldots, r_{j-1}, r_i, r_{j+1}, \ldots, r_{s-1})$. There is also specular symmetry on each argument: the expected cost with rank vector $\mathbf{r}$ is the same as with rank vector $\mathbf{r}' = (r_0, \ldots, r_{i-1}, n - r_i, r_{i+1}, \ldots, r_{s-1})$, for any i, $0 \le i < s$.

Our goal is to show that if, for all i, $0 \le i < s$, $r_i = z_i n + o(n)$ with $0 < z_i < 1$ then the expected cost of a partial match with rank vector $\mathbf{r}$ in a random relaxed K-d tree of size n is

$$P_{n,\mathbf{r}} = f(z_0, \ldots, z_{s-1}) \cdot n^\alpha + o(n^\alpha),$$

where $\rho = s/K$, $\alpha = \alpha(\rho)$, and $f(z_0, \ldots, z_{s-1})$ is a bounded function in $[0,1]^s$, which also depends on s and K. Because of the symmetries discussed above, we must have $f(z_0, \ldots, z_{s-1}) = f(z'_0, \ldots, z'_{s-1})$ for any permutation $(z'_0, \ldots, z'_{s-1})$ of $(z_0, \ldots, z_{s-1})$, and $f(z_0, \ldots, z_i, \ldots, z_{s-1}) = f(z_0, \ldots, 1 - z_i, \ldots, z_{s-1})$, for any i, $0 \le i < s$.

Before going into the proof of Theorem 1, we will start with the analysis of a partial match with s coordinates specified, s_0 of which are exactly 0 (or, equivalently, 1), and the other $s - s_0$ are randomly drawn from $(0, 1)$. This is a generalization of the analysis of random partial matches where $s_0 = 0$.

Theorem 2 *The expected cost $\tilde{P}_n := \tilde{P}_{n,s,s_0,K}$ of a partial match in a random relaxed K-d tree of size n where s_0 specified coordinates of the query are identically 0, $0 \leq s_0 \leq s$, and the remaining $s - s_0$ specified coordinates are randomly drawn from $(0, 1)$, satisfies*

$$\tilde{P}_n = \tilde{\beta} n^{\tilde{\alpha}} + o(n^{\tilde{\alpha}}),$$

where the exponent $\tilde{\alpha}$ and the leading factor $\tilde{\beta}$ depend on the ratios $\rho = s/K$ and $\rho_0 = s_0/K$, namely,

$$\tilde{\alpha} := \tilde{\alpha}(\rho, \rho_0) = \frac{1}{2}\left(\sqrt{(3-\rho_0)^2 - 8(\rho - \rho_0)} - 1 - \rho_0\right), \tag{6}$$

and

$$\tilde{\beta} := \tilde{\beta}(\rho, \rho_0) = \frac{1}{(1-\rho)} \frac{\Gamma(2\tilde{\alpha} + 1 + \rho_0)}{(\tilde{\alpha}+1)\Gamma(\tilde{\alpha} + 1 + \rho_0)\tilde{\alpha}^2\Gamma^2(\tilde{\alpha})}.$$

Proof: The proof relies on fairly standard tools of Analytic Combinatorics [FS09], although it involves somewhat lengthy calculations. The first step is to set up a recurrence for $\tilde{P}_{n,}$

$$\tilde{P}_n = 1 + \frac{2(s-s_0)}{K}\frac{1}{n}\sum_{j=0}^{n-1}\frac{j+1}{n+1}\tilde{P}_j + \frac{2(K-s)+s_0}{K}\frac{1}{n}\sum_{j=0}^{n-1}\tilde{P}_j$$

and then translate the recurrence into a differential equation for the corresponding generating function. In particular, if $\tilde{P}(z) = \sum_{n\geq 0}\tilde{P}_n z^n$ then

$$\tilde{P}''(z) + \tilde{P}'(z)\frac{2-(4-\rho_0)z}{z(1-z)} - \tilde{P}(z)\frac{4-2\rho-(2-\rho_0)z}{z(1-z)^2} = \frac{2}{z(1-z)^3},$$

a second order linear differential equation with initial conditions $\tilde{P}(0) = 0$ and $\tilde{P}'(0) = 1$. The solution is

$$\tilde{P}(z) = \frac{1}{2}\left(\frac{{}_2F_1\left(\begin{smallmatrix}1-\tilde{\alpha}-\rho_0, -\tilde{\alpha}\\ 2\end{smallmatrix}\,\middle|\, z\right)}{(1-z)^{\tilde{\alpha}+1}} - \frac{1}{1-z}\right),$$

where ${}_2F_1\left(\begin{smallmatrix}a,b\\ c\end{smallmatrix}\,\middle|\, z\right)$ denotes the hypergeometric function. To get the asymptotic estimate for $\tilde{P}_n = [z^n]\tilde{P}(z)$ we need only to study the asymptotic behavior of $\tilde{P}(z)$ near its dominant singularity at $z = 1$, and using the transfer lemma of Flajolet and Odlyzko [FS09] the result follows. □

Let us observe that $\tilde{\alpha} = \alpha$ and $\tilde{\beta} = \beta$ if $s_0 = 0$; moreover, $\tilde{\alpha}(\rho, \rho_0) < \tilde{\alpha}(\rho, 0) = \alpha(\rho)$, for any $\rho > 0$.

Theorem 3 *If $r_i = o(n)$ or $r_i = n - o(n)$, for $0 \leq i < s_0$, and the remaining $s - s_0$ specified coordinates are randomly drawn from $(0, 1)$, then*

$$P_{n,\mathbf{r}} = \Theta\left(n^{\tilde{\alpha}}\right),$$

where $\tilde{\alpha}$ is as given in Theorem 2.

This result is actually an immediate consequence of a more general result:

$$P_{n,\mathbf{r}} = \tilde{\nu}_{s,s_0,K} \left(\prod_{i=s_0}^{s-1} \left(\frac{r_i}{n}\right)\left(1-\frac{r_i}{n}\right) \right)^{\tilde{\alpha}/2} \cdot n^{\tilde{\alpha}} + o(n^{\tilde{\alpha}}) \tag{7}$$

for some strictly positive constant $\tilde{\nu}_{s,s_0,K}$. Let us observe that the r_i's, with $s_0 \leq i \leq s-1$, are the ones that do not satisfy neither $r_i = o(n)$ nor $r_i = n - o(n)$.

Indeed, the result above generalizes our Theorem 4 later, which only holds for $s_0 = 0$. The proof of this more general result follows the same steps as the proof of Theorem 4. However, we must proceed inductively for a given s: the case $s_0 = s$, $s - s_0 = 0$ is very easy to prove and then we have to apply the result for the pair $(s_0, s - s_0)$ inductively to show that it is also true for $(s_0 - 1, s - s_0 + 1)$, reaching that way the interesting case $(0, s)$. But only the weaker statement of Theorem 3 is necessary to prove the initial conditions satisfied by the function $f(z_0, \ldots, z_{s-1}) = \lim_{n\to\infty} n^{-\alpha} P_{n,\mathbf{r}}$. We omit the details of the proof of (7) here because lack of space, but Theorem 2 makes reasonable to assume that the asymptotic behavior of the expected cost of a partial match with fixed specified coordinates should be of the same order of magnitude (namely, $n^{\tilde{\alpha}}$, Theorem 3) as the asymptotic behavior when the non-null specified coordinates are drawn at random (Theorem 2).

The important point here is that, for any s, if one or more of the s specified coordinates has rank either $o(n)$ or $n - o(n)$ then the expected cost of the partial match will be of an order of magnitude ($n^{\tilde{\alpha}}$) which is asymptotically smaller than the expected cost of a partial match when none of the s specified coordinates has rank either $o(n)$ or $n - o(n)$—in that case the order of magnitude is n^{α}.

From Theorem 3 and the continuity of the function $f(z_0, \ldots, z_{s-1}) = \lim_{n\to\infty} \frac{P_{n,\mathbf{r}}}{n^{\alpha}}$ (so far hypothesized), with $z_i = \lim_{n\to\infty} \frac{r_i}{n}$, it follows that $f = 0$ if any $z_i = 0$ (and, by symmetry, if any $z_i = 1$).

Lemma 1 *Let $z_i = \lim_{n\to\infty} \frac{r_i}{n}$, with $0 < z_i < 1$, for all i, $0 \leq i < s < K$. The limit*

$$f(z_0, \ldots, z_{s-1}) = \lim_{n\to\infty} \frac{P_{n,\mathbf{r}}}{n^{\alpha}},$$

with $\alpha = \alpha(\rho) = \alpha(s/K)$, exists if and only if it is the unique solution of the integral equation

$$f(z_0, \ldots, z_{s-1}) = \frac{\alpha+2}{2s} \sum_{i=0}^{s-1} \left\{ z_i^{\alpha+1} \int_{z_i}^{1} f(z_0, \ldots, z_{i-1}, u, z_{i+1}, \ldots, z_{s-1}) \frac{du}{u^{\alpha+2}} + (1-z_i)^{\alpha+1} \int_{0}^{z_i} f(z_0, \ldots, z_{i-1}, u, z_{i+1}, \ldots, z_{s-1}) \frac{du}{(1-u)^{\alpha+2}} \right\},$$

satisfying the following conditions:

(a) The function f is symmetric with respect to any permutation of its arguments.

(b) For any i, $0 \leq i < s$, and $z_i \in (0,1)$, $f(\ldots, z_i, \ldots) = f(\ldots, 1 - z_i, \ldots)$.

(c) For any i, $0 \leq i < s$, $f(z_0, \ldots, z_{i-1}, 0, z_{i+1}, \ldots) = f(z_0, \ldots, z_{i-1}, 1, z_{i+1}, \ldots) = 0$.

(d)

$$\int_0^1 \int_0^1 \cdots \int_0^1 f(z_0, \cdots, z_{s-1})\, dz_0\, dz_1 \cdots dz_{s-1} = \beta,$$

where β is the constant factor that multiplies n^α in the expected cost of a random partial match with s specified coordinates, given in (4)*.*

Proof: If the limit exists (and given the properties of $P_{n,\mathbf{r}}$ and Theorem 3) then the integral equation satisfied by f and the additional constraints follow, as we will show below. On the other hand, by exhibiting a function f which satisfies the integral equation and all the conditions and proving it is the unique such function, one can readily prove that $f(r_0/n, \ldots, r_{s-1}/n)n^\alpha - P_{n,\mathbf{r}} = o(n^\alpha)$ (that is, that the sought limit exists) by simply plugging in the value of f and using the recurrence for $P_{n,\mathbf{r}}$ that we give below; further details will be omitted in this extended abstract because of space constraints.

We start with a "case analysis" to obtain the recurrence satisfied by $P_{n,\mathbf{r}}$. Using the total probability formula,

$$P_{n,\mathbf{r}} = \frac{1}{K} \sum_{i=0}^{K-1} \mathbb{E}\{\mathcal{P}_{n,\mathbf{r}} \,|\, \text{the root discriminates w.r.t. } i\}.$$

We have to consider two different situations: 1) when $0 \leq i < s$, that is, when the discriminant of the root is one of the specified coordinates of the partial match, and 2) when it is not. In the second case, we will recursively continue the partial match in both subtrees of the tree, while in the first case, only one of the subtrees will be recursively explored; if the root is the $(r+1)$-th smallest element along the discriminant coordinate i and $r_i \leq r$ then the partial match will proceed into the left subtree, whereas if $r+1 \leq r_i$ then the partial match continues into the right subtree. In order to stress the different behavior of the partial match, we will denote

$$A_i = \mathbb{E}\{\mathcal{P}_{n,\mathbf{r}} \,|\, \text{the root discriminates w.r.t. } i\}.$$

when $0 \leq i < s$, and A'_i the same quantity when $s \leq i < K$. Of course the A_i's and A'_i's depend on n and $\mathbf{r}$ but we will not make this dependency explicit to keep the notation simple.

We can write thus

$$\frac{P_{n,\mathbf{r}}}{n^\alpha} = \frac{1}{Kn^\alpha}\Big(A_0 + A_1 + \cdots + A_{s-1} + A'_s + \cdots + A'_{K-1}\Big).$$

For $s \leq i < K$, let denote as $\mathbf{x}^{(i;j)}$ the $(j+1)$-th smallest element along coordinate i, then

$$A'_i = \frac{1}{n} \sum_{j=0}^{n-1} \mathbb{E}\{\mathcal{P}_{n,\mathbf{r}} \,|\, \text{the root discriminates w.r.t. } i \text{ and contains } \hat{\mathbf{x}} = \mathbf{x}^{(i;j)}\}$$

Or equivalently,

$$A'_i = \frac{1}{n} \sum_{j=0}^{n-1} \sum_{\boldsymbol{\delta}=(\delta_0,\ldots,\delta_{s-1})} \prod_{\ell=0}^{s-1} \frac{(1-\delta_\ell)(n-r_\ell) + \delta_\ell r_\ell}{n} \Big(1 + \sum_{\mathbf{r}'} \Pi^{n,j,i}_{\mathbf{r},\mathbf{r}',\boldsymbol{\delta}} \left(P_{j,\mathbf{r}'} + P_{n-1-j,\mathbf{r}-\mathbf{r}'-\boldsymbol{\delta}}\right)\Big) \quad (8)$$

where $\delta_\ell = 1$ if $\hat{x}_\ell < q_\ell$ and $\delta_\ell = 0$ if $\hat{x}_\ell \geq q_\ell$, and $\Pi^{n,j,i}_{\mathbf{r},\mathbf{r}',\boldsymbol{\delta}}$ is the probability that $\mathbf{r}'$ is the rank vector with respect to the j points in the left subtree and $\mathbf{r}-\mathbf{r}'-\boldsymbol{\delta}$ is the rank vector with respect to the $n-1-j$ points in the right subtree, for a random relaxed K-d tree of size n where the root discriminates with respect to coordinate i and contains $\mathbf{x}^{(i;j)}$, and when the query has rank vector $\mathbf{r}$.

By considering the partition of F into the 2^s sets created by the hyperplanes $x_i = q_i$, $0 \leq i < s$ and how the hyperplane $x_i = \hat{x}_i$ splits each of those sets we obtain a multivariate hypergeometric distribution. From that distribution and the linearity of expectations we obtain that the expected value of $\mathbf{r}'$ is $\sim \bar{\mathbf{r}} = \frac{j}{n}\mathbf{r}$; Furthermore, the distribution of $\mathbf{r}'$ is highly concentrated around the mean; for $n \to \infty$, the variance goes to zero. Therefore

$$\sum_{\mathbf{r}'=(r'_0,\ldots,r'_{s-1})} \Pi^{n,j,i}_{\mathbf{r},\mathbf{r}',\boldsymbol{\delta}} \left(P_{j,\mathbf{r}'} + P_{n-1-j,\mathbf{r}-\mathbf{r}'-\boldsymbol{\delta}}\right) \sim P_{j,\bar{\mathbf{r}}} + P_{n-1-j,\mathbf{r}-\bar{\mathbf{r}}}$$

Since the terms for the different $\boldsymbol{\delta}$ in (8) are asymptotically equal they can all be combined to obtain

$$A'_i \sim \frac{1}{n}\sum_{j=0}^{n-1}\left(1 + P_{j,\bar{\mathbf{r}}} + P_{n-1-j,\mathbf{r}-\bar{\mathbf{r}}}\right) = 1 + \frac{1}{n}\sum_{j=0}^{n-1}\left(P_{j,\bar{\mathbf{r}}} + P_{n-1-j,\mathbf{r}-\bar{\mathbf{r}}}\right).$$

Replacing the sum by an integral, passing to the limit $n \to \infty$, using that $\frac{r_j}{n} \to z_j$ and making $\frac{j}{n} \to z$:

$$\begin{aligned}\frac{A'_i}{n^\alpha} &\sim \frac{P_{0,\bar{\mathbf{r}}} + P_{n-1,\mathbf{r}-\bar{\mathbf{r}}} + P_{n-1,\bar{\mathbf{r}}} + P_{0,\mathbf{r}-\bar{\mathbf{r}}}}{n^{\alpha+1}} + \frac{1}{n}\sum_{j=1}^{n-2}\left[\frac{P_{j,\bar{\mathbf{r}}}}{j^\alpha}\left(\frac{j}{n}\right)^\alpha + \frac{P_{n-1-j,\mathbf{r}-\bar{\mathbf{r}}}}{(n-1-j)^\alpha}\left(\frac{n-1-j}{n}\right)^\alpha\right] \\ &\sim f(z_0,\ldots,z_{s-1})\int_0^1 \Big(z^\alpha + (1-z)^\alpha\Big)dz = \frac{2}{\alpha+1}f(z_0,\ldots,z_{s-1}).\end{aligned}$$

Let us observe that for the second step of the previous equation we are using the hypothesis that $f(z_0,\ldots,z_{s-1}) = \lim_{n\to\infty}\frac{P_{n,\mathbf{r}}}{n^\alpha}$. Therefore, using (2) for the second equality below

$$\begin{aligned}f(z_0,\ldots,z_{s-1}) &= \frac{1}{K}\lim_{n\to\infty}\frac{1}{n^\alpha}\left(A_0 + A_1 + \ldots + A_{s-1}\right) + \frac{K-s}{K}\frac{2}{\alpha+1}f(z_0,\ldots,z_{s-1}) \\ &= \frac{\alpha+2}{2s}\lim_{n\to\infty}\frac{1}{n^\alpha}\left(A_0 + A_1 + \ldots + A_{s-1}\right).\end{aligned}$$

On the other hand, for $0 \leq i < s$,

$$\begin{aligned}A_i &= \frac{1}{n}\sum_{j=0}^{n-1}\mathbb{E}\{\mathcal{P}_{n,\mathbf{r}} \mid \text{the root discriminates w.r.t. } i \text{ and contains } \hat{\mathbf{x}} = \mathbf{x}^{(i;j)}\} \\ &= \frac{1}{n}\sum_{j=0}^{r_i-1}\sum_{\boldsymbol{\delta}=(\ldots,\delta_{i-1},1,\delta_{i+1}\ldots)}\prod_{\substack{\ell=0\\ \ell\neq i}}^{s-1}\frac{(1-\delta_\ell)(n-r_\ell)+\delta_\ell r_\ell}{n}\Big(1 + \sum_{\mathbf{r}'=(\ldots,r'_{i-1},j,r'_{i+1},\ldots)}\Pi^{n,j,i}_{\mathbf{r},\mathbf{r}',\boldsymbol{\delta}}P_{n-1-j,\mathbf{r}-\mathbf{r}'-\boldsymbol{\delta}}\Big) \\ &+ \frac{1}{n}\sum_{j=r_i}^{n-1}\sum_{\boldsymbol{\delta}=(\ldots,\delta_{i-1},0,\delta_{i+1}\ldots)}\prod_{\substack{\ell=0\\ \ell\neq i}}^{s-1}\frac{(1-\delta_\ell)(n-r_\ell)+\delta_\ell r_\ell}{n}\Big(1 + \sum_{\mathbf{r}'=(\ldots,r'_{i-1},r_i,r'_{i+1},\ldots)}\Pi^{n,j,i}_{\mathbf{r},\mathbf{r}',\boldsymbol{\delta}}P_{j,\mathbf{r}'}\Big).\end{aligned}$$

A similar proof to the case $s \leq i < K$, with $\mathbf{r}' = (r_0 - \bar{r}_0, \ldots, r_{i-1} - \bar{r}_{i-1}, r_i - j - 1, r_{i+1} - \bar{r}_{i+1}, \ldots, r_{s-1} - \bar{r}_{s-1})$, $\mathbf{r}'' = (\bar{r}_0, \ldots, \bar{r}_{i-1}, r_i, \bar{r}_{i+1}, \ldots, \bar{r}_{s-1})$ and $\bar{r}_t = \frac{j}{n} r_t$, leads to conclude that

$$A_i \sim 1 + \frac{1}{n}\left[\sum_{j=0}^{r_i-1} P_{n-1-j,\mathbf{r}'} + \sum_{j=r_i}^{n-1} P_{j,\mathbf{r}''}\right].$$

Hence

$$\frac{A_i}{n^\alpha} \sim \frac{1}{n}\left[\sum_{j=0}^{r_i-1} \frac{P_{n-1-j,\mathbf{r}'}}{(n-1-j)^\alpha}\left(\frac{n-1-j}{n}\right)^\alpha + \sum_{j=r_i}^{n-1} \frac{P_{j,\mathbf{r}''}}{j^\alpha}\left(\frac{j}{n}\right)^\alpha\right].$$

Replacing the sums by integrals, passing to the limit $n \to \infty$, using that $\frac{r_j}{n} \to z_j$ and making $\frac{j}{n} \to z$ we get $\frac{r_i-1-j}{n-1-j} \to \frac{z_i - z}{1-z}$ and $\frac{r_i}{j} \to \frac{z_i}{z}$, therefore:

$$\begin{aligned}\frac{A_i}{n^\alpha} \sim &\int_0^{z_i} f\left(z_0, \ldots, z_{i-1}, \frac{z_i - z}{1-z}, z_{i+1} \ldots, z_{s-1}\right)(1-z)^\alpha dz \\ &+ \int_{z_i}^1 f\left(z_0, \ldots, z_{i-1}, \frac{z_i}{z}, z_{i+1} \ldots, z_{s-1}\right) z^\alpha dz\end{aligned}$$

Finally

$$\begin{aligned}f(z_0, \ldots, z_{s-1}) = \frac{\alpha+2}{2s}\sum_{i=0}^{s-1}\Bigg\{&\int_0^{z_i} f\left(z_0, \ldots, z_{i-1}, \frac{z_i - z}{1-z}, z_{i+1} \ldots, z_{s-1}\right)(1-z)^\alpha dz \\ &+ \int_{z_i}^1 f\left(z_0, \ldots, z_{i-1}, \frac{z_i}{z}, z_{i+1} \ldots, z_{s-1}\right) z^\alpha dz\Bigg\}.\end{aligned}$$

The equation given in the statement of the lemma follows by making the changes of variables $u = z_i/z$ and $u = (z_i - z)/(1-z)$ in the corresponding integrals. The conditions (a – c) that f must satisfy follow from the properties of $P_{n,\mathbf{r}}$ and from Theorem 3, and we have already discussed them. Averaging $P_{n,\mathbf{r}}$ for all the $(n+1)^s$ possible rank vectors must give us the expected value of the cost with a random query, that is, $\bar{P}_n$ in (1)–(4). Condition (d) is a direct consequence. □

Theorem 4 *For a query q with rank vector $\mathbf{r} = (r_0, \ldots, r_{s-1})$ such that $r_i = z_i n + o(n)$, $0 < z_i < 1$, for all i, $0 \leq i < s$, the expected cost of the partial match with query q in a random relaxed K-d tree of size n is*

$$P_{n,\mathbf{r}} = \nu_{s,K}\left(\prod_{i=0}^{s-1} z_i(1-z_i)\right)^{\alpha/2} \cdot n^\alpha + o(n^\alpha),$$

where $\rho = s/K$, $\alpha = \alpha(\rho)$ is given in (3) *and $\nu_{s,K}$ is:*

$$\nu_{s,K} = \frac{\Gamma(2\alpha+1)}{(1-\rho)(\alpha+1)\alpha^3\Gamma^3(\alpha)} \frac{\Gamma^s(\alpha+2)}{\Gamma^{2s}(\alpha/2+1)}.$$

Proof: To prove this result we need only to find the solution of the integral equation of Lemma 1.

For any function $f(z_0, z_1, \ldots, z_{s-1})$ let

$$L_i[f] := z_i^{\alpha+1} \int_{z_i}^{1} f(z_0, \ldots, z_{i-1}, u, z_{i+1}, \ldots, z_{s-1}) \, \frac{du}{u^{\alpha+2}},$$

and, similarly

$$R_i[f] := (1 - z_i)^{\alpha+1} \int_{0}^{z_i} f(z_0, \ldots, z_{i-1}, u, z_{i+1}, \ldots, z_{s-1}) \, \frac{du}{(1-u)^{\alpha+2}}.$$

If we set $T := \lambda \sum_{i=0}^{s-1} (L_i + R_i)$ where $\lambda = \frac{\alpha+2}{2s}$ then the function f is a non-trivial solution to the fix-point equation $f = T[f]$ with the additional constraints mentioned in Lemma 1.

Let us now assume that the solution to the integral equation is a function in separable variables, namely $f(z_0, z_1, \ldots, z_{s-1}) = \phi_0(z_0) \cdot \phi_1(z_1) \cdots \phi_{s-1}(z_{s-1})$ and that $\phi_0 = \phi_1 = \cdots = \phi_{s-1} = \phi$. We must also have $\phi(z) = \phi(1 - z)$ for any $z \in (0, 1)$ and $\lim_{z \to 0} \phi(z) = 0$ to satisfy $f(\ldots, 0, \ldots) = 0$.

Going back to the integral equation, if we denote $\phi_i = \phi(z_i)$ we must have

$$\phi_0 \cdot \phi_1 \cdots \phi_{s-1} = \lambda \sum_{i=0}^{s-1} \phi_0 \cdots \phi_{i-1} \cdot \phi_{i+1} \cdots \phi_{s-1} \Big(L_i[\phi_i] + R_i[\phi_i] \Big).$$

If, for all i, $0 \leq i < s$,

$$\phi_i = s\lambda \Big(L_i[\phi_i] + R_i[\phi_i] \Big), \tag{9}$$

then

$$\lambda \sum_{i=0}^{s-1} \phi_0 \cdots \phi_{i-1} \cdot \phi_{i+1} \cdots \phi_{s-1} \cdot \Big(L_i[\phi_i] + R_i[\phi_i] \Big) = \lambda \sum_{i=0}^{s-1} \frac{\phi_0 \cdots \phi_{s-1}}{s\lambda} = \phi_0 \cdots \phi_{s-1}.$$

The solution of (9) can be obtained by solving the equivalent ordinary differential equation that we obtain applying the operator

$$\Phi_i[g(z_i)] := z_i(1 - z_i) \frac{d^2 g}{dz_i^2} + \alpha(2z_i - 1) \frac{dg}{dz_i} - \alpha(\alpha + 1) g(z_i),$$

to both sides.

In particular, we obtain the following ODE for $\phi(z)$, after rearranging:

$$z(1 - z)\phi''(z) + (\alpha - s\lambda)(2z - 1)\phi'(z) - \alpha(\alpha + 1 - 2s\lambda)\phi(z) = 0;$$

with the initial condition $\phi(0) = 0$. Again we have a second order linear ODE and we can get without too much effort the solution $\phi(z) = \mu \left(z(1 - z) \right)^{\alpha/2}$, for some constant μ and $\alpha = \alpha(s/K)$. We have thus $f(z_0, \ldots, z_{s-1}) = \nu_{s,K} \left(\prod_{i=0}^{s-1} z_i(1 - z_i) \right)^{\alpha/2}$, with $\nu_{s,K} := \mu^s$. This family of solutions (parameterized by the "arbitrary" $\nu_{s,K}$) obviously satisfies conditions (1-3). The last condition yields the sought function, as we impose

$$\nu_{s,K} \frac{\Gamma^{2s}(\alpha/2 + 1)}{\Gamma^s(\alpha + 2)} = \beta.$$

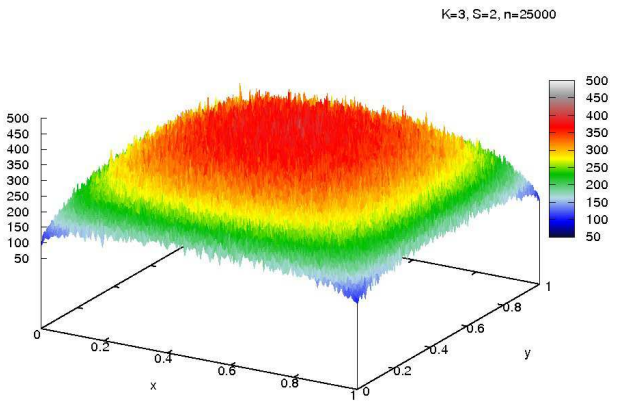

Fig. 1: The average cost of fixed partial match queries for $K = 3$ and $s = 2$.

□

To conclude this section we sketch the proof of Theorem 1.

Proof of Theorem 1: By conditioning, for a query $\mathbf{q} = (z_0, \ldots, z_{s-1}, *, \ldots)$ such that $0 < z_i < 1$ for all i, $0 \leq i < s$, we have

$$P_{n,\mathbf{q}} = \sum_{\mathbf{r}} \mathbb{E}\{\mathcal{P}_{n,\mathbf{r}}\} \Pr\{\mathbf{r}(\mathbf{q}) = \mathbf{r}\}.$$

The probability that $\mathbf{r}(\mathbf{q}) = \mathbf{r}$ is highly concentrated around its mean value $\bar{\mathbf{r}} = (z_0 \cdot n, z_1 \cdot n, \ldots)$; hence $P_{n,\mathbf{q}} \sim P_{n,\bar{\mathbf{r}}}$ and the statement of Theorem 1 follows. □

3 Experiments

In order to show graphically the behavior of our results and to see how they match in practice we have conducted the preliminary set of experiments that we present in this section.

For dimension $K = 3$, we generate $M = 100$ random relaxed K-d trees of size n. In each tree we performed a fixed partial match with $s = 2$ specified coordinates and 200 fixed values in every specified coordinate, counting the total number of visited nodes and taking the corresponding averages.

Figure 1 contains the experimental results regarding the average total number of visited nodes for a fixed partial match with coordinates x and y specified. The theoretical prediction for this plot is the function $6.9294(x(1-x)y(1-y))^{0.2287}n^{0.4574}$. The plot exhibits the symmetrical behavior of the cost function along every specified coordinate. It also shows how looking for specified coordinates with values near the median is more expensive than looking for specified coordinates whose values are near to 0 or to 1.

Figure 2 shows the behavior of the average cost for queries with two specified coordinates, say x and y, showing the variation of the average cost w.r.t. y as x takes several distinct values ($x = 0, 0.05, 0.25, 0.5$). For each considered value of x we show in brown the theoretical prediction and in a different color (one per

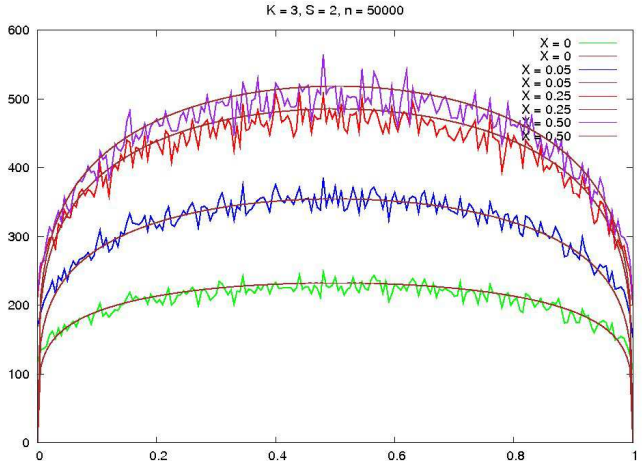

Fig. 2: The behavior along a single coordinate of fixed partial match queries for $K = 3$ and $s = 2$.

value) the experimental values (the ragged lines in the figure). As it can be appreciated, the experiments match quite well the predicted costs that are: $6.9294(x(1-x)y(1-y))^{0.2287}n^{0.4574}$ for $x \neq 0$ and $4.5959(y(1-y))^{0.1937}n^{0.3874}$ for $x = 0$ (this last calculated using Theorem 3). The experiments also exhibit that the average cost of a fixed partial match query with a fixed value equal to 0 or 1 is significantly smaller than the cost for bigger values.

Although our theoretical results apply in the asymptotic regime, the experiments show that these results are already useful for moderate values of n, e.g., $n = 1000$.

All the programs are written in the `C++` programming language and compiled with the `gnu gcc` compiler version `v4.4.3`. The experiments were run on a Pentium Genuine Intel `x86_64` double 32K core processor of 64 bits.

4 Conclusions

We have shown here that, albeit the recurrences involved are considerably more intrincate, the analysis of partial matches with fixed queries is feasible and the expected cost has a simple form, namely,

$$P_{n,\mathbf{q}} = \nu_{s,K}\left(\prod_{i=0}^{s-1} z_i(1-z_i)\right)^{\alpha/2} \cdot n^{\alpha} + o(n^{\alpha}).$$

We have also shown that the formula holds when some of the specified coordinates are 0 (or 1), only the coefficient $\nu_{s,K}$ and the exponent α change. We have also a proof (not given here) that an analogous for Theorem 1 holds for standard K-d trees, with the exponent α corresponding to standard K-d trees and the constant factor $\nu_{\mathbf{w}}$ now depending on the order of specified and unspecified coordinates in the query.

We conjecture that the result is fairly general, it will apply for other multidimensional data structures, such as quadtrees or K-d tries, as well.

Directions for future research include analyzing partial matches with fixed queries in other multidimensional data structures (hence providing further evidence for our conjecture or disproving it), analyzing the distribution of $n^{-\alpha}\mathcal{P}_{n,\mathbf{q}}$ (we conjecture that a limiting distribution $\mathcal{P}(z_0,\ldots,z_{s-1})$ exists), and applying these results about partial match to other associative queries.

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No Shannon Effect Induced by `And/Or` *Trees* †

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Abstract. Quantitative logic has been the subject of an increasing interest since a seminal paper by Chauvin et al. in 2004, which presented the first Analytic Combinatorics approach of the subject. Since then, the understanding of random Boolean trees has been deeply widened, even if the question of Shannon effect remains open for the majority of the models. We focus in this paper on the original case of Catalan `And/Or` trees and propose a new specification of those objects that implies easier ways to describe large families of trees. Equipped with this specification, we prove that the model of Catalan `And/Or` binary trees do not exhibit Shannon effect, i.e. there exists a family of functions with small complexities, that have a positive probability.

Keywords: Boolean functions; Probability distribution; Random Boolean formulas; Random trees; Asymptotic ratio; Analytic combinatorics.

1 Introduction

Pick up at random a Boolean formula of a given size: what is the distribution of the random Boolean function it represents? Defining models in which this question has a meaning and answering it in these models is the domain of quantitative logic. To our knowledge, the first attempts in this direction go back to the 90's, by Paris et al. [PVW94] and later Lefmann and Savický [LS97]. The framework they propose is to use the representation of Boolean formulas by plane binary trees and then rely on the good combinatorial properties of these trees. The domain has then strongly developed after the seminal contribution of Chauvin et al. [CFGG04], proposing the first Analytic Combinatorics approach of the question. Since 2004, many different models have been studied via Analytic Combinatorics, leading to a better understanding of random Boolean trees.

The first approaches [PVW94, LS97, CFGG04] focused on the `And/Or` logical system, i.e. on Boolean formulas built with the connectives AND and OR and with the negation. They pick up a binary plane Boolean tree uniformly at random among all trees with m leaves, and then let m tend to infinity: the induced distribution on the set of Boolean functions is called the *Catalan tree distribution*. Their initial

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results have been deeply improved by Kozik [Koz08], via Analytic Combinatorics and a very powerful *ad hoc* machinery called the *pattern theory*. Equivalent results have been shown for the implicational system by Fournier et al. [FGGG12], but there a different approach was required. The theory has then been extended to many directions: for example by considering non plane and non binary trees in order to take into account the logical properties of the logical connectives (for example the commutativity and associativity of AND and OR) [GGKM12, GGKM]; or by considering different distributions on Boolean trees [CFGG04, CGM11].

In this paper, however, we aim at revisiting the original `And/Or` Catalan tree distribution in order to prove that this model does not exhibit the *Shannon effect*. Riordan and Shannon have proved, in the paper [RS42], that a uniformly distributed random Boolean function on n variables is almost surely of exponential *complexity*: we say that the uniform distribution on Boolean functions of fixed size exhibits the Shannon effect. We prove in the present paper that the Catalan tree distribution does not. To prove this new result, we needed to develop a new framework: a new way to specify `And/Or` trees and thus a new way to count them.

We would like to point out, that the study of the Shannon effect in random Boolean tree models is only done in very few models [GG10, GGKM12], both models based on the connective of IMPLICATION, in the case of plane or non-plane trees. There is thus a need to progress in this direction. Moreover, we think that it is important to find universal methods to study those models, i.e. methods that could be used for both the `And/Or` and the implicational logical systems (note that Kozik's pattern theory does not apply for implicational trees). This was successfully done in the case of branching processes as underlying tree model [GG10]. The new proof happens to be very similar to the ones used in the implicational system [GG10, GGKM12]. The method we use has some common base with the expansion tools, developped for example in [FGGG12], but it is very different in the way the tools are used.

This paper is organised in two sections. The first one, Section 2, is devoted to the definition of the Catalan tree model and to the introduction of our new point of view on `And/Or` trees. The second one, Section 3, states and prove our main result on Shannon effect in the Catalan tree model and its proof.

2 Description of the model and specifications

2.1 Context

Definition 1 *A* **Catalan tree** *is a rooted full binary plane tree (meaning that each node has either 0 or 2 children). We define the* **size** *of a Catalan tree as the number of its leaves. The combinatorial class of Catalan trees is denoted by $\mathcal{C}$. The corresponding ordinary generating function is $C(z) = \sum_{m>0} C_m z^m$, where C_m is the number of Catalan trees of size m.*

It is well known that $C(z) = \dfrac{1-\sqrt{1-4z}}{2}$ and $C_m = \dfrac{1}{m} \cdot \binom{2m-2}{m-1}$.

Definition 2 *An `And/Or` tree on n variables is a Catalan tree whose internal nodes are labelled by a connective from the set $\{\wedge, \vee\}$ (resp.* AND *and* OR*) and whose leaves are labelled by a literal from $\{x_1, \bar{x}_1, \ldots, x_n, \bar{x}_n\}$, where $\bar{x}_i$ denotes the negation of x_i. The combinatorial class of `And/Or` trees on n variables is denoted by $\mathcal{T}_n$, the number of such trees of size m by $T_{m,n}$.*

Each `And/Or` tree is equivalent to a Boolean expression and thus *represents*, or *computes*, a Boolean function with n variables, i.e. a function from $\{0,1\}^n$ into $\{0,1\}$. An example is given in Fig. 1. We will from now denote the set of Boolean functions with n variables by $\mathcal{F}_n$.

Definition 3 *The* **complexity** $L(f)$ *of a non constant Boolean function* $f \in \mathcal{F}_n$ *is the size of the smallest trees calculating it. We call the trees realizing this complexity the* **minimal trees** *of* f*. The complexity of the constant functions* $\mathrm{true} : (x_1, \ldots, x_n) \mapsto 1$ *and* $\mathrm{false} : (x_1, \ldots, x_n) \mapsto 0$ *is defined to be 0.*

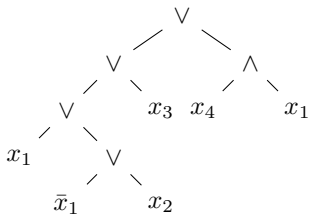

Fig. 1: The above tree is equivalent to the Boolean formula $([x_1 \vee (\bar{x}_1 \vee x_2)] \vee x_3) \vee (x_4 \wedge x_1)$ and represents the constant Boolean function $\mathrm{true} : (x_1, \ldots, x_n) \mapsto 1$.

The idea of quantitative logic is historically the following: Equip the set of `And/Or` trees of size m with the uniform distribution and denote by $\mu_{m,n}$ the induced distribution on the set of Boolean functions in n variables. Can we prove that the sequence $(\mu_{m,n})_{m \geq 1}$ converges? And what are the properties of the limiting distribution (if it exists)?

Since this model has already been studied in the literature, where it is sometimes called the **Catalan model**, we already know the following result:

Theorem 4 ([LS97, CFGG04]) *The sequence of distributions* $(\mu_{m,n})_{m \geq 1}$ *converges to a limiting distribution on the set of Boolean function with* n *variables. This distribution is denoted by* μ_n *and called the* **Catalan distribution**.

Moreover, we have the following inequalities: for all Boolean functions $f \in \mathcal{F}_n$*,*

$$\frac{1}{4}\left(\frac{1}{8n}\right)^{L(f)+1} \leq \mu_n(f) \leq (1 + O(1/n))\mathsf{e}^{-c\frac{L(f)+1}{n^2}},$$

asymptotically when n *tends to* $+\infty$*.*

This is the best result, in full generality, up to now. Kozik [Koz08] has proven the following more precise result:

Theorem 5 ([Koz08]) *Let* $f = f(x_1, \ldots, x_{n_0})$ *be a Boolean function and* $\mu_n(f)$ *denote the proportion of all* `And/Or` *trees on* n *which represent* f (cf. *Definition 8). Then there exists a constant* $\lambda_f > 0$ *such that, for* n *tending to infinity,*

$$\mu_n(f) = \frac{\lambda_f}{n^{L(f)+1}} + O\left(\frac{1}{n^{L(f)+2}}\right).$$

This result suggests that the Catalan distribution *gives more weight to low complexity functions*, but this result is too weak to claim that the Catalan distribution *does not exhibit the Shannon effect*. One has to consider sequences of functions indexed on n.

Definition 6 *We say that a sequence of distributions $(\nu_n)_{n\geq 1}$, respectively defined on the sets $(\mathcal{F}_n)_{n\geq 1}$,* **exhibit the Shannon effect** *if, for all $\varepsilon > 0$,*

$$\nu_n\left(\left\{f \text{ such that } L(f) \geq \frac{2^n(1-\varepsilon)}{\log_2 n}\right\}\right) \to 1,$$

when n tends to $+\infty$.

Remark: It is shown (see [Lup62] that the maximal complexity of a Boolean function with n variables is less than $\frac{2^n}{\log_2 n}(1+o(1))$. Thus, the sequence $(\nu_n)_{n\geq 1}$ exhibit the Shannon effect if, asymptotically when n tends to $+\infty$, almost all Boolean functions (under ν_n) have almost maximal complexity.

To prove that a sequence of distributions $(\nu_n)_{n\geq 1}$ does not exhibit the Shannon effect, it is enough to find a sub-exponential function $g(n)$ and a constant $\alpha > 0$ such that, for all $n \geq 1$,

$$\nu_n\left(\{f \text{ such that } L(f) \leq g(n)\}\right) \geq \alpha > 0.$$

The approach is thus very different from the proof of Theorem 5 since one has to consider a set of Boolean functions, among them functions whose complexity does depend on n. This explains why the Shannon effect has only been studied in a few models: the implicational model [GG10], the general implicational model [GGKM12], and the models based on branching processes [GG10]. The successful approach in those two articles is based on a very careful Analytic Combinatorics study.

Corollary 7 (of Theorem 5) *If K is some constant which is independent of n. Then the set of all Boolean functions up to complexity K is not sufficiently large to refute the Shannon effect.*

Proof: The number of functions of complexity k is bounded by $\alpha \cdot n^k$ (where α is a constant), and therefore, by using Theorem 5, the probability of functions of complexity smaller or equal to k is $O(1/n)$. Thus, we need a class of functions of complexity up to some bound K_n tending to infinity as n tends to infinity to have a chance to prove that there is no Shannon effect. □

Our aim in the present paper is to introduce a new specification for `And/Or` trees which simplifies the Analytic Combinatorics involved in their study and therefore allows us to tackle the Shannon effect question in this context.

2.2 New specification of `And/Or` trees

The historical specification of `And/Or` trees is the following [CFGG04]: there are $2n$ different trees of size one (one for each literal $\{x_1, \bar{x}_1, \ldots, x_n, \bar{x}_n\}$), and an `And/Or` tree is either a tree of size one ($2n \cdot \mathcal{Z}$) or an internal node (two choices) with two subtrees from $\mathcal{T}$. Namely,

$$\mathcal{T} = 2 \cdot (\mathcal{T} \times \mathcal{T}) + 2n \cdot \mathcal{Z}.$$

We propose here another point of view that simplifies the descriptions of the subfamilies of trees needed later on and therefore the technical calculations. Maybe, with this new description we could rederive the results of [Koz08] while circumventing the pattern theory but keeping the key ideas of the proofs.

Let us denote by $\mathcal{A}$ the family of `And/Or` trees that are rooted by an $\wedge$ label, and by $\mathcal{O}$ the family of trees that are rooted by an $\vee$ label. We have $\mathcal{T} = 2n\mathcal{Z} + \mathcal{A} + \mathcal{O}$, and we describe the $\wedge$-rooted trees

as follows: it is a Catalan tree of $\wedge$-labels (of size at least two), whose leaves are substituted either by (Boolean decorated) leaves ($2n\mathcal{Z}$) or by $\vee$-rooted trees. Namely,

$$\mathcal{A} = (\mathcal{C} \setminus \mathcal{Z}) \circ (2n \cdot \mathcal{Z} + \mathcal{O}).$$

Thus, in terms of generating functions, we have via the symbolic method (see [FS09] for an introduction to this method)

$$A(z) = K(O(z) + 2nz), \tag{1}$$

where $K(z) = C(z) - z$ is the generating function of Catalan trees of size at least 2, $A(z)$ (resp. $O(z)$) is the generating function of $\wedge$-rooted trees (resp. $\vee$-rooted trees). By symmetry $A(z) = O(z)$, thus

$$A(z) = \frac{1 - 8nz - \sqrt{1 - 16nz}}{8}.$$

Obviously, we again obtain the classical generating enumerating all trees,

$$T(z) = 2nz + 2A(z) = \frac{1 - \sqrt{1 - 16nz}}{4},$$

which is directly translated from the classical specification: $\mathcal{T} = 2n \cdot \mathcal{Z} + 2 \cdot (\mathcal{T} \times \mathcal{T})$.

Observe that an `And/Or` tree can be seen in the following way: Instead of looking at it node by node, we partition the set of internal nodes into clusters of nodes carrying the same label. For example, if the root is labelled by $\vee$, then we take all nodes labelled by $\vee$ and connected to the root by an $\vee$-only path into a super-$\vee$-node. Repeat this procedure recursively. Then, we arrive at a tree consisting of such supernodes, which we will call $\wedge$- and $\vee$-**clusters** in the sequel, and leaves. This tree is not binary any more, and on each path the labels of the clusters are alternating. We will refer to this viewpoint as the **cluster tree** of a given `And/Or` tree. Equation (1) corresponds to this way of looking at an `And/Or` tree.

2.3 Distribution on `And/Or` trees in details

Let us recall the notions and notations which have become common in quantitative logics (cf. [FGGG12] for example).

Definition 8 *Let $\mathcal{X}$ be a subfamily of $\mathcal{T}$, we define its* **limiting ratio** $[\mathcal{X}]_n$ *as the following limit, if it exists:*

$$[\mathcal{X}]_n := \lim_{m \to +\infty} \frac{X_{m,n}}{T_{m,n}},$$

where $T_{m,n}$ is the number of `And/Or` *trees of size m and $X_{m,n}$ is the number of elements of $\mathcal{X}$ of size m.*

Remark: Let f be a Boolean function in $\mathcal{F}_n$, and let $\mathcal{X}(f)$ be the family of `And/Or` trees that compute f. Then $[\mathcal{X}(f)]_n$ exists and we set $\mu_n(f) = [\mathcal{X}(f)]_n$.

Fact 9 *Let $\mathcal{X}$ be a subfamily of $\mathcal{T}$. If the dominant singularity of the generating function $X(z) = \sum_{m \geq 0} X_{m,n} z^m$ of $\mathcal{X}$ is $\rho = 1/16n$ and if this singularity is a square-root singularity, then*

$$[\mathcal{X}]_n = \lim_{z \to \rho} \frac{X'(z)}{T'(z)}.$$

3 No Shannon effect in And/Or trees

Theorem 10 *The Catalan distribution does not exhibit the Shannon effect.*

Let us mention here a difference in the approach that we will use in this paper than the one used in [GG10]. The generating functions that appear there are not as intricate as the one we get in the And/Or tree model. So, in the implicational model the authors have tried to obtain the best possible lower bound for the probability of a well-chosen family of functions. In this paper, our goal is to prove that there is no Shannon effect. We will not care for the final value for the probability of a suitably chosen family of functions, but only prove that it is positive.

Definition 11 *Let t be an And/Or tree and ν_α be a leaf labelled by the literal α in t. Denote by η the root of the cluster containing ν_α. The subtree rooted by η is denoted u.*
Let ν be a node of u, and v the subtree with root ν.

- *If ν_α belongs to an $\vee$-cluster, then replace v by $(v \vee t_e)$ or $(t_e \vee v)$ in t, where t_e is a tree with a root labelled by $\wedge$ and such that at least one of the leaves that are attached to the topmost $\wedge$-cluster is labelled by α.*
- *If ν_α belongs to an $\wedge$-cluster, then replace v by $(v \wedge t_e)$ or $(t_e \wedge v)$ in t, where t_e is a tree with a root labelled by $\vee$ and such that at least one of the leaves that are attached to the topmost $\vee$-cluster is labelled by α.*

The obtained tree $\tilde{t}$ is called an α-expansion *of t.*

Remark: In every node of u we can do an expansion according to the label of ν_α.

Lemma 12 *If t is a tree computing a Boolean function f, then for all literals α, all α-expansions of t are trees computing f.*

Proof: A proof by case is relatively straightforward. Assume that ν_α belongs to an $\vee$-cluster. Then u computes a function of the form $\alpha \vee f$. If $\alpha = \texttt{True}$, then the value of f is irrelevant and thus an expansion can do no harm. If $\alpha = \texttt{False}$, then observe that t_e is rooted by an $\wedge$-cluster which has a leaf α. Thus t_e attains the value False and replacing v by $v \vee t_e$ has no effect, either. The other cases are analogous. □

To prove Theorem 10, we will enumerate a subfamily of the expansions of all trees of size at most $g(n)$, for all literals α. We will constrain the expansion-structures in order to be able to retrieve the node in an expansion where the grafting has been done. This avoids double counting. We constrain the shapes in the following way: the grafted tree t_e has a shape $\alpha \vee (t_1 \vee t_2)$ (resp. $\alpha \wedge (t_1 \wedge t_2)$) where t_1 and t_2 are two subtrees of size at least $g(n)$ (we denote by $G(z)$ the generating function of such trees). Thus, given an expansion, find the topmost node that has two subtrees of size at least $g(n)$; its parent is the root of the grafted subtree t_e, denoted by ν in Fig. 2.

Fix a literal α. Let $\hat{N}(z,u)$ (resp. $\check{N}(z,u)$) be the generating function of $\wedge$-rooted (resp. $\vee$-rooted) And/Or trees, where z marks the size and u marks the number of nodes allowing an α-expansion. It is given by

$$\check{N}(z,u) = K((2n-1)z + \hat{N}(z,u)) + \sum_{p\geq 1} \frac{u^{2p-1}z^p}{p!} K^{(p)}(A(u^2 z) + u^2(2n-1)z),$$

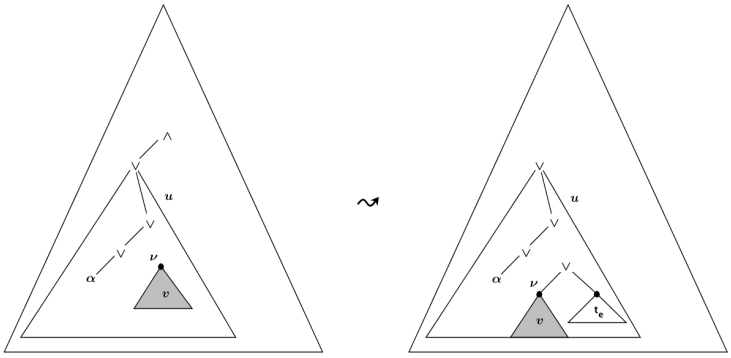

Fig. 2: On the right, the `And/Or` tree is an expansion from the tree represented on the left.

where

- the first term $K((2n-1)z + \hat{N}(z,u))$ stands for the case where there is no leaf of the topmost $\vee$-cluster that is labelled by α;
- the term $u^{2p-1}z^p K^{(p)}(A(u^2z)+u^2(2n-1)z)/p!$ stands for the case, where exactly p leaves of the topmost $\vee$-cluster are labelled by α: in this case, the choice of those p leaves yields the derivative and an expansion is possible at every node in the tree. Thus, a tree having k leaves contributes $z^k u^{2k-1}$ to the generating function $\check{N}(z,u)$.

By symmetry, we have an analogous equation for $\hat{N}(z,u)$, thus let us define $N(z,u) := \check{N}(z,u) = \hat{N}(z,u)$. Consequently we obtain:

$$N(z,u) = K((2n-1)z + N(z,u)) + \sum_{p\geq 1} \frac{u^{2p-1}z^p}{p!} K^{(p)}(A(u^2z) + u^2(2n-1)z), \tag{2}$$

Since we have avoided multiple-counting, we get the following inequality:

$$\mu_n(\{f \text{ such that } L(f) \leq g(n)\}) \geq \lim_{m\to+\infty} 4n \cdot \sum_{r=1}^{g(n)} [z^r]\partial_u N(z,1)\, \frac{[z^{m-r}]G(z)}{[z^m]T(z)}. \tag{3}$$

The factor $4n$ represents the choice of the literal α (with respect to which the expansions are done) and the label of the root of the tree; the sum is over all r from 1 to $g(n)$, where r represents the size of the original trees that are then expanded); the factor $[z^r]\partial_u N(z,1)$ counts the sum over all trees of size r of the different places where an α-expansion is possible; and the factor $[z^{m-r}]G(z)$ represents the number of different grafts that can be realized at each node.

Let us first focus on the generating function $G(z)$:

$$G(z) = z\left(\sum_{m\geq g(n)} T_{m,n} z^m\right)^2.$$

Lemma 13 *The generating function $G(z)$ satisfies:*

$$\lim_{m\to+\infty}\frac{[z^m]G(z)}{[z^m]T(z)}\geq\frac{1}{2\sqrt{\pi g(n)}}\,\frac{1}{16n}.$$

Proof: Let $P(z)$ be the polynomial such that $G(z)=z\cdot(T(z)-P(z))^2$. Since $P(z)$ is a polynomial, the generating functions $T(z)$ and $G(z)$ have the same dominant singularity $\rho=\frac{1}{16n}$, and both singularities are of squareroot type. Therefore, using a transfer lemma, one can prove that

$$\lim_{m\to+\infty}\frac{[z^m]G(z)}{[z^m]T(z)}=\lim_{z\to\rho}\frac{G'(z)}{T'(z)}=2\rho\left(T(\rho)-P(\rho)\right).$$

Let us find a lower bound for $T(\rho)-P(\rho)$:

$$T(\rho)-P(\rho)=\sum_{m\geq g(n)}\frac{(4n)^m}{2}C_m\rho^m.$$

Since $C_m\geq\frac{4^{m-1}}{\sqrt{\pi m^3}}$, for all $m>0$, we get $T(\rho)-P(\rho)\geq\sum_{m\geq g(n)}\frac{1}{8\sqrt{\pi m^3}}$. The function $m\mapsto m^{-3/2}$ is decreasing. Using a Riemann approximation, we get

$$T(\rho)-P(\rho)\geq\frac{1}{8\sqrt{\pi}}\int_{g(n)-1}^{\infty}\frac{du}{\sqrt{u^3}}\geq\frac{1}{4\sqrt{\pi g(n)}},$$

which concludes the proof. □

Now, let us come back to $N(z,u)$ by differentiating Equation (2) according to u and then by taking $u=1$. We get:

$$\begin{aligned}N_u(z,1)=&\sum_{p\geq1}(2p-1)\frac{z^p}{p!}K^{(p)}(A(z)+(2n-1)z)+\\&\sum_{p\geq1}\frac{z^p}{p!}(2zA'(z)+2(2n-1)z)K^{(p+1)}(A(z)+(2n-1)z)+\\&N_u(z,1)K'(N(z,1)+(2n-1)z).\end{aligned}$$

Observing that $N(z,1)=A(z)$ and isolating $N_u(z,1)$, we obtain

$$\begin{aligned}N_u(z,1)=&\frac{zK'((2n-1)z+A(z))}{1-K'((2n-1)z+A(z))}+\\&\frac{\sum_{p\geq2}[(2p-1)z^p+z^{p-1}(2zA'(z)+2(2n-1)z)]/p!\;K^{(p)}((2n-1)z+A(z))}{1-K'((2n-1)z+A(z))}.\end{aligned}$$

All generating functions in the numerator of $N_u(z,1)$ have non-negative coefficients, therefore,

$$[z^m]N_u(z,1)\geq[z^m]\frac{[z^2+z(zA'(z)+(2n-1)z)]K''((2n-1)z+A(z))}{1-K'((2n-1)z+A(z))}.$$

Note that the generating function $K''((2n-1)z + A(z))$ has only non negative integer coefficients. Therefore, omitting it causes a further decrease of the coefficients of the generating function. So, after all these reductions we can conclude that

$$[z^m]N_u(z,1) \geq [z^m]\frac{2z^2A'(z)}{1-K'((2n-1)z+A(z))} =: [z^m]F(z). \tag{4}$$

Recall that:

$$A(z) = \frac{1-8nz-\sqrt{1-16nz}}{8}, \qquad A'(z) = n\left(\frac{1}{\sqrt{1-16nz}}-1\right), \quad \text{and} \quad K'(z) = \frac{1}{\sqrt{1-4z}}-1.$$

Thus,

$$F(z) = 2nz^2\left(\frac{1}{\sqrt{1-16nz}}-1\right)\ \frac{1}{2-\frac{1}{\sqrt{\frac{1}{2}-4(n-1)z+\frac{1}{2}\sqrt{1-16nz}}}}.$$

Thus, for all $r \geq 0$, substituting z by $z/16n$ yields

$$[z^r]F(z) = n\,(16n)^{r-2}\,[z^r]z^2\left(\frac{1}{\sqrt{1-z}}-1\right)\frac{2}{2-\frac{1}{\sqrt{\frac{1}{2}-\frac{1}{4}\left(1-\frac{1}{n}\right)z+\frac{1}{2}\sqrt{1-z}}}}. \tag{5}$$

Let us first focus on the last factor: Set

$$H(z) := \frac{2}{2-\frac{1}{\sqrt{\frac{1}{2}-\frac{1}{4}\left(1-\frac{1}{n}\right)z+\frac{1}{2}\sqrt{1-z}}}} = \frac{1}{1-\frac{1}{\sqrt{2-\left(1-\frac{1}{n}\right)z+2\sqrt{1-z}}}}$$

and observe that the shape of $H(z)$ implies that all its coefficients are non-negative and thus its dominant singularity must lie on the positive real axis. For $0 \leq z \leq 1$, the radicand $R := 2-\left(1-\frac{1}{n}\right)z+2\sqrt{1-z}$ is obviously always positive and strictly larger than 1. Thus, the denominator of $H(z)$ never vanishes and hence the dominant singularity of $H(z)$ is $z=1$, originating from the term $\sqrt{1-z}$ of R. Hence, $H(z)$ admits a Puiseux expansion

$$H(z) = c_0 + c_1\sqrt{1-z} + c_2(1-z) + c_3(1-z)^{3/2} + \ldots \tag{6}$$

around $z=1$, and all the coefficients c_k depend on n.

Lemma 14 *For all $k \geq 0$, $c_k \sim (-1)^k(2n)^{k+1}$, as n tends to infinity.*

Proof: Let $X = \sqrt{1-z}$, we have

$$\begin{aligned}
H(z) &= \frac{1}{1-\frac{1}{(1+1/n)+2X+(1-1/n)X^2}} \\
&= \frac{1}{1-\frac{1}{\sqrt{1+1/n}}\sum_{k\geq 0}\binom{-1/2}{k}\left(\frac{2X+(1-1/n)X^2}{1+1/n}\right)^k} \\
&= \sum_{p\geq 0}\left(\frac{1}{1-\frac{1}{\sqrt{1+1/n}}}\right)^{p+1}\left(\sum_{k\geq 1}\binom{-1/2}{k}\frac{X^k}{(1+1/n)^k}\left(\frac{2+(1-1/n)X}{1+1/n}\right)^k\right)^p.
\end{aligned}$$

Observing that

$$\frac{1}{1-\frac{1}{\sqrt{1+1/n}}} \sim 2n \quad \text{when } n \to +\infty$$

completes the proof. □

Now, let us turn to (3) and prove the desired lower bound. The following lemma immediately implies Theorem 10.

Lemma 15 *Let $\varepsilon > 0$. If $g(n) = \Omega(n^{2+\varepsilon})$, then there is a constant $C > 0$ such that*

$$\mu_n(\{f \text{ such that } L(f) \leq g(n)\}) \geq C \tag{7}$$

for sufficiently large n.

Proof: First observe that

$$\frac{[z^{m-r}]G(z)}{[z^m]T(z)} = \frac{[z^{m-r}]G(z)}{[z^{m-r}]T(z)}\frac{[z^{m-r}]T(z)}{[z^m]T(z)} = \frac{[z^{m-r}]G(z)}{[z^{m-r}]T(z)}(16n)^{-r}.$$

Starting from (3), then applying Lemma 13, (4), and (5), we arrive at

$$\begin{aligned}
\mu_n(\{f \text{ such that } L(f) \leq g(n)\}) &\geq \lim_{m\to+\infty} 4n \cdot \sum_{r=1}^{g(n)} [z^r]\partial_u N(z,1)\,\frac{[z^{m-r}]G(z)}{[z^m]T(z)} \\
&\geq \frac{2n}{\sqrt{\pi g(n)}} \cdot \sum_{r=1}^{g(n)} [z^r]\partial_u N(z,1)\,\frac{1}{(16n)^{r+1}} \\
&\geq \frac{1}{2^{11}n\sqrt{\pi g(n)}} \cdot \sum_{r=0}^{g(n)-2} [z^r]\left(\frac{1}{\sqrt{1-z}} - 1\right) H(z) \\
&\geq \frac{1}{2^{12}n\sqrt{\pi g(n)}} [z^{g(n)-2}]\frac{1}{(1-z)^{3/2}} H(z) \qquad \text{for } n \text{ sufficiently large.}
\end{aligned}$$

Using the Puiseux expansion (6) then the classical transfer lemma yielding $[z^\ell](1-z)^{-\alpha} \sim {\ell^{\alpha-1}}/{\Gamma(\alpha)}$, we obtain

$$[z^{g(n)}]\frac{H(z)}{(1-z)^{3/2}} = c_0\frac{2\sqrt{g}(n)}{\sqrt{\pi}} + c_2\frac{1}{\sqrt{\pi g(n)}} + O(g(n)^{-3/2}).$$

The constant hidden in the error term depends on n, but using the knowledge on the growth rate of the c_k in (6), we conclude that

$$\mu_n(\{f \text{ such that } L(f) \leq g(n)\}) \geq \frac{1}{1024\pi} + \frac{n^2}{512\pi g(n)} + R_n$$

with $|R_n| = O\left({n^4}/{g(n)^2}\right)$; and here the O-constant is independent of n. □

4 Conclusion

The new specification for `And/Or` trees presented in the present paper has permitted us estimate the number of valid expansions of trees of size at most $n^{2+\epsilon}$. We have shown by precise analytic combinatorics that the asymptotic proportion of such expanded trees is positive, implying that the `And/Or` tree distribution do not exhibit Shannon effect.

It is interesting to note that, as in the implicational systems, we need a subset of functions of quadratic complexity in order to disprove the presence of the Shannon effect.

Note that we have shown that the asymptotic probability of functions of almost quadratic complexity is positive, but we have not proven that it is equal to one. In view of the absence of the Shannon effect and Kozik's result on the limiting distributions it seems reasonable that asymptotically almost all functions have polynomial complexity. It appears reasonable to conjecture that the asymptotic proportion of the class we used to prove our result is one, but proving this conjecture would need further arguments.

To be more precise, it would be interesting to extend Lemma 15 in two directions: showing that it still holds if ε is 0; and proving that $C = 1$.

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Persisting randomness in randomly growing discrete structures: graphs and search trees

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Abstract. The successive discrete structures generated by a sequential algorithm from random input constitute a Markov chain that may exhibit long term dependence on its first few input values. Using examples from random graph theory and search algorithms we show how such persistence of randomness can be detected and quantified with techniques from discrete potential theory. We also show that this approach can be used to obtain strong limit theorems in cases where previously only distributional convergence was known.

Keywords: Boundary theory, Markov chains, random graphs, search trees

1 Introduction

Given a sequence $t_1, t_2, \ldots$ of input values, a sequential algorithm produces an output sequence $x_1, x_2, \ldots$, where the next output x_{n+1} depends on the current state x_n and the next input t_{n+1} only. For cases where x_n is a discrete structure, such as a permutation or a graph, and where the input values are realizations of independent random variables with the same distribution, the output sequence is a Markov chain $X = (X_n)_{n\in\mathbb{N}}$ that is adapted to a combinatorial family $\mathbb{F}$ in the sense that X_n takes its values in the subset $\mathbb{F}_n \subset \mathbb{F}$ of objects with base parameter n. Markov chains of this type often exhibit *persisting randomness*: Informally, this means that the influence of early values does not go away as time goes by; formally, it means that the tail σ-field $\mathscr{T}(X)$ associated with X is not trivial. Further, such chains eventually leave every fixed finite subset of $\mathbb{F}$ with probability 1, which leads to the related problem of finding a state space completion that captures the information contained in $\mathscr{T}(X)$.

Discrete potential theory provides a general method for the construction of such state space boundaries. This was initiated by the fundamental paper [Doo59]. A recent textbook treatment is given in [Woe09]; see also the survey [Saw97]. Many authors have used boundary theory for the analysis of random walks on discrete structures; see the monograph [Woe00].

In the present extended abstract we regard the discrete structures themselves as states of a stochastic process. Some standard search algorithms have recently been investigated from this point of view

in [EGW12], and the results have been used in [Grü14] to prove strong limit theorems for functionals of the output sequence, such as the path length or Wiener index of search trees, that have attracted the attention of many researchers from the AofA community. We address the phenomenon of randomness persistence with these tools, specifically in connection with some popular models for random graphs, and for search algorithms. Further, we show that the method can be used to obtain almost sure convergence for the structures themselves or for functionals of the structures in cases where previously only convergence in distribution was known.

In the next section we provide some background on discrete potential theory and the Doob-Martin compactification. In order to keep this short we restrict ourselves to combinatorial Markov chains, where the state space is graded by the time parameter. Section 3 gives two simple examples from random graph theory; the present author is not aware of any previous use of the Doob-Martin compactification in connection with (general) graph limits. In Section 4 we consider search trees, where we can build on [EGW12] and [Grü14]. Proofs and some additional results and explanations are given in the full version of the paper.

We hope that the approach presented here contributes to the theoretical understanding of the growth models and algorithms. From an entirely practical point of view persisting randomness should be of interest as a strong dependence on the first few input values may be an entirely unwelcome aspect of an algorithm that the practitioner may have to address, for example by an additional randomization step.

2 An ultrashort summary of Markov chain boundary theory

A Markov chain is a sequence $X = (X_n)_{n\in\mathbb{N}}$ of random variables that take their values in some countable set $\mathbb{F}$, the state space, such that the Markov property holds,

$$P(X_{n+1} = x_{n+1}|X_n = x_n,\dots,X_1 = x_1) \;=\; P(X_{n+1} = x_{n+1}|X_n = x_n) \tag{1}$$

for all $n \in \mathbb{N}$, $x_1,\dots,x_{n+1} \in \mathbb{F}$. In the cases we are interested in there will be a canonical state $e \in \mathbb{F}$ with $X_1 = e$, and the transitions are homogeneous in time, which means that for some function $p : \mathbb{F}\times\mathbb{F} \to [0,1]$,

$$P(X_{n+1} = y|X_n = x) = p(x,y) \quad \text{for all } x,y \in \mathbb{F},\ n \in \mathbb{N}.$$

These are the transition probabilities; together with the starting point e they determine the distribution of the stochastic process X. We also assume that

$$P(X_n = x \text{ for some } n \in \mathbb{N}) > 0 \text{ for all } x \in \mathbb{F}. \tag{2}$$

In words: Every state has a chance to be visited—the chain is weakly irreducible.

Boundary theory provides an approach to the asymptotics of chains that 'leave the state space' in the sense that $\lim_{n\to\infty} P(X_n \in S) = 0$ for every finite set $S \subset \mathbb{F}$. It gives the 'right' extension (completion, compactification) $\bar{\mathbb{F}}$ of the state space, in the sense that

$$X_n \to X_\infty \text{ as } n \to \infty \text{ with probability 1} \tag{3}$$

for some random variable X_∞ with values in the boundary $\partial\mathbb{F}$ of $\mathbb{F}$ in $\bar{\mathbb{F}}$, and that

$$\sigma(X_\infty) =_{\text{a.s.}} \mathscr{T}(X) := \bigcap_{n=1}^{\infty} \sigma\big(\{X_m : m \ge n\}\big). \tag{4}$$

In words: The limit generates the tail σ-field of the process, up to null sets. For property (4) we assume that X has the space-time property, by which we mean that each state can be visited at one particular point in time only. The combinatorial Markov chains in Section 1 are such space-time processes.

This feat is achieved by the Doob-Martin compactification, where we regard a sequence $(y_n)_{n\in\mathbb{N}} \subset \mathbb{F}$ as convergent if the conditional probabilities $P(X_1 = x_1, \dots, X_m = x_m | X_n = y_n)$ converge as $n \to \infty$ for all fixed $m \in \mathbb{N}$, $x_1, \dots, x_m \in \mathbb{F}$. Due to the Markov property (1) the construction can be based on the Martin kernel K,

$$K(x,y) := \frac{P(X_n = y | X_m = x)}{P(X_n = y)}, \quad x, y \in \mathbb{F}, n > m,$$

where m and n are the time values associated with the states x and y respectively; here weak irreducibility (2) is important. Indeed, manipulations of elementary conditional probabilities lead to

$$P(X_1 = x_1, \dots, X_m = x_m | X_n = y_n) = K(x_m, y_n)\, P(X_1 = x_1, \dots, X_m = x_m),$$

which connects the convergence condition on the conditional probabilities to the convergence of the values of the Martin kernel.

A standard procedure, either via a completion of a metric space or by a variant of the Stone-Čech compactification, leads to $\bar{\mathbb{F}}$ as the smallest compact space that contains (a copy of) the discrete space $\mathbb{F}$ and allows for a continuous extension of the functions $y \mapsto K(x,y)$, $x \in \mathbb{F}$. We use the same symbol for the extended functions and denote boundary elements by lower case Greek letters. With this construction, (3) and (4) are satisfied. In addition, we have the following remarkable properties: First, all non-negative harmonic functions $h : \mathbb{F} \to \mathbb{R}$ can be written as mixtures of the functions $K(\cdot, \alpha)$, $\alpha \in \partial\mathbb{F}$. To be precise we recall that $h : \mathbb{F} \to \mathbb{R}$ is harmonic if $h(x) = \sum_{y\in\mathbb{F}} p(x,y)h(y)$ for all $x \in \mathbb{F}$. Then for each such h with $h \geq 0$ and $h(e) = 1$ there is a probability measure μ_h on (the Borel subsets of) the boundary $\partial\mathbb{F}$ such that

$$h(x) = \int K(x,\alpha)\, \mu_h(d\alpha) \quad \text{for all } x \in \mathbb{F}. \tag{5}$$

The distribution μ_1 of the limit X_∞ represents the (trivial) harmonic function $h \equiv 1$. Secondly, conditioned on a limit value $X_\infty = \alpha$, the process is again a Markov chain, with transition probabilities p^h given by

$$p^h(x,y) = \frac{1}{K(x,\alpha)}\, p(x,y) K(y,\alpha). \tag{6}$$

This is an instance of Doob's h-transform, with $K(\cdot,\alpha)$ the corresponding harmonic function h. Of course, the interpretation of these transforms as a conditioning on the final value is a natural consequence of the initial idea of conditioning on the values y_n at time n and then letting n tend to ∞.

3 Graph limits

Our basis in this section is the recent monograph [Lov12], which also gives references to the original research articles. Let $\mathbb{G}[n]$ be the set of simple graphs $G = (V,E)$ with vertex set $V = [n] := \{1, \dots, n\}$. The set $\mathbb{G}[1]$ has only one element, the graph $e = G_1$ with the single node 1 and no edges. A number of popular models for randomly growing graphs fits into the framework of combinatorial Markov chains, with state space $\mathbb{F} = \mathbb{G} := \bigcup_{n=1}^{\infty} \mathbb{G}[n]$ and start at G_1. We work out the boundary for two of them, the uniform attachment process, and the Erdős-Rényi graphs. We note that the state space compactifications

are abstract constructions so that the only uniqueness that we may expect is up to homeomorphisms; usually there are many possibilites for a concrete description.

On its own the question of how to define limits of finite graphs, interpreted as the search for a completion or compactification of the countable set $\mathbb{G}$, does not involve any probability and, of course, it can have quite different answers depending on the specific circumstances. For example, we might distinguish between sparse and dense graphs, referring to the rate of growth of the number $e(G_n)$ of edges $E(G_n)$ in relation to the number $v(G_n)$ of vertices $V(G_n)$ of G_n in a sequence $(G_n)_{n\in\mathbb{N}} \subset \mathbb{G}$. For the dense case the notion of subgraph sampling has turned out to be important (there are several equivalent definitions): For two graphs $G,H \in \mathbb{G}$ let $t(H,G)$ be the number of possibilities to embed H into G or, more formally, with $\Gamma(H,G)$ the set of injective functions $\phi : V(H) \to V(G)$, let

$$T(H,G) := \big\{\phi \in \Gamma(H,G) : \{\phi(i),\phi(j)\} \in E(G) \Leftrightarrow \{i,j\} \in E(H)\big\}, \tag{7}$$

$$t(H,G) := \#T(H,G), \quad \rho(H,G) := \frac{(v(G)-v(H))!}{v(G)!}\, t(H,G). \tag{8}$$

We then say that a sequence $(G_n)_{n\in\mathbb{N}}$ converges if for all $H \in \mathbb{G}$ the relative number $\rho(H,G_n)$ of these possibilities converges as a sequence of real numbers. The values $\rho(H,G_n)$ can be interpreted as the probability that, choosing $m = v(H)$ elements of $V(G_n)$ randomly and without replacement, the subgraph of G_n induced on these nodes is isomorphic to H. The convergence may be rephrased in a somewhat abstract manner: We define an embedding of $\mathbb{G}$ into the set $[0,1]^{\mathbb{G}}$ of functions on $\mathbb{G}$ with values in the unit interval by

$$G \mapsto \big(H \mapsto \rho(H,G)\big), \quad G \in \mathbb{G}, \tag{9}$$

and then consider the closure of the range of the embedding as a compactification of $\mathbb{G}$. Note that the function space is compact with respect to pointwise convergence by Tychonov's theorem. Viewed this way, the similarity to the Doob-Martin compactification becomes apparent, where we use the embedding

$$y \mapsto \big(x \mapsto K(x,y)\big), \quad y \in \mathbb{F}, \tag{10}$$

based on the Martin kernel instead.

Returning to the Markov chain models of randomly growing graphs, we first consider the *uniform attachment* model; see [Lov12, Example 11.39]. In order to describe its dynamics suppose that we are in state $G_n \in \mathbb{G}[n]$ at time n. We then construct $G_{n+1} \in \mathbb{G}[n+1]$ by adding those edges $\{i,j\} \subset [n+1]$ not (yet) in G_n with probability $1/(n+1)$, independently of each other. Let $X = (X_n)_{n\in\mathbb{N}}$ be the corresponding Markov chain, which has state space $\mathbb{G}$ and starts at G_1.

Let $\Delta := \{\{i,j\} \in \mathbb{N}\times\mathbb{N} : 1 \le i < j\}$. For each $\{i,j\} \in \Delta$ we define the edge indicator $1_{\{i,j\}} : \mathbb{G} \to \{0,1\}$ to have the value 1 for a graph G if $\{i,j\}$ is an element of the edge set $E(G)$ of G, and 0 otherwise.

Theorem 1 (a) *The Doob-Martin boundary of the uniform attachment process X consists of the set $\{0,1\}^\Delta$, where convergence of a sequence $(G_n)_{n\in\mathbb{N}}$ of graphs $G_n \in \mathbb{G}[n]$ to a limit $M \in \{0,1\}^\Delta$ means that the edge indicators $1_{\{i,j\}}(G_n)$ converge to $M(i,j)$ as $n \to \infty$, for each $(i,j) \in \Delta$.*

(b) *With probability 1, X_∞ is equal to $M \equiv 1$.*

As a consequence of part (b) of the theorem, the tail σ-field of the uniform attachment process is trivial. Further, using (6), the chain conditioned on some limit value $M \in \{0,1\}^\Delta$ can easily be described as follows: We proceed as before, but only edges $\{i,j\} \in \Delta$ with $M(i,j) = 1$ are allowed to enter.

Remark (a) An embedding interpretation as in (9) and (10) of the topology in Theorem 1 results if we identify a graph with the values of the edge indicators,

$$G \mapsto \big(\{i,j\} \mapsto 1_{\{i,j\}}(G)\big), \quad G \in \mathbb{G}. \tag{11}$$

Here the boundary is the full function space $\{0,1\}^{\Delta}$, which is usually not the case.

(b) The graph sequence generated by the uniform attachment model converges in the sampling topology too, and in fact to what is arguably a more interesting limit; see [Lov12, Proposition 11.40]. However, this 'more global' topology does not capture the tail information. To be specific, consider a random variable ξ with values in $\mathbb{N}$ and define a random element α of the boundary by $\alpha(i,j) = 0$ if $j = \xi$ and $\alpha(i,j) = 1$ otherwise, and let Y be the corresponding h-transform. In Y the random node ξ remains isolated forever. Then $\mathscr{T}(Y) =_{\text{a.s.}} \sigma(\xi)$, which means that some randomness persists. The 'local' topology in Theorem 1 detects this, whereas from the global point of view Y and the original chain X are asymptotically indistinguishable.

(c) Whereas (11) is an embedding in the strict sense of being one-to-one, (9) is not: If G and G' are of the same isomorphism type, then the functions $\rho(\cdot, G)$ and $\rho(\cdot, G')$ coincide; see also Theorem 5.29 and its proof in [Lov12]. ◁

The second model that we consider is perhaps the most famous of all random discrete structures: To obtain the Erdős-Rényi-Gilbert graph [Lov12, p.8] or binomial random graph [JŁR00, p.2] Y_n with node set $[n]$ and parameter $\theta \in [0,1]$ we include each of the $\binom{n}{2}$ possible edges with probability θ, independently of each other. In contrast to the uniform attachment model discussed above the variables Y_n are now defined for each n separately, with

$$P(Y_n = G_n) \;=\; \theta^{e(G_n)}(1-\theta)^{\binom{n}{2}-e(G_n)} \quad \text{for all } G_n \in \mathbb{G}[n], \tag{12}$$

but there is a well-known and canonical method to combine these into a Markov chain $Y = (Y_n)_{n\in\mathbb{N}}$: In order to move from Y_n to Y_{n+1} we add the node $n+1$ and then, independently of each other, each of the edges $\{i, n+1\}$, $1 \le i \le n$, with probability θ.

A moment's thought reveals that, in this model, none of the randomness will ever go away, which is the other extreme as compared with tail triviality. Indeed, it is possible to reconstruct the complete sequence $G_1, \dots, G_n$ from its last element G_n, which implies that $\mathscr{T}(Y) = \sigma(Y)$. Roughly, for such chains with perfect memory 'the sequence is the limit'; see also [EGW12, Section 9]. This can be formalized by projective limits. There is a slightly different point of view that connects this to the material in the next section and that is also useful for the description of probability measures on the projective limit: The transition graph of a combinatorial Markov chain on $\mathbb{G}$ is a rooted and locally finite tree, with root G_1 and directed edges (G_n, G_{n+1}), where G_n arises from G_{n+1} by deleting node $n+1$ and the incident edges. The projective limit then coincides with the ends compactification of the transition tree. For a node G of this tree with k vertices let

$$A_G := \big\{(G_n)_{n\in\mathbb{N}} \in \mathbb{G}_{\text{proj}} : G_k = G\big\}$$

be the set paths through G. It is easy to see that a probability measure μ on the ends compactification is completely specified by the values $\mu(A_G)$, $G \in \mathbb{G}$.

The perfect memory property is a consequence of the labelling of the nodes in the order of their appearance and the fact that in the step from n to $n+1$ only edges incident to $n+1$ are added. Uniform

attachment graphs do not have this property; for example, if $\{1,2\} \in E(X_3)$ then it is not clear whether this edge has been added at time 2 or 3.

We now show that in the perfect memory case random relabelling may lead to a more interesting topology. We recall that the group $\mathbb{S}[n]$ of permutations of $[n]$ acts on $\mathbb{G}[n]$, meaning that each $\pi_n \in \mathbb{S}[n]$ defines a function on and to $\mathbb{G}[n]$ by mapping $G = ([n], E(G))$ to

$$\pi_n(G) := \big([n], \big\{\{\pi_n(i), \pi_n(j)\} : \{i,j\} \in E(G)\big\}\big). \tag{13}$$

Now let Π_n, $n \in \mathbb{N}$, be a sequence of independent random variables, with Π_n uniformly distributed on $\mathbb{S}[n]$. We define $X = (X_n)_{n\in\mathbb{N}}$ inductively by $X_1 \equiv G_1$, $X_{n+1} = \Pi_{n+1}(\tilde{X}_{n+1})$, where $\tilde{X}_{n+1}$ is constructed from X_n as in the chain Y above. In view of the fact that the transition from X_n to X_{n+1} only involves X_n and quantities that are independent of X_n the process $X = (X_n)_{n\in\mathbb{N}}$ is again a Markov chain and it continues to be adapted to $\mathbb{G}$. Also, the distribution (12) is invariant under $\mathbb{S}[n]$ as the action (13) does not change the number of edges. This implies that X_n and the variable Y_n from the perfect memory version without random relabelling have the same distribution. Below, we will refer to the sequence X as the Erdős-Rényi chain with parameter θ.

The following result shows that the Doob-Martin compactification for this model leads to the sampling topology mentioned at the beginning of this section; see (7) and (8).

Theorem 2 *Let X be the Erdős-Rényi chain with parameter θ, $0 < \theta < 1$.*

(a) *A sequence $(G_n)_{n\in\mathbb{N}}$ with $G_n \in \mathbb{G}[n]$ for all $n \in \mathbb{N}$ converges in the Doob-Martin compactification associated with X if and only if the sequences $\big(\rho(H, G_n)\big)_{n\in\mathbb{N}}$ converge for every fixed $H \in \mathbb{G}$.*

(b) *With probability 1, X_∞ is equal to the function*

$$H \mapsto \theta^{e(H)}(1-\theta)^{\binom{v(H)}{2}-e(H)}, \quad H \in \mathbb{G}.$$

Again, part (b) implies that the tail σ-field of X is trivial. Further, the Erdős-Rényi chains with different parameter values are easily seen to be h-transforms of each other.

Theorem 2 identifies the Doob-Martin boundary of the Erdős-Rényi chain as a subset of the set of all functions $G_\infty : \mathbb{G} \to [0,1]$. For a concise description of this subset, by 'graphons', we refer the reader to [Lov12].

4 Search trees

The nodes of the complete binary tree $\mathbb{V} = \{0,1\}^\star$ are finite 0-1 sequences (or words) $u = (u_1, \ldots, u_k)$; we write $u0 = (u_1, \ldots, u_k, 0)$ and $u1 = (u_1, \ldots, u_k, 1)$ for the left and right child of u respectively and, if $k = |u| > 0$, $\bar{u} = (u_1, \ldots, u_{k-1})$ for its direct ancestor. The concatenation of $u = (u_1, \ldots, u_k)$ and $v = (v_1, \ldots, v_l)$ is given by $u + v = (u_1, \ldots, u_k, v_1, \ldots, v_l)$. We further write $\partial\mathbb{V} = \{0,1\}^\infty$ for the ends compactification of the tree $\mathbb{V}$.

By a binary tree we mean a subset $x \subset \mathbb{V}$ that is prefix-stable or, equivalently, contains the ancestor of each of its non-root elements. If $u \notin x$, $\bar{u} \in x$, then we call u external, and we write ∂x for the set of external nodes of x. The (fringe) subtree of x rooted at u is given by $x(u) := \{v \in \mathbb{V} : u + v \in x\}$. Let $\mathbb{B}_n$ be the set of binary trees with n nodes; $\mathbb{B} := \bigcup_{n=1}^\infty \mathbb{B}_n$. Prefix stability implies that any $x \in \mathbb{B}$ can be regarded as a contiguous subset of $\mathbb{V}$ and hence be described by its *boundary function*

$$B_x : \partial\mathbb{V} \to \mathbb{N}, \quad (u_i)_{i\in\mathbb{N}} \mapsto \min\big\{k \in \mathbb{N} : (u_1, \ldots, u_k) \notin x\big\}.$$

(This seems to be the most natural term, but in view of all the other occurrences of boundaries in the present extended abstract, 'frontier' may be a sensible alternative.)

Given a sequence $(t_n)_{n\in\mathbb{N}}$ of pairwise distinct real numbers the binary search tree (BST) algorithm generates a sequence $(x_n)_{n\in\mathbb{N}}$ of labelled binary trees as follows: The first value is stored at the root node; given x_n the next value t_{n+1} is stored at the first empty node found when travelling through x_n, moving from u to $u0$ if the new value is smaller that the label of an occupied node and to $u1$ otherwise. This is one of the standard algorithm for searching and also arises in the context of sorting; see [Knu73], [Mah92] and [Drm09]. Suppose that the t_i's are realizations of independent random variables η_i, $i \in \mathbb{N}$, with the same continuous distribution. Then the random binary trees X_n obtained for $\eta_1, \ldots, \eta_n$, $n \in \mathbb{N}$, can be collected into a Markov chain $X = (X_n)_{n\in\mathbb{N}}$ with a simple transition structure: X_1 is the tree that consists of the root node $\emptyset$ only, and in the transition from X_n to X_{n+1} one of the $n+1$ external nodes of X_n is chosen uniformly at random and incorporated into the tree. The BST chain has $\mathbb{B}$ as its state space, and $P(X_n \in \mathbb{B}_n) = 1$ for all $n \in \mathbb{N}$.

The Doob-Martin compactification of $\mathbb{B}$ with respect to X and the distribution of the limit X_∞ were obtained in [EGW12] and can be described as follows: $\partial\mathbb{B}$ is the set of probability measures μ on $\partial\mathbb{V}$. Convergence to $\mu \in \partial\mathbb{B}$ of a sequence $(x_n)_{n\in\mathbb{N}} \subset \mathbb{B}$ means that $a_n := \#x_n \to \infty$ and that the relative number $\#x_n(u)/a_n$ of nodes in the subtree rooted at $u \in \mathbb{V}$ converges to $\mu(A_u)$ for all $u \in \mathbb{V}$, where A_u consists of all infinite 0-1 sequences with prefix u. As with the transition tree in the previous section, the values $\mu(A_u)$, $u \in \mathbb{V}$, determine μ. With probability 1, the distribution of X_∞, which is a random probability measure, is diffuse in the sense that $X_\infty(A_u) > 0$ for all $u \in \mathbb{V}$, and it has the (characterizing) property that the random variables

$$\xi_u := \frac{X_\infty(A_{u0})}{X_\infty(A_u)}, \quad u \in \mathbb{V}, \tag{14}$$

are independent and uniformly distributed on the unit interval. This in turn implies that $X_\infty(A_u)$ can be written as the product of independent, identically distributed random variables, a fact that we will use repeatedly below.

In the present section we apply this to the asymptotics of the random functions B_{X_n}, $n \in \mathbb{N}$. The idea of describing randomly growing sets by their boundary appears in connection with models now known under the acronym 'IDLA' (internal diffusion limited aggregation). This subject area was initiated in [DF91], an early important contribution is [LBG92]. Both papers deal with integer lattices, but the basic model has since then been applied to various other infinite discrete background sets, for example to the 'comb' in [HS12]. BST chains may be seen as an IDLA variant on the background set $\mathbb{V}$, where the exploration process is a reinforced random walk in the sense that the probabilities of moving from u to $u0$ and $u1$ respectively depend on the number of previous particles that have travelled along the respective edge. The BST boundary functions have earlier been investigated under the name of 'silhouette' in [Grü05] and [Grü09], where they were regarded as functions on the unit interval via

$$\partial\mathbb{V} \ni u = (u_k)_{k\in\mathbb{N}} \;\mapsto\; \beta(u) := \frac{1}{2} + \sum_{k=1}^{\infty} \frac{2u_k - 1}{2^{k+1}} \in [0,1] \tag{15}$$

(binary rationals do not matter as X_∞ has no atoms). Figure 1 shows the boundary functions of X_n for various n, with pseudorandom data, where (15) has been used to display B_{X_n} as a function on $[0,1]$.

We begin with two real-valued functionals of the boundary functions. First we consider the growth of the trees along a fixed path through the infinite binary tree.

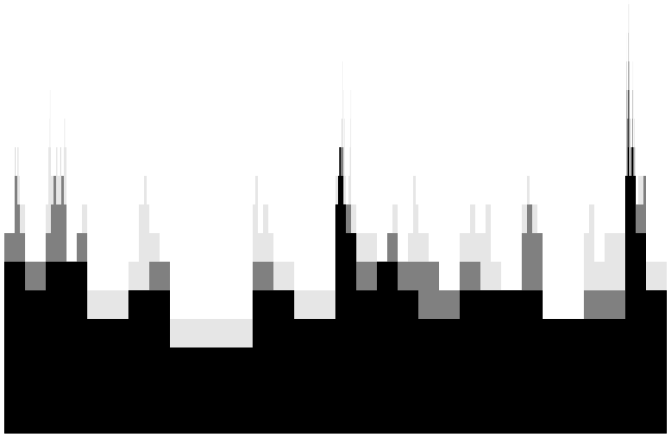

Fig. 1: The subgraph of B_{X_n}, for $n = 50$ (black), $n = 100$ (gray) and $n = 200$ (light gray).

Theorem 3 *Let $u \in \partial\mathbb{V}$ be fixed. Then the tail σ-field of the sequence $(B_{X_n}(u))_{n\in\mathbb{N}}$ is P-trivial.*

Let

$$H(0) = 0, \quad H(n) = \sum_{k=1}^{n} 1/k \ \text{ for } n \in \mathbb{N},$$

be the harmonic numbers. From the representation of $B_{X_n}(u)$ as a sum of independent Bernoulli variables we obtain $EB_{X_n}(u) = H(n)$ and, using $H(n) \sim \log n$, the distributional convergence

$$\frac{1}{\sqrt{\log n}}\big(B_{X_n}(u) - \log n\big) \ \to_{\text{distr}} \ Z \ \text{ as } n \to \infty, \tag{16}$$

where Z has a standard normal distribution. However, by Theorem 3, there is no transformation of the random variables $B_{X_n}(u)$, $u \in \partial\mathbb{V}$ fixed, that leads to strong convergence with a non-degenerate limit.

For the second functional we integrate the boundary functions with respect to the measure ν on $\partial\mathbb{V}$ given by $\nu(A_u) = 2^{-|u|}$. This is the unique normalized Haar measure if we regard the set of infinite 0-1 sequences as a compact group under the pointwise addition modulo 2. Recall from (14) that $\xi_u = X_\infty(A_{u0})/X_\infty(A_u)$, and let

$$C(t) \ = \ 1 + \frac{1}{2}\big(\log(t) + \log(1-t)\big), \quad 0 < t < 1.$$

Lemma 4 *The sequence $L_{\infty,k} := \sum_{|u|<k} 2^{-|u|} C(\xi_u)$ converges almost surely and in L^2 as $k \to \infty$.*

We write $L_\infty = \sum_{v\in\mathbb{V}} 2^{-|v|} C(\xi_v)$ for the limit of $L_{\infty,k}$ as $k \to \infty$. In this series we do not have absolute convergence: For $k \in \mathbb{N}$ fixed the mean of the random variable $\sum_{|u|=k} 2^{-|u|}|C(\xi_u)|$ is a positive value that does not depend on k.

Theorem 5 *Let* $L_n := \int B_{X_n}\, d\nu$. *Then* $L_n - H(n) \to L_\infty$ *with probability 1 as* $n \to \infty$.

As a sum of independent and non-degenerate random variables the limit L_∞ is not almost surely constant; in particular, the tail σ-field of the L-sequence is not P-trivial.

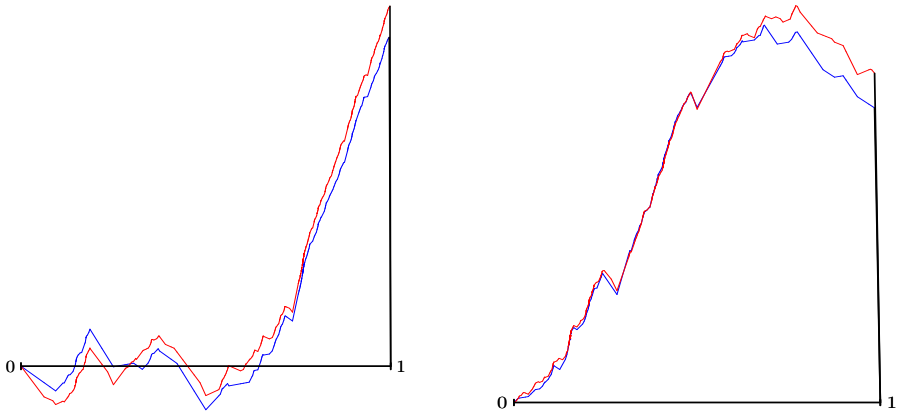

Fig. 2: Two values of Y_n, with $n = 500$ (blue) and $n = 1000$ (red).

We return to the boundary functions. From Theorem 3 it is clear that we cannot expect these to converge pointwise; see also Figure 1. Further, the asymptotic normality in (16) shows that, at a specific point, the functions increase roughly as $\log n$ but that there are fluctuations of the order $\sqrt{\log n}$. Hence, apart from shifting, some smoothing is needed, as has already been noticed in [Grü09]. We first adapt the smoothing procedure introduced [Grü09] to $\partial\mathbb{V}$ instead of $[0,1]$ as domain of the random functions. For this we define a total order on $\partial\mathbb{V}$ by setting $u \prec v$ for $u = (u_k)_{k\in\mathbb{N}}$, $v = (v_k)_{k\in\mathbb{N}}$, with $u \neq v$, if and only if $u_l = 0$ and $v_l = 1$ in the first position l where the sequences differ. With the IDLA connection in mind we are now led to normalizing and smoothing B_{X_n} to Y_n given by

$$Y_n(u) := \int_{v\prec u} \big(B_{X_n}(v) - H(n)\big)\, \nu(dv)$$

(recall that the nth harmonic number is the expectation of $B_{X_n}(v)$ for each $v \in \partial\mathbb{V}$). It is easy to deduce from [Grü09, Theorem 8] that Y_n converges in distribution to a process with continuous paths. However, as the Y_n's are all defined on the same probability space, it makes sense to ask whether these variables themselves converge.

Figure 2 shows the values of $Y_n(\omega)$ for two ω's, with $n = 500$ and $n = 1000$ respectively, where instead of two such ω's in the left and the right part of the figure two separate streams of numbers were used that the present author regards as plausible substitutes for truly random numbers: The two sequences were generated from alternating blocks of ten digits in the decimal expansion of $\pi - 3$, so that the left stream begins with $t_1 = 0.1415926535$, $t_2 = 0.2643383279$, ..., whereas the right stream has $t_1 = 0.8979323846$, $t_2 = 0.5028841971$ and so on. As in Figure 1, $\partial\mathbb{V}$ is mapped to $[0,1]$ by the function β defined in (15) in order to be able to draw the functions.

The figure supports the conjecture that the random functions Y_n themselves converge, and that the limit is not a fixed function. Incidentally, it also demonstrates the influence of the first few values on the output of the BST algorithm: The long-term proportion $\#X_n((0))/n$ of nodes in the left subtree is equal to the value of the first input variable, for example, and for the above π-data the t_1-values are quite different.

The theorem below confirms this conjecture. The theorem also provides a representation of the limit process in terms of the Doob-Martin limit X_∞ of the BST sequence and, in fact, its proof is closely connected to this representation.

We need to specify what convergence of the random functions Y_n means. For this, we define a metric d on $\partial\mathbb{V}$ by $d(u,v) = 2^{-l+1}$ for $u, v \in \partial\mathbb{V}$, $u \neq v$, where l is the first coordinate in which the two sequences differ as in the definition of the total order on $\partial\mathbb{V}$; also, $l-1 = |u \wedge v|$ where $u \wedge v$ denotes the longest common prefix (last common ancestor) of u and v. This turns $\partial\mathbb{V}$ into a compact metric space; we write $C(\partial\mathbb{V})$ for the set of continuous functions on $(\partial\mathbb{V}, d)$. Endowed with the supremum norm, $\|f\|_\infty = \sup_{u\in\mathbb{V}} |f(u)|$, $C(\partial\mathbb{V})$ becomes a Banach space.

Further, for $u = (u_k)_{k\in\mathbb{N}} \in \partial\mathbb{V}$ let $K(u) := \{k \in \mathbb{N} : u_k = 1\}$, and $u(k) := (u_1, \ldots, u_{k-1}, 0)$ for $k \in K(u)$. Generalizing the notation introduced above in connection with the second functional of the boundary functions we write

$$L_\infty(u) := \sum_{v \geq u} 2^{-|v|} C(\xi_v), \quad u \in \mathbb{V}, \tag{17}$$

where '$\geq$' now refers to prefix order. Clearly, $L_\infty(u)$ has the same distribution as $2^{-|u|}L_\infty(\emptyset)$, and we know from Lemma 4 that $L_\infty(\emptyset) = L_\infty$ has zero mean and finite variance. It can be shown that it makes sense to define two random functions $Y'_\infty = (Y'_\infty(u))_{u\in\partial\mathbb{V}}$ and $Y''_\infty = (Y''_\infty(u))_{u\in\partial\mathbb{V}}$ on $\partial\mathbb{V}$ by

$$Y'_\infty(u) = \sum_{k\in K(u)} L_\infty(u(k)), \quad Y''_\infty(u) = \sum_{k\in K(u)} 2^{-k} \log\bigl(2^k X_\infty(A_{u(k)})\bigr). \tag{18}$$

The random functions Y'_∞ and Y''_∞ may also be regarded as stochastic processes with time parameter $u \in \partial\mathbb{V}$. It can be shown that they have continuous paths with probability 1 and that they are integrable in the sense that $E\|Y'_\infty\|_\infty < \infty$ and $E\|Y''_\infty\|_\infty < \infty$.

Theorem 6 *With probability 1, Y_n converges in $\bigl(C(\partial\mathbb{V}), \|\cdot\|_\infty\bigr)$ to $Y_\infty := Y'_\infty + Y''_\infty$ as $n \to \infty$.*

The proof makes use of infinite-dimensional martingales; see [Nev75, Chapter V-2]. These are obtained by projecting Y'_∞ and Y''_∞ on the natural filtration of the BST chain.

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Counting Terms in the Binary Lambda Calculus

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Abstract. In a paper entitled *Binary lambda calculus and combinatory logic*, John Tromp presents a simple way of encoding lambda calculus terms as binary sequences. In what follows, we study the numbers of binary strings of a given size that represent lambda terms and derive results from their generating functions, especially that the number of terms of size n grows roughly like $1.963447954\ldots^n$.

Keywords: lambda calculus, combinatorics, functional programming, test, random generator, ranking, unranking

1 Introduction

In recent years growing attention has been given to quantitative research in logic and computational models. Investigated objects (e.g., propositional formulae, tautologies, proofs, programs) can be seen as combinatorial structures, providing therefore the inspiration for combinatorists and computer scientists. In particular, several works have been devoted to studying properties of lambda calculus terms. On a practical point of view, generation of random lambda terms is the core of debugging functional programs using random tests [3] and the present paper offers an answer to an open question (see introduction of [3]) since we are able to generate closed typable terms following a uniform distribution. This work applies beyond λ-calculus to any system with bound variables, like first order predicate calculus (quantifiers are binders like λ) or block structures in programming languages.

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First traces of the combinatorial approach to lambda calculus date back to the work of Jue Wang [19], who initiated the idea of enumerating λ-terms. In her report, Wang defined the size of a term as the total number of abstractions, applications and occurrences of variables, which corresponds to the number of all vertices in the tree representing the given term.

This size model, although natural from the combinatorial viewpoint, turned out to be difficult to handle. The question that arises immediately concerns the number of λ-terms of a given size. This task has been done for particular classes of terms by Bodini, Gardy, and Gittenberger in [2] and Lescanne in [14].

The approach applied in the latter paper has been extended in [9] by the authors of the current paper to the model in which applications and abstractions are the only ones that contribute to the size of a λ-term. The same model has been studied in [4] by David et al., where several properties satisfied by random λ-terms are provided.

When dealing with the two described models, it is not difficult to define recurrence relations for the number of λ-terms of a given size. However, by applying standard tools of the theory of generating functions one obtains generating functions that are expressed in the form of infinitely nested radicals. Moreover, the radii of convergence are in both cases equal to zero, which makes the analysis of those functions very difficult to cope with.

In this paper, we study the binary encoding of lambda calculus introduced by John Tromp in [18]. This representation results in another size model. It comes from the binary lambda calculus he defined in which he builds a minimal self interpreter of lambda calculus[(i)] as a basis of algorithmic complexity theory [15]. Set as a central question of theoretical computer science and mathematics, this approach is also more realistic for functional programming. Indeed for compiler builders it is counter-intuitive to assign the same size to all the variables, because in the translation of a program written in Haskell, Ocaml or LISP variables are put in a stack. A variable deep in the stack is not as easily reachable as a variable shallow in the stack. Therefore the weight of the former should be larger than the weight of the latter. Hence it makes sense to associate a size with a variable proportional to its distance to its binder. In this model, recurrence relations for the number of terms of a given size are built using this specific notion of size. From that, we derive corresponding generating functions defined as infinitely nested radicals. However, this time the radius of convergence is positive and allows us a further analysis of the functions. We are able to compute the asymptotics for the number of all (not necessarily closed) terms and we also prove the upper bound for the asymptotics for the number of closed ones. Moreover, we define an unranking function, i.e., a generator of terms from their indices from which we derive a uniform generator of λ-terms (general and typable). This allows us to provide outcomes of computer experiments in which we estimate the number of simply typable λ-terms of a given size.

2 Lambda calculus and its binary representation

Lambda calculus is a model of computation that is equivalent to Turing machines or recursive functions, serving as a powerful tool in the development of the programming theory [16]. Furthermore, it constitutes the basis for functional programming languages and has many applications in automated theorem provers.

Basic objects of the lambda calculus are λ-terms, which are regarded as denotation for functions or computer programs. In order to eliminate names of variables from the notation of λ-terms, de Bruijn introduced an alternative way of representing equivalent terms.

[(i)] an alternative to universal Turing machine

Let us assume that we are given a countable set $\{\underline{1}, \underline{2}, \underline{3}, \ldots\}$, elements of which are called de Bruijn indices. We define de Bruijn terms (called terms for brevity) in the following way:

(i) each de Bruijn index $\underline{\mathrm{i}}$ is a term,

(ii) if M is a term, then (λM) is a term (called an abstraction),

(iii) if M and N are terms, then (MN) is a term (called an application).

For the sake of clarity, we will omit the outermost parentheses. Moreover, we sometimes omit other parentheses according to the convention that application associates to the left, and abstraction associates to the right. Therefore, instead of $(MN)P$ we will write MNP, and instead of $\lambda(\lambda M)$ we will write $\lambda\lambda M$.

Given a term λN we say that the λ encloses all indices occuring in the term N. Given a term M, we say that an occurence of an index $\underline{\mathrm{i}}$ in the term M is *free* in M if the number of λ's in M enclosing the occurrence of $\underline{\mathrm{i}}$ is less than i. Otherwise, we say the given occurrence of $\underline{\mathrm{i}}$ is bound by the i-th lambda enclosing it. A term M is called closed if there are no free occurrences of indices.

For instance, given a term $\lambda\lambda\underline{1}(\lambda\underline{14})$, the first occurrence of $\underline{1}$ is bound by the second λ, the second occurrence of $\underline{1}$ is bound by the third λ, and the occurrence of $\underline{4}$ is free. Therefore, the given term is not closed.

Following John Tromp, we define the binary representation of de Bruijn indices in the following way:

$$\begin{aligned} \widehat{\lambda M} &= 00\widehat{M}, \\ \widehat{MN} &= 01\widehat{M}\widehat{N}, \\ \widehat{\underline{\mathrm{i}}} &= 1^i 0. \end{aligned}$$

However, notice that unlike Tromp [18] and Lescanne [13], we start the de Bruijn indices at 1 like de Bruijn [5]. Given a de Bruijn term, we define its size as the length of the corresponding binary sequence, i.e.,

$$\begin{aligned} |\underline{\mathrm{n}}| &= n + 1, \\ |\lambda M| &= |M| + 2, \\ |M\,N| &= |M| + |N| + 2. \end{aligned}$$

For example, the de Bruijn term $\lambda\lambda\underline{1}(\lambda\underline{14})$ is represented by the sequence 00000110001011110 and hence its length is 17.

In contrast to previously studied models, the number of all (not necessarily closed) λ-terms of a given size is always finite. This is due to the fact that the size of each variable depends on the distance from its binder.

3 Combinatorial facts

In order to determine the asymptotics of the number of all/closed λ-terms of a given size, we will use the following combinatorial notions and results.

We say that a sequence $(F_n)_{n\geq 0}$ is of

- order G_n, for some sequence $(G_n)_{n\geq 0}$ (with $G_n \neq 0$), if

$$\lim_{n\to\infty} F_n/G_n = 1,$$

and we denote this fact by $F_n \sim G_n$;

- exponential order A^n, for some constant A, if

$$\limsup_{n\to\infty} |F_n|^{1/n} = A,$$

and we denote this fact by $F_n \bowtie A^n$.

Given the generating function $F(z)$ for the sequence $(F_n)_{n\geq 0}$, we write $[z^n]F(z)$ to denote the n-th coefficient of the Taylor expansion of $F(z)$, therefore $[z^n]F(z) = F_n$.

The theorems below (Theorem IV.7 and Theorem VI.1 of [8]) serve as powerful tools that allow to estimate coefficients of certain functions that frequently appear in combinatorial considerations.

Fact 1 *If $F(z)$ is analytic at 0 and R is the modulus of a singularity nearest to the origin, then*

$$[z^n]F(z) \bowtie (1/R)^n.$$

Fact 2 *Let α be an arbitrary complex number in $\mathbb{C} \setminus \mathbb{Z}_{\leq 0}$. The coefficient of z^n in*

$$f(z) = (1-z)^\alpha$$

admits the following asymptotic expansion:

$$[z^n]f(z) \quad \sim \quad \frac{n^{\alpha-1}}{\Gamma(\alpha)}\left(1 + \frac{\alpha(\alpha-1)}{2n} + \frac{\alpha(\alpha-1)(\alpha-2)(3\alpha-1)}{24n^2} + O\left(\frac{1}{n^3}\right)\right),$$

where Γ is the Euler Gamma function.

4 The sequences $S_{m,n}$

Let us denote the number of λ-terms of size n with at most m distinct free indices by $S_{m,n}$.

First, let us notice that there are no terms of size 0 and 1. Let us consider a λ-term of size $n+2$ with at most m distinct free variables. Then we have one of the following cases.

- The term is a de Bruijn index $\underline{\mathsf{n}+1}$, provided m is greater than or equal to $n+1$.
- The term is an abstraction whose binary representation is given by $00\widehat{M}$, where the size of M is n and M has at most $m+1$ distinct free variables.
- The term is an application whose binary representation is given by $01\widehat{M}\widehat{N}$, where M is of size i and N is of size $n-i$, with $i \in \{0,\ldots,n\}$, and each of the two terms has at most m distinct free variables.

This leads to the following recursive formula[(ii)]:

$$S_{m,0} = S_{m,1} = 0, \tag{1}$$

$$S_{m,n+2} = [m \geq n+1] + S_{m+1,n} + \sum_{k=0}^{n} S_{m,k} S_{m,n-k}. \tag{2}$$

The sequence $S_{0,n}$, i.e., the sequence of numbers of closed λ-terms of size n, can be found in the *On-line Encyclopedia of Integer Sequences* under the number **A114852**. Its first 20 values are as follows:

$$0,\ 0,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1,\ 2,\ 1,\ 6,\ 5,\ 13,\ 14,\ 37,\ 44,\ 101,\ 134,\ 298,\ 431.$$

Now let us define the family of generating functions for sequences $(S_{m,n})_{n\geq 0}$:

$$\mathbb{S}_m(z) = \sum_{n=0}^{\infty} S_{m,n}\, z^n.$$

Most of all, we are interested in the generating function for the number of closed terms, i.e.,

$$\mathbb{S}_0(z) = \sum_{n=0}^{\infty} S_{0,n}\, z^n.$$

Applying the recurrence on $S_{m,n}$, we get

$$\begin{aligned}
\mathbb{S}_m(z) &= z^2 \sum_{n=0}^{\infty} S_{m,n+2} z^n \\
&= z^2 \sum_{n=0}^{\infty} [m \geq n+1] z^n + z^2 \sum_{n=0}^{\infty} S_{m+1,n}\, z^n + z^2 \sum_{n=0}^{\infty} \sum_{k=0}^{n} S_{m,k} S_{m,n-k}\, z^n \\
&= z^2 \sum_{k=0}^{m-1} z^k + z^2 \mathbb{S}_{m+1}(z) + z^2 \mathbb{S}_m(z)^2 \\
&= \frac{z^2\,(1-z^m)}{1-z} + z^2 \mathbb{S}_{m+1}(z) + z^2 \mathbb{S}_m(z)^2.
\end{aligned}$$

Solving the equation

$$z^2 \mathbb{S}_m(z)^2 - \mathbb{S}_m(z) + \frac{z^2\,(1-z^m)}{1-z} + z^2 \mathbb{S}_{m+1}(z) = 0 \tag{3}$$

gives us

$$\mathbb{S}_m(z) = \frac{1 - \sqrt{1 - 4z^4 \left(\frac{1-z^m}{1-z} + \mathbb{S}_{m+1}(z)\right)}}{2z^2}. \tag{4}$$

[(ii)] Given a predicate P, $[P(\vec{x})]$ denotes the Iverson symbol, i.e., $[P(\vec{x})] = 1$ if $P(\vec{x})$ and $[P(\vec{x})] = 0$ if $\neg P(\vec{x})$.

This means that the generating function $\mathbb{S}_m(z)$ is expressed by means of infinitely many nested radicals, a phenomenon which has already been encountered in previous research papers on enumeration of lambda terms, see e.g., [1]. However, in Tromp's binary lambda calculus we are able to provide more results than in other representations of lambda terms.

First of all, let us notice that the number of lambda terms of size n has to be less than 2^n, the number of all binary sequences of size n. This means that in the considered model of lambda terms the radius of convergence of the generating function enumerating closed lambda terms is positive (it is at least $1/2$), which is not the case in other models, where the radius of convergence is equal to zero.

5 The number of all λ-terms

Let us now consider the sequence enumerating all binary λ-terms, i.e., including terms that are not closed. Let $S_{\infty,n}$ denote the number of all such terms of size n. Repeating the reasoning from the previous section, we obtain the following recurrence relation:

$$\begin{aligned} S_{\infty,0} &= S_{\infty,1} = 0, \\ S_{\infty,n+2} &= 1 + S_{\infty,n} + \sum_{k=0}^{n} S_{\infty,k} S_{\infty,n-k}. \end{aligned}$$

The sequence $(S_{\infty,n})_{n\in\mathbb{N}}$ can be found in *On-line Encyclopedia of Integer Sequences* with the entry number **A114851**. Its first 20 values are as follows:

$$0,\ 0,\ 1,\ 1,\ 2,\ 2,\ 4,\ 5,\ 10,\ 14,\ 27,\ 41,\ 78,\ 126,\ 237,\ 399,\ 745,\ 1292,\ 2404,\ 4259.$$

Obviously, we have $S_{m,n} \leq S_{\infty,n}$ for every $m, n \in \mathbb{N}$. Moreover, $\lim_{m\to\infty} S_{m,n} = S_{\infty,n}$.

Let $\mathbb{S}_\infty(z)$ denote the generating function for the sequence $(S_{\infty,n})_{n\in\mathbb{N}}$, that is

$$\mathbb{S}_\infty(z) = \sum_{n=0}^{\infty} S_{\infty,n} z^n.$$

Notice that for $m \geq n-1$ we have $S_{m,n} = S_{\infty,n}$. Therefore

$$\mathbb{S}_\infty(z) = \sum_{n=1}^{\infty} S_{n,n} z^n,$$

which yields that $[z^n]\mathbb{S}_{n,n} = [z^n]\mathbb{S}_{\infty,n}$. Furthermore, $\mathbb{S}_\infty(z) = \lim_{m\to\infty} \mathbb{S}_m(z)$ for all $z \in [0, \rho]$.

Theorem 1 *The number of all binary λ-terms of size n satisfies*

$$S_{\infty,n} \sim (1/\rho)^n \cdot \frac{C}{n^{3/2}},$$

where $\rho \doteq 0.509308127$ and $C \doteq 1.021874073$.

The proof is in the full version of the paper [10]. Notice that $1/\rho \doteq 1.963447954$.

6 The number of closed λ-terms

Proposition 1 *Let ρ_m denote the dominant singularity of $\mathbb{S}_m(z)$. Then for every natural number m we have*

$$\rho_m = \rho_0,$$

which means that all functions $\mathbb{S}_m(z)$ have the same dominant singularity.

The proof is in the full version of the paper [10].

Proposition 2 *The dominant singularity of $\mathbb{S}_0(z)$ is equal to the dominant singularity of $\mathbb{S}_\infty(z)$, i.e.,*

$$\rho_0 \;=\; \rho \;\doteq\; 0.509308127.$$

Proof: Since the number of closed binary λ-terms is not greater than the number of all binary terms of the same size, we conclude immediately that $\rho_0 \geq \rho$.

Let us now consider the functionals

$$\begin{aligned}
\Phi_m(F) &= \frac{1-\sqrt{1-4z^4(\frac{1-z^m}{1-z}+F)}}{2z^2},\\
\Phi_\infty(F) &= \frac{1-\sqrt{1-4z^4(\frac{1}{1-z}+F)}}{2z^2}.
\end{aligned}$$

In particular, when $m=0$, we have

$$\Phi_0(F) \;=\; \frac{1-\sqrt{1+4z^4F}}{2z^2}.$$

We have also

$$\mathbb{S}_m(z) \;=\; \Phi_m(\mathbb{S}_{m+1}(z)).$$

The Φ_m's and Φ_∞ are increasing over functions over $[0,1)$, which means that for every $z \in [0,1)$ we have

$$\begin{aligned}
F(z) \leq G(z) &\;\Rightarrow\; \Phi_m(F(z)) \leq \Phi_m(G(z)),\\
F(z) \leq G(z) &\;\Rightarrow\; \Phi_\infty(F(z)) \leq \Phi_\infty(G(z)).
\end{aligned}$$

For each $m \in \mathbb{N}$, let us consider the function $\widetilde{\mathbb{S}}_m(z)$ defined as the fixed point of Φ_m. In other words, $\widetilde{\mathbb{S}}_m(z)$ is defined as the solution of the following equation:

$$\widetilde{\mathbb{S}}_m(z) \;=\; \Phi_m(\widetilde{\mathbb{S}}_m(z)).$$

Notice that since $S_{m,n}(z) \leq S_{m+1,n}(z) \leq S_{\infty,n}(z)$ for $z \in [0,\rho]$ we can claim that $\mathbb{S}_m(z) \leq \mathbb{S}_{m+1}(z) \leq \mathbb{S}_\infty(z)$. Therefore, for $z \in [0,\rho]$, we have

$$\Phi_m(\mathbb{S}_m(z)) \;\leq\; \mathbb{S}_m(z), \tag{5}$$

$$\widetilde{\mathbb{S}}_m(z) \;\leq\; \mathbb{S}_m(z) \;\leq\; \mathbb{S}_\infty(z). \tag{6}$$

Since $\widetilde{\mathbb{S}}_m(z)$ satisfies

$$2z^2\widetilde{\mathbb{S}}_m(z) \quad = \quad 1-\sqrt{1-4z^4\Big(\frac{1-z^m}{1-z}+\widetilde{\mathbb{S}}_m(z)\Big)},$$

we get

$$z^2\widetilde{\mathbb{S}}_m^2(z)-(1-z^2)^2\widetilde{\mathbb{S}}_m(z)+\frac{z^2(1-z^m)}{1-z}=0.$$

The discriminant of this equation is:

$$\Delta_m \quad = \quad (1-z^2)^2-\frac{4z^4(1-z^m)}{1-z}.$$

The values for which $\Delta_m = 0$ are the singularities of $\widetilde{\mathbb{S}}_m(z)$. Let us denote the main singularity of $\widetilde{\mathbb{S}}_m(z)$ by σ_m. From Equation (6) we see that

$$\sigma_m \geq \rho_m \geq \rho.$$

The value of σ_m is equal to the root of smallest modulus of the following polynomial:

$$P_m(z) \ := \ (z-1)\Delta_m \ = \ 4z^4(1-z^m)-(1-z)^3(1+z)^2.$$

In the case of the function $\widetilde{\mathbb{S}}_\infty(z)$, we get the polynomial

$$P_\infty(z) \quad = \quad z^5+3z^4-2z^3+2z^2+z-1 \ = \ \frac{R_\infty(z)}{z-1},$$

whose root of smallest modulus is, like in the case of $R_\infty(z)$, equal to ρ.

Now let us show that the sequence $(\sigma_m)_{m\in\mathbb{N}}$ of roots of polynomials $P_m(z)$ is decreasing (see Figure 1) and that it converges to ρ.

Notice that $P_m(z) = P_\infty(z) - 4z^{m+4}$. Given a value ζ such that $\rho < \zeta < 1$ (for instance $\zeta = 0.8$), $P_m(z)$ converges uniformly to $P_\infty(z)$ in the interval $[0,\zeta]$. Therefore $\sigma_m \to \rho$ when $m \to \infty$. By $\sigma_m \geq \rho_m \geq \rho$, we get $\rho_m \to \rho$, as well. Since all the ρ_m's are equal, we obtain that $\rho_m = \rho$ for every natural m. □

The number of closed terms of a given size cannot be greater than the number of all terms. Therefore, we immediately obtain what follows.

Theorem 2 *The number of closed binary λ-terms of size n is of exponential order $(1/\rho)^n$, i.e.,*

$$S_{0,n} \bowtie 1.963448\ldots^n.$$

Figure 2 shows values $S_{m,n}\cdot\rho^n\cdot n^{3/2}$ for a few initial values of m and n up to 600.

These numerical experiments allow us to state the following conjecture.

Conjecture 1 *For every natural number m, we have*

$$S_{m,n} \sim o\big(1.963448\ldots^n\cdot n^{-3/2}\big).$$

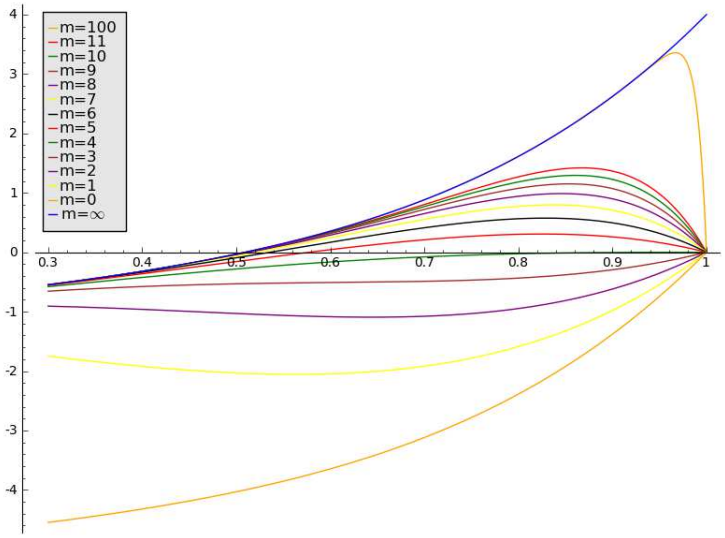

Fig. 1: Roots of the P_m's

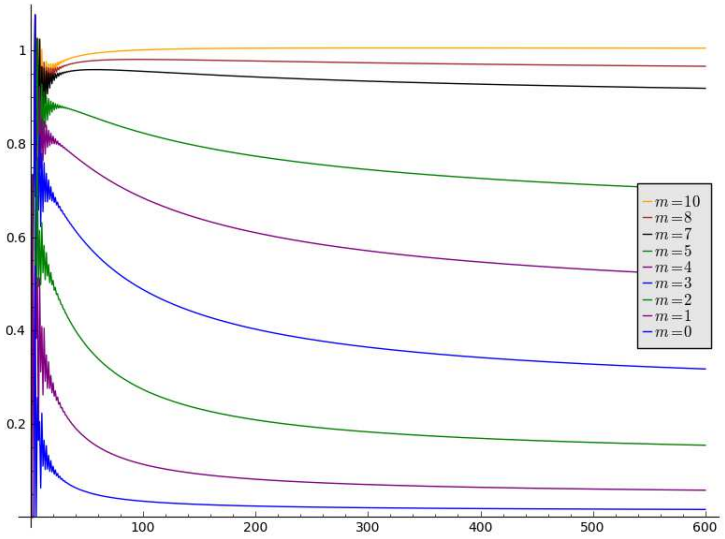

Fig. 2: $S_{m,n}\rho^n n^{3/2}$ up to $n = 600$ for $m = 0$ to 10

7 Unrankings

The recurrence relation (2) for $S_{m,n}$ allows us to define the function generating λ-terms. More precisely, we construct bijections $s_{m,n}$, called *unranking* functions, between all non-negative integers not greater than $S_{m,n}$ and binary λ-terms of size n with at most m distinct free variables [7]. This approach is also known as the *recursive method*, originating with Nijenhuis and Wilf [17] (see especially Chapter 13). In order to describe unranking functions, we make use of the Cantor pairing function.

Let us recall that for $n \geq 2$ we have, by (2),

$$S_{m,n} \quad = \quad S_{m+1,n-2} + \sum_{j=0}^{n-2} S_{m,j} S_{m,n-2-j} + [m \geq n-1].$$

The encoding function $s_{m,n}$ takes an integer $k \in \{1, \ldots, S_{m,n}\}$ and returns the term built in the following way.

- If $m \geq n-1$ and k is equal to $S_{m,n}$, the function returns the string $1^{n-1}0$.
- If k is less than or equal to $S_{m+1,n-2}$, then the corresponding term is in the form of abstraction $00\widehat{M}$, where $\widehat{M}$ is the value of the unranking function $s_{m+1,n-2}$ on k.
- Otherwise (i.e., k is greater than $S_{m+1,n-2}$ and less than $S_{m,n}$ if $m \geq n+1$ or less than or equal to $S_{m,n}$ if $m < n+1$) then the corresponding term is in the form of application $01\widehat{M}\widehat{N}$. In order to get strings $\widehat{M}$ and $\widehat{N}$, we compute the maximal value $\ell \in \{0, \ldots, n-2\}$ for which

$$k - S_{m+1,n-2} = \sum_{j=0}^{\ell-1} S_{m,j} S_{m,n-2-j} + r \qquad \text{with } r \leq S_{m,\ell} S_{m,n-2-\ell}.$$

  The strings $\widehat{M}$ and $\widehat{N}$ are the values $s_{m,\ell}(k')$ and $s_{m,n-2-\ell}(k'')$, respectively, where (k', k'') is the pair of integers encoded by r by the Cantor pairing function.

In Figure 3 the reader may find a Haskell program [12] which computes the values $s_{m,n}(k)$. In this program, the function $s_{m,n}(k)$ is written as `unrankT m n k` and the sequence $S_{m,n}$ is written as `tromp m n`.

8 Number of typable terms

The unranking function allows us to traverse all the closed terms of size n and to filter those that are typable (see [11] and appendix) in order to count them and similarly to traverse all the terms of size n to count those that are typable. [10] provides tables of the numbers of typable terms of size n.

Thanks to the unranking function, we can build a *uniform generator of λ-terms* and, using this generator, we can build a *uniform generator of simply typable λ-terms*, which works by sieving the uniformly generated plain terms through a program that checks their typability (see for instance [9]). This way, it is possible to generate uniformly typable closed terms up to size 450 which is rather good since Tromp was able to build a self interpreter[(iii)] for the λ-calculus of size 210.

[(iii)] Which is not typable by definition!

```
unrankT :: Int -> Int -> Integer -> Term
unrankT m n k
  | m >= n - 1 && k == (tromp m n) = Index $ fromIntegral (n - 1)
  | k <= (tromp  (m+1) (n-2)) = Abs (unrankT (m+1) (n-2) k)
  | otherwise = unrankApp (n-2) 0 (k - tromp  (m+1) (n-2))
    where unrankApp n j r
            | r <=  tmjtmnj  = let (dv,rm) = (r-1) `divMod` tmnj
                              in App (unrankT m j (dv+1)) (unrankT  m (n-j) (rm+1))
            | otherwise = unrankApp n (j + 1) (r -tmjtmnj)
            where tmnj = tromp m (n-j)
                  tmjtmnj = (tromp m j) * tmnj
```

Fig. 3: A Haskell program for computing values of the function $s_{m,n}$

9 Conclusion

We have shown that if we use the size yielded by the binary lambda calculus [18], we get an exponential growth of the number of λ-terms of size n when n goes to infinity. This applies to closed λ-terms, to λ-terms with a bounded number of free variables, and to all λ-terms of size n. Except for the size of all λ-terms, the question of finding the non-exponential factor of the asymptotic approximation of these numbers is still open. Since the generating functions are not standard, we were lead to devise new methods for computing these approximations. Beside, we describe unranking functions (recursive methods) for generating λ-terms from which we derive tools for their uniform generation and for the enumeration of typable λ-terms. The generation of random (typable) terms is limited by the performance of the generators based on the recursive methods aka unranking which needs to handle huge number. Boltzmann samplers [6] should allow us to generate terms of larger size.

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Asymptotic analysis of the sum of the output of transducers

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Abstract. As a generalization of the sum of digits function and other digital sequences, we asymptotically analyze sequences defined as the sum of the output of a transducer when reading a random integer in $[0, N)$. Analogues in higher dimensions are also considered. We show that sequences defined by a certain class of recursions can be written in this framework.

Depending on properties of the transducer, we give the main term, the periodic fluctuation and an error term of the expected value and the variance of this sequence. In many cases, the periodic fluctuation of the expected value is continuous and nowhere differentiable. We give a general formula for the Fourier coefficients of this periodic function. Furthermore, the sequence is asymptotically normally distributed for many transducers. As an example, we analyze the abelian complexity function of the paperfolding sequence, which has recently been studied by Madill and Rampersad.

Keywords: Central limit theorem, periodic fluctuation, Fourier coefficient, transducer, automatic sequence, non-differentiability.

1 Introduction

Over the last decades, asymptotic properties of digital sequences have been studied by many authors. The simplest example is the q-ary sum of digits, see Delange [Del75]. This has been generalized to various other number systems (cf. [Kir83], [KP84], [Thu99], [GT00], [BG01], [GHP03], [GHP04], [HM07], [HK14]). Similar results have been obtained for other digital sequences (cf. [Cat92] and [BK95]). Frequently observed phenomena in the asymptotic analysis of these sequences include periodic fluctuations in the second order term and asymptotic normality (see also [DG10]).

The purpose of this article is to use finite state machines as a uniform framework to derive such asymptotic results. The results mentioned above will follow as corollaries from our main results, see the end of

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Section 2 for more details. As an example of a new result fitting into this framework, we study the abelian complexity function of the paperfolding sequence (cf. [MR13]), see Example 6.1.

Our main focus lies on transducers: these finite state machines transform input words to output words using a finite memory (see Section 2 for a more precise definition). In our case, the input is the q-ary digit expansion of a random integer in the interval $[0, N)$. We then asymptotically study the sum of the output of the transducer for $N \to \infty$. This is also extended to higher dimensions.

While some of the examples can easily be formulated by transducers, other examples are more readily expressed in terms of recursions of the shape

$$a(q^\kappa n + \lambda) = a(q^{\kappa_\lambda} n + r_\lambda) + t_\lambda \quad \text{for} \quad 0 \le \lambda < q^\kappa, \quad n \ge 0 \tag{1}$$

with fixed κ, κ_λ, $r_\lambda \in \mathbb{Z}$, $t_\lambda \in \mathbb{R}$ and $\kappa_\lambda < \kappa$. We reduce these recursions to transducers in Section 6. This reduction can be performed algorithmically by a Sage [S$^+$13] program using the finite state machine package described in [HKK].

Several notions abstracting the sum-of-digits and related problems have been studied. One of them is the notion of completely q-additive functions $a : \mathbb{N}_0 \to \mathbb{R}$ with

$$a(qn + \lambda) = a(n) + a(\lambda) \tag{2}$$

for $0 \le \lambda < q$ (cf. [BK95]). These have been generalized to digital sequences as defined in [AS03, Cat92]: A sequence $a(n)$ is a digital sequence if it is the sum, over all windows of a fixed length κ of the q-ary digit representation of n, of a given function of these windows. These digital sequences can easily be formulated by a recursion as in (1).

For a transducer $\mathcal{T}$, let $\mathcal{T}(n)$ be the sum of the output labels of $\mathcal{T}$ when reading the q-ary expansion of n. For a positive integer N, we study the behavior of $\mathcal{T}(n)$ for a uniformly chosen random n in $\{0, \dots, N-1\}$. Assuming suitable connectivity properties of the graph underlying the transducer, we obtain the following results.

- The expected value is given by $\mathbb{E}(\mathcal{T}(\boldsymbol{n})) = e_{\mathcal{T}} \log_q N + \Psi_1(\log_q N) + o(\log N)$ for a constant $e_{\mathcal{T}}$ and a periodic, continuous function Ψ_1 (Theorem 1).
- The variance is $\mathbb{V}(\mathcal{T}(n)) = v_{\mathcal{T}} \log_q N - \Psi_1^2(\log_q N) + \Psi_2(\log_q N) + o(\log N)$ with constant $v_{\mathcal{T}}$ and a periodic, continuous function $\Psi_2(x)$ (Theorem 1).
- After suitable renormalization, $\mathcal{T}(n)$ is asymptotically normally distributed (Theorem 1).
- The Fourier coefficients of Ψ_1 are given explicitly (Theorem 2).
- The function Ψ_1 is nowhere differentiable provided that $e_{\mathcal{T}}$ is not an integer (Theorem 3).

The exact assumptions for the various results are given in detail in the corresponding theorems. Results for higher dimensional input are available for expectation, variance and normal distribution.

In the following, we discuss the relation of our setting and our results with the notion of q-regular sequences introduced in [AS03].

A sequence is q-regular if it is the first coordinate of a vector $\boldsymbol{v}(n)$ and there exist matrices V_0, …, V_{q-1} such that

$$\boldsymbol{v}(qn + \varepsilon) = V_\varepsilon \boldsymbol{v}(n) \tag{3}$$

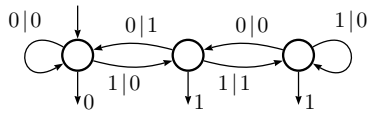

Figure 1: Transducer defining the Hamming weight of the non-adjacent form.

for $\varepsilon \in \{0, 1, \ldots, q-1\}$.

The concept of q-regular sequences is more general than our setting, but a broader variety of asymptotic behavior is observed which precludes any generalization of our results to general q-regular sequences.

While $\mathcal{T}(n)$ is a q-regular sequence for any transducer $\mathcal{T}$, the converse is not necessarily true: Obviously, the sum of the output of a transducer reading the input n is always bounded by $\mathcal{O}(\log n)$. However, the 2-regular sequence

$$a(n) = \begin{cases} n & \text{if } n \text{ is a power of 2,} \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

can clearly not be bounded by $\mathcal{O}(\log n)$.

Asymptotic estimates of q-regular sequences are given by Dumas [Dum13a, Dum13b]. By restricting our attention to sequences defined by transducers, we also obtain an asymptotic estimate of the variance, explicit expressions for the Fourier coefficients of the fluctuation in the second term of the expected value, non-differentiability of this fluctuation as well as a central limit theorem.

2 Preliminaries and Results

We consider complete, deterministic, subsequential transducers. In our case, we use the input alphabet $\{0, \ldots, q-1\}^d$ for a positive integer d and the output alphabet $\mathbb{R}$. A transducer is said to be *deterministic* and *complete* if for every state and every digit of the input alphabet, there is exactly one transition starting in this state with this input label. A *subsequential* transducer $\mathcal{T}$ is defined to be a finite deterministic automaton with one initial state, an output label for every transition and a final output label for every state.

In Figure 1, we show an example of a complete, deterministic, subsequential transducer. The label of a transition with input ε and output δ is written as $\varepsilon \mid \delta$.

The input of the transducer is the standard q-ary joint digit representation of an integer vector $\boldsymbol{n} \in \mathbb{N}_0^d$, i.e. the standard q-ary digit representation in each coordinate of the vector $\boldsymbol{n}$. The input is read from right (least significant digit) to left (most significant digit), without leading zeros. Then the output of the transducer is the sequence of the outputs of the transitions along the unique path with the given input and the final output of the last state of this path. The element $\mathcal{T}(\boldsymbol{n})$ of the sequence defined by the transducer $\mathcal{T}$ is the sum of this output sequence.

Using final output labels is convenient for our purposes because we do not have to care about a sufficient number of leading zeros in the input digit expansion to ensure that all carries are fully processed. Clearly, it would also be possible to model the final output labels by using an "end-of-input" marker and additional transitions.

We use the following probability space for computing the expected value, the variance and the limit distribution. The sample space is the set $\Omega_N = \{0, 1, \ldots, N-1\}^d$ and the probability measure is the equidistribution on this set.

For the different results, we need different properties of the complete, deterministic, subsequential transducer and its underlying digraph. The underlying digraph is assumed to be weakly connected and consists of strongly connected components C_j. Contracting each strongly connected component of the underlying digraph gives an acyclic digraph. A strongly connected component is said to be *final strongly connected* if it corresponds to a leaf (i.e., a vertex with outdegree 0) in this acyclic digraph. Let c be the number of final strongly connected components. We call a transducer or a digraph *finally connected* if $c = 1$.

For the asymptotic expressions, only the final strongly connected components are important. All other strongly connected components only influence the error term. Thus, we are not interested in the periodicity of the whole underlying digraph, but in the periodicity of the final strongly connected components. The *period* of a digraph is defined as the greatest common divisor of all lengths of directed cycles of the digraph. For $j = 1, \dots, c$, we define p_j as the period of the final strongly connected component C_j. The *final period* p of the digraph is defined to be the least common multiple of p_j, $j = 1, \dots, c$. We call a digraph *finally aperiodic* if $p = 1$. If the underlying digraph is strongly connected, its final period is equal to its period.

For proving the non-differentiability of the fluctuation, we not only need a finally aperiodic, finally connected digraph ($p = c = 1$), but also a reset sequence. A *reset sequence* is an input sequence such that starting at any state and reading this sequence leads to a specific state s. If the transducer is not finally aperiodic and finally connected, then there cannot exist a reset sequence.

In Section 3, we sketch the proof of the main part of the following theorem.

Theorem 1 *Let $d \geq 1$, $\mathcal{T}$ be a complete, deterministic, subsequential transducer with input alphabet $\{0, 1, \dots, q-1\}^d$, output alphabet $\mathbb{R}$ and final period p. Let $\mathcal{T}(\boldsymbol{n})$ be the sum of the output labels of $\mathcal{T}$ when reading the q-ary joint digit representation of the integer vector $\boldsymbol{n}$, including the corresponding final output. We consider the probability space $\Omega_N = \{0, 1, \dots, N-1\}^d$ with equidistribution for a fixed N.*

Then $\mathcal{T}(\boldsymbol{n})$ has the expected value

$$\mathbb{E}(\mathcal{T}(\boldsymbol{n})) = e_{\mathcal{T}} \log_q N + \Psi_1(\log_q N) + \mathcal{O}(N^{-\xi} \log N) \tag{5}$$

where $e_{\mathcal{T}}$, $\xi > 0$ are constants and $\Psi_1(x)$ is a p-periodic, continuous function. The variance is bounded by

$$\mathbb{V}(\mathcal{T}(\boldsymbol{n})) = \mathcal{O}(\log^2 N). \tag{6}$$

If $\mathcal{T}$ is finally connected, then $\mathcal{T}(\boldsymbol{n})$ has the variance

$$\mathbb{V}(\mathcal{T}(\boldsymbol{n})) = v_{\mathcal{T}} \log_q N - \Psi_1^2(\log_q N) + \Psi_2(\log_q N) + \mathcal{O}(N^{-\xi} \log^2 N) \tag{7}$$

with constant $v_{\mathcal{T}} \in \mathbb{R}$ and a p-periodic, continuous function $\Psi_2(x)$.

If furthermore $v_{\mathcal{T}} \neq 0$, then $\mathcal{T}(\boldsymbol{n})$ is asymptotically normally distributed. In particular, we have

$$\mathbb{P}\left(\frac{\mathcal{T}(\boldsymbol{n}) - \mathbb{E}(\mathcal{T}(\boldsymbol{n}))}{\sqrt{\mathbb{V}(\mathcal{T}(\boldsymbol{n}))}} < x\right) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{\frac{-y^2}{2}} dy + \mathcal{O}\left(\log^{-\frac{1}{4}} N\right) \tag{8}$$

for all $x \in \mathbb{R}$.

Assume that the transducer is finally connected, finally aperiodic and $d = 1$. Then the Fourier coefficients of $\Psi_1(x)$ are stated in Theorem 2. Furthermore assume that the transducer has a reset sequence, the output alphabet is $\mathbb{Z}$ and that $e_{\mathcal{T}} \notin \mathbb{Z}$. Then $\Psi_1(x)$ is non-differentiable for every $x \in \mathbb{R}$ (see Theorem 3).

In Theorem 2 in Section 4, we state the Fourier coefficients of the periodic fluctuation $\Psi_1(x)$ of the expected value in the one dimensional case. We discuss the non-differentiability of $\Psi_1(x)$ in Theorem 3 in Section 5.

In the last section, we consider a sequence satisfying the recursion (1). We construct a transducer computing this sequence in Theorem 4. Thus, from Theorem 1, the expected value, the variance and the limit distribution follow in many cases. This construction and the computations for the constants $e_{\mathcal{T}}$, $v_{\mathcal{T}}$ and the Fourier coefficients can be done algorithmically by a computer algebra system.

Theorem 1 is a generalization of the following known results.

- For the sum of digits of the standard q-ary digit representations (cf. [Del75]), we obtain an asymptotic normal distribution, the Fourier coefficients and the non-differentiability (for even q). The error term vanishes, as stated in Remark 3.1. Therefore, the formula is not only asymptotic but also exact.

- The occurrence of subblocks in standard and non-standard digit representations is defined by a strongly connected, aperiodic transducer. Thus we obtain the expected value, the variance and the limit law (cf. [Kir83, KP84, GHP03] for the expected value). For one dimensional digit representations, we also obtain the Fourier coefficients and the non-differentiability (assuming $e_{\mathcal{T}} \notin \mathbb{Z}$).

- The Hamming weight is a special case of the occurrence of subblocks. Thus, Theorem 1 is a generalization of the results about the width-w nonadjacent form [HK14], the simple joint sparse [GHP04] and the asymmetric joint sparse form [HK14].

- The transducer defining a completely q-additive function consists of only one state. Therefore, we obtain an asymptotic normal distribution (as in [BK95]), the Fourier coefficients and the non-differentiability (assuming $e_{\mathcal{T}} \notin \mathbb{Z}$ and integer output). Here, the error term vanishes, too.

- A digital sequence is defined by a finally connected, finally aperiodic transducer. Thus, digital sequences are asymptotically normally distributed. Assuming $e_{\mathcal{T}} \notin \mathbb{Z}$ and integer output, the periodic fluctuation $\Psi_1(x)$ is non-differentiable. The Fourier coefficients can be computed by Theorem 2. See [Cat92] for results about the expected value.

- Automatic sequences [AS03] also are defined by transducers: the output labels of all transitions are 0 and the final output labels are like in the definition of such sequences. Theorem 1 gives the expected value with $e_{\mathcal{T}} = 0$ (see also [Pet03]) and depending on the transducer also the variance with $v_{\mathcal{T}} = 0$. In many cases, the Fourier coefficients of the periodic fluctuation of the expected value are given explicitly in Theorem 2.

- In [GT00], Grabner and Thuswaldner investigate the sum of digits function for negative bases $\nu_{-q}(n)$. They give a transducer to compute the function $\nu_{-q}(n) - \nu_{-q}(-n)$. Their result about the limit law follows directly from our Theorem 1.

As an example of a new result obtained by Theorem 1, we give an asymptotic estimate of the abelian complexity function of the paperfolding sequence in Example 6.1. In [MR13], the authors prove that this sequence satisfies a recursion of type (1). As consequences of Theorem 1, the expected value of $\rho(n)$ is $\sim \frac{8}{13}\log_2 N$, the variance is $\sim \frac{432}{2197}\log_2 N$ and the sequence is asymptotically normally distributed.

3 Asymptotic Distribution

We briefly sketch the proof of Theorem 1 in this section. Details can be found in the full version of this article.

For a transducer $\mathcal{T}$, we consider the exponential sum

$$F(N) = \sum_{\boldsymbol{n}\in\Omega_N} e^{it\mathcal{T}(\boldsymbol{n})}. \tag{9}$$

The function $F(N)$ also depends on the complex variable t, but for simplicity, we do not state it in the notation.

We define transition matrices M_ε for $\varepsilon \in \{0,\dots,q-1\}^d$. We label the states of the transducer with contiguous positive integers starting with the initial state 1. The (s_1,s_2)-th entry of the matrix M_ε is $e^{it\delta}$ if there is a transition from state s_1 to state s_2 with input label ε and output label δ, and 0 otherwise. Let M be the sum of all these transition matrices.

Then we can rewrite the summands in (9) as a matrix product

$$e^{it\mathcal{T}(\boldsymbol{n})} = \boldsymbol{e}_1^\top \prod_{l=0}^{L} M_{\varepsilon_l} \boldsymbol{u} \tag{10}$$

where $(\varepsilon_L \dots \varepsilon_0)_q$ is the standard q-ary joint digit representation of $\boldsymbol{n}$, $\varepsilon_L \neq 0$, $\boldsymbol{e}_1 = (1,0,\dots,0)^\top$ and the vector $\boldsymbol{u}$ has entries $e^{itb(s)}$ where $b(s)$ is the final output of the state s. Here $^\top$ denotes transposition.

For the next steps, we only consider the matrix product without the vectors. We define $G(N) = \sum_{\boldsymbol{n}\in\Omega_N} g(\boldsymbol{n})$ with

$$g(\boldsymbol{n}) = \prod_{l=0}^{L} M_{\varepsilon_l}. \tag{11}$$

The function $G(N)$ satisfies the recursion $G(qN+\varepsilon) = MG(N) + H_\varepsilon(N)$ where $H_\varepsilon(N)$ are certain known functions. Thus, we obtain

$$G((\varepsilon_L \dots \varepsilon_0)_q) = \sum_{m=0}^{L} M^m H_{\varepsilon_m}((\varepsilon_L \dots \varepsilon_{m+1})_q) \tag{12}$$

by induction.

Next, we investigate the dominant eigenvalues of the matrix M at $t=0$. The absolute value of the dominant eigenvalues is at most q^d. Furthermore, q^d is an eigenvalue. We then split up (12) into two parts. The first part corresponds to the dominant eigenvalues. The second part is the error term.

Thus, we have an asymptotic expression for $G(N)$ and also for $F(N)$. The first and second derivative of $F(N)$ with respect to t at $t=0$ give asymptotic expressions for the expected value and the variance. The constants $e_\mathcal{T}$ and $v_\mathcal{T}$ depend on the first and second derivatives of the dominant eigenvalues of M and can be computed by a computer algebra system. For the periodic fluctuations $\Psi_1(x)$ and $\Psi_2(x)$, we obtain representations as infinite sums.

The Berry-Esseen inequality implies the asymptotic normal distribution.

Remark 3.1 *If there are only dominant eigenvalues, then there is no remainder term and thus no error term. This case occurs in the case of the sum of digits of the standard q-ary digit representation and other completely q-additive functions.*

4 Fourier Coefficients

In this section, we state the formulas for the Fourier coefficient of the periodic fluctuation $\Psi_1(x)$.

The computation is rather lengthy and is not stated here. It starts with the representation for $\Psi_1(x)$ obtained in the proof of Theorem 1. See the full version of this article for the corresponding calculations.

Theorem 2 *Let $\mathcal{T}$ be a finally aperiodic, finally connected transducer and $d = 1$. Then the Fourier coefficients of the 1-periodic fluctuation $\Psi_1(x)$ are*

$$\begin{aligned} c_0 &= -e_{\mathcal{T}}\Big(\frac{1}{2} + \frac{1}{\log q}\Big) - i\boldsymbol{w}'^{\top}\mathbf{1} + \operatorname{Res}_{z=1} \boldsymbol{w}^{\top}\boldsymbol{H}(z), \\ c_l &= \frac{e_{\mathcal{T}}}{\chi_l(1+\chi_l)\log q} + \frac{1}{1+\chi_l}\operatorname{Res}_{z=1+\chi_l} \boldsymbol{w}^{\top}\boldsymbol{H}(z) \end{aligned} \tag{13}$$

for $l \neq 0$. In these formulas, we use the following definitions. We have $\chi_l = \frac{2\pi i l}{\log q}$, $\zeta(z)$ the Riemann zeta function, $\zeta(z,a)$ the Hurwitz zeta function, defined as

$$\zeta(z,a) = \sum_{r>-a} (r+a)^{-z}, \tag{14}$$

and $\mathbf{1}$ a vector whose entries are all 1.

Furthermore, $\boldsymbol{w}^{\top}$ is the normalized (i.e. $\boldsymbol{w}^{\top}\mathbf{1} = 1$) left eigenvector of the transition matrix M at $t = 0$ corresponding to the eigenvalue q. For general t, let $\boldsymbol{w}^{\top}(t)$ be the left eigenvector $\boldsymbol{e}_1^{\top}\boldsymbol{v}_r(t)\boldsymbol{v}_l^{\top}(t)$ where $\boldsymbol{v}_l^{\top}(t)$ is a left eigenvector, $\boldsymbol{v}_r(t)$ is an eigenvector of M corresponding to the dominant eigenvalue with $\boldsymbol{v}_l^{\top}(t)\boldsymbol{v}_r(t) = 1$ and $\boldsymbol{v}_r(0) = \mathbf{1}$. Then $\boldsymbol{w}'^{\top}$ is defined to be the derivative of $\boldsymbol{w}^{\top}(t)$ at $t = 0$.

The (s_1, s_2)-th entry of the matrix Δ_ε is the output label of the transition from state s_1 to state s_2 with input label ε if it exists, and 0 otherwise. The matrix Δ is the sum of all matrices Δ_ε, $\varepsilon \in \{0, \ldots, q-1\}$. The vector-valued function $\boldsymbol{H}(z)$ is defined by the Dirichlet series

$$\boldsymbol{H}(z) = \sum_{r\geq 1} (\boldsymbol{b}(r) - e_{\mathcal{T}}\lfloor \log_q r \rfloor \mathbf{1}) r^{-z} \tag{15}$$

and has simple poles at $z = 1 + \chi_l$ for $l \in \mathbb{Z}$. The s-th coordinate of the vector $\boldsymbol{b}(r)$ is the sum of the output of the transducer $\mathcal{T}$ if starting in state s with input r, in particular, $\boldsymbol{b}(0)$ is the vector of final outputs.

For $\Re z > 1$, the Dirichlet series $\boldsymbol{H}(z)$ satisfies the following infinite recursion

$$\begin{aligned} (1 - q^{-z}M)\boldsymbol{H}(z) = \mathbf{1}e_{\mathcal{T}} \sum_{\varepsilon=1}^{q-1} \varepsilon^{-z} + \sum_{\varepsilon=1}^{q-1} M_\varepsilon \boldsymbol{b}(0)\varepsilon^{-z} - \mathbf{1}e_{\mathcal{T}}\zeta(z) + q^{-z}\sum_{\varepsilon=0}^{q-1} \Delta_\varepsilon \mathbf{1}\zeta\left(z, \frac{\varepsilon}{q}\right) \\ + \sum_{\varepsilon=0}^{q-1} M_\varepsilon \sum_{m\geq 1} \binom{-z}{m} q^{-z-m}\varepsilon^m \boldsymbol{H}(z+m). \end{aligned} \tag{16}$$

We can use (16) to numerically evaluate the Dirichlet series $\boldsymbol{H}(z)$ with arbitrary precision (cf. [GH05]) and compute its residues at $z = 1 + \chi_l$. In Example 6.1, we computed the first 24 Fourier coefficients of the abelian complexity function $\rho(n)$ of the paperfolding sequence.

5 Non-differentiability

In this section, we again consider the periodic fluctuation $\Psi_1(x)$ of the expected value. We prove that for certain transducers, it is nowhere differentiable. We follow the method presented by Tenenbaum [Ten97], see also Grabner and Thuswaldner [GT00]. The details can be found in the full version of this article.

Theorem 3 *Let $d = 1$. Assume that $e_{\mathcal{T}} \notin \mathbb{Z}$ and that the transducer $\mathcal{T}$ has a reset sequence and output alphabet $\mathbb{Z}$. Then the function $\Psi_1(x)$ is non-differentiable for any $x \in \mathbb{R}$.*

In [Ten97, GT00], the reset sequence consists only of 0's. If working with digit expansions, it is often possible to choose such a reset sequence. However, in the context of recursions, this is not always possible, see Example 6.1. There the reset sequence is (10000). For a general finally aperiodic, finally connected transducer, the existence of a reset sequence cannot be guaranteed.

6 Recursions

In this section, we describe how to reduce a recursion to a transducer computing the given sequence.

Theorem 4 *Let $a(n)$ be a sequence satisfying the recursion*

$$a(q^\kappa n + \lambda) = a(q^{\kappa_\lambda} n + r_\lambda) + t_\lambda \quad \text{for} \quad 0 \le \lambda < q^\kappa, \quad n \ge 0 \tag{17}$$

with fixed q, κ, κ_λ, $r_\lambda \in \mathbb{Z}$, $t_\lambda \in \mathbb{R}$ and $0 \le \kappa_\lambda < \kappa$. A suitable set of initial values of $a(n)$ has to be given. Then there exists a subsequential, complete, deterministic transducer whose input is the q-ary expansion of n and the sum of the output is $a(n)$, that is $\mathcal{T}(n) = a(n)$.

Together with Theorem 1, we obtain an asymptotic expansion of the expected value $\frac{1}{N}\sum_{n<N} a(n)$ of the sequence $a(n)$. Depending on the properties of the transducer, we also obtain the variance and a Gaussian limit law. It is also possible to compute the Fourier coefficients of the periodic fluctuation and prove its non-differentiability, as in Example 6.1. Moreover, all this can be performed algorithmically by a Sage program.

We just give the idea of the construction of the transducer. For more details, see the full version of this article.

For simplicity, assume here that $0 \le r_\lambda < q^{\kappa_\lambda}$. The first part of the transducer is a rooted q-ary tree of depth $\kappa - 1$. We start in the root at depth 0. Each vertex of the tree corresponds to exactly one equivalence class modulo q^j for $j = 0, \dots, \kappa - 1$. The input label of a transition starting in a leaf of this tree defines an equivalence class $\lambda \bmod q^\kappa$. Thus we know which case we have to use in the recursion (17). This transition has output label t_λ and leads to the vertex of the tree corresponding to the equivalence class $r_\lambda \bmod q^{\kappa_\lambda}$.

The final output of a state is the value of $a(l)$ where l is a minimal non-negative representative of the corresponding equivalence class.

Note that the transducer also encodes for which indices an initial value has to be given: in each cycle of the sub-transducer induced by the transitions with input label 0, an initial value has to be given for one of its states because in this instance, leading zeros are admissible.

Example 6.1 *Consider the abelian complexity function $\rho(n)$ of the paperfolding sequence. The paperfolding sequence is obtained by repeatedly folding a strip of paper in half in the same direction. Then we open the strip and encode a right turn by 1 and a left turn by 0. The abelian complexity function $\rho(n)$ gives*

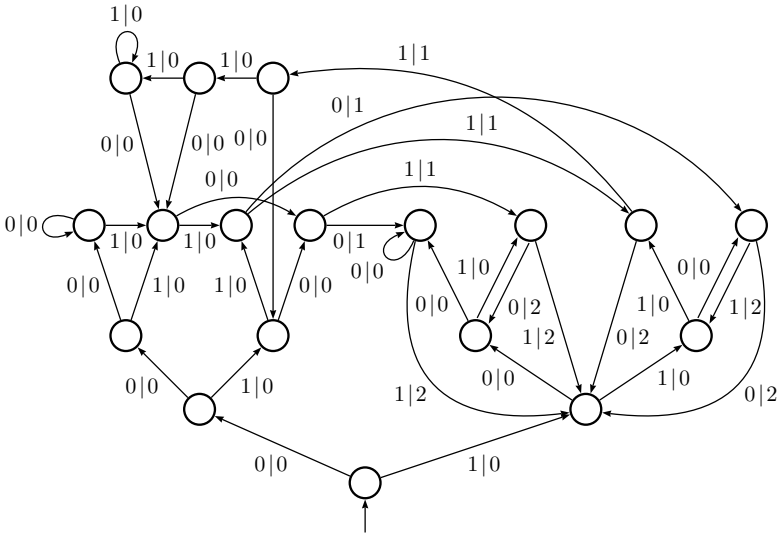

Figure 2: Transducer computing the abelian complexity function $\rho(n)$ of the paperfolding sequence. For simplicity, we neglect the final output labels in this figure.

the number of abelian equivalence classes of subsequences of length n of the paperfolding sequence. Two subsequences of length n are equivalent if they are permutations of each other. In [MR13], the authors prove that this sequence satisfies the recursion

$$\begin{aligned}
\rho(4n) &= \rho(2n),\\
\rho(4n+2) &= \rho(2n+1)+1,\\
\rho(16n+1) &= \rho(8n+1),\\
\rho(16n+3) &= \rho(2n+1)+2,\\
\rho(16n+5) &= \rho(4n+1)+2,\\
\rho(16n+7) &= \rho(2n+1)+2,\\
\rho(16n+9) &= \rho(2n+1)+2,\\
\rho(16n+11) &= \rho(4n+3)+2,\\
\rho(16n+13) &= \rho(2n+1)+2,\\
\rho(16n+15) &= \rho(2n+2)+1
\end{aligned} \tag{18}$$

with $\rho(1)=2$ and $\rho(0)=0$. The constructed transducer is shown in Figure 2. For simplicity, we do not state the final output labels in this figure. The expected value and the variance are

$$\begin{aligned}
\mathbb{E}(\rho(n)) &= \frac{8}{13}\log_2 N + \Psi_1(\log_2 N) + \mathcal{O}(N^{-\xi}\log N),\\
\mathbb{V}(\rho(n)) &= \frac{432}{2197}\log_2 N - \Psi_1^2(\log_2 N) + \Psi_2(\log_2 N) + \mathcal{O}(N^{-\xi}\log^2 N)
\end{aligned} \tag{19}$$

l	c_l	l	c_l
0	0.9154305133	12	$-0.0002297481 + 0.0009687657\,i$
1	$-0.0162585750 + 0.0478637218\,i$	13	$0.0006425378 + 0.0006516706\,i$
2	$0.0054521982 + 0.0075023586\,i$	14	$0.0000413217 - 0.0003867709\,i$
3	$-0.0028294724 + 0.0086495903\,i$	15	$-0.0005632948 - 0.0001843541\,i$
4	$0.0036818110 + 0.0021908312\,i$	16	$0.0009051717 - 0.0000476354\,i$
5	$-0.0028244495 + 0.0014519078\,i$	17	$-0.0004621780 - 0.0000594551\,i$
6	$-0.0008962222 + 0.0030512180\,i$	18	$-0.0000127264 - 0.0003100797\,i$
7	$0.0015033904 + 0.0013217107\,i$	19	$0.0004112716 + 0.0001954204\,i$
8	$-0.0006766166 - 0.0015392566\,i$	20	$-0.0000011706 + 0.0004183253\,i$
9	$0.0016074870 - 0.0000503663\,i$	21	$-0.0001027596 + 0.0004091624\,i$
10	$-0.0006908394 + 0.0018753575\,i$	22	$-0.0004725451 + 0.0004237489\,i$
11	$-0.0008974336 + 0.0007658455\,i$	23	$-0.0000596181 + 0.0002323317\,i$

Table 1: First 24 Fourier coefficients of the abelian complexity function $\rho(n)$ of the paperfolding sequence.

for $\xi > 0$ and the sequence $\rho(n)$ is asymptotically normally distributed. The functions $\Psi_1(x)$ and $\Psi_2(x)$ are 1-periodic, continuous and $\Psi_1(x)$ is nowhere differentiable. The reset sequence of the transducer is (10000). The first 24 Fourier coefficients of $\Psi_1(x)$ are listed in Table 1. In Figure 3, the trigonometric polynomial formed with these Fourier coefficients is compared with the function $\Psi_1(x)$.

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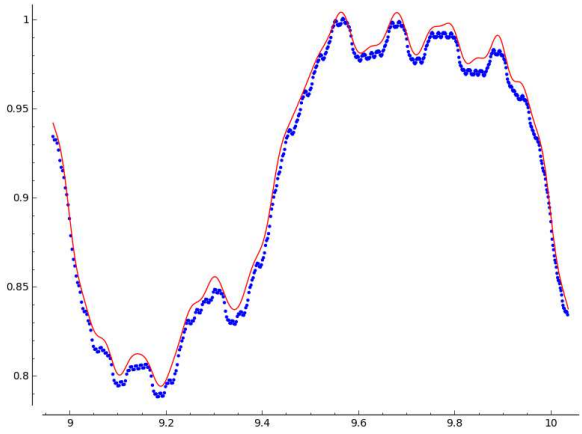

Figure 3: Trigonometric polynomial formed with the first 24 Fourier coefficients in Table 1 compared with empirical values of $\Psi_1(x)$ in the range $[9, 10]$.

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On the distribution of parameters in random weighted staircase tableaux

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Abstract. In this paper, we study staircase tableaux, a combinatorial object introduced due to its connections with the asymmetric exclusion process (ASEP) and Askey-Wilson polynomials. Due to their interesting connections, staircase tableaux have been the object of study in many recent papers. More specific to this paper, the distribution of various parameters in random staircase tableaux has been studied. There have been interesting results on parameters along the main diagonal, however, no such results have appeared for other diagonals. It was conjectured that the distribution of the number of symbols along the kth diagonal is asymptotically Poisson as k and the size of the tableau tend to infinity. We partially prove this conjecture; more specifically we prove it for the second main diagonal.

Keywords: staircase tableau, asymmetric exclusion process, Poisson distribution, weak convergence

1 Introduction

In this paper, we study staircase tableaux, a combinatorial object introduced (in [10], [11]) due to connections with the asymmetric exclusion process (ASEP) and Askey-Wilson polynomials. The ASEP can be defined as a Markov chain with n sites, with at most one particle occupying each site. Particles may jump to any neighboring empty site with rate u to the right and rate q to the left. Particles may enter and exit at the first site with rates α and γ respectively. Similarly, particles may enter and exit the last site with rates δ and β. The ASEP is an interesting particle model that has been studied extensively in mathematics and physics. It has also been studied in many other fields, including computational biology [3], and biochemistry, specifically as a primitive model for protein synthesis [16]. Staircase tableaux were introduced per a connection between the steady state distribution of the ASEP and the generating function for staircase tableaux [11]. See Section 2 for a discussion of the ASEP and its connection with staircase tableaux.

In addition to interest in its own right, the ASEP has been known to have interesting connections in combinatorics and analysis. Consequently, staircase tableaux have similarly been connected to many combinatorial objects and a family of polynomials. In fact, the generating function for staircase tableaux has been used to give a formula for the moments of Askey-Wilson polynomials [11], [7]. Staircase tableaux have also inherited many interesting properties from other types of tableaux (See [1], [5], [6], [11], [8], [9], [15], [17]). We refer to [14, Table 1] for a description of some of the bijections between the various

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types of the tableaux.

Due to all these interesting connections, staircase tableaux have been the object of study in many recent papers. In [12], a probabilistic approach was developed and the distributions of various parameters were studied. In fact, it was shown in [12] that the distribution of the number of α's and β's in a staircase tableau are asymptotically normal, and distributions regarding the main diagonal were also given (see Section 4). In [14], the distribution of each box in a staircase tableau was given, and it was conjectured that the distribution of the number of symbols along the kth diagonal is asymptotically Poisson as k and the size of the tableau tend to infinity. The main result of this paper is the proof of this in a special case when $k = n - 1$. That is, we show that the distribution of the number of symbols along the second main diagonal is asymptotically Poisson with parameter 1, see Theorem 8. Similarly, we show that the number of α's (resp. β's) along the second main diagonal is asymptotically Poisson with parameter $1/2$, see Theorem 5 and Corollary 6.

2 Definitions and Notation

Staircase tableaux were first introduced in [10] and [11] as follows:

Definition 1 *A staircase tableau of size n is a Young diagram of shape (n, n-1, ..., 1) such that:*

1. *The boxes are empty or contain an α, β, γ, or δ.*
2. *All boxes in the same column and above an α or γ are empty.*
3. *All boxes in the same row and to the left of an β or δ are empty.*
4. *Every box on the diagonal contains a symbol.*

The rows and columns in a staircase tableau are numbered from 1 through n, beginning with the box in the NW-corner and continuing south and east respectively. Each box is numbered (i, j) where $i, j \in \{1, 2, ..., n\}$. Note that $i + j \leq n + 1$. We refer to the collection of boxes $(n - i + 1, i)$ such that $i = 1, 2, ..., n$ as the main diagonal, and the collection of boxes $(n - i, i)$ such that $i = 1, 2, ..., n - 1$ as the second main diagonal.

Following the conventions of [14], $\mathcal{S}_n$ is the set of all staircase tableaux of size n. For a given $S \in \mathcal{S}_n$, the number of α's, γ's, β's and δ's in S are denoted by $N_\alpha, N_\beta, N_\gamma$, and N_δ respectively. The weight of S is the product of all symbols in S:

$$wt(S) = \alpha^{N_\alpha}\beta^{N_\beta}\gamma^{N_\gamma}\delta^{N_\delta}.$$

It was known (see e.g. [4]) that the generating function $Z_n(\alpha, \beta, \gamma, \delta) := \sum_{S\in\mathcal{S}_n} wt(S)$ is equal to the product:

$$Z_n(\alpha, \beta, \gamma, \delta) = \prod_{i=0}^{n-1}(\alpha + \beta + \delta + \gamma + i(\alpha + \gamma)(\beta + \delta)). \tag{1}$$

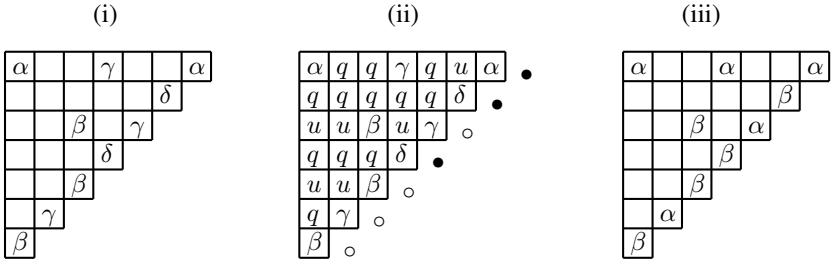

Fig. 1: A staircase tableau of size 7 with weight $\alpha^2\beta^3\delta^2\gamma^3$. (ii) The extension of (i) to a staircase tableau of weight $\alpha^2\beta^3\delta^2\gamma^3u^6q^{13}$ and type $\bullet\bullet\circ\bullet\circ\circ\circ$. (iii) The α/β-staircase tableau obtained from (i) by replacing γ's with α's and δ's with β's. It's weight is $\alpha^5\beta^5$.

Notice that there is an involution on the staircase tableaux of a given size obtained by interchanging the rows and the columns, α's and β's, and γ's and δ's, see further [4]. In particular, the fact that α's and β's are identical up to this involution allows us to extend results for α's to results for β's.

The connection between staircase tableaux and the ASEP requires an extension of this preceding definition. After following the rules from Definition 1, we then fill all the empty boxes with u's and q's, the rates at which particles in the ASEP jump to the right and left respectively. We do so by first filling all boxes to the left of a β with a u and to the left of a δ with a q. Then, we fill the empty boxes with a u if it is above an α or a δ, and q otherwise. The weight of a staircase tableau filled as such is defined in the same way, the product of the parameters in each box. Also, the total weight of all such staircase tableaux, which we denote by $\mathcal{S}_n^{'}$, is given by:

$$Z_n(\alpha,\beta,\gamma,\delta,q,u) := \sum_{S\in\mathcal{S}_n'} wt(S).$$

Then, each staircase tableau of size n is associated with a state of the ASEP with n sites (See Figure 1). This is done by aligning the Markov chain with the diagonal entries of the staircase tableau. A site is filled if the corresponding diagonal entry is an α or a γ and a site is empty if the corresponding diagonal entry is a β or a δ. Each staircase tableau's associated state of the ASEP is called its type.

Using this association, it was shown in [11] that the steady state probability that the ASEP is in state η is given by:

$$\frac{\sum_{T\in\mathfrak{T}} wt(T)}{Z_n},$$

where $\mathfrak{T}$ is the set of all staircase tableau of type η.

For the purposes of this paper, we will consider more simplified staircase tableaux, namely α/β-staircase tableaux as introduced in [14], which are staircase tableaux limited to the symbols α and β. The set $\overline{\mathcal{S}}_n \subset \mathcal{S}_n$ denotes the set of all such staircase tableaux. Since the symbols α and γ follow the same rules in the definition, as do β and δ, any $S \in \mathcal{S}_n$ can be obtained from an $S^{'} \in \overline{\mathcal{S}}_n$ by replacing the appropriate α's with γ's and β's with δ's.

The generating function of α/β-staircase tableaux is:

$$Z_n(\alpha,\beta) := \sum_{S\in\overline{\mathcal{S}}_n} wt(S) = Z_n(\alpha,\beta,0,0)$$

and it follows from (1) that it is simply:

$$Z_n(\alpha,\beta) = \alpha^n \beta^n (a+b)^{\overline{n}}$$

where $a := \alpha^{-1}$ and $b := \beta^{-1}$, a notation that will be used frequently throughout this paper, and $(a+b)^{\overline{n}}$ is the rising factorial of $(a+b)$, i.e. $(a+b)^{\overline{n}} = (a+b)((a+b)+1)\cdots((a+b)+n-1)$.

We wish to consider random staircase tableaux as was done in [12] but it suffices to study random α/β-staircase tableaux, denoted by $S_{n,\alpha,\beta}$, as was done in [14]. All of our results for random α/β-staircase tableaux can be extended to random staircase tableaux with all four parameters, $\alpha, \gamma, \beta, \delta$. This is done by considering $S_{n,\alpha+\gamma,\beta+\delta}$ and randomly replacing each α with γ with probability $\frac{\gamma}{\alpha+\gamma}$ and similarly, each β with δ with probability $\frac{\delta}{\beta+\delta}$ independently for each occurrence. Notice that $Z_n(\alpha,\beta,\gamma,\delta) = Z_n(\alpha+\gamma,\beta+\delta)$. We also allow all parameters to be arbitrary positive real numbers, i.e. $\alpha, \beta \in (0,\infty)$, allowing $\alpha = \infty$ by fixing β and taking the limit or vice versa, or $\alpha = \beta = \infty$ by taking the limit. The following is a formal definition as in [14]:

Definition 2 *For all $n \geq 1$, $\alpha, \beta \in [0,\infty)$ with $(\alpha,\beta) \neq (0,0)$, $S_{n,\alpha,\beta}$ is defined to be a random α/β-staircase tableau in $\overline{\mathcal{S}}_n$ with respect to the probability distribution on $\overline{\mathcal{S}}_n$ given by:*

$$\forall S \in \overline{\mathcal{S}}_n, \qquad \mathbb{P}(S_{n,\alpha,\beta} = S) = \frac{wt(S)}{Z_n(\alpha,\beta)} = \frac{\alpha^{N_\alpha}\beta^{N_\beta}}{Z_n(\alpha,\beta)}.$$

We will also write is as

$$\mathcal{L}(S_{n,\alpha,\beta}) = \frac{\alpha^{N_\alpha}\beta^{N_\beta}}{Z_n(\alpha,\beta)}.$$

Using this definition, Hitczenko and Janson presented the distribution of a given box in a random staircase tableau. If a box is on the main diagonal, the distribution is (see [14, Theorem 7.1]):

$$\mathbb{P}(S_{n,\alpha,\beta}(i,n+1-i) = \alpha) = \frac{n-i+b}{n+a+b-1}. \tag{2}$$

Since a box on the main diagonal is never empty, the β case follows trivially.

If a box is not on the main diagonal, its distribution is (see [14, Theorem 7.2]):

$$\mathbb{P}(S_{n,\alpha,\beta}(i,j) = \alpha) = \frac{j-1+b}{(i+j+a+b-1)(i+j+a+b-2)} \tag{3}$$

$$\mathbb{P}(S_{n,\alpha,\beta}(i,j) = \beta) = \frac{i-1+a}{(i+j+a+b-1)(i+j+a+b-2)}. \tag{4}$$

3 Subtableaux and Preliminaries

For an arbitrary $S \in \overline{\mathcal{S}}_n$ and an arbitrary box (i,j) in S, define $S[i,j]$ to be the subtableau in $\overline{\mathcal{S}}_{n-i-j+2}$ obtained by deleting the first $i-1$ rows and $j-1$ columns, see [14]. The following statement was proven in [14, Theorem 6.1] and is a useful tool in our results:

$$S_{n,\alpha,\beta}[i,j] \stackrel{d}{=} S_{n-i-j+2,\hat{a},\hat{b}}, \text{ with } \hat{a} = a+i-1 \text{ and } \hat{b} = b+j-1. \tag{5}$$

The following two lemmas consider the probability of an arbitrary staircase tableau in $\overline{\mathcal{S}}_n$ that is conditioned on having an α or a β in the box $(n-1,1)$. The statements follow almost immediately from the definition of a staircase tableau, but will be used frequently throughout the paper.

Lemma 1 *If $S_{n,\alpha,\beta}$ is conditioned on $S_{n,\alpha,\beta}(n-1,1)=\alpha$, then the subtableau $S_{n,\alpha,\beta}[1,3] \stackrel{d}{=} S_{n-2,\alpha,\beta}$, that is*

$$\mathcal{L}(S_{n,\alpha,\beta} \mid S_{n,\alpha,\beta}(n-1,1)=\alpha) = \mathcal{L}(S_{n-2,\alpha,\beta}).$$

Proof: If $S_{n,\alpha,\beta}$ is a staircase tableau such that the box $S_{n,\alpha,\beta}(n-1,1)=\alpha$, then the box, $S_{n,\alpha,\beta}(n,1)=\beta$ and $S_{n,\alpha,\beta}(n-1,2)=\alpha$ by the rules of a staircase tableau. The first and second column are otherwise empty by those same rules. The remainder, $S_{n,\alpha,\beta}[1,3]$, is an arbitrary staircase tableau of size $n-2$. Therefore, the lemma follows. □

Lemma 2 *Let $(S_{n,\alpha,\beta})_{i,j}$ be a tableau $S_{n,\alpha,\beta}$ with the ith row and the jth column removed. If $S_{n,\alpha,\beta}$ is conditioned on $S_{n,\alpha,\beta}(n-1,1)=\beta$, then the subtableau $(S_{n,\alpha,\beta})_{n-1,2} \stackrel{d}{=} \widetilde{S}_{n-1,\alpha,\beta}$ where $\widetilde{S}_{n-1,\alpha,\beta}$ is random tableau of size $n-1$ conditioned on having a β in the $(n-1,1)$ box. In other words*

$$\mathcal{L}(S_{n,\alpha,\beta} \mid S_{n,\alpha,\beta}(n-1,1)=\beta) = \mathcal{L}(S_{n-1,\alpha,\beta} \mid S_{n-1,\alpha,\beta}(n-1,1)=\beta).$$

Proof: If $S_{n,\alpha,\beta}$ is a staircase tableau such that the box $S_{n,\alpha,\beta}(n-1,1)=\beta$, then the box $S_{n,\alpha,\beta}(n-1,2)=\alpha$ and $S_{n,\alpha,\beta}(n-1,1)=\beta$ by the rules of a staircase tableau. The second column is otherwise empty by those same rules. The nth row only has one box, $(n,1)$, which must be a β. The remainder is an arbitrary staircase tableau of size $n-1$ conditioned to have a β in box $(n-1,1)$. Therefore, the lemma follows. □

4 Distribution of parameters along the second main diagonal

The asymptotic distribution of parameters along the main diagonal is known. The number of α/γ symbols and the number of β/δ symbols along the main diagonal were proven to be asymptotically normal in [12], and the distribution of boxes along the main diagonal was given in [14]. However, the distributions of parameters on the other diagonals have not been studied specifically. The expected values were computed in [14] and it was conjectured there that the asymptotic distribution for the symbols on the kth diagonal is Poisson as $k=k_n$ goes to infinity with n going to infinity. As the first step towards proving that conjecture we now present results concerning the second main diagonal. In order to simplify notation, let $S_{n,\alpha,\beta}(i)$ be the symbol contained in second main diagonal box $(n-i,i)$ of $S_{n,\alpha,\beta}$. As our first result, the following is the distribution of boxes along the second main diagonal.

Theorem 3 *Let $1 \le j_1 < ... < j_r \le n-1$. If*

$$j_k \le j_{k+1}-2, \quad \forall k = 1,2,...,r-1 \tag{6}$$

then

$$\mathbb{P}(S_{n,\alpha,\beta}(j_1) = ... = S_{n,\alpha,\beta}(j_r) = \alpha) = \prod_{k=1}^{r} \frac{b + j_{r-k+1} - 2r + 2k - 1}{(a+b+n-2r+2k-1)(a+b+n-2r+2k-2)}.$$

(For $r=1$, this is (3)). Otherwise,

$$\mathbb{P}(S_{n,\alpha,\beta}(j_1) = ... = S_{n,\alpha,\beta}(j_r) = \alpha) = 0.$$

Proof: First note that when (6) fails there exists j_k such that $j_k = j_{k+1} - 1$ and thus there must be two α's in boxes side by side on the $(n-i, i)$ diagonal. But this is impossible by the rules of a staircase tableau as no symbol can be put in the diagonal box $(n - j_k, j_{k+1})$ adjacent to these two boxes. Therefore the probability is 0.

Suppose now that (6) holds. We proceed by induction on r. By (5), $S_{n,\alpha,\beta}[1, j_1] \stackrel{d}{=} S_{n-j_1+1,\alpha,\hat{\beta}}$ with $\hat{\beta}^{-1} = \beta^{-1} + j_1 - 1$ which yields:

$$\begin{aligned}\mathbb{P}(S_{n,\alpha,\hat{\beta}}(j_1) = ... = S_{n,\alpha,\hat{\beta}}(j_r) = \alpha) &= \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) = ... = S_{n-j_1+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) = \alpha) \\ &= \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(j_2 - j_1 + 1) = ... = S_{n-j_1+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) = \alpha \mid S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha) \\ &\quad \cdot \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha).\end{aligned}$$

By Lemma 1 and the induction hypothesis:

$$\begin{aligned}&\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(j_2 - j_1 + 1) = ... = S_{n-j_1+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) = \alpha \mid S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha) \\ &= \mathbb{P}(S_{n-j_1-1,\alpha,\hat{\beta}}(j_2 - j_1 - 1) = ... = S_{n-j_1-1,\alpha,\hat{\beta}}(j_r - j_1 - 1) = \alpha) \\ &= \prod_{k=1}^{r-1} \frac{\hat{b} + j_{r-k+1} - j_1 - 2r + 2k}{(a + \hat{b} + n - j_1 - 2r + 2k)(a + \hat{b} + n - j_1 - 2r + 2k - 1)}.\end{aligned}$$

By (3):

$$\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha) = \frac{\hat{b}}{(n - j_1 + a + \hat{b})(n - j_1 + a + \hat{b} - 1)}.$$

Therefore,

$$\begin{aligned}&\mathbb{P}(S_{n,\alpha,\hat{\beta}}(j_1) = ... = S_{n,\alpha,\hat{\beta}}(j_r) = \alpha) \\ &= \prod_{k=1}^{r} \frac{\hat{b} + j_{r-k+1} - j_1 - 2r + 2k}{(a + \hat{b} + n - j_1 - 2r + 2k)(a + \hat{b} + n - j_1 - 2r + 2k - 1)} \\ &= \prod_{k=1}^{r} \frac{b + j_{r-k+1} - 2r + 2k - 1}{(a + b + n - 2r + 2k - 1)(a + b + n - 2r + 2k - 2)}\end{aligned}$$

which proves the result. □

Our second main result is the distribution of the number of α's (and β's) along the second main diagonal. The proof requires a lemma.

Lemma 4 *Let*

$$J_{r,m} := \{1 \le j_1 < ... < j_r \le m : \ j_k \le j_{k+1} - 2, \ \ \forall k = 1, 2, ..., r-1\}.$$

Then

$$\sum_{J_{r,m}} \left(\prod_{k=1}^{r} j_{r-k+1} \right) = \frac{(m+1)_{2r}}{2^r r!},$$

where $(x)_r = x(x-1)\dots(x-(r-1))$ *is the falling factorial.*

Proof: By induction on r. When $r = 1$:

$$\sum_{J_{1,m}} \left(\prod_{k=1}^{1} j_{1-k+1} \right) = \sum_{j_1=1}^{m} j_1 = \frac{(m+1)m}{2}.$$

Assume the statement holds for $r-1$. Then:

$$\begin{aligned} \sum_{J_{r,m}} \left(\prod_{k=1}^{r} j_{r-k+1} \right) &= \sum_{j_r=2r-1}^{m} j_r \left(\sum_{J_{r-1,j_r-2}} \prod_{k=2}^{r} j_{r-k+1} \right) = \sum_{j_r=2r-1}^{m} j_r \frac{(j_r-1)_{2(r-1)}}{2^{r-1}(r-1)!} \\ &= \frac{1}{2^{r-1}(r-1)!} \sum_{j_r=2r-1}^{m} (j_r)_{2r-1} \end{aligned}$$

where the second equality is by the induction hypothesis. Since

$$\sum_{j_r=2r-1}^{m} (j_r)_{2r-1} = \sum_{j_r=0}^{m} (j_r)_{2r-1}$$

the lemma will be proved once we verify that

$$\sum_{j=0}^{m} (j)_t = \frac{(m+1)_{t+1}}{t+1},$$

for any non-negative integer t (and apply it with $t = 2r-1$). Using the identity

$$\sum_{j=0}^{m} \binom{j}{t} = \binom{m+1}{t+1}$$

(see, e.g. [13, Formula (5.10)]) we see that

$$\sum_{j=0}^{m} (j)_t = \sum_{j=0}^{m} \frac{j!}{(j-t)!} = t! \sum_{j=0}^{m} \binom{j}{t} = t! \binom{m+1}{t+1} = t! \frac{(m+1)_{t+1}}{(t+1)!} = \frac{(m+1)_{t+1}}{m+1},$$

as asserted. □

Finally, define A_n and B_n to be the number of α's and β's on the second main diagonal, i.e. $A_n := \sum_{j=1}^{n-1} I_{S_n,\alpha,\beta(j)=\alpha}$ and $B_n := \sum_{j=1}^{n-1} I_{S_n,\alpha,\beta(j)=\beta}$. Then, the asymptotic distribution of A_n and B_n is given in the following theorem and corollary.

Theorem 5 *Let $Pois(\lambda)$ be a Poisson random variable with parameter λ. Then, as $n \to \infty$,*

$$A_n \xrightarrow{d} Pois\left(\frac{1}{2}\right). \tag{7}$$

Proof: By [2, Theorem 20, Chapter 1] it suffices to show that the rth factorial moment of A_n satisfies:

$$\mathbb{E}(A_n)_r \to \left(\frac{1}{2}\right)^r \quad \text{as } \to \infty. \tag{8}$$

For the ease of notation let $I_j := I_{S_{n,\alpha,\beta}(j)=\alpha}$ and consider

$$\begin{aligned} z^{A_n} &= z^{\sum_{j=1}^{n-1} I_j} = \prod_{j=1}^{n-1} z^{I_j} = \prod_{j=1}^{n-1} (1+(z-1))^{I_j} = \prod_{j=1}^{n-1} (1+I_j(z-1)) \\ &= 1 + \sum_{r=1}^{n-1} \left(\sum_{1\le j_1<\ldots<j_r\le n-1} \left(\prod_{k=1}^{r} I_{j_k} \right) \right) (z-1)^r \\ &= 1 + \sum_{r=1}^{n-1} (z-1)^r \left(\sum_{1\le j_1<\ldots<j_r\le n-1} \left(\prod_{k=1}^{r} I_{j_k} \right) \right). \end{aligned}$$

Thus,

$$\mathbb{E}(z^{A_n}) = 1 + \sum_{r=1}^{n-1} (z-1)^r \left(\sum_{1\le j_1<\ldots<j_r\le n-1} \mathbb{P}(I_{j_1} \cap \ldots \cap I_{j_r}) \right).$$

Hence

$$\mathbb{E}(A_n)_r = \frac{d^r}{dz^r} (\mathbb{E}z^{A_n})|_{z=1} = r! \left(\sum_{1\le j_1<\ldots<j_r\le n-1} \mathbb{P}(I_{j_1} \cap \ldots \cap I_{j_r}) \right).$$

By Theorem 3 and Lemma 4

$$\begin{aligned} \mathbb{E}(A_n)_r &= r! \sum_{J_{r,n-1}} \left(\prod_{k=1}^{r} \frac{b + j_{r-k+1} - 2r + 2k - 1}{(a+b+n-2r+2k-1)(a+b+n-2r+2k-2)} \right) \\ &\approx r! \sum_{J_{r,n-1}} \left(\prod_{k=1}^{r} \frac{j_{r-k+1}}{n^2} \right) = \frac{r!}{n^{2r}} \frac{(n)_{2r}}{2^r r!} \to \left(\frac{1}{2}\right)^r, \quad \text{as } n \to \infty. \end{aligned}$$

□

Corollary 6 *The rth factorial moment of the number B_n of β's on the second main diagonal of a random staircase tableau of size n satisfies:*

$$\mathbb{E}(B_n)_r \to \left(\frac{1}{2}\right)^r \quad \textit{as } n \to \infty. \tag{9}$$

Furthermore,

$$B_n \xrightarrow{d} Pois\left(\frac{1}{2}\right) \quad \textit{as } n \to \infty. \tag{10}$$

Proof: This follows by symmetry, see Section 1. □

Remark 1 *Theorem 5 and Corollary 6 hold regardless of the values of α and β including the cases discussed earlier when $\alpha = \infty$, $\beta = \infty$, or $\alpha = \beta = \infty$. As noted in [14, Examples 3.6 and 3.7] these cases correspond to staircase tableaux with the maximal number of α's (or β's) and the maximal number of symbols, respectively.*

5 Distribution of Non-Empty Boxes

The number of α's and the number of β's, N_a and N_b, are not independent random variables, and the second main diagonal may have empty boxes. Therefore, in order to completely describe the second main diagonal, we must consider both symbols collectively. First, we present the distribution of non-empty boxes along the second main diagonal.

Theorem 7 *Let $1 \leq j_1 < ... < j_r \leq n-1$. If (6) holds then*

$$\mathbb{P}(S_{n,\alpha,\beta}(j_1) \neq 0, ..., S_{n,\alpha,\beta}(j_r) \neq 0) = \prod_{k=1}^{r} \frac{1}{(n+a+b-r+k-1)}.$$

(For $r = 1$, this is obtained by adding (3) and (4)). Otherwise,

$$\mathbb{P}(S_{n,\alpha,\beta}(j_1) \neq 0, ..., S_{n,\alpha,\beta}(j_r) \neq 0) = 0.$$

Proof: Suppose (6) holds. We proceed by induction on r.

By (5), $S_{n,\alpha,\beta}[1, j_1] \stackrel{d}{=} S_{n-j_1+1,\alpha,\hat{\beta}}$ with $\hat{\beta}^{-1} = \beta^{-1} + j_1 - 1$ which yields:

$$\begin{aligned}&\mathbb{P}(S_{n,\alpha,\hat{\beta}}(j_1) \neq 0, ..., S_{n,\alpha,\beta}(j_r) \neq 0)\\ &\quad = \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) \neq 0, ..., S_{n-j_r+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) \neq 0).\end{aligned}$$

Further

$$\begin{aligned}&\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) \neq 0, ..., S_{n-j_r+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) \neq 0)\\ &= \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha, S_{n-j_1+1,\alpha,\hat{\beta}}(j_2 - j_1 + 1) \neq 0, ..., S_{n-j_1+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) \neq 0)\\ &\quad + \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \beta, S_{n-j_1+1,\alpha,\hat{\beta}}(j_2 - j_1 + 1) \neq 0, ..., S_{n-j_1+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) \neq 0)\\ &= \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(j_2 - j_1 + 1) \neq 0, ..., S_{n-j_1+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) \neq 0) \mid S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha)\\ &\quad \cdot \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha)\\ &\quad + \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(j_2 - j_1 + 1) \neq 0, ..., S_{n-j_1+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) \neq 0 \mid S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \beta)\\ &\quad \cdot \mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \beta).\end{aligned}$$

Now consider two cases:

Case 1: $S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha$. By Lemma 1 and the induction hypothesis:

$$\begin{aligned}&\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(j_2 - j_1 + 1) \neq 0, ..., S_{n-j_1+1,\alpha,\hat{\beta}}(j_r - j_1 + 1) \neq 0) \mid S_{n-j_1+1,\alpha,\hat{\beta}}(1) = \alpha)\\ &\quad = \mathbb{P}(S_{n-j_1-1,\alpha,\hat{\beta}}(j_2 - j_1 - 1) \neq 0, ..., S_{n-j_1-1,\alpha,\hat{\beta}}(j_r - j_1 - 1) \neq 0)\\ &\quad = \prod_{k=1}^{r-1} \frac{1}{(n-j_1+a+\hat{b}-r+k-1)}.\end{aligned}$$

Also, by (3),

$$\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1)=\alpha)=\frac{\hat{b}}{(n-j_1+a+\hat{b})(n-j_1+a+\hat{b}-1)}.$$

Therefore,

$$\begin{aligned}&\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1)=\alpha, S_{n-j_1+1,\alpha,\hat{\beta}}(j_2-j_1+1)\neq 0,...,S_{n-j_r+1,\alpha,\hat{\beta}}(j_r-j_1+1)\neq 0)\\ &=\frac{\hat{b}}{(n-j_1+a+\hat{b})(n-j_1+a+\hat{b}-1)}\cdot\prod_{k=1}^{r-1}\frac{1}{(n-j_1+a+\hat{b}-r+k-1)}.\end{aligned}$$

Case 2: $S_{n-j_1+1,\alpha,\hat{\beta}}(1)=\beta$. By Lemma 2

$$\begin{aligned}&\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(j_2-j_1+1)\neq 0,...,S_{n-j_1+1,\alpha,\hat{\beta}}(j_r-j_1+1)\neq 0\mid S_{n-j_1+1,\alpha,\hat{\beta}}(1)=\beta)\\ &=\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(j_2-j_1)\neq 0,...,S_{n-j_{1r},\alpha,\hat{\beta}}(j_r-j_1)\neq 0\mid S_{n-j_1,\alpha,\hat{\beta}}(n-j_1,1)=\beta)\\ &=\frac{\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(j_2-j_1)\neq 0,...,S_{n-j_1,\alpha,\hat{\beta}}(j_r-j_1)\neq 0,\ S_{n-j_1,\alpha,\hat{\beta}}(n-j_1,1)=\beta)}{\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(n-j_1,1)=\beta)}.\end{aligned}$$

The numerator is equal to

$$\begin{aligned}&\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(j_2-j_1)\neq 0,...,S_{n-j_1,\alpha,\hat{\beta}}(j_r-j_1)\neq 0)\\ &\quad-\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(j_2-j_1)\neq 0,...,S_{n-j_1,\alpha,\hat{\beta}}(j_r-j_1)\neq 0,\ S_{n-j_1,\alpha,\hat{\beta}}(n-j_1,1)=\alpha)\\ &\quad=\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(j_2-j_1)\neq 0,...,S_{n-j_1,\alpha,\hat{\beta}}(j_r-j_1)\neq 0)\\ &\quad-\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(j_2-j_1)\neq 0,...,S_{n-j_1,\alpha,\hat{\beta}}(j_r-j_1)\neq 0\mid S_{n-j_1,\alpha,\hat{\beta}}(n-j_1,1)=\alpha)\\ &\qquad\cdot\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(n-j_1,1)=\alpha).\end{aligned}$$

By [14, Lemma 7.5] and the induction hypothesis the conditional probability above is

$$\mathbb{P}(S_{n-j_1-1,\alpha,\hat{\beta}}(j_2-j_1-1)\neq 0,...,S_{n-j_1-1,\alpha,\hat{\beta}}(j_r-j_1-1)\neq 0)=\prod_{k=1}^{r-1}\frac{1}{n-j_1+a+\hat{b}-r+k-1}. \tag{11}$$

By (4), (2) (and some algebra), the induction hypothesis, and (3), respectively,

$$\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(1)=\beta)=\frac{n-j_1+a-1}{(n-j_1+a+\hat{b})(n-j_1+a+\hat{b}-1)} \tag{12}$$

$$\frac{1}{\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(n-j_1,1)=\beta)}=\frac{n-j_1+a+\hat{b}-1}{n-j_1+a-1} \tag{13}$$

$$\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(j_2-j_1)\neq 0,...,S_{n-j_1+1,\alpha,\hat{\beta}}(j_r-j_1)\neq 0)=\prod_{k=1}^{r-1}\frac{1}{n-j_1+a+\hat{b}-r+k} \tag{14}$$

$$\mathbb{P}(S_{n-j_1,\alpha,\hat{\beta}}(n-j_1,1)=\alpha)=\frac{\hat{b}}{(n-j_1+a+\hat{b}-1)}. \tag{15}$$

Combining (11) - (15):

$$\begin{aligned}&\mathbb{P}(S_{n-j_1+1,\alpha,\hat{\beta}}(j_2-j_1+1)\neq 0,...,S_{n-j_1+1,\alpha,\hat{\beta}}(j_r-j_1+1)\neq 0, S_{n-j_1+1,\alpha,\hat{\beta}}(1)=\beta)\\ &=\frac{1}{n-j_1+a+\hat{b}}\cdot\Big(\prod_{k=1}^{r-1}\frac{1}{n-j_1+a+\hat{b}-r+k}\\ &\quad-\frac{\hat{b}}{n-j_1+a+\hat{b}-1}\prod_{k=1}^{r-1}\frac{1}{n-j_1+a+\hat{b}-r+k-1}\Big).\end{aligned}$$

Adding Case 1 and Case 2:

$$\begin{aligned}&\mathbb{P}(S_{n,\alpha,\hat{\beta}}(j_1)\neq 0,...,S_{n,\alpha,\hat{\beta}}(j_r)\neq 0)=\frac{1}{n-j_1+a+\hat{b}}\cdot\prod_{k=1}^{r-1}\frac{1}{n-j_1+a+\hat{b}-r+k}\\ &=\prod_{k=1}^{r}\frac{1}{n-j_1+a+\hat{b}-r+k}=\prod_{k=1}^{r}\frac{1}{n+a+b-r+k-1}\end{aligned}$$

which proves our assertion when (6) holds.

If there exists j_k such that $j_k=j_{k+1}-1$, then $\{S_{n,\alpha,\beta}(j_1)\neq 0,...,S_{n,\alpha,\beta}(j_r)\neq 0\}$ implies that two boxes side by side on the $(n-i,i)$ diagonal are non-empty, which is impossible by the rules of a staircase tableau. Therefore the probability is 0. □

As our final result, we consider the number of symbols on the second main diagonal, which we denote by X_n. Then $X_n=\sum_{j=1}^{n-1}I_j$ where $I_j:=I_{S_{n,\alpha,\beta}(j)\neq 0}$. The asymptotic distribution of the number of symbols on the second main diagonal is given by:

Theorem 8 *As $n\to\infty$,*

$$X_n\xrightarrow{d}Pois\,(1)\,. \tag{16}$$

Proof: By Theorem 7 and the same argument as in Theorem 5

$$\begin{aligned}&\mathbb{E}(X_n)_r=r!\sum_{1\leq j_1<\ldots<j_r\leq n-1}\mathbb{P}(I_{j_1}\cap\ldots\cap I_{j_r})=r!|J_{r,n-1}|\prod_{k=1}^{r}\frac{1}{n+a+b-r+k-1}\\ &=r!\left(\binom{n-1}{r}+O(n^{r-1})\right)\prod_{k=1}^{r}\frac{1}{n+a+b-r+k-1}\approx r!\cdot\frac{(n-1)^r}{r!n^r}\to 1\quad\text{as } n\to\infty.\end{aligned}$$

The result then follows by [2, Theorem 20], as discussed in the proof of Theorem 5. □

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Using Stein's Method to Show Poisson and Normal Limit Laws for Fringe Subtrees

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Abstract. We consider sums of functions of fringe subtrees of binary search trees and random recursive trees (of total size n).

The use of Stein's method and certain couplings allow provision of simple proofs showing that in both of these trees, the number of fringe subtrees of size $k < n$, where $k \to \infty$, can be approximated by a Poisson distribution. Combining these results and another version of Stein's method, we can also show that for $k = o(\sqrt{n})$, the number of fringe subtrees in both types of random trees has asymptotically a normal distribution as $n \to \infty$. Furthermore, using the Cramér–Wold device, we show that a random vector with components corresponding to the random number of copies of certain fixed fringe subtrees T_i, has asymptotically a multivariate normal distribution. We can then use these general results on fringe subtrees to obtain simple solutions to a broad range of problems relating to random trees; as an example, we can prove that the number of protected nodes in the binary search tree has asymptotically a normal distribution.

Keywords: Fringe subtrees. Stein's method. Couplings. Limit laws. Binary search trees. Recursive trees.

1 Introduction

In this paper we consider fringe subtrees of the random binary search tree, as well as of the random recursive tree; recall that a fringe subtree is a subtree consisting of some node and all its descendants, see Aldous [1] for a general theory, and note that fringe subtrees typically are "small" compared to the whole tree. This is an extended abstract of [9] where further details are given.

We will use a representation of Devroye [4, 5] for the binary search tree, and a well-known bijection between binary trees and recursive trees, together with different applications of Stein's method for both normal and Poisson approximation to give both new general results on the asymptotic distributions for random variables depending on fringe subtrees, and more direct proofs of several earlier results in the field.

The *binary search tree* is the tree representation of the sorting algorithm Quicksort, see e.g. [11]. Starting with n distinct numbers called keys, we draw one of the keys at random and associate it to the root.

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Then we draw one of the remaining keys. We compare it with the root, and associate it to the left child if it is smaller than the key at the root, and to the right child if it is larger. We continue recursively by drawing new keys until the set is exhausted. The comparison for each new key starts at the root, and at each node the key visits, it proceeds to the left/right child if it is smaller/larger than the key associated to that node; eventually, the new key is associated to the first empty node it visits. In the final tree, all the n ordered numbers are sorted by size, so that smaller numbers are in left subtrees, and larger numbers are in right subtrees.

We use the representation of the binary search tree by Devroye [4, 5]. We may clearly assume that the keys are $1, \dots, n$. We assign, independently, each key k a uniform random variable U_k in $(0, 1)$ which we regard as a time stamp indicating the time when the key is drawn. (We may and will assume that the U_k are distinct.) The random binary search tree constructed by drawing the keys in this order, i.e., in order of increasing U_k, then is the unique binary tree with nodes labelled by $(1, U_1), \dots, (n, U_n)$ with the property that it is a binary search tree with respect to the first coordinates in the pairs, and along every path down from the root the values U_i are increasing. We will also use a cyclic version of this representation described in Section 2.3.

Recall that the *random recursive tree* is constructed recursively, by starting with a root with label 1, and at stage i ($i = 2, \dots, n$) a new node with label i is attached uniformly at random to one of the previous nodes $1, \dots, i-1$. We let Λ_n denote a random recursive tree with n nodes.

There is a well-known bijection between ordered trees of size n and binary trees of size $n-1$, see e.g. Knuth [12, Section 2.3.2] who calls this *the natural correspondence* (the same bijection is also called the rotation correspondence): Given an ordered tree with n nodes, eliminate first the root, and arrange all its children in a path from left to right, as right children of each other. Continue recursively, with the children of each node arranged in a path from left to right, with the first child attached to its parent as the left child. This yields a binary tree with $n-1$ nodes, and the transformation is invertible.

As noted by Devroye [4], see also Fuchs, Hwang and Neininger [8], the natural correspondence extends to a coupling between the random recursive tree Λ_n and the binary search tree $\mathcal{T}_{n-1}$; the probability distributions are equal by induction because the n possible places to add a new node to Λ_n correspond to the n possible places (external leaves) to add a new node to $\mathcal{T}_{n-1}$, and these places have equal probabilities for both models.

Note that a left child in the binary search tree corresponds to an eldest child in the random recursive tree, while a right child corresponds to a sibling. We say that a proper subtree in a binary tree is left-rooted [right-rooted] if its root is a left [right] child. Thus, for $1 < k < n$, fringe subtrees of size k in the random recursive tree Λ_n, correspond to left-rooted fringe subtrees of size $k-1$ in the binary search tree $\mathcal{T}_{n-1}$, while fringe subtrees of size 1 (i.e., leaves) correspond to nodes without a left child.

We consider first only the sizes of the fringe subtrees. The results in the following two theorems, except the explicit rate in (3)–(4), were shown by Feng, Mahmoud and Panholzer [6] and Fuchs [7] by using variants of the method of moments. Theorem 1.3 was earlier proved for fixed k by Devroye [4] (using the central limit theorem for m-dependent variables), see also Aldous [1]. The part (5) of Theorem 1.3 was proved for a smaller range of k by Devroye [5] using Stein's method. (The mean (1) is also found in [5].) In the present paper we continue this approach, and use Stein's method for both Poisson and normal approximations to provide simple proofs for the full range.

We recall the definition of the total variation distance between two probability measures.

Definition 1.1 *Let $(\mathcal{X}, \mathcal{A})$ be any measurable space. The total variation distance d_{TV} between two prob-*

ability measures μ_1 and μ_2 on $\mathcal{X}$ is defined to be

$$d_{TV}(\mu_1, \mu_2) := \sup_{A \in \mathcal{A}} |\mu_1(A) - \mu_2(A)|.$$

Let $\mathcal{L}(X)$ denote the distribution of a random variable X. $\mathrm{Po}(\mu)$ denotes the Poisson distribution with mean μ, and $\mathcal{N}(0,1)$ the standard normal distribution. Convergence in distribution is denoted by $\xrightarrow{\mathrm{d}}$.

Theorem 1.2 *Let $X_{n,k}$ be the number of fringe subtrees of size k in the random binary search tree $\mathcal{T}_n$ and similarly let $\hat{X}_{n,k}$ be the number of fringe subtrees in the random recursive tree Λ_n. Let $k = k_n$ where $k < n$. Furthermore, let*

$$\mu_{n,k} := \mathbb{E}(X_{n,k}) = \frac{2(n+1)}{(k+1)(k+2)}, \tag{1}$$

$$\hat{\mu}_{n,k} := \mathbb{E}(\hat{X}_{n,k}) = \frac{n}{k(k+1)}. \tag{2}$$

Then, for the binary search tree,

$$d_{TV}(\mathcal{L}(X_{n,k}), \mathrm{Po}(\mu_{n,k})) = \frac{1}{2}\sum_{l\geq 0}\Big|\mathbb{P}(X_{n,k} = l) - e^{-\mu_{n,k}}\frac{(\mu_{n,k})^l}{l!}\Big| = O\Big(\frac{1}{k}\Big), \tag{3}$$

and for the random recursive tree,

$$d_{TV}(\mathcal{L}(\hat{X}_{n,k}), \mathrm{Po}(\hat{\mu}_{n,k})) = \frac{1}{2}\sum_{l\geq 0}\Big|\mathbb{P}(\hat{X}_{n,k} = l) - e^{-\hat{\mu}_{n,k}}\frac{(\hat{\mu}_{n,k})^l}{l!}\Big| = O\Big(\frac{1}{k}\Big). \tag{4}$$

Consequently, if $n \to \infty$ and $k \to \infty$, then

$$d_{TV}(\mathcal{L}(X_{n,k}), \mathrm{Po}(\mu_{n,k})) \to 0 \qquad \text{and} \qquad d_{TV}(\mathcal{L}(\hat{X}_{n,k}), \mathrm{Po}(\hat{\mu}_{n,k})) \to 0.$$

Theorem 1.3 *Let $X_{n,k}$ be the number of fringe subtrees of size k in the binary search tree $\mathcal{T}_n$ and similarly let $\hat{X}_{n,k}$ be the number of fringe subtrees of size k in the random recursive tree Λ_n. Let $k = k_n = o(\sqrt{n})$. Then, as $n \to \infty$, for the binary search tree*

$$\frac{X_{n,k} - \mathbb{E}(X_{n,k})}{\sqrt{\mathrm{Var}(X_{n,k})}} \xrightarrow{\mathrm{d}} \mathcal{N}(0,1) \tag{5}$$

and, similarly, for the random recursive tree

$$\frac{\hat{X}_{n,k} - \mathbb{E}(\hat{X}_{n,k})}{\sqrt{\mathrm{Var}(\hat{X}_{n,k})}} \xrightarrow{\mathrm{d}} \mathcal{N}(0,1). \tag{6}$$

Remark 1.4 *If $k/\sqrt{n} \to \infty$, then $\mu_{n,k}, \hat{\mu}_{n,k} \to 0$, and the convergence result in Theorem 1.2 reduces to the trivial $X_{n,k} \xrightarrow{\mathrm{p}} 0$ and $\hat{X}_{n,k} \xrightarrow{\mathrm{p}} 0$; the rate of convergence in* (3)–(4) *is still of interest.*

If $k/\sqrt{n} \to c \in (0,\infty)$, then $\mu_{n,k} \to 2c^{-2}$ and $\hat{\mu}_{n,k} \to c^{-2}$; and we obtain the Poisson distribution limits $X_{n,k} \xrightarrow{\mathrm{d}} \mathrm{Po}(2c^{-2})$ and $\hat{X}_{n,k} \xrightarrow{\mathrm{d}} \mathrm{Po}(c^{-2})$ [6, 7].

We also consider the number of fringe subtrees that are equal to a fixed tree T in the binary search tree $\mathcal{T}_n$, which we denote by X_n^T. Combining the Cramér–Wold device [3, Theorem 7.7] and Stein's method we show that random vectors of fringe subtrees are multivariate normally distributed. These results are also useful for proving general theorems for sums of functions of fringe subtrees.

Theorem 1.5 *Let T be a binary tree of size k and let T' be a binary tree of size m where $m \leq k$. Let X_n^T be the number of fringe subtrees T and let $X_n^{T'}$ be the number of fringe subtrees T' in the binary search tree $\mathcal{T}_n$ with n nodes. Let $p_{k,T} := \mathbb{P}(\mathcal{T}_k = T)$ and $p_{m,T'} := \mathbb{P}(\mathcal{T}_m = T')$, and let $q_{T'}^T$ be the number of fringe subtrees of T that are copies of T'. If $n > k + m + 1$, then the covariance between X_n^T and $X_n^{T'}$ is equal to*

$$\operatorname{Cov}(X_n^T, X_n^{T'}) = (n+1)\sigma_{T,T'}, \tag{7}$$

where,

$$\sigma_{T,T'} := \frac{2}{(k+1)(k+2)} q_{T'}^T p_{k,T} - \gamma(k,m) p_{k,T} p_{m,T'}, \tag{8}$$

with

$$\gamma(k,m) := \frac{4(k+m+3)}{(k+1)(k+2)(m+1)(m+2)} - \frac{4(k^2+3km+m^2+4k+4m+3)}{(k+1)\,(m+1)\,(k+m+1)\,(k+m+2)\,(k+m+3)}\,. \tag{9}$$

Theorem 1.6 *Let X_n^T be the number of fringe subtrees T in the random binary search tree $\mathcal{T}_n$. Let $T^1, \dots, T^d$ be a fixed sequence of distinct binary trees and let $\bar{\mathcal{X}}_n^d = (X_n^{T^1}, X_n^{T^2}, \dots, X_n^{T^d})$. Let*

$$\mu_n^d := \Big(\mathbb{E}(X_n^{T^1}), \mathbb{E}(X_n^{T^2}), \dots, \mathbb{E}(X_n^{T^d}) \Big)$$

and let $\Gamma = (\gamma_{ij})_{i,j=1}^d$ denote the matrix with elements

$$\gamma_{ij} = \lim_{n\to\infty} \frac{1}{n} \operatorname{Cov}(X_n^{T^i}, X_n^{T^j}) = \sigma_{T^i,T^j}, \tag{10}$$

with notation as in (7)–(8)*. Then Γ is non-singular and*

$$n^{-1/2}(\bar{\mathcal{X}}_n^d - \mu_n^d) \xrightarrow{\mathrm{d}} \mathcal{N}(0,\Gamma). \tag{11}$$

In [9] there are corresponding multivariate-normal distribution results for the number of fringe subtrees Λ in the random recursive tree Λ_n.

In Section 5 we explain how Theorem 1.6 can be used to prove that the number of the so called *protected* nodes in the binary search trees asymptotically has a normal distribution.

2 Representations using uniform random variables

2.1 Devroye's representation for the binary search tree

We use the representation of the binary search tree $\mathcal{T}_n$ by Devroye [4, 5] described in Section 1, using i.i.d. random time stamps $U_i \sim U(0,1)$ assigned to the keys $i = 1, \dots, n$. Write, for $1 \le k \le n$ and $1 \le i \le n-k+1$,

$$\sigma(i,k) = \{(i,U_i), \dots, (i+k-1, U_{i+k-1})\}, \tag{12}$$

i.e., the sequence of k labels (j, U_j) starting with $j = i$. For every node $u \in \mathcal{T}_n$, the fringe subtree $\mathcal{T}_n(u)$ rooted at u consists of the nodes with labels in a set $\sigma(i,k)$ for some such i and k, where $k = |\mathcal{T}_n(u)|$, but note that not every set $\sigma(i,k)$ is the set of labels of the nodes of a fringe subtree; if it is, we say simply that $\sigma(i,k)$ *is a fringe subtree*. We define the indicator variable

$$I_{i,k} := \mathbf{1}\{\sigma(i,k) \text{ is a fringe subtree in } \mathcal{T}_n\}.$$

It is easy to see that, for convenience defining $U_0 = U_{n+1} = 0$,

$$I_{i,k} = \mathbf{1}\big\{U_{i-1} \text{ and } U_{i+k} \text{ are the two smallest among } U_{i-1}, \dots, U_{i+k}\big\}. \tag{13}$$

Note that if $i = 1$ or $i = n-k+1$, this reduces to

$$I_{1,k} = \mathbf{1}\big\{U_{k+1} \text{ is the smallest among } U_1, \dots, U_{k+1}\big\}, \tag{14}$$

$$I_{n-k+1,k} = \mathbf{1}\big\{U_{n-k} \text{ is the smallest among } U_{n-k}, \dots, U_n\big\}. \tag{15}$$

For $k = n$, when we only consider $i = 1$, we have $I_{1,n} = 1$.

Let $f(T)$ be a function from the set of (unlabelled) binary trees to $\mathbb{R}$. We are interested in the functional

$$X_n := \sum_{u \in \mathcal{T}_n} f(\mathcal{T}_n(u)), \tag{16}$$

summing over all fringe subtrees of $\mathcal{T}_n$.

For example, one obtains the number of fringe subtrees that are equal (up to labelling) to a given binary tree T' by choosing $f(T) = \mathbf{1}\{T \approx T'\}$ (where $\approx$ denotes equality when we ignore labels), and one obtains the number of fringe subtrees with exactly k nodes by letting $f(T) = \mathbf{1}\{|T| = k\}$. We refer to Devroye [5] for several other examples showing the generality of this representation.

Since a permutation $(\sigma_1, \dots, \sigma_k)$ defines a binary search tree (by drawing the keys in order $\sigma_1, \dots, \sigma_k$), we can also regard f as a function of permutations (of arbitrary length). Moreover, any set $\sigma(i,k)$ defines a permutation $(\sigma_1, \sigma_2, \dots, \sigma_k)$ where the values j, $1 \le j \le k$, are ordered according to the order of U_{i+j-1}. We can thus also regard f as a mapping from the collection of all sets $\sigma(i,k)$. Note that if $\sigma(i,k)$ corresponds to a fringe subtree $\mathcal{T}_n(u)$ of $\mathcal{T}_n$, then, ignoring labels, $\mathcal{T}_n(u)$ is the binary search tree defined by the permutation defined by $\sigma(i,k)$, and thus $f\big(\mathcal{T}_n(u)\big) = f\big(\sigma(i,k)\big)$. Consequently, see [5],

$$X_n := \sum_{u \in \mathcal{T}_n} f(\mathcal{T}_n(u)) = \sum_{k=1}^{n} \sum_{i=1}^{n-k+1} I_{i,k} f(\sigma(i,k)). \tag{17}$$

2.2 The random recursive tree

Consider now instead the random recursive tree Λ_n. Let $f(T)$ be a function from the set of ordered rooted trees to $\mathbb{R}$. In analogy with (16), we define

$$Y_n := \sum_{u\in\Lambda_n} f(\Lambda_n(u)), \tag{18}$$

summing over all fringe subtrees of Λ_n.

As said in the introduction, the natural correspondence yields a coupling between the random recursive tree Λ_n and the binary search tree $\mathcal{T}_{n-1}$. The subtrees in Λ_n correspond to the left subtrees at the nodes in $\mathcal{T}_{n-1}$ together with the whole tree, including an empty left subtree $\emptyset$ at every node in $\mathcal{T}_{n-1}$ without a left child, corresponding to a subtree of size 1 (a leaf) in Λ_n. Thus, as noted by [4], the representation in Section 2.1 yields a similar representation for the random recursive tree, which can be described as follows.

Define $\bar f$ as the functional on binary trees corresponding to f by $\bar f(T) := f(T')$, where T' is the ordered tree corresponding to the binary tree T by the natural correspondence. (Thus $|T'| = |T| + 1$.) We regard the empty binary tree $\emptyset$ as corresponding to the (unique) ordered tree $\bullet$ with only one vertex, and thus we define $\bar f(\emptyset) := f(\bullet)$.

Assume first $1 < k < n$ and recall that subtrees of size k in the random recursive tree Λ_n correspond to left-rooted subtrees of size $k-1$ in the binary search tree $\mathcal{T}_{n-1}$. As said in Section 2.1, a subtree of size $k-1$ in $\mathcal{T}_{n-1}$ corresponds to a set $\sigma(i,k-1)$ for some $i \in \{1,\dots,n-k+1\}$. The parent of the root of this subtree is either $i-1$ or $i+k-1$; it is $i-1$, and the subtree is right-rooted, if $U_{i-1} > U_{i+k-1}$, and it is $i+k-1$, and the subtree is left-rooted, if $U_{i-1} < U_{i+k-1}$. We define

$$I^{\mathrm{L}}_{i,k-1} := \mathbf{1}\{\sigma(i,k-1) \text{ is a left-rooted subtree in } \mathcal{T}_{n-1}\}. \tag{19}$$

Using (13) it follows that, in analogy with (17),

$$Y_n := \sum_{u\in\Lambda_n} f(\Lambda_n(u)) = \sum_{k=1}^{n}\sum_{i=1}^{n-k+1} I^{\mathrm{L}}_{i,k-1}\bar f(\sigma(i,k-1)). \tag{20}$$

This is easily extended to $k = 1$ too.

2.3 Cyclic representations

The representation (17) of X_n using a linear sequence $U_1,\dots,U_n$ of i.i.d. random variables is natural and useful, but it has the (minor) disadvantage that terms with $i = 1$ or $i = n-k+1$ have to be treated specially because of boundary effects, as seen in (14)–(15). It will be convenient to use a related cyclic representation, where we take $n+1$ i.i.d. uniform variables $U_0,\dots,U_n \sim U(0,1)$ and extend them to an infinite periodic sequence of random variables by

$$U_i \;:= U_{i \bmod (n+1)}, \qquad i \in \mathbb{Z}, \tag{21}$$

where $i \bmod (n+1)$ is the remainder when i is divided by $n+1$, i.e., the integer $\ell \in [0,n]$ such that $i \equiv \ell \pmod{n+1}$. (We may and will assume that $U_0,\dots,U_n$ are distinct.) We define further $I_{i,k}$ as in (13), but now for all i and k. Similarly, we define $\sigma(i,k)$ by (12) for all i and k. We then have the following cyclic representation of X_n. (We are indebted to Allan Gut for suggesting a cyclic representation.)

Lemma 2.1 *Let $U_0, \dots, U_n \sim U(0,1)$ be independent and extend this sequence periodically by* (21)*. Then, with notations as above,*

$$X_n := \sum_{u \in \mathcal{T}_n} f(\mathcal{T}_n(u)) \stackrel{\mathrm{d}}{=} \tilde{X}_n := \sum_{k=1}^{n} \sum_{i=1}^{n+1} I_{i,k} f(\sigma(i,k)). \tag{22}$$

Proof: The double sum in (22) is invariant under a cyclic shift of $U_0, \dots, U_n$. If we shift these values so that U_0 becomes the smallest, we obtain the same distribution of $(U_0, \dots, U_n)$ as if we instead condition on the event that U_0 is the smallest U_i, i.e., on $\{U_0 = \min_i U_i\}$. Hence,

$$\tilde{X}_n \stackrel{\mathrm{d}}{=} \bigl(\tilde{X}_n \mid U_0 = \min_i U_i\bigr). \tag{23}$$

Furthermore, the variables $I_{i,k}$ depend only on the order relations among $\{U_i\}$, so if U_0 is minimal, they remain the same if we put $U_0 = 0$. Moreover, in this case also $U_{n+1} = U_0 = 0$ and it follows from (13) that $I_{i,k} = 0$ if $i \le n+1 \le i+k-1$; hence the terms in (22) with $n-k+1 < i \le n+1$ vanish. Note also that in the remaining terms, $f(\sigma(i,k))$ does not depend on U_0. Consequently,

$$\tilde{X}_n \stackrel{\mathrm{d}}{=} \Bigl(\sum_{k=1}^{n} \sum_{i=1}^{n-k+1} I_{i,k} f(\sigma(i,k)) \;\Big|\; U_0 = 0\Bigr) = X_n, \tag{24}$$

by (17), showing that the cyclic and linear representations in (17) and (22) are equivalent. □

Since U_i is defined for all $i \in \mathbb{Z}$ and has period $n+1$, it is natural to regard the index i as an element of $\mathbb{Z}_{n+1}$; similarly, $I_{i,k}$ is defined for all $i \in \mathbb{Z}$ with period $n+1$ in i, so we can regard it as defined for $i \in \mathbb{Z}_{n+1}$. When discussing these variables, we will use the natural metric on $\mathbb{Z}_{n+1}$ defined by

$$|i-j|_{n+1} := \min_{\ell \in \mathbb{Z}} |i - j - \ell \cdot (n+1)|. \tag{25}$$

For the random recursive tree Λ_n we argue in the same way, now using (20); for further details see [9].

The cyclic representations lead to simple exact calculations of means and variances. In [9] we use the cyclic representation to show general results for sums of functions of fringe subtrees.

3 Poisson approximations by Stein's method and couplings

To prove Theorems 1.2 we use Stein's method with couplings as described by Barbour et al. [2].

In general, let $\mathcal{A}$ be a finite index set and let $(I_\alpha,\ \alpha \in \mathcal{A})$ be indicator random variables. We write $W := \sum_{\alpha \in \mathcal{A}} I_\alpha$ and $\lambda := \mathbb{E}(W)$. To approximate W with a Poisson distribution $\mathrm{Po}(\lambda)$, this method uses a coupling for each $\alpha \in \mathcal{A}$ between W and a random variable W_α which is defined on the same probability space as W and has the property

$$\mathcal{L}(W_\alpha) = \mathcal{L}(W - I_\alpha \mid I_\alpha = 1). \tag{26}$$

A common way to construct such a coupling (W, W_α) is to find random variables $(J_{\beta\alpha},\ \beta \in \mathcal{A})$ defined on the same probability space as $(I_\alpha,\ \alpha \in \mathcal{A})$ in such a way that for each $\alpha \in \mathcal{A}$, and jointly for all $\beta \in \mathcal{A}$,

$$\mathcal{L}(J_{\beta\alpha}) = \mathcal{L}(I_\beta \mid I_\alpha = 1). \tag{27}$$

Then $W_\alpha = \sum_{\beta\neq\alpha} J_{\beta\alpha}$ is defined on the same probability space as W and (26) holds.

Suppose that $J_{\beta\alpha}$ are such random variables, and that, for each α, the set $\mathcal{A}_\alpha := \mathcal{A}\backslash\{\alpha\}$ is partitioned into $\mathcal{A}_\alpha^-$ and $\mathcal{A}_\alpha^0$ in such a way that

$$J_{\beta\alpha} \le I_\beta \quad \text{if } \beta \in \mathcal{A}_\alpha^-, \tag{28}$$

with no condition if $\beta \in \mathcal{A}_\alpha^0$. We will use the following result from [2] (with a slightly simplified constant). ([2] also contain similar results using a third part $\mathcal{A}_\alpha^+$ of $\mathcal{A}_\alpha$, where (28) holds in the opposite direction; we will not need them and note that it is always possible to include $\mathcal{A}_\alpha^+$ in $\mathcal{A}_\alpha^0$ and then use the following result.)

Theorem 3.1 ([2, Corollary 2.C.1]) *Let $W = \sum_{\alpha\in\mathcal{A}} I_\alpha$ and $\lambda = \mathbb{E}(W)$. Let $\mathcal{A}_\alpha = \mathcal{A}\backslash\{\alpha\}$ and $\mathcal{A}_\alpha^-, \mathcal{A}_\alpha^0$ be defined as above. Then*

$$d_{TV}(\mathcal{L}(W), \mathrm{Po}(\lambda)) \le (1\wedge\lambda^{-1})\Bigl(\lambda - \mathrm{Var}(W) + 2\sum_{\alpha\in\mathcal{A}}\sum_{\beta\in\mathcal{A}_\alpha^0}\mathbb{E}(I_\alpha I_\beta)\Bigr).$$

□

Couplings for proving Theorem 1.2

Returning to the binary search tree, we use the cyclic representation in Section 2.3 to prove the following lemma where we give exact expressions for the expected value and the variance of $X_{n,k}$.

Lemma 3.2 *Let $1 \le k < n$. For the random binary search tree $\mathcal{T}_n$,*

$$\mathbb{E}(X_{n,k}) = \frac{2(n+1)}{(k+1)(k+2)} \tag{29}$$

and

$$\mathrm{Var}(X_{n,k}) = \begin{cases} \mathbb{E}\,X_{n,k} - (n+1)\frac{22k^2+44k+12}{(k+1)(k+2)^2(2k+1)(2k+3)}, & k < \frac{n-1}{2}, \\ \mathbb{E}\,X_{n,k} + \frac{2}{n} - \frac{64}{(n+3)^2}, & k = \frac{n-1}{2}, \\ \mathbb{E}\,X_{n,k} - (\mathbb{E}\,X_{n,k})^2 = \mathbb{E}\,X_{n,k} - \frac{4(n+1)^2}{(k+1)^2(k+2)^2}, & k > \frac{n-1}{2}. \end{cases} \tag{30}$$

Hence,

$$\mathrm{Var}(X_{n,k}) = \mathbb{E}(X_{n,k}) + O\Bigl(\frac{n}{k^3}\Bigr), \tag{31}$$

except when $k = (n-1)/2$; in this case

$$\mathrm{Var}(X_{n,k}) = \mathbb{E}(X_{n,k}) + \frac{2}{n} + O\Bigl(\frac{n}{k^3}\Bigr) = \mathbb{E}(X_{n,k}) + O\Bigl(\frac{1}{n}\Bigr). \tag{32}$$

To prove this lemma, we use the cyclic representation (22), which in this case is

$$X_{n,k} \stackrel{\mathrm{d}}{=} \sum_{i=1}^{n+1} I_{i,k}, \tag{33}$$

where now $I_{i,k}$ are defined by (13) with U_i given by (21). By (13) and symmetry, for any i and $1 \le k < n$, $\mathbb{E}(I_{i,k}) = \frac{2}{(k+2)(k+1)}$, and thus (29) follows directly from (33). Using the cyclic representation we can also simply prove that (30) holds; however for Poisson approximation we only need the weak asymptotics in (31)–(32).

Recall the construction of $I_{i,k}$ in (13) and the distance $|i-j|_{n+1}$ on $\mathbb{Z}_{n+1}$ given by (25).

Lemma 3.3 *Let $k \in \{1,\dots,n-1\}$ and let $I_{i,k}$ be as in Section 2.3. Then for each $i \in 1,\dots,n+1$, there exists a coupling $((I_{j,k})_j, (Z^k_{ji})_j)$ such that $\mathcal{L}(Z^k_{ji}) = \mathcal{L}(I_{j,k} \mid I_{i,k} = 1)$ jointly for all $j \in 1,\dots,n+1$. Furthermore,*

$$\begin{cases} Z^k_{ji} = I_{j,k} & \text{if} \quad |j-i|_{n+1} > k+1, \\ Z^k_{ji} \ge I_{j,k} & \text{if} \quad |j-i|_{n+1} = k+1, \\ Z^k_{ji} = 0 \le I_{j,k} & \text{if} \quad 0 < |j-i|_{n+1} \le k. \end{cases}$$

Proof: We define Z^k_{ji} as follows. (Indices are taken modulo $n+1$.) Let m and m' be the indices in $i-1,\dots,i+k$ such that U_m and $U_{m'}$ are the two smallest of $U_{i-1},\dots,U_{i+k}$; if one of these is $i-1$ we choose $m = i-1$, and if one of them is $i+k$ we choose $m' = i+k$, otherwise, we randomize the choice of m among these two indices so that $\mathbb{P}(m < m') = \frac12$, independently of everything else. Now exchange $U_{i-1} \leftrightarrow U_m$ and $U_{i+k} \leftrightarrow U_{m'}$, i.e., let $U'_{i-1} := U_m$, $U'_m := U_{i-1}$, $U'_{i+k} := U_{m'}$, $U'_{m'} := U_{i+k}$, and $U'_l := U_l$ for all other indices l. Finally, let, cf. (13),

$$Z^k_{ji} = \mathbf{1}\bigl\{U'_{j-1} \text{ and } U'_{j+k} \text{ are the two smallest among } U'_{j-1},\dots,U'_{j+k}\bigr\}. \tag{34}$$

Then, $\mathcal{L}\bigl(U'_1,\dots,U'_n\bigr) = \mathcal{L}\bigl((U_1,\dots,U_n) \mid I_{i,k} = 1\bigr)$ and thus $\mathcal{L}(Z^k_{ji}) = \mathcal{L}(I_{j,k} \mid I_{i,k} = 1)$ jointly for all j.

Note that $U'_l = U_l$ if $l \notin \{i-1,\dots,i+k\}$ and thus $Z^k_{ji} = I_{j,k}$ if $|j-i|_{n+1} > k+1$. On the other hand, if $0 < j-i < k+1$, then $Z^k_{ji} = 0$ since $i+k$ lies in $\{j,\dots,j+k-1\}$ and U'_{i+k} is smaller than U'_{j-1} by construction; the case $-k-1 < j-i < 0$ is similar. (This says simply that two different fringe subtrees of the same size cannot overlap, which is obvious.)

Finally, if $j = i+k+1$ with $j+k+1 < i+n+1$ (i.e., $k+1 < (n+1)/2$), then $j-1 = i+k$ and thus $U'_{j-1} \le U_{j-1}$ while $U'_l = U_l$ for $l \in j,\dots,j+k$; hence $Z^k_{ji} \ge I_{j,k}$. The cases $j = i+k+1$ with $j+k+1 = i+n+1$ and $j = i-k-1$ with $j-k-1 > i-n-1$ are similar. □

See Figures 1–2 that illustrate an example for such a coupling in the case $k = 3$.

Proof of Theorem 1.2:

We prove the result for the binary search tree, using the representation $X_{n,k} = \sum_{i=1}^{n+1} I_{i,k}$ in (33). (For the random recursive tree the proof is similar and uses the representation $\hat{X}_{n,k} \overset{\mathrm{d}}{=} \sum_{i=1}^{n} I^{\mathrm{L}}_{i,k-1}$; see [9].)

Let $\mathcal{A} := \{1,\dots,n+1\}$. From Lemma 3.3 we see that for each $i \in \mathcal{A}$ we can apply Theorem 3.1 with

$$\mathcal{A}_i^- := \mathcal{A} \setminus \{i, i \pm (k+1)\}, \qquad \mathcal{A}_i^0 := \{i \pm (k+1)\};$$

this yields, using Lemma 3.2 and the fact that $\mathbb{E}(I_{i,k}I_{i+k+1,k}) = O\bigl(\frac{1}{k^3}\bigr)$ (which is shown easily),

$$\begin{aligned} d_{TV}(\mathcal{L}(X_{n,k}), \mathrm{Po}(\mu_{n,k})) &\le \bigl(1 \wedge \mu_{n,k}^{-1}\bigr)\Bigl(\mu_{n,k} - \mathrm{Var}(X_{n,k}) + 4 \sum_{1 \le i \le n+1} \mathbb{E}(I_{i,k}I_{i+k+1,k})\Bigr) \\ &= O\Bigl(\frac{1}{\mu_{n,k}} \cdot \frac{n}{k^3}\Bigr) = O\Bigl(\frac{1}{k}\Bigr), \end{aligned}$$

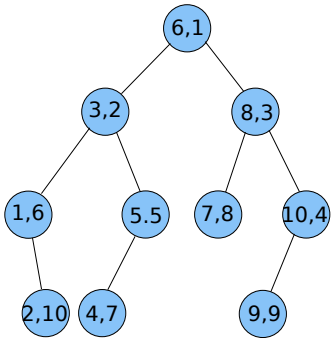

Fig. 1: A binary search tree with no fringe subtree of size three containing the keys $\{4, 5, 6\}$.

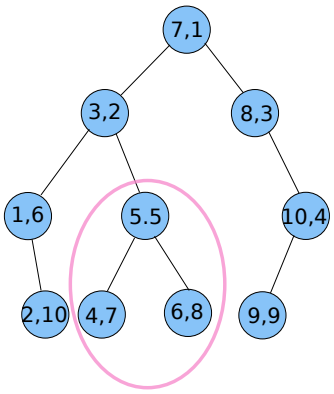

Fig. 2: A coupling forcing a fringe subtree of size three containing the keys $\{4, 5, 6\}$ in the tree in Fig. 1.

which shows (3).

□

4 Normal approximations by Stein's method

In this section we will prove Theorem 1.6. As in [5, Theorem 5] we will apply the following result, see [10, Theorem 6.33] for a proof, and for the definition of a dependency graph.

Lemma 4.1 *Suppose that $(S_n)_1^\infty$ is a sequence of random variables such that $S_n = \sum_{\alpha\in V_n} Z_{n\alpha}$, where for each n, $\{Z_{n\alpha}\}_\alpha$ is a family of random variables with dependency graph (V_n, E_n). Let $N(\cdot)$ denote the closed neighborhood of a node or set of nodes in this graph. Suppose further that there exist numbers M_n and Q_n such that $\sum_{\alpha\in V_n} \mathbb{E}(|Z_{n\alpha}|) \le M_n$ and for every $\alpha, \alpha' \in V_n$,*

$$\sum_{\beta\in N(\alpha,\alpha')} \mathbb{E}(|Z_{n\beta}| \mid Z_{n\alpha}, Z_{n\alpha'}) \le Q_n \, .$$

Let $\sigma_n^2 = \mathrm{Var}(S_n)$. If $\lim_{n\to\infty} \frac{M_n Q_n^2}{\sigma_n^3} = 0$, then it holds that $\frac{S_n - \mathbb{E}(S_n)}{\sqrt{\mathrm{Var}(S_n)}} \xrightarrow{\mathrm{d}} \mathcal{N}(0,1)$.

Proof of Theorem 1.6: Recall that $\bar{\mathcal{X}}_n^d = (X_n^{T^1}, X_n^{T^2}, \dots, X_n^{T^d})$ and let $\mathcal{Z}_d = (Z_1, \dots, Z_d)$, where $\mathcal{Z}_d$ is multivariate normal with the distribution $\mathcal{N}(0, \Gamma)$, where Γ is the matrix with elements $\gamma_{ij} = \lim_{n\to\infty} \frac{1}{n} \mathrm{Cov}(X_n^{T^i}, X_n^{T^j})$, see (10) above.

By the Cramér–Wold device [3, Theorem 7.7], to show that $n^{-\frac{1}{2}}(\bar{\mathcal{X}}_n^d - \mu_n^d)$ converges in distribution to $\mathcal{Z}_d$, it is enough to show that for every fixed vector $(t_1, \dots, t_d) \in \mathbb{R}^d$ we have

$$\frac{\sum_{j=1}^d t_j X_n^{T^j} - \mathbb{E}\left(\sum_{j=1}^d t_j X_n^{T^j}\right)}{\sqrt{n}} \xrightarrow{\mathrm{d}} \sum_{j=1}^d t_j Z_j, \tag{35}$$

where $\sum_{j=1}^{d} t_j Z_j \sim \mathcal{N}\big(0,\gamma^2\big)$ with $\gamma^2 := \sum_{j,k=1}^{d} t_j t_k \gamma_{ij}$.

Let $S_n := \sum_{j=1}^{d} t_j X_n^{T^j}$. Theorem 1.5 implies that, as $n \to \infty$,

$$\mathrm{Var}(S_n) \sim n \sum_{j,k=1}^{d} t_j t_k \sigma_{T^i,T^j} = n \sum_{j,k=1}^{d} t_j t_k \gamma_{ij} = n\gamma^2. \tag{36}$$

In particular, if $\gamma^2 = 0$, then (35) is trivial, with the limit 0.

To show that (35) holds when $\gamma^2 > 0$, we will use the same method as was used in [5, Theorem 5] for proving this theorem (in a more general form) in the 1-dimensional case $d = 1$. Let $I_{i,k}^T = \mathbf{1}\{\sigma(i,k) \approx T\}$. Let $|T^j| = k_j$, $1 \le j \le d$. We use the cyclic representation (22), which in this case can be written as $X_n^{T^j} = \sum_{i=1}^{n+1} I_i^j$, for some indicator variable $I_i^j = I_{i,k_j} I_{i,k_j}^{T^j}$ depending only on $U_{i-1},\dots,U_{i+k_j}$. We define

$$V_n := \{(i,j) : 1 \le i \le n+1, 1 \le j \le d\}$$

and let for each $(i,j) \in V_n$, $A_{i,j}$ be the set $\{i-1,\dots,i+k_j\}$, regarded as a subset of $\mathbb{Z}_{n+1}$. Thus I_i^j depends only on $\{U_k : k \in A_{i,j}\}$, and thus we can define a dependency graph L_n with vertex set V_n by connecting (i,j) and (i',j') when $A_{i,j} \cap A_{i',j'} \neq \emptyset$.

Let $K := \max\{k_1,k_2,\dots,k_d\}$ and $M := \max\{t_1,t_2,\dots,t_d\}$. It is easy to see that for the sum

$$S_n := \sum_{j=1}^{d} t_j X_n^{T^j} = \sum_{i=1}^{n+1}\sum_{j=1}^{d} t_j I_i^j = \sum_{(i,j)\in V_n} t_j I_i^j,$$

we can choose the numbers M_n and Q_n in Lemma 4.1 as $M_n = (n+1)dM$ and

$$Q_n = 2M \sup_{(i,j)\in V_n} |N((i,j))| \le 2Md(2K+3).$$

Since $\sigma_n \sim n^{1/2}$ by (36), it holds that $\lim_{n\to\infty} \frac{M_n Q_n^2}{\sigma_n^3} = 0$, and Lemma 4.1 shows that (35) holds.

It is shown in [9] that the matrix Γ is non-singular. □

The proof of Theorem 1.3 when $k = o(\sqrt{n})$ and k tends to infinity follows directly from Theorem 1.2 and (31), since then $\mathbb{E}(X_{n,k})$ and $\mathrm{Var}(X_{n,k})$ tend to infinity as n tends to infinity. For the case $k = O(1)$ we can apply Lemma 4.1 similarly to the proof of Theorem 1.6 and repeat the arguments used in [5, Theorem 5]; see [9] for details.

5 Protected nodes

We consider the number of protected nodes. A node is *protected* if the shortest distance to a leaf is at least two, i.e., it is neither a leaf or the parent of a leaf. The following theorem was shown by Mahmoud and Ward [13, Theorem 3.1] using generating functions.

Theorem 5.1 *Let X_n denote the number of protected nodes in a binary search tree $\mathcal{T}_n$. Then it holds that*

$$\frac{X_n - \frac{11}{30}n}{\sqrt{n}} \xrightarrow{d} \mathcal{N}\Big(0, \frac{29}{225}\Big).$$

We can show this result from a simple application of Theorem 1.6. Using the formulation of fringe subtrees, we note that the number of unprotected nodes in the binary search tree equals twice the number of leaves (counting all the leaves and all the parents of the leaves) minus the number of cherry subtrees, i.e., subtrees consisting of a root with one left and one right child that both are leaves (since these are the only cases when a parent is counted twice). Hence, since any linear combination of the components in a random vector with a multivariate normal distribution is normal, Theorem 5.1 follows from Theorem 1.6.

Moreover, our approach using fringe subtrees also allows us to provide a simple proof of the following result which was conjectured in [13, Conjecture 2.1]. See [9] for detailed proofs of Theorems 5.1–5.2.

Theorem 5.2 *Let X_n denote the number of protected nodes in a binary search tree $\mathcal{T}_n$. For each fixed integer $k \geq 1$, there exists a polynomial $p_k(n)$ of degree k, the leading term of which is $(\frac{11}{30})^k$, such that $\mathbb{E}(X_n^k) = p_k(n)$ for all $n \geq 4k$.*

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Trie structure for Graph Sequences

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Abstract. We present a data structure extending trie structure, that we call *graph tries* that allows to store label functions defined on a graph. In this paper we analyze the performance of such structure (size, insertion costs) for labels in acyclic regular graphs such as infinite trees and lattices. We analyze means and variance of this parameters. We also show an interesting theorem that establishes the equivalence between dePoissonization and analytic continuation of coefficients.

Keywords: Data structure, combinatorics, Poissonization, asymptotic analysis, graph pattern matching

1 Introduction

Trie structures [1] have been invented in order to efficiently store and retrieve digital string sequences. They are nowadays intensively used in data storage, IP routing and DNA sequencing. In this paper we introduce a new data structure where linear string sequences are replaced by label functions in a graph. We call this new structure a *graph trie* (in short G-trie). Given an (infinite) graph $G = G(V, E)$ of vertices set V and edge set E, we define a graph sequence as a function $X\colon V \to \mathcal{A}$ where $\mathcal{A}$ is a finite alphabet. In other words X is a function that gives a label in $\mathcal{A}$ to each vertex of G. The classic trie structure on string sequence is a special case where the graph G is a directed infinite chain: $G = G(\mathbb{N}, E)$ where $E = \{(j, j+1), j \in \mathbb{N}\}$. In this paper we will focus on the case where G is an acyclic graph such as a directed M-ary lattice or a directed infinite M-ary tree, but the concept can be as well applied to graph containing cycles.

The main applications of G-trie are about space-time pattern matching in graphs. For example let's consider the graph G made of a static graph G_S where each vertex is replaced by an infinite chain. More precisely, let v be a vertex in G_S and let $v_n \in V$ be the nth element of the chain in v, let v' be another vertex in G_S; there is an edge from v_n to v'_{n+1} in G iff $v = v'$ or if there is an edge between v and v' in G_S. As an application, the static vertices could be routers in a network and the labels in a router chain be the alarm sequence the router has generated. The use of G-trie can help to detect interesting spatial correlations between alarms that could not be detected by only considering router alarm logs separately. In this case a structure generalizing suffix graph trees can be derived from G-tries.

Our aim is to analyse the asymptotic performance of G-trie build from n i.i.d label functions (each of them are a collection of i.i.d labels). We consider two parameters of interest: the size $\mathbf{S}_n$ and the insertion

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cost $\mathbf{C}_n$. We show that for regular graph of degree larger than one, the average of these quantities are respectively in n^ρ, and $n^{\rho-1}$ for some $1 < \rho < 2$. For classic tries, when G is of degree 1, these quantities are respectively in n and $\log n$. In the case where G is a regular tree, we respectively get variance estimates of $\mathbf{S}_n$ and $\mathbf{C}_n$ respectively in $n^{2\rho-1}$ and $n^{\rho-1}$ instead of n and $\log n$ for the classic tries.

The techniques used so far are analytic combinatorics [3], generating functions and asymptotic analysis via Mellin transform [2], dePoissonization [4]. Regarding the later, we show an interesting theorem that establishes an equivalence between dePoissonization and analytic continuation of coefficient functions. The plan of the paper is the following:

- A section on G-trie definition;
- A section on average size of G-tries and insertion cost in G-tries;
- A section on distribution and variance with a new theorem about dePoissonization;

2 Graph Trie specifications and structure

One vertex in V is selected to be the *anchor* vertex. The graph trie associated to the graph G is a tree where each node is associated with a path T in G starting from the anchor, and a string sequence w of labels that will be the sequence of labels encountered on this path in G. The length of w is equal to the length of T. The root of the G-trie is the null path staying on the anchor. Let $X_1, \ldots, X_n$ be a sequence of n label functions and we define the graph tries as follow. A node in the graph trie is defined by a path T and a sequence w. It exists in the graph trie iff there are at least two label functions, say X_i and X_j such that the sequences of labels reading each label functions when following the path T, are both equal to the sequence w. We take the example of the grid graph displayed in figure 1, with $\mathcal{A} = \{A, G, C, T\}$, and an example of label function. The anchor vertex is the bottom left node. Let assume that another label function shares the same values AGATTACATTC on the bottom line, then all nodes corresponding to the bottom line path associated with the prefixes of AGATTACATTC will be in the graph trie. Due to the tree like structure of both the path set in G and the string set, the graph trie has a natural tree structure. If the graph G is a regular graph of degree M and the alphabet $\mathcal{A}$ is of size A, then the graph trie is a $M \times A$-ary tree.

Like in classic tries we can insert a new label function X_{n+1} in the G-trie made of n previously inserted label functions $X_1, \ldots, X_n$. For this purpose we consider all paths in G. For each path T one proceeds in the graph trie according to the sequence of labels provided by X_{n+1}. One progresses on the path T until one reaches a leaf in the G-trie that corresponds to a single previously inserted label function, say label function X_i. At this point, one creates new nodes in the graph trie continuing the path until X_{n+1} and X_i finds a different label. Like classic tries, the G-trie is indifferent of the insertion order. We can extend to b graph tries, for b integer, by extending the definition when leaves can contain up to b label functions.

If G is a regular M-ary regular graph, and X a single label function we can define a suffix graph tree as the trie made of the label functions obtained by translating the label function X by taking different vertices as anchor. The suffix graph tree can help to find repeated patterns in space-time sequences. In particular by identifying the path with the longest common path sequence with past labels functions one can detect spatial correlations of events.

3 Analysis in the average case

In this section we assume that each label function is a set of i.i.d. random variables over $\mathcal{A}$. Let $a \in \mathcal{A}$, we denote p_a the probability that a label is identical to symbol a. Let $w \in \mathcal{A}^*$ we define $\Pr(w)$ as the

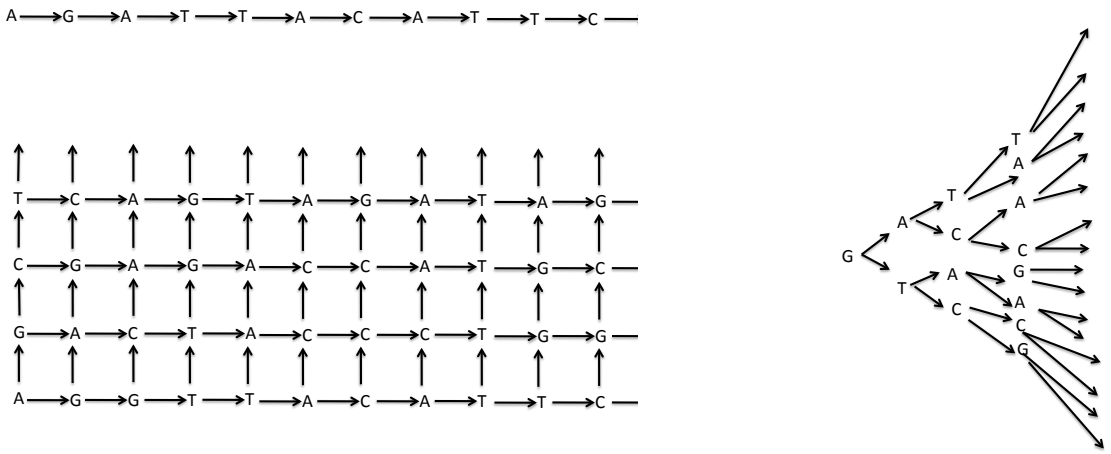

Fig. 1: (left) Label functions on regular graph, linear sequence (top), grid (bottom). (right) Label function on a binary tree, the alphabet is $\{A, G, C, T\}$.

product of the individual probabilities of its symbols. We assume that we have n i.i.d. label functions. We also assume that the graph G is acyclic. We first study the average size of the graph trie. We can see that under some parameters the average size can be infinite. We second study the distribution of its insertion cost.

3.1 The average size

Let T_k be the number of paths of length k from the anchor vertex in G. If the graph is M-ary regular, then $T_k = M^k$. Let $\mathbf{S}_n$ be the random variable denoting the size of graph trie built over n independent label functions; we define the size as the number of internal nodes. Let $S_n = E(\mathbf{S}_n)$, we have

$$S_n = \sum_k T_k \sum_{w \in \mathcal{A}^k} (1 - (1 - \Pr(w))^n - n\Pr(w)(1 - \Pr(w))^{n-1}) \,. \tag{1}$$

Notice that $S_0 = S_1 = 0$. In passing the above identity does not hold when the graph contains cycle. Indeed looping path would need to be associated with sequences w containing repeated patterns and the independence between path and i.i.d. sequences would not hold. Let $H(s) = \sum_{a \in \mathcal{A}} (p_a)^{-s}$ and $T(z) = \sum_k T_k z^k$ for z complex. We have the obvious lemma:

Lemma 1 *if* $T(H(-2)) = \infty$ *then* $S_n = \infty$ *for all* $n \geq 2$.

Proof: Since $S_n \geq S_2$ and $S_2 = T(H(-2))$. □

The case where $T(H(-2)) = \infty$ is called the *explosive case*. In the remaining of the paper we assume that we are not in the explosive case and thus $T(H(-2)) < \infty$. Notice that this implies that $M < A$ in the M-ary regular case. Let $S(z) = \sum_n S_n \frac{z^n}{n!} e^{-z}$ the Poisson generating function of the sequence S_n:

$$S(z) = \sum_k T_k \sum_{w \in \mathcal{A}^k} (1 - e^{-\Pr(w)z} - \Pr(w) z e^{-\Pr(w)z}) . \tag{2}$$

The Mellin transform $S^*(s) = \int_0^\infty S(x) x^{s-1} dx$ is defined for $\Re(s) > -2$ and satisfies $S^*(s) = -(1+s)\Gamma(s)T(H(s))$ (see [2]). If the graph is M-ary regular then $T(z) = (1 - Mz)^{-1}$. and $S(z) = 1 - (1+z)e^{-z} + M \sum_{a \in \mathcal{A}} S(p_a z)$. We get the classic asymptotic estimate, displayed in theorem 1, defining ρ such that $H(-\rho) = \frac{1}{M}$. Notice that $1 < \rho < 2$, for example when $M = 2$ and $A = 3$, uniform case: $\rho = 1 + \frac{\log 2}{\log 3}$. In passing we notice that when $M = 1$ we get the equation of classic tries [5] with $\rho = 1$.

Theorem 1 *When the graph is M-ary regular with $M > 1$ and $MH(2) < 1$ (non explosive case), we have $S_n = S(n) + O(n^{\rho-1})$ and for $z \to +\infty$ $S(z) = \sum_{k \in \mathbb{Z}} B_k z^{\beta_k} + O(z^{\beta'})$ for some arbitrary $\beta' < \beta$, $\beta_0 = \beta$ and $\forall k \in \mathbb{Z}$: $\rho' < \Re(\beta_k) \leq \rho$, the B_k is an absolutely convergent series with $B_0 = \frac{(1-\rho)\Gamma(-\rho)}{MH'(-\rho)}$. The β_k's are the roots of $MH(-s) = 1$ in the strip $\rho' < \Re(s) \leq \rho$.*

Proof: This is a retroactive application of theorems 3 and 5 and lemma 4, noticing that $1 - (1+z)e^{-z}$ satisfies the $\mathcal{JS}$ condition. □

Remark When the $\log p_a$'s are commensurable we have an infinite number of β_k such that $\Re(\beta_k) = \rho$ and this leads to classic oscillating factor of z^ρ. Otherwise $\forall k \neq 0$: $\Re(\beta_k) < \rho$, erasing the oscillations, for more details the reader can refer to [8].

3.2 Average insertion cost in a graph trie

The insertion cost is the number of nodes one must visit or create to insert a new label function in the graph trie. Those nodes form a sub-tree in the resulting graph trie. In a regular trie formed on a linear sequence, this is a branch. In a general graph G the visited nodes is also isomorphic to a connected subgraph of G. Let $\mathbf{C}_n$ be the insertion cost of a random label function in a graph trie made from n label functions (thus the new label function is the $n+1$th label function). Let $C_n = E(\mathbf{C}_n)$, we have

$$C_n = \sum_k T_k \sum_{w \in \mathcal{A}^k} \Pr(w)(1 - (1 - \Pr(w))^n) . \tag{3}$$

and the Poisson generating function $C(z) = \sum_n C_n \frac{z^n}{n!} e^{-z}$:

$$C(z) = \sum_k T_k \sum_{w \in \mathcal{A}^k} \Pr(w)(1 - e^{-\Pr(w)z}) , \tag{4}$$

with Mellin transform $C^*(s) = -\Gamma(s)T(H(s-1))$.

Theorem 2 *When G is M-ary regular, with $M > 1$ and $MH(2) < 1$, $C(z) = 1 - e^{-z} + M \sum_{a \in \mathcal{A}} p_a C(p_a z)$ and $C_n = C(n) + O(n^{\rho-2})$ with*

$$C(z) = \sum_{k \in \mathbb{Z}} D_k z^{\beta_k - 1} + O(z^{\rho' - 1}) \tag{5}$$

with D_k an absolutely convergent series with $D_0 = \frac{\Gamma(1-\rho)}{MH'(-\rho)}$.

Proof: Direct application of theorems 3 and 6 and lemma 5. □

Remark We have C_n of order $n^{\rho-1}$. The case $M = 1$ (classic tries) shows a real difference since C_n is of order $\log n$ in this case.

4 Distribution and moments

4.1 A Poisson DePoissonization equivalence

First we show an interesting generalization of the dePoissonization theorem which will greatly help our technical analysis. In [4] the authors show the following theorem;

Theorem 3 *Let an absolutely convergent series for all $z \in \mathbb{C}$ $f(z) = \sum_n a_n \frac{z^n}{n!} e^{-z}$ for some complex sequence $\{a_n\}_{n\in\mathbb{N}}$. We show that if there exists $\theta \in]0, \frac{\pi}{2}[$ and B and α such that $\forall z \in \mathbb{C}$, when $|z| \to \infty$:*

- *(i) there exists $\beta > 0$ such:*
$$|\arg(z)| \leq \theta \Rightarrow |f(z)| = O(|z|^\beta) \tag{6}$$
- *(o) there exists $\alpha < 1$ such:*
$$|\arg(z)| > \theta \Rightarrow |f(z)e^z| = O(e^{\alpha|z|}) \,, \tag{7}$$

then when $n \to \infty$:
$$a_n = f(n) - \frac{n}{2} f''(n) + O(n^{\beta-2}) \,. \tag{8}$$

The conditions (i) and (o) are also called the $\mathcal{JS}$ condition in [9]. In [6] the authors proves the following partially reverse theorem.

Theorem 4 *Let $a(x)$ an analytic function defined for $x \in \mathbb{C}$ and let $\theta \in]0, \frac{\pi}{2}[$, such that there exist β such that when $|x| \to \infty$:*
$$|\arg(x)| \leq \theta \Rightarrow |a(x)| = O(|x|^\beta) \,, \tag{9}$$

then there exists a cone for variable z such that $f(z) = \sum_n a(n) \frac{z^n}{n!} e^{-z}$ satisfies the $\mathcal{JS}$ conditions and for z the cone when $|z| \to \infty$
$$f(z) = a(z) + \frac{z}{2} a''(z) + O(z^{\beta-2}) \,. \tag{10}$$

In fact we can prove the full reverse theorem by the following lemma:

Lemma 2 *Let $f(z) = \sum_n a_n \frac{z^n}{n!} e^{-z}$, the function $f(z)$ satisfies the $\mathcal{JS}$ depoissonization conditions* **iff** *there exists a function $a(x)$ such that $\forall n \in \mathbb{N}$: $a_n = a(n)$ and $a(x)$ has a polynomial growth in a cone around the real positive axis.*

Proof: From [6] we know that the reverse is true, namely that when $a(x)$ has a polynomial growth in a cone then the Poisson generating function satisfies the $\mathcal{JS}$ depoissonization conditions. We will now prove the direct implication. To simplify the notation we denote the cone for function $a(x)$ the x-cone, and for function $f(z)$ the z-cone. We have

$$a_n = \frac{n!}{2i\pi} \oint f(z) e^z z^{-n} \frac{dz}{z} , \tag{11}$$

that can be analytically continued into

$$a(x) = \frac{\Gamma(1+x)}{2\pi} x^{-x} \int_{-\pi}^{\pi} f(xe^{i\theta}) \exp((e^{i\theta} - i\theta)x) d\theta . \tag{12}$$

The integral part is clearly an analytical function of x on the whole complex plan, and the function $\Gamma(1+x)x^{-x}e^x$ is clearly analytical in any closed x-cone of angle smaller than π (excluding an open cut for non positive real x).

Using the fact that $f(z)e^z = O(e^{\alpha|z|})$ for some $\alpha < 1$ for z outside the z-cone, and taking an x-cone of angle θ_0 such that $\cos\theta_0 > \alpha$ the contribution of $f(xe^{i\theta})e^{xe^{i\theta}}$ for $xe^{i\theta}$ outside the interval z-cone is of order $\Gamma(1+x)e^{\alpha|x|}|x^{-x}|$ which is exponentially small when we take the Stirling approximation $\Gamma(1+x) = \sqrt{2\pi x} x^x e^{-\cos\theta_0 x}(1+O(x^{-1}))$. Therefore *modulo* an exponentially small term $a(x)$ is equal to

$$a(x) = \frac{\Gamma(1+x)}{2\pi} x^{-x} e^x \int_{-\theta_1 - \arg(x)}^{\theta_1 - \arg(x)} f(xe^{i\theta}) \exp(x(e^{i\theta} - 1 - i\theta)) d\theta \tag{13}$$

with θ_1 the angle of the z-cone.

Whatever the value of $\theta_1 < \frac{\pi}{2}$, we have $\Re(e^{i\theta} - 1 - i\theta) = \cos\theta - 1 \leq -\frac{\theta^2}{2}$ and since $\Im(e^{i\theta} - 1 - i\theta) = \sin\theta - \theta = O(\theta^3)$. Thus we can take θ_0 small enough such that $\Re(x(e^{i\theta} - 1 - i\theta)) \leq -|x|\frac{\theta^2}{4}$ and therefore using $|f(z)| \leq B|z|^\beta$ for some B and β as specified in the first dePoissonization condition:

$$\left| \int_{-\theta_1 - \arg(x)}^{\theta_1 - \arg(x)} f(xe^{i\theta}) \exp(x(e^{i\theta} - 1 - i\theta)) d\theta \right| \leq B|x|^\beta \int_{-\infty}^{\infty} e^{-|x|\theta^2/4} d\theta \tag{14}$$

$$= B\frac{\sqrt{2}}{\sqrt{\pi|x|}} |x|^\beta . \tag{15}$$

Combining with the Stirling approximation of $\Gamma(1+x)$ we get $a(x) = O(x^\beta)$ for x in the x-cone, as claimed. □

This lemma is important since it basically close the loop of depoissonization theorems by giving a strict equivalence between poissonization and depoissonization. In particular we have the following corollary on Hadamard products:

Corollary 1 *Let $f(z) = \sum_n a_n \frac{z^n}{n!} e^{-z}$ and $g(z) = \sum_n b_n \frac{z^n}{n!} e^{-z}$ that both satisfy the $\mathcal{JS}$ conditions (on same cone), then $f(z) \star g(z) = \sum_n a_n b_n \frac{z^n}{n!} e^{-z}$ satisfies the $\mathcal{JS}$ condition and for z in the cone when $|z| \to \infty$:*

$$f(z) \star g(z) = f(z)g(z) + zf'(z)g'(z) + O(z^{\beta-2}) . \tag{16}$$

The author refers to [9] for an alternative handling of Hadamard products in Poisson generating functions and dePoissonization. Regarding the G-trie size and cost moment analysis we will summarize our main analytical tolls in two theorems that we will state after the following technical lemmas.

We denote $\mathcal{T}$ the operator on a function $f(z)$ such that $\mathcal{T}f(z) = \sum_{a\in\mathcal{A}} f(p_a z)$ and $\mathcal{S}$ the operator such that $\mathcal{S}f(z) = \sum_{a\in\mathcal{A}} p_a f(p_a z)$.

Lemma 3 *Let the functional equation $f(z) - M\mathcal{T}f(z) = g(z)$. If $g(z) = z^\beta$ for some $\Re(\beta) > \rho$ then $f(z) = \frac{z^\beta}{1-MH(-\beta)}$. When $g(z)$ is a function such that $|g(z)| \leq B|z|^\beta$ in a complex cone with $\beta > \rho$ then $f(z)$ satisfies $|f(z)| \leq \frac{B}{1-MH(-\beta)}|z|^\beta$ in the cone.*

Proof: We have $f(z) = \sum_{n\geq 0} M^n\mathcal{T}^n g(z)$ which converges to $\frac{z^\beta}{1-MH(-\beta)}$ when $g(z) = z^\beta$. When $|g(z)| \leq B|z|^\beta$ we get the upper bound $|f(z)| \leq \sum_{n\geq 0} M^n(H(-\beta))^n|z|^\beta$. □

Lemma 4 *Let the functional equation $f(z) - M\mathcal{T}f(z) = g(z)$. If $g(z) = O(|z|^\beta)$ when $|z| \to \infty$ and $g(z) = O(z^2)$ when $z \to 0$, in a cone for some $\beta < \rho$, then for arbitrarily chosen $\rho' < \rho$ and z in the cone we have*

$$f(z) = \sum_{k\in\mathbb{Z}} g^*(\beta_k)\frac{z^{\beta_k}}{MH'(-\beta_k)} + O(z^{\rho'}) \tag{17}$$

with the β_k, the root of $1 - MH(-s) = 0$ in the strip $\rho' < \Re(\beta_k) \leq \beta_0 = \rho$ and $g^*(s)$ is the Mellin transform of function $g(z)$.

Proof: Since $g(z) = O(z^2)$ when $z \to 0$ the series $f(z) = \sum_{n\geq 0} M^n\mathcal{T}^n g(z)$ absolutely converge and is therefore a solution. The Mellin transform $g^*(s) = \int_0^\infty g(z)z^{s-1}dz$ exists [2] for $-2 < \Re(s) < -\beta$. Since the Mellin transform $f^*(s)$ of function $f(z)$ satisfies

$$f^*(s) = \frac{g^*(s)}{1 - MH(s)} \tag{18}$$

it exists for $-2 < \Re(s) < -\rho$ and is singular on the roots of $1 - MH(s)$. The classic application of singularity on the inverse Mellin: $f(z) = \int_{c-\infty}^{c+i\infty} f^*(s)z^{-s}ds$ for $-2 < c < -\rho$ gives

$$f(z) = \sum_{k\in\mathbb{Z}} g^*(\beta_k)\frac{z^{\beta_k}}{MH'(-\beta_k)} + \int_{-\rho'-\infty}^{-\rho'+i\infty} f^*(s)z^{-s}ds \tag{19}$$

□

Lemma 5 *Let the functional equation $f(z) - M\mathcal{S}f(z) = g(z)$. If $g(z) = z^{\beta-1}$ with $\Re(\beta) > \rho$ then $f(z) = \frac{z^{\beta-1}}{1-MH(-\beta)}$. When $|g(z)| \leq B|z|^{\beta-1}$, then $f(z)$ satisfies $|f(z)| \leq \frac{B}{1-MH(-\beta)}|z|^{\beta-1}$. If $g(z) = O(z)$ when $z \to 0$ and $g(z) = O(z^{\beta-1})$ when $z \to \infty$ with $\beta < \rho$ then*

$$f(z) = \sum_{k\in\mathbb{Z}} g^*(\beta_k)\frac{z^{\beta_k-1}}{MH'(-\beta_k)} + O(z^{\rho'-1}) \tag{20}$$

Proof: It suffices to notice that $zf(z)$ is solution of $zf(z) - M\mathcal{T}zf(z) = zg(z)$ and then to apply the previous lemma. □

Theorem 5 *Let $f(z)$ be an analytic function which is $O(z^2)$ when $z \to 0$ and which satisfies the $\mathcal{JS}$ conditions for some cone θ. Then the function $g(z)$ such that $g(z) - M\mathcal{T}g(z) = f(z)$ satisfies the $\mathcal{JS}$ conditions.*

Proof: First we check the condition (i). Without loss of generality we can assume that for z in the cone: $|f(z)| \leq B|z|^\beta$ with $\beta > \rho$. Since $|\mathcal{T}f(z)| \leq B(\sum_{a\in\mathcal{A}} p_a^\beta)|z|^\beta$ and $|g(z)| \leq \frac{B}{1-MH(-\beta)}|z|^\beta$ as stated by lemma 3.

Second we check he condition (o). For z outside the cone we have $|f(z)e^z| \leq A_0|z|^2 e^{\alpha|z|}$ uniformly for some $A_0 > 0$ and $\alpha < 1$, since $f(z) = O(z^2)$ when $z \to 0$. Without loss of generality we assume that $\alpha > \cos\theta$. We have

$$|\mathcal{T}f(z)e^z| \leq A_0 \sum_{a\in\mathcal{A}} p_a^2|z|^2 e^{(\alpha p_a + (1-p_a)\cos\theta)|z|} \leq A_0(\sum_{a\in\mathcal{A}} p_a^2)|z|^2 e^{\alpha|z|} \,. \tag{21}$$

Thus $|g(z)e^z| \leq \frac{A_0}{1-MH(-2)}|z|^2 e^{\alpha|z|}$. □

We have the theorem similar to the previous theorem.

Theorem 6 *Let $f(z)$ be an analytic function which is $O(z)$ when $z \to 0$ and which satisfies the $\mathcal{JS}$ conditions for some cone θ. Then the function $g(z)$ such that $g(z) - M\mathcal{S}g(z) = f(z)$ satisfies the $\mathcal{JS}$ conditions.*

Proof: The proof is very similar to the previous proof and is not detailed here. □

4.2 Moment generating functions

Further moments and distribution are more delicate to handle, in particular when the graph G has semi-cycles (two path with same end points). Therefore we assume that G is a M-ary tree with $M > 1$.Let $P_n(u) = E(u^{\mathbf{S}_n})$ the p.g.f. of the graph trie size built from n independent label functions in a graph trie. We have

$$P_n(u) = u\left(\sum_{\mathbf{n}\in\mathbb{N}^A} \binom{n}{\mathbf{n}} \prod_{a\in\mathcal{A}} p_a^{n_a} P_{n_a}(u)\right)^M \tag{22}$$

where $\mathbf{n} = (n_a)_{a\in\mathcal{A}}$ is a A tuple of integers and $\binom{n}{\mathbf{n}}$ is the multinomial $\frac{n!}{\prod_{a\in\mathcal{A}} n_a!}$ when $\sum_{a\in\mathcal{A}} n_a = n$ or zero otherwise. Now introducing the Poisson generating function $P(z,u) = \sum_n P_n(u)\frac{z^n}{n!}e^{-z}$ it comes that

$$P(z,u) = u\left(\prod_{a\in\mathcal{A}} P(p_a z, u)\right)^{\star M} + (1-u)(1+z)e^{-z} \tag{23}$$

Regarding the insertion cost, denoting $D_n(u) = E(u^{\mathbf{C}_n})$ its p.g.f., we have for $n \geq 1$ a simpler identity:

$$D_n(u) = u\left(\sum_{a\in\mathcal{A}}\sum_{k\leq n} \binom{n}{k} p_a^k (1-p_a)^{n-k} D_k(u)\right)^M \tag{24}$$

which leads to the functional equation with the Poisson generating functions:

$$D(z,u) = u\left(\sum_{a\in\mathcal{A}} p_a D(p_a z,u)\right)^{\star M} + (1-u)e^{-z}\ . \tag{25}$$

4.3 Variances

Let $Q_n = E((S_n)^2) = P_n''(1) + P'(1)$, its Poisson generating function $Q(z)$ satisfies:

$$\begin{aligned} Q(z) &= M\mathcal{T}Q(z) + M\left(-\mathcal{T}S^2(z) + (\mathcal{T}S(z))^2\right) \\ &\quad +2M\mathcal{T}S(z) + M(M-1)\left(\mathcal{T}S(z)\right)^{\star 2} + 1 - (1+z)e^{-z}\ . \end{aligned} \tag{26}$$

Lemma 6 *Function $Q(z)$ satisfies the $\mathcal{JS}$ conditions.*

Proof: We have $Q(z)$ which satisfies $Q(z) = \mathcal{T}Q(z) + f(z)$ splitting $f(z) = f_1(z) + f_2(z)$ such

$$f_1(z) = 2M\mathcal{T}S(z) + M(M-1)\left(\mathcal{T}S(z)\right)^{\star 2} + 1 - (1+z)e^{-z} \tag{27}$$

$$f_2(z) = M\left(-\mathcal{T}S^2(z) + (\mathcal{T}S(z))^2\right)\ . \tag{28}$$

Function $f_1(z)$ although containing an Hadamard product satisfies $\mathcal{JS}$ conditions thanks to corollary 1 and is $O(z^2)$ when $z\to 0$. Function $f_2(z)$ is $O(z^2)$ when $z\to 0$ and satisfies condition (i). We rewrite

$$f_2(z) = 2M\sum_{\{a,b\}\subset\mathcal{A}} S(p_a z)S(p_b z)\ . \tag{29}$$

Under this form $\mathcal{JS}$ condition comes from the closure property in [9]. In particular to check condition (o); notice that always $a\neq b$ in the summation. Let $\alpha<1$ such that when $|z|\to\infty$ outside of the cone $|S(z)e^z| = O(e^{\alpha|z|})$, without loss of generality we assume $\alpha > \cos\theta$ where θ is the angle of the cone. We have

$$|S(p_a z)S(p_b z)e^z| = O\left(\exp\left(((p_a+p_b)\alpha) + (1-p_a-p_b)\cos\theta)|z|\right)\right)\ . \tag{30}$$

Since $p_a+p_b\leq 1$ since $a\neq b$ we have $|S(p_a z)S(p_b z)e^z| = O(e^{\alpha|z|})$. Thus $f(z)$ is $O(z^2)$ when $z\to 0$ and satisfies the $\mathcal{JS}$ conditions; by application of theorem 5. □

Using the classic Poisson variance [4][9] defined as $V(z) = Q(z) - S^2(z)$ we get

$$\begin{aligned} V(z) &= M\mathcal{T}V(z) - 2S(z)(1+z)e^{-z} + (1+z)^2e^{-2z} - (1+z)e^{-z} \\ &\quad +M(M-1)\left(\left(\mathcal{T}S(z)\right)^{\star 2} - \left(\mathcal{T}S(z)\right)^2\right) \end{aligned} \tag{31}$$

Lemma 7 *For z in a cone around the real positive axis we have*

$$\left(\mathcal{T}S(z)\right)^{\star 2} - \left(\mathcal{T}S(z)\right)^2 = \sum_{k\in\mathbb{Z}} \frac{1}{M^2} F_k z^{\gamma_k} + O(z^{\rho+\rho'-1}) \tag{32}$$

with $\forall k\in\mathbb{Z}:\ \rho+\rho'-1 < \Re(\gamma_k) \leq \gamma_0 = 2\rho-1$ and $\{F_k\}_{i\in\mathbb{N}}$ is an absolute convergent series obtained from the expansion of $\left(\sum_{k\in\mathbb{Z}}\beta_k B_k z^{\beta_k-1}\right)^2 z$.

Remark Thus the left hand side function is $O(z^{2\rho-1})$. Notice that $2\rho-1 \geq \rho$.

Proof: Since the function $f(z) = \mathcal{T}S(z)$ satisfies the $\mathcal{JS}$ conditions, corollary 1 applies, *i.e.* ,

$$(\mathcal{T}S(z))^{\star 2} - (\mathcal{T}S(z))^2 = z(f'(z))^2 + O(z^{2\rho-2}) \; . \tag{33}$$

We know that $M(\mathcal{T}S(z))' + ze^{-z} = S'(z)$, and $S(z) = \sum_{k\in\mathbb{Z}} B_k z^{\beta_k} + O(z^{\rho'})$. Thus

$$(f'(z))^2 = \frac{1}{M^2} \sum_{(k,k')\in\mathbb{Z}^2} \beta_k B_k \beta_{k'} B_{k'} z^{\beta_k+\beta_{k'}-2} + O(z^{\rho'+\rho-2}) \; . \tag{34}$$

Rewriting in $(f'(z))^2 = \frac{1}{M^2}\sum_{i\in\mathbb{Z}} F_i z^{\gamma_i - 1} + O(z^{\rho'+\rho-2})$ with $\gamma_0 = 2\rho - 1$, yields the result. □

Theorem 7 *For z in a cone around the real axis we have*

$$V(z) = \frac{M^2 - M}{M^2} \sum_i \frac{F_i}{1 - MH(-\gamma_i)} z^{\gamma_i} + O(z^{\rho+\rho'-1}) \tag{35}$$

with $1 < \rho' < \rho$.

Remark Thus the Poisson variance $V(z)$ is of order $z^{2\rho-1}$ greater than the order of the Poisson mean $S(z)$. However the standard deviation is in $z^{\rho-1/2}$ is smaller than $S(z)$ thus we conjecture a normal limiting distribution here.

Proof: We have $\rho < \rho + \rho' - 1$, which is always possible since $\rho < 2\rho - 1$. We have basically

$$V(z) = M\mathcal{T}V(z) + \frac{(M-1)M}{M^2} \sum_i F_i z^{\gamma_i} + g(z) \tag{36}$$

with $g(z)$ which is $O(z^{\rho+\rho'-1})$ when $z \to \infty$ in a cone and is $O(z^{2\rho-1})$ when $z \to 0$, in fact in $O(z^{\min\{2,2\rho-1\}})$. Therefore we have

$$V(z) = \frac{(M-1)M}{M^2} \sum_i \frac{F_i}{1 - MH(-\gamma_i)} z^{\gamma_i} + h(z) \tag{37}$$

with $h(z)$ the solution of $h(z) = M\mathcal{T}h(z) + g(z)$. Using lemma 3 we have $h(z) = O(z^{\rho+\rho'-1})$. □

Therefore we can conclude our variance analysis by the following theorem

Theorem 8 *The variance V_n of the size satisfies*

$$V_n = \sum_{k\in\mathbb{Z}} \left(\frac{(M-1)M}{M^2(1 - MH(-\gamma_k))} - 1 \right) F_k n^{\gamma_k} + O(n^{\rho'+\rho-1}) \tag{38}$$

For some $1 < \rho' < \rho$.

In the particular case where the p_a are all identical then the n^{γ_k} terms cancel and V_n expands in n^{β_k} with coefficients expressed as a calculable convergent series and the error term is in $n^{2\rho-2}$.

Remark The variance V_n is in general of order $n^{2\rho-1}$, but when the probabilities p_a's are uniforms it is in n^ρ.

Proof: This a basic application of [4] regarding variance, and also [9]. Since $Q(z)$ satisfies the $\mathcal{JS}$ conditions we have

$$Q_n = Q(n) - \frac{n}{2}Q'(n) + O(n^{2\rho-2}) \tag{39}$$

since $Q(n) = V(n) + S^2(n)$ is $O(n^{2\rho})$, it is proven in [4] and [9] that $V_n = V(n) - n(S'(n))^2 + O(n^{2\rho-2})$ and thus we get the expansion displayed in the theorem. In general we don't expect a systematic cancelation of the coefficients. Anyhow such cancelation occurs when the p_a's are all equal to $\frac{1}{A}$. Indeed, in this case $H(s) = A^{1-s}$ and since the γ_i are all of the form $\beta_k + \beta_{k'} - 1$, we have $H(-\gamma_i) = A^{1-\beta_k} \times A^{1-\beta_{k'}}$. Since $\forall k \in \mathbb{Z}$: $A^{1-\beta_k} = \frac{1}{M}$, then $M^2(1 - MH(-\gamma_i)) = M(M-1)$.

To get the expansion in the uniform case we borrow some methodology of [9] and define $V_B(z) = V(z) - z(S'(z))^2$. When the probabilities p_a's are uniform we have the functional equations:

$$\begin{aligned} V_B(z) &= M\mathcal{T}V_B(z) - 2S(z)(1+z)e^{-z} + (1+z)^2e^{-2z} - (1+z)e^{-z} + z^3e^{-2z} + 2z^2S'(z)e^{-z} \\ &\quad M(M-1)\left(A^2(S(\frac{z}{A}))^{*2} - A^2(S(\frac{z}{A}))^2 - z(S'(\frac{z}{A}))^2\right) . \end{aligned} \tag{40}$$

Since $A^2(S(\frac{z}{A}))^{*2} - A^2(S(\frac{z}{A}))^2 = z(S'(\frac{z}{A}))^2 + O(z^{2\rho-2})$ it turns out that $V_B(z) - MV_B(z) = g(z)$ with $g(z) = O(z^{2\rho-2})$. Since $g(z) = O(z^2)$ when $z \to 0$ and $2\rho - 2 < \rho$ we can apply lemma 4 to get that $V_B(z) = O(z^\rho)$ and $V_n = O(n^\rho)$. □

Remark The variance V_n is in general in $O(n^{2\rho-1})$ a greater order than the mean S_n, but the standard deviation $\sqrt{V_n}$ is of order smaller than the mean, thus there is hope to get a normal limiting distribution. For the uniform case mean and variance are of same order n^ρ and in this case the central limit theorem should held via a standard application of the contraction method; see Theorem 5.2 in [7].

Theorem 9 *The variance W_n of the insertion cost in a G-trie already containing n label functions has the asymptotic expansion*

$$W_n = \sum_{k\in\mathbb{Z}} G_k n^{\beta_k - 1} + O(n^{\rho'+\rho-2}) \tag{41}$$

with the G_k's a calculable absolutely convergent series.

Remark The variance of insertion cost W_n is of order $n^{\rho-1}$, thus of the same order of the mean, the contraction method of [7] can apply for proving the normal limiting convergence.

Proof: Let $R_n = E((C_n)^2) = D_n''(1) + D'(1)$, its Poisson generating function $R(z)$ satisfies:

$$R(z) = \mathcal{S}R(z) - 2\mathcal{S}C(z) + M(M-1)\left(\sum_{a\in\mathcal{A}} \mathcal{S}C(z)\right)^{\star 2} \tag{42}$$

By using theorem 6 we know that $R(z)$ is $O(z)$ when $z \to 0$ and is $O(z^{2\rho-2})$ satisfies the $\mathcal{JS}$ conditions.

The Poisson variance $W(z)$ satisfies

$$W(z) = M\mathcal{S}W(z) + e^{2z} - e^{-z} - 2C(z)e^{-z} + M(M-1)\left((\mathcal{S}C(z))^{\star 2} - (\mathcal{S}C(z))^2\right) \tag{43}$$

but since $(\mathcal{S}C(z))^{\star 2} - (\mathcal{S}C(z))$ is in $z^{2\rho-3}$ when $z \to \infty$, an order smaller than $z^{\rho-1}$, by virtue of lemma 5 we have the expansion displayed in the theorem. The coefficients G_k are obtained by the Mellin transform of the right-hand side of (43). The expansion $W_n = W(n) - n(C'(n))^2 + O(n^{2\rho-4})$ does not change these coefficients since the order of $n(C'(n))^2$ is $n^{2\rho-3}$. □

5 Conclusion

We have introduced a new data structure, called graph trie, that mixes graphs and sequences. It is a generalization of classic trie. The evaluation of the performance via generating function, mean and variance, gives rise to an interesting combination of difference equations and Hadamard products of Poisson generating functions. The order of magnitude of mean and variance are significantly different than their counterpart in classic tries. In passing we close the loop of analytic depoisssonization by showing that the dePoissonization conditions are strictly equivalent to the polynomial growth of the analytic continuation of the coefficients in a cone. We give an expression of the moment generating functions and we conjecture that they give rise to limiting normal distribution like with classic regular tries.

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Asymptotic normality of fringe subtrees and additive functionals in conditioned Galton–Watson trees.

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Abstract. We consider conditioned Galton–Watson trees and show asymptotic normality of additive functionals that are defined by toll functions that are not too large. This includes, as a special case, asymptotic normality of the number of fringe subtrees isomorphic to any given tree, and joint asymptotic normality for several such subtree counts. The offspring distribution defining the random tree is assumed to have expectation 1 and finite variance; no further moment condition is assumed.

Keywords: Fringe subtrees; conditioned Galton–Watson trees; random trees; asymptotic normality; toll functions.

1 Introduction

Given a rooted tree T and a node v in T, let T_v be the subtree of T rooted at v, i.e., the subtree consisting of v and all its descendents. Such subtrees are called *fringe subtrees*. The *random fringe subtree* T_* is the random rooted tree obtained by taking the subtree T_v at a uniformly random node v in T, see **(author?)** [1].

We let, for $T, T' \in \mathfrak{T}$,

$$n_{T'}(T) := \bigl|\{v \in T' : T_v = T'\}\bigr|, \tag{1.1}$$

i.e., the number of subtrees of T that are equal (i.e., isomorphic to) to T'. Then the distribution of T_* is given by

$$\mathbb{P}(T_* = T') = n_{T'}(T)/|T|, \qquad T' \in \mathfrak{T}. \tag{1.2}$$

Thus, to study the distribution of T_* is equivalent to studying the numbers $n_{T'}(T)$.

A related point of view is to let f be a functional of rooted trees, i.e., a function $f : \mathfrak{T} \to \mathbb{R}$, and for a tree $T \in \mathfrak{T}$ consider the sum

$$F(T) = F(T; f) := \sum_{v \in T} f(T_v). \tag{1.3}$$

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Thus,

$$F(T)/|T| = \mathbb{E}\, f(T_*). \tag{1.4}$$

One important example of this is to take $f(T) = \mathbf{1}\{T = T'\}$, the indicator function that T equals some given tree $T' \in \mathfrak{T}$; then $F(T) = n_{T'}(T)$ and (1.4) reduces to (1.2). Conversely, for any f,

$$F(T) = \sum_{T' \in \mathfrak{T}} f(T') n_{T'}(T); \tag{1.5}$$

hence any $F(T)$ can be written as a linear combination of the subtree counts $n_{T'}(T)$, so the two points of views are essentially equivalent.

Remark 1.1 Functionals F that can be written as (1.3) for some f are called *additive functionals*. The definition (1.3) can also be written recusively as

$$F(T) = f(T) + \sum_{i=1}^{d} F(T_i), \tag{1.6}$$

where $T_1, \dots, T_d$ are the branches (i.e., the subtrees rooted at the children of the root) of T. In this context, $f(T)$ is often called a *toll function*. (One often considers toll functions that depend only on the size $|T|$ of T, but that is not always the case. We emphasise that we allow more general functionals f.)

Note that when T is a random tree, as it was in [1] and will be in the present paper, $F(T)$ is a random variable. In particular, $n_{T'}(T)$ is a random variable for each $T' \in \mathfrak{T}$, and thus the distribution of T_*, which is given by (1.2), is a random probability distribution on $\mathfrak{T}$. Note that (1.2) now reads

$$\mathbb{P}\big(T_* = T' \mid T\big) = n_{T'}(T)/|T| \tag{1.7}$$

and that similarly (1.4) then has to be replaced by

$$F(T)/|T| = \mathbb{E}\big(f(T_*) \mid T\big). \tag{1.8}$$

The random trees that we consider in this paper are conditioned Galton–Watson trees. (Related results for some other random trees are given by Fill and Kapur [9, 10] (m-ary search trees under different models) and Holmgren and Janson [11] (random binary search trees and random recursive trees).) The Galton–Watson trees are defined using an offspring distribution ξ and we assume throughout the paper that $\mathbb{E}\,\xi = 1$ and $\sigma^2 := \operatorname{Var}\xi$ is finite (and non-zero). We denote the probability distribution of ξ by $(p_k)_0^\infty$, i.e., $p_k := \mathbb{P}(\xi = k)$.

The results in **(author?)** [1] focus on convergence (in probability), as $|T| \to \infty$, of the fringe subtree distribution for suitable classes of random trees T, which by (1.8) is equivalent to convergence of $F(T)/|T|$ or $\mathbb{E}\, F(T)/|T|$ for suitable functionals f. For the conditioned Galton–Watson trees studied here, this is stated in the following theorem from [15, Theorem 7.12], improving earlier results by **(author?)** [1] and Bennies and Kersting [2].

Theorem 1.2 (Aldous, et al.) *Let $\mathcal{T}_n$ be a conditioned Galton–Watson tree with n nodes, defined by an offspring distribution ξ with $\mathbb{E}\,\xi = 1$, and let $\mathcal{T}$ be the corresponding unconditioned Galton–Watson tree. Then, as $n \to \infty$: For every fixed tree T,*

$$\frac{n_T(\mathcal{T}_n)}{n} = \mathbb{P}(\mathcal{T}_{n,*} = T \mid \mathcal{T}_n) \xrightarrow{\mathrm{p}} \mathbb{P}(\mathcal{T} = T). \tag{1.9}$$

Equivalently, for any bounded functional f on $\mathfrak{T}$,

$$\frac{F(\mathcal{T}_n)}{n} = \mathbb{E}\, f\big(\mathcal{T}_{n,*} \mid \mathcal{T}_n\big) \xrightarrow{\mathrm{p}} \mathbb{E}\, f(\mathcal{T}). \tag{1.10}$$

Theorem 1.2 is a law of large numbers for $F(\mathcal{T}_n)$. In the present paper we take the next step and give a central limit theorem. This includes, as a special case, (joint) normal convergence of the subgraph counts $n_{T'}(T)$, see Corollary 1.4.

Theorem 1.3 *Let $\mathcal{T}_n$ be a conditioned Galton–Watson tree of order n with offspring distribution ξ, where $\mathbb{E}\,\xi = 1$ and $0 < \sigma^2 := \operatorname{Var}\xi < \infty$, and let $\mathcal{T}$ be the corresponding unconditioned Galton–Watson tree. Suppose that $f : \mathfrak{T} \to \mathbb{R}$ is a functional of rooted trees such that $\mathbb{E}\,|f(\mathcal{T})| < \infty$, and let $\mu := \mathbb{E}\, f(\mathcal{T})$.*

(i) *If $\mathbb{E}\, f(\mathcal{T}_n) \to 0$ as $n \to \infty$, then*

$$\mathbb{E}\, F(\mathcal{T}_n) = n\mu + o\big(\sqrt{n}\big). \tag{1.11}$$

(ii) *If*

$$\mathbb{E}\, f(\mathcal{T}_n)^2 \to 0 \tag{1.12}$$

as $n \to \infty$, and

$$\sum_{n=1}^{\infty} \frac{\sqrt{\mathbb{E}(f(\mathcal{T}_n)^2)}}{n} < \infty, \tag{1.13}$$

then

$$\operatorname{Var} F(\mathcal{T}_n) = n\gamma^2 + o(n) \tag{1.14}$$

where

$$\gamma^2 := 2\,\mathbb{E}\Big(f(\mathcal{T})\big(F(\mathcal{T}) - |\mathcal{T}|\mu\big)\Big) - \operatorname{Var} f(\mathcal{T}) - \mu^2/\sigma^2 \tag{1.15}$$

is finite; moreover,

$$\frac{F(\mathcal{T}_n) - n\mu}{\sqrt{n}} \xrightarrow{\mathrm{d}} N(0, \gamma^2). \tag{1.16}$$

By (1.11), we may replace $n\mu$ by the exact mean $\mathbb{E}\, F(\mathcal{T}_n)$ in (1.16).

Special cases of Theorem 1.3 have been proved before, by various methods. A simple example is the number of leaves in $\mathcal{T}_n$, shown to be normal by Kolchin [19], see Example 2.1. (See also **(author?)** [1, Remark 7.5.3].) Wagner [26] considered random labelled trees (the case $\xi \sim \mathrm{Po}(1)$) and showed Theorem 1.3 (and convergence of all moments) for this case, assuming further that f is bounded and $\mathbb{E}\,|f(\mathcal{T}_n)| = O(c^n)$ for some $c < 1$ (a stronger assumption that our (1.12)–(1.13)).

Theorem 1.3 is stated for a single functional F, but joint convergence for several different F (each satisfying the conditions in the theorem) follows immediately by the Cramér–Wold device. One example is the following corollary for the subtree counts (1.1). (We state the result as asymptotic normality for the infinite family of all subtree counts; by definition, this is the same as asymptotic normality for any finite subfamily.)

Corollary 1.4 *The subtree counts $n_T(\mathcal{T}_n)$, $T \in \mathfrak{T}$, are asymptotically jointly normal. More precisely, let $\pi_T := \mathbb{P}(\mathcal{T} = T)$,*

$$\gamma_{T,T} := \pi_T - \bigl(2|T| - 1 + \sigma^{-2}\bigr)\pi_T^2, \tag{1.17}$$

and, for $T_1 \neq T_2$,

$$\gamma_{T_1,T_2} := n_{T_2}(T_1)\pi_{T_1} + n_{T_1}(T_2)\pi_{T_2} - \bigl(|T_1| + |T_2| - 1 + \sigma^{-2}\bigr)\pi_{T_1}\pi_{T_2}. \tag{1.18}$$

Then, for any trees $T, T_1, T_2 \in \mathfrak{T}$,

$$\mathbb{E}\, n_T(\mathcal{T}_n) = n\pi_T + o\bigl(\sqrt{n}\bigr), \tag{1.19}$$

$$\operatorname{Cov}\bigl(n_{T_1}(\mathcal{T}_n), n_{T_2}(\mathcal{T}_n)\bigr) = n\gamma_{T_1,T_2} + o(n), \tag{1.20}$$

$$\frac{n_T(\mathcal{T}_n) - n\pi_T}{\sqrt{n}} \xrightarrow{\mathrm{d}} Z_T, \tag{1.21}$$

the latter jointly for all $T \in \mathfrak{T}$, where Z_T are jointly normal with mean $\mathbb{E}\, Z_T = 0$ and covariances $\operatorname{Cov}\bigl(Z_{T_1}, Z_{T_2}\bigr) = \gamma_{T_1,T_2}$.

We say that the functional f has *finite support* if $f(T) \neq 0$ only for finitely many trees $T \in \mathfrak{T}$; equivalently, there exists a constant K such that $f(T) = 0$ unless $|T| \leqslant K$. Note that a functional with finite support necessarily is bounded. By (1.5), the additive functionals F that arise from functionals f with finite support are exactly the finite linear combinations of subgraph counts $n_{T'}(T)$. Hence Corollary 1.4 is equivalent to asymptotic normality (with convergence of mean and variance) for $F(\mathcal{T}_n)$ whenever f has finite support. The asymptotic variance $\gamma^2 = \lim_{n\to\infty} \operatorname{Var} F(\mathcal{T}_n)/n$ is given by (1.15) or, equivalently, follows from (1.17)–(1.18).

Remark 1.5 The condition (1.12) in Theorem 1.3(ii) is equivalent to $\mathbb{E}\, f(\mathcal{T}_n) \to 0$ and $\operatorname{Var} f(\mathcal{T}_n) \to 0$, and it implies $\mathbb{E}\,|f(\mathcal{T}_n)| \to 0$ as assumed in (i). Both this condition and (1.13) say that $f(T)$ is (on the average, at least) decreasing as $|T| \to \infty$, but a rather slow decrease is sufficient; for example, the theorem applies when $f(T) = 1/\log^2 |T|$ (for $|T| > 1$). In particular, it is *not* enough to assume that f is a bounded functional. For a trivial example, let $f(T) = 1$ for all trees T; then $F(T) = |T|$ so $F(\mathcal{T}_n) = n$ is constant, with mean n and variance 0. However, the first two terms on the right-hand side of (1.15) vanish, so $\gamma^2 = -\sigma^{-2} < 0$, which is absurd for an asymptotic variance, and (1.14) and (1.16) fail.

Remark 1.6 If we go further and allow $f(T)$ that grow with the size $|T|$, we cannot expect the results to hold. Fill and Kapur [8] have made an interesting and illustrative study (for certain f) of the case of binary trees, which is the case $\xi \sim \mathrm{Bin}(2, 1/2)$ of conditioned Galton–Watson tree, and presumably typical for other conditioned Galton–Watson trees as well. They show that for $f(T) = \log |T|$, $F(\mathcal{T}_n)$ is asymptotically normal, but with a variance of the order $n \log n$. And if $f(T)$ increases more rapidly, with $f(T) = |T|^\alpha$ for some $\alpha > 0$, then the variance is of order $n^{1+2\alpha}$, and $F(\mathcal{T}_n)$ has, after normalization, a non-normal limiting distribution.

Intuitively, our conditions are such that the sum (1.3) is dominated by the many small subtrees T_v; since different parts of our trees are only weakly dependent on each other, this makes asymptotic normality plausible. For a toll function f that grows too rapidly with the size of T, the sum (1.3) will on the contrary be dominated by large subtrees, which are more strongly dependent, and then other limit distributions will appear.

Remark 1.7 For the m-ary search tree ($2 \leqslant m \leqslant 26$) and random recursive tree a similar theorem holds, but there $f(T)$ may grow almost as $|T|^{1/2}$, see Hwang and Neininger [13] (binary search tree, f depends on $|T|$ only), Fill and Kapur [9] (m-ary search tree, f depends on $|T|$ only), Holmgren and Janson [11] (binary search tree and random recursive tree, general f). A reason for this difference is that for a conditioned Galton–Watson tree, the limit distribution of the size of the fringe subtree, which by Theorem 1.2 is the distribution of $|\mathcal{T}|$, decays rather slowly, with $\mathbb{P}(|\mathcal{T}| = n) \asymp n^{-3/2}$. while the corresponding limit distribution for fringe subtrees in a binary search tree or random recursive tree decays somewhat faster, as n^{-2}, see **(author?)** [1]. Cf. also the related results in Fill, Flajolet and Kapur [7, Theorem 13 and 14], showing a similar contrast (but at orders $n^{1/2}$ and n) between uniform binary trees (an example of a conditioned Galton–Watson tree) and binary search trees for the asymptotic expectation of an additive functional.

We can weaken the conditions on the size of f if we assume that f is "nice". We say that a functional $f(T)$ on $\mathfrak{T}$ is *local* (with *cut-off* M) if it depends only on the first M generations of T, for some $M < \infty$, i.e., if we let $T^{(M)}$ denote T truncated at height M, then $f(T) = f(T^{(M)})$. More generally, we say that f is *weakly local* (with *cut-off* M) if $f(T)$ depends on $|T|$ and $T^{(M)}$ for some M.

Theorem 1.8 *Let $\mathcal{T}_n$ be a conditioned Galton–Watson tree as in Theorem 1.3. Suppose that $f : \mathfrak{T} \to \mathbb{R}$ is a bounded and local functional. Then the conclusions* (1.11)*,* (1.14) *and* (1.16) *hold for some $\gamma^2 < \infty$.*

More generally, the same holds if f is a bounded and weakly local functional such that $\mathbb{E}\, f(\mathcal{T}_n) \to 0$ and $\sum_n |\mathbb{E}\, f(\mathcal{T}_n)|/n < \infty$.

Remark 1.9 The asymptotic variance γ^2 equals 0 in two trivial cases:

(i) $f(\mathcal{T}) = F(\mathcal{T}) = F(\mathcal{T}_n) = 0$ a.s.;

(ii) $\{k : p_k > 0\} = \{0, r\}$ for some $r > 1$ and $f(\mathcal{T}) = a\mathbf{1}\{|\mathcal{T}| = 1\}$ for some real a; then $F(\mathcal{T}_n) = a(n - (n-1)/r)$ is deterministic.

We can show, using [17], that if f has finite support, then $\gamma^2 > 0$ except in these trivial cases. For general f, we do not know whether $\gamma^2 = 0$ is possible except in such trivial cases. (See Example 2.2 for another trivial case. For some f, it may be possible to use the simple criterion in [6] to show $\gamma^2 > 0$, but in general, our f is not of the type studied there so more research is needed.)

This is an extended abstract of [16], where proofs and further details are given.

2 Examples

Example 2.1 The perhaps simplest non-trivial example is to take $f(T) = \mathbf{1}\{|T| = 1\}$. Then $F(T)$ is the number of leaves in T. We have $\mathbb{E}\, f(\mathcal{T}) = \mathbb{P}(|\mathcal{T}| = 1) = \mathbb{P}(\xi = 0) = p_0$.

Theorems 1.3 and 1.8 both apply and show asymptotic normality of $F(\mathcal{T}_n)$, and so does Corollary 1.4 since $F(T) = n_\bullet(T)$, where $\bullet$ is the tree of order 1; (1.15) yields

$$\gamma^2 = 2p_0(1-p_0) - p_0(1-p_0) - p_0^2/\sigma^2 = p_0 - (1+\sigma^{-2})p_0^2, \tag{2.1}$$

which also is seen directly from (1.17). The asymptotic normality in this case (and a local limit theorem) was proved by Kolchin [19, Theorem 2.3.1]. By Remark 1.9, or by a simple calculation directly from (2.1), $\gamma^2 > 0$ except in the case $p_r = 1 - p_0 = 1/r$ for some $r \geqslant 2$ when all nodes in $\mathcal{T}_n$ have 0 or r children (full r-ary trees) and $n_\bullet(\mathcal{T}_n) = n - (n-1)/r$ is deterministic.

Example 2.2 A natural extension is to consider the number of nodes of outdegree r, for some given integer $r \geqslant 1$; we denote this by $n_r(T)$. Then $n_r(T) = F(T)$ with $f(T) = 1$ if the root of T has degree r, and $f(T) = 0$ otherwise. Asymptotic normality of $n_r(\mathcal{T}_n)$ too was proved by Kolchin [19, Theorem 2.3.1], with

$$n^{-1/2}\bigl(F(\mathcal{T}_n) - np_r\bigr) \xrightarrow{\mathrm{d}} N\bigl(0, \gamma_r^2\bigr) \tag{2.2}$$

where

$$\gamma_r^2 = p_r(1-p_r) - (r-1)^2 p_r^2/\sigma^2, \tag{2.3}$$

see also Janson [14] (joint convergence and moment convergence, assuming at least $\mathbb{E}\,\xi^3 < \infty$), Minami [23] and Drmota [5, Section 3.2.1] (both assuming an exponential moment) for different proofs.

It is easily checked that for $r > 0$, $\gamma_r > 0$ except in the two trivial cases $p_r = 0$, when $n_r(\mathcal{T}_n) = 0$, and $p_r = 1 - p_0 = 1/r$, when all nodes have 0 or r children (full r-ary trees) and $n_r(\mathcal{T}_n) = (n-1)/r$ is deterministic.

In this example,

$$\mathbb{E}\, f(\mathcal{T}_n) = \mathbb{P}(\text{the root of } \mathcal{T}_n \text{ has degree } r) \to r p_r. \tag{2.4}$$

see [18] and [15, Theorem 7.10]. Hence (1.12) and (1.13) both fail, and we cannot apply Theorem 1.3. (It does not help to subtract a constant, since $f(\mathcal{T}_n)$ is an indicator variable.) However, f is a bounded local functional. Hence Theorem 1.8 applies and yields (2.2), together with convergence of mean and variance, for some γ_r. It is immediate from the definition of the Galton–Watson tree $\mathcal{T}$ that

$$\mu := \mathbb{E}\, f(\mathcal{T}) = \mathbb{P}(\text{the root of } \mathcal{T} \text{ has degree } r) = p_r. \tag{2.5}$$

Similarly, we obtain joint convergence for different r by Theorem 1.8 and the Cramér–Wold device. (It seems that joint convergence has not been proved before without assuming at least $\mathbb{E}\,\xi^3 < \infty$.)

Nevertheless, this result is a bit disappointing, since we do not obtain the explicit formula (2.3) for the variance. Theorem 1.8 shows existence of γ^2 but the formula (3.19) given by the proof is rather involved, and we do not know any way to derive (2.3) from it. In this example, because of the simple structure of f, we can use a special argument and derive both (2.3) and the asymptotic covariance γ_{rs} for two different outdegrees $r, s \geqslant 0$:

$$\gamma_{rs} = -p_r p_s - (r-1)(s-1)p_r p_s/\sigma^2, \qquad r \neq s, \tag{2.6}$$

(as proved by [14] provided $\mathbb{E}\,\xi^3 < \infty$).

Note that by (2.2), $\liminf_{n\to\infty} n^{-1/2}\,\mathbb{E}\,|F(\mathcal{T}_n) - n\mu| \geqslant (2/\pi)^{1/2}\gamma_r$, so assuming $\gamma_r > 0$, $\mathbb{E}\,|F(\mathcal{T}_n) - n\mu| \geqslant c_1 n^{1/2}$, at least for large n. It is easily seen that also $\mathbb{E}\, f(\mathcal{T}_n)|F(\mathcal{T}_n) - n\mu| \geqslant c_2 n^{1/2}$, at least for large n; hence, using $\mathbb{P}(|\mathcal{T}| = n) \sim cn^{-3/2}$,

$$\mathbb{E}\bigl|f(\mathcal{T})\bigl(F(\mathcal{T}) - |T|\mu\bigr)\bigr| = \sum_{n=1}^{\infty} \mathbb{P}(|\mathcal{T}| = n)\,\mathbb{E}\bigl|f(\mathcal{T}_n)\bigl(F(\mathcal{T}_n) - n\mu\bigr)\bigr| = \infty,$$

which shows that the expectation in (1.15) does not exist, so γ^2 is not given by (1.15).

Example 2.3 A node in a (rooted) tree is said to be *protected* if it is neither a leaf nor the parent of a leaf. Asymptotics for the expected number of protected nodes in various random trees, including several examples of conditioned Galton–Watson trees, have been given by e.g. Cheon and Shapiro [3] and Mansour

[22], and convergence in probability of the fraction of protected nodes is proved for general conditioned Galton–Watson trees by Devroye and Janson [4].

We can now extend this to asymptotic normality of the number of protected nodes, in any conditioned Galton–Watson tree $\mathcal{T}_n$ with $\mathbb{E}\,\xi = 1$ and $\sigma^2 < \infty$. We define $f(T) := \mathbf{1}\{\text{the root of } T \text{ is protected}\}$, and then $F(T)$ is the number of protected nodes in T. Since f is a bounded and local functional, Theorem 1.8 applies and shows asymptotic normality of $F(\mathcal{T}_n)$.

The asymptotic mean $\mu = \mathbb{E}\, f(\mathcal{T})$ is easily calculated, see [4] where also explicit values are given for several examples of conditioned Galton–Watson trees. However, as in Example 2.2, we do not see how to find an explicit value of γ^2 from (3.19) (although it ought to be possible to use these for numerical calculation for a specific offspring distribution). It seems possible that there is some other argument to find γ^2, but we have not pursued this and we leave it as an open problem to find the asymptotic variance γ^2, for example for uniform labelled trees or uniform binary trees.

Example 2.4 Wagner [26] studied the number $s(T)$ of arbitrary subtrees (not necessarily fringe subtrees) of the tree T, and the number $s_1(T)$ of such subtrees that contain the root. He noted that if T has branches $T_1, \dots, T_d$, then $s_1(T) = \prod_{i=1}^{d}(1 + s_1(T_i))$ and thus

$$\log\bigl(1 + s_1(T)\bigr) = \log\bigl(1 + s_1(T)^{-1}\bigr) + \sum_{i=1}^{d} \log\bigl(1 + s_1(T_i)\bigr), \tag{2.7}$$

so $\log\bigl(1 + s_1(T)\bigr)$ is an additive functional with toll function $f(T) = \log\bigl(1 + s_1(T)^{-1}\bigr)$, see (1.6). Wagner [26] used this and the special case of Theorem 1.3 shown by him to show asymptotic normality of $\log\bigl(1 + s_1(\mathcal{T}_n)\bigr)$ (and thus of $\log s_1(\mathcal{T}_n)$) for the case of uniform random labelled trees (which is $\mathcal{T}_n$ with $\xi \sim \mathrm{Po}(1)$). We can generalize this to arbitrary conditioned Galton–Watson trees with $\mathbb{E}\,\xi = 1$ and $\mathbb{E}\,\xi^2 < \infty$ by Theorem 1.3, noting that $|f(\mathcal{T}_n)| \leqslant s_1(\mathcal{T}_n)^{-1} \leqslant n^{-1}$ (since $s_1(T) \geqslant |T|$ by considering only paths from the root); hence (1.12)–(1.13) hold. Consequently,

$$\bigl(\log s_1(\mathcal{T}_n) - n\mu\bigr)/\sqrt{n} \xrightarrow{\mathrm{d}} N(0, \gamma^2) \tag{2.8}$$

for some $\mu = \mathbb{E}\log\bigl(1 + s_1(\mathcal{T})^{-1}\bigr)$ and γ^2 given by (1.15) (both depending on the distribution of ξ); Wagner [26] makes a numerical calculation of μ and σ^2 for his case.

Furthermore, as noted in [26], $s_1(T) \leqslant s(T) \leqslant |T| s_1(T)$ for any tree (an arbitrary subtree is a fringe subtree of some subtree containing the root), and thus the asymptotic normality (2.8) holds for $\log s(\mathcal{T}_n)$ too.

Similarly, the example by Wagner [26, pp. 78–79] on the average size of a subtree containg the root generalizes to arbitrary conditioned Galton–Watson trees (with $\mathbb{E}\,\xi^2 < \infty$), showing that the average size is asymptotically normal with expectation $\sim \mu n$ and variance $\sim \gamma^2 n$ for some $\mu > 0$ and γ^2; we omit the details. We conjecture that the same is true for the average size of an arbitrary subtree, as shown in [26] for the case considered there. (Note that a uniformly random arbitrary subtree thus is much larger than a uniformly random fringe subtree.)

3 Sketch of proofs

We let $\xi_1, \xi_2, \dots$ be a sequence of independent copies of ξ, and let

$$S_n := \sum_{i=1}^{n} \xi_i. \tag{3.1}$$

3.1 A useful representation

A tree in $\mathfrak{T}$ is uniquely described by its degree sequence $(d_1, \dots, d_n)$. We may thus define the functional f also on finite nonnegative integer sequences $(d_1, \dots, d_n)$, $n \geqslant 1$, by

$$f(d_1, \dots, d_n) := \begin{cases} f(T), & (d_1, \dots, d_n) \text{ is the degree sequence of a tree } T, \\ 0, & \text{otherwise.} \end{cases} \tag{3.2}$$

If T has degree sequence $(d_1, \dots, d_n)$, and its nodes are numbered $v_1, \dots, v_n$ in depth-first order so d_i is the degree of v_i, then the subtree T_{v_i} has degree sequence $(d_i, d_{i+1}, \dots, d_{i+k-1})$, where $k \leqslant n-i+1$ is the unique index such that $(d_i, \dots, d_{i+k-1})$ is a degree sequence of a tree. By the definition (3.2), we thus can write (1.3) as

$$F(T) = \sum_{1 \leqslant i \leqslant j \leqslant n} f(d_i, \dots, d_j) = \sum_{k=1}^{n} \sum_{i=1}^{n-k+1} f(d_i, \dots, d_{i+k-1}). \tag{3.3}$$

Moreover, if we regard $(d_1, \dots, d_n)$ as a cyclic sequence and allow wrapping around by defining $d_{n+i} := d_i$, we also have the more symmetric formula

$$F(T) = \sum_{k=1}^{n} \sum_{i=1}^{n} f(d_i, \dots, d_{i+k-1}). \tag{3.4}$$

The difference from (3.3) is that we have added some terms $f(d_i, \dots, d_{i+k-1-n})$ where the indices wrap around, but these terms all vanish by definition because $(d_i, \dots, d_{i+k-1-n})$ is never a degree sequence. (The subtree with root v_i is completed at the latest by v_n.)

It is a well-known fact, see e.g. [15, Corollary 15.4], that up to a cyclic shift, the degree sequence $(d_1, \dots, d_n)$ of the conditioned Galton–Watson tree $\mathcal{T}_n$ has the same distribution as $\big((\xi_1, \dots, \xi_n) \mid S_n = n-1\big)$. Since (3.4) is invariant under cyclic shifts of $(d_1, \dots, d_n)$, it follows that, recalling (3.1),

$$F(\mathcal{T}_n) \stackrel{\mathrm{d}}{=} \left(\sum_{k=1}^{n} \sum_{i=1}^{n} f(\xi_i, \dots, \xi_{i+k-1 \bmod n}) \;\middle|\; S_n = n-1 \right), \tag{3.5}$$

where $j \bmod n$ denotes the index in $\{1, \dots, n\}$ that is congruent to j modulo n.

3.2 More notation

We let, for $k \geqslant 1$, f_k be f restricted to $\mathfrak{T}_k$; more precisely, we define f_k for all trees $T \in \mathfrak{T}$ by $f_k(T) := f(T)$ if $|T| = k$ and $f_k(T) := 0$ otherwise. In other words,

$$f_k(T) := f(T) \cdot \mathbf{1}\{|T| = k\}. \tag{3.6}$$

Extended to integer sequences as in (3.2), this means that

$$f_k(d_1,\dots,d_n) = f(d_1,\dots,d_n)\cdot \mathbf{1}\{n=k\}. \tag{3.7}$$

Note that $\mathfrak{T}_k$ is a finite set; thus f_k is always a bounded function for each k.

We further let, for $k \geqslant 1$ and any tree T, with degree sequence $(d_1,\dots,d_n)$,

$$F_k(T) := F(T; f_k) = \sum_{i=1}^{n-k+1} f_k(d_i,\dots,d_{i+k-1}). \tag{3.8}$$

(We can also let the sum extend to n, wrapping around d_i as in (3.4).) Obviously,

$$f(T) = \sum_{k=1}^{\infty} f_k(T) \qquad \text{and} \qquad F(T) = \sum_{k=1}^{\infty} F_k(T) \tag{3.9}$$

for any tree T, where in both sums it suffices to consider $k \leqslant |T|$ since the summands vanish for $k > |T|$.

3.3 Expectations

We calculate the expectation $\mathbb{E}\, F(\mathcal{T}_n)$ using (3.5), which converts this into a problem on expectations of functionals of a sequence of i.i.d. variables conditioned on their sum. Results of this type have been studied before under various conditions, see for example Zabell [27, 28, 29], Swensen [25] and Janson [14].

By (3.5) and symmetry,

$$\mathbb{E}\, F(\mathcal{T}_n) = n\sum_{k=1}^{n} \mathbb{E}\big(f(\xi_1,\dots,\xi_k) \mid S_n = n-1\big). \tag{3.10}$$

We consider first the expectation of each $F_k(\mathcal{T}_n)$ separately, recalling (3.9). Note that each f_k is bounded, and thus trivially $\mathbb{E}\,|f_k(\mathcal{T})| < \infty$. A simple argument yields the following.

Lemma 3.1 *If $1 \leqslant k \leqslant n$, then*

$$\mathbb{E}\, F_k(\mathcal{T}_n) = n\frac{\mathbb{P}(S_{n-k}=n-k)}{\mathbb{P}(S_n=n-1)}\,\mathbb{E}\, f_k(\mathcal{T}). \tag{3.11}$$

We use this in combination with the following estimates, which are shown using the local limit theorem and the methods used to prove it. (Cf. [24, Theorem VII.13].)

Lemma 3.2 (i) *Uniformly for all k with $1 \leqslant k \leqslant n/2$, as $n \to \infty$,*

$$\frac{\mathbb{P}(S_{n-k}=n-k)}{\mathbb{P}(S_n=n-1)} = 1 + O\left(\frac{k}{n}\right) + o\big(n^{-1/2}\big). \tag{3.12}$$

(ii) *If $n/2 < k \leqslant n$, then*

$$\frac{\mathbb{P}(S_{n-k}=n-k)}{\mathbb{P}(S_n=n-1)} = O\left(\frac{n^{1/2}}{(n-k+1)^{1/2}}\right). \tag{3.13}$$

3.4 Variances and covariances

We next consider the variance of $F(\mathcal{T}_n)$. As in Section 3.3, we consider first the different $F_k(\mathcal{T}_n)$ separately; thus we study variances and covariances of these sums. We begin with an exact formula (omitted here), corresponding to Lemma 3.1; then the terms in it are estimated similarly to Lemma 3.2, but with more care since there typically is important cancellation between different terms. In particular, this leads to a simple asymptotic result for fixed k and m.

Lemma 3.3 *For any fixed k and m with $k \geqslant m$, as $n \to \infty$,*

$$\frac{1}{n}\operatorname{Cov}(F_k(\mathcal{T}_n), F_m(\mathcal{T}_n)) \to \mathbb{E}\big(f_k(\mathcal{T})F_m(\mathcal{T})\big) - (k+m-1+\sigma^{-2})\,\mathbb{E}\,f_k(\mathcal{T})\,\mathbb{E}\,f_m(\mathcal{T}).$$

Corollary 3.4 *Suppose that f has finite support. Then, as $n \to \infty$,*

$$\frac{1}{n}\operatorname{Var} F(\mathcal{T}_n) \to \mathbb{E}\Big(f(\mathcal{T})\big(2F(\mathcal{T}) - f(\mathcal{T})\big)\Big) - 2\,\mathbb{E}\big(|\mathcal{T}|f(\mathcal{T})\big)\,\mathbb{E}\,f(\mathcal{T}) + \big(1-\sigma^{-2}\big)\big(\mathbb{E}\,f(\mathcal{T})\big)^2.$$

For general f, we first show a uniform bound valid for all n.

Theorem 3.5 *For any functional $f : \mathfrak{T} \to \mathbb{R}$,*

$$\operatorname{Var}\big(F(\mathcal{T}_n)\big)^{1/2} \leqslant C_1 n^{1/2}\left(\sup_k \sqrt{\mathbb{E}\,f(\mathcal{T}_k)^2} + \sum_{k=1}^{\infty}\frac{\sqrt{\mathbb{E}\,f(\mathcal{T}_k)^2}}{k}\right), \tag{3.14}$$

with C_1 independent of f.

Using this bound, (1.14)–(1.15) follow easily.

3.5 Asymptotic normality

To prove asymptotic normality, we first consider functionals f with finite support. We use the representation (3.5), where now it suffices to sum over $k \leqslant m$ for some $m < \infty$. We define

$$g(x_1,\dots,x_m) := \sum_{k=1}^{m} f(x_1,\dots,x_k) = \sum_{k=1}^{m} f_k(x_1,\dots,x_k). \tag{3.15}$$

Then (3.5) can be written (assuming $n \geqslant m$)

$$F(\mathcal{T}_n) \overset{\mathrm{d}}{=} \left(\sum_{i=1}^{n} g(\xi_i,\dots,\xi_{i+m-1 \bmod n}) \;\Big|\; S_n = n-1\right). \tag{3.16}$$

Asymptotic normality now follows by a method by Le Cam [21] and Holst [12], see also Kudlaev [20].

For general f in Theorems 1.3 and 1.8 we define the truncation

$$f^{(N)}(T) := \sum_{k=1}^{N} f_k(T) = f(T)\mathbf{1}\{|T| \leqslant N\} \tag{3.17}$$

and the corresponding sum $F^{(N)}(T)$. The result follow from the case of finite support, using Theorem 3.5 and a similar but sharper estimate for weakly local functionals.

More precisely, with $\mu^{(N)} := \mathbb{E}\, f^{(N)}(\mathcal{T})$ and

$$(\gamma^{(N)})^2 := 2\,\mathbb{E}\Big(f^{(N)}(\mathcal{T})\big(F^{(N)}(\mathcal{T}) - |\mathcal{T}|\mu^{(N)}\big)\Big) - \operatorname{Var} f^{(N)}(\mathcal{T}) - (\mu^{(N)})^2/\sigma^2, \tag{3.18}$$

this proof yields asymptotic normality with the asymptotic variance

$$\gamma^2 := \lim_{N\to\infty} (\gamma^{(N)})^2. \tag{3.19}$$

In Theorem 1.3, this leads to (1.15). In Theorem 1.8, we do not know any simple general formula for γ^2.

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A unified approach to linear probing hashing

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Abstract. We give a unified analysis of linear probing hashing with a general bucket size. We use both a combinatorial approach, giving exact formulas for generating functions, and a probabilistic approach, giving simple derivations of asymptotic results. Both approaches complement nicely, and give a good insight in the relation between linear probing and random walks. A key methodological contribution, at the core of Analytic Combinatorics, is the use of the symbolic method (based on q-calculus) to directly derive the generating functions to analyze.

Keywords: hashing; linear probing; buckets; generating functions; analytic combinatorics

1 Motivation

Linear probing hashing, defined below, is certainly the simplest "in place" hashing algorithm [10].

> *A table of length m, $T[1\,..\,m]$, with buckets of size b is set up, as well as a hash function h that maps keys from some domain to the interval $[1\,..\,m]$ of table addresses. A collection of n elements with $n \leqslant bm$ are entered sequentially into the table according to the following rule: Each element x is placed at the first bucket that is not full starting from $h(x)$ in cyclic order, namely the first of $h(x), h(x)+1, \dots, m, 1, 2, \dots, h(x)-1$.*

In [9] Knuth motivates his paper in the following way: "The purpose of this note is to exhibit a surprisingly simple solution to a problem that appears in a recent book by Sedgewick and Flajolet [12]:

Exercise 8.39 Use the symbolic method to derive the EGF of the number of probes required by linear probing in a successful search, for fixed M."

Moreover, at the end of the paper in his personal remarks he declares: "None of the methods available in 1962 were powerful enough to deduce the expected square displacement, much less the higher moments, so it is an even greater pleasure to be able to derive such results today from other work that has enriched the field of combinatorial mathematics during a period of 35 years." In this sense, he is talking about the powerful methods based on Analytic Combinatorics that has been developed for the last decades, and are presented in [6].

In this paper we present in a unified way the analysis of several random variables related with linear probing hashing with buckets, giving explicit and exact trivariate generating functions in the combinatorial

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model, together with generating functions in the asymptotic Poisson model that provide limit results, and relations between the two types of results. Linear probing has been shown to have strong connections with several important problems (see [9, 5, 2] and the references therein). The derivations in the asymptotic Poisson model are probabilistic and use heavily the relation between random walks and the profile of the table. Moreover, the derivations in the combinatorial model are based in combinatorial specifications that directly translate into multivariate generating functions. As far as we know, this is the first unified presentation of the analysis of linear probing hashing with buckets based on Analytic Combinatorics ("if you can specify it, you can analyze it").

We will see that results can easily be translated between the exact combinatorial model and the asymptotic Poisson model. Nevertheless, we feel that it is important to present independently derivations for the two models, since the methodologies complement very nicely. Moreover, they heavily rely in the deep relations between linear probing and other combinatorial problems like random walks, and the power of Analytic Combinatorics.

The derivations based on Analytic Combinatorics heavily rely on a lecture presented by Flajolet whose notes can be accessed in [4]. Since these ideas have only been partially published in the context of the analysis of hashing in [6], we briefly present here some constructions that lead to q-analogs of their corresponding exponential generating functions. Proofs will be given in the full version [8] of this paper.

1.1 Some notation

We study tables with m buckets of size b and n elements, where $b \geqslant 1$ is a constant. We often consider limits as $m, n \to \infty$ with $n/bm \to \alpha$ with $\alpha \in (0, 1)$. We consider also the Poisson model with $n \sim \mathrm{Po}(\alpha bm)$, and thus $\mathrm{Po}(b\alpha)$ elements hashed to each bucket; in this model we can also take $m = \infty$ which gives a natural limit object, see Section 4 and Lemma 5.1.

A *cluster* or *block* is a (maximal) sequence of full buckets ended by a non-full one. The *tree function* is $T(z) := \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} z^n$, which converges for $|z| \leqslant e^{-1}$. Let $\omega = \omega_b := e^{2\pi \mathrm{i}/b}$ be a primitive b:th unit root.

2 Combinatorial characterization of linear probing

As a combinatorial object, a non-full linear probing hash table is a sequence of almost full tables (or clusters) [9, 5, 13]. As a consequence, any random variable related with the table itself (like block lengths, or the overflow in the parking problem) or with a random element (like its search cost) can be studied in a cluster (that we may assume to be the last one in the sequence), and then use the sequence construction. Figure 1 presents an example of such a decomposition.

We briefly recall here some of the definitions presented in [13]. Let F_{bi+d} be the number of ways to construct an almost full table of length $i + 1$ and size $bi + d$ (that is, there are $b - d$ empty slots in the last bucket). Define also

$$F_d(u) := \sum_{i \geq 0} F_{bi+d} \frac{u^{bi+d}}{(bi+d)!}, \qquad N_d(z, w) := \sum_{s=0}^{b-1-d} w^{b-s} F_s(zw), \quad 0 \leq d \leq b-1. \tag{2.1}$$

In this setting $N_d(z, w)$ is the generating function for the number of almost full tables with more than d empty locations in the last bucket. More specifically $N_0(z, w)$ is the generating function for all the almost

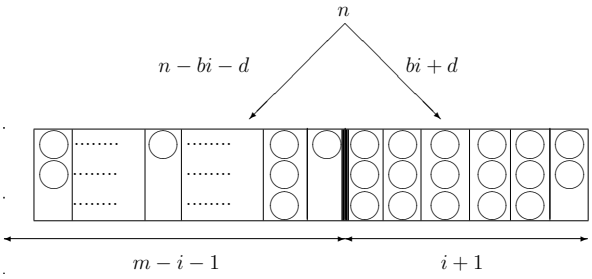

Fig. 1: A decomposition for $b = 3$ and $d = 2$.

full tables. We borrow from [13] the following identities:

$$\sum_{d=0}^{b-1} F_d(bz)x^d = x^b - \prod_{j=0}^{b-1}\left(x - \frac{T(\omega^j z)}{z}\right), \tag{2.2}$$

$$N_0(bz, w) = 1 - \prod_{j=0}^{b-1}\left(1 - \frac{T(\omega^j zw)}{z}\right), \tag{2.3}$$

$$\sum_{d=0}^{b-1} N_d(bz, w)x^d = \frac{\prod_{j=0}^{b-1}\left(1 - x\frac{T(\omega^j zw)}{z}\right) - \prod_{j=0}^{b-1}\left(1 - \frac{T(\omega^j zw)}{z}\right)}{1 - x}. \tag{2.4}$$

Let also $Q_{m,n,d}$ be the number of ways of inserting n elements into a table with m buckets of size b, so that a given (say the last) bucket of the table contains more than d empty slots. In this setting, by a direct application of the sequence construction as presented in [6] we derive a result presented in [1]:

$$\Lambda_0(z, w) := \sum_{m\geq 0}\sum_{n\geq 0} Q_{m,n,0}\frac{z^n}{n!}w^{bm} = \frac{1}{1 - N_0(z, w)}. \tag{2.5}$$

Then, $\Lambda_0(z, w)$ is the generating function for the number of ways to construct hash tables such that their last bucket is not full.

Consider a hash table of length m and n keys, where collisions are resolved by linear probing. Let P be a property (e.g. cost of a successful search or block length), related with the last cluster of the sequence, or with a random element inside it. Let $p_{bi+d}(q)$ be the probability generating function of P calculated in the cluster of length $i + 1$ and with $bi + d$ elements. We may express $p_{m,n}(q)$, the generating function of P for a table of length m and n elements with at least one empty spot in the last bucket, as the sum of the conditional probabilities:

$$p_{m,n}(q) = \sum_{d=0}^{b-1}\sum_{i\geqslant 0} \#\{\text{tables where last cluster has size } i + 1 \text{ and } bi + d \text{ elements}\}\; p_{bi+d}(q). \tag{2.6}$$

There are $Q_{m-i-1,n-bi-d,0}$ ways to insert $n-bi-d$ elements in the leftmost hash table of length $m-i-1$, leaving their rightmost bucket not full. Moreover, there are F_{bi+d} ways to insert $bi + d$ elements in the

almost full table of length $i+1$. Furthermore, there are $\binom{n}{bi+d}$ ways to choose which $bi+d$ elements go to the last cluster. Therefore,

$$p_{m,n}(q) = \sum_{d=0}^{b-1} \sum_{i\geq 0} \binom{n}{bi+d} Q_{m-i-1,n-bi-d,0}\ F_{bi+d} p_{bi+d}(q). \tag{2.7}$$

Then, the trivariate generating function for $p_{m,n}(q)$ is

$$P(z,w,q) := \sum_{m,n\geq 0} p_{m,n}(q)\ w^{bm} \frac{z^n}{n!} = \frac{\hat{N}_0(z,w,q)}{1-N_0(z,w)}, \qquad \text{with} \tag{2.8}$$

$$\hat{N}_0(z,w,q) := \sum_{d=0}^{b-1} w^{b-d} \sum_{i\geq 0} F_{bi+d}\ \frac{(zw)^{bi+d}}{(bi+d)!}\ p_{bi+d}(q), \tag{2.9}$$

which could be directly derived with the sequence construction [6]. Notice that, as expected, $\hat{N}_0(z,w,1) = N_0(z,w)$ and $P(z,w,1) = \Lambda_0(z,w)-1$, since we consider only $m \geq 1$ (we have a last, non-filled bucket).

Moreover the Poisson Transform of $p_{m,n}(q)/m^n$ is, with $Q_{m,d}(u) := \sum_{n\geqslant 0} Q_{m,n,d} u^n/n!$,

$$\begin{aligned}\mathbf{P}_m[p_{m,n}(q)/m^n; b\alpha] &:= e^{-mb\alpha} \sum_{n\geq 0} p_{m,n}(q)\ \frac{(mb\alpha)^n}{m^n n!} \\ &= \sum_{d=0}^{b-1} e^{-(b-d)\alpha}\ \sum_{i\geq 0} F_{bi+d}\ \frac{(b\alpha e^{-\alpha})^{bi+d}}{(bi+d)!}\ p_{bi+d}(q)\ e^{-(m-i-1)b\alpha}\ Q_{m-i-1,0}(b\alpha). \end{aligned} \tag{2.10}$$

Furthermore, $Q_{m-i-1,0}(b\alpha) = [T_0(b\alpha)\ e^{(m-i-1)b\alpha}]_{b(m-i-1)-1}$ where $T_0(b\alpha)$ is, in the asymptotic Poisson model, the probability that a given bucket is not full [13]. It is proven in [1, 13] that

$$\lim_{m\to\infty} \mathbf{P}_m[Q_{m,n,0}/m^n; b\alpha] = \lim_{m\to\infty} e^{-mb\alpha} Q_{m,0}(b\alpha) = T_0(b\alpha) = \frac{b(1-\alpha)}{\prod_{j=1}^{b-1}\left(1-\frac{T(\omega^j \alpha e^{-\alpha})}{\alpha}\right)}. \tag{2.11}$$

As a consequence, (2.10) and (2.9) yield

$$\lim_{m\to\infty} \mathbf{P}_m[p_{m,n}(q)/m^n; b\alpha] \quad = \quad T_0(b\alpha)\hat{N}_0(b\alpha, e^{-\alpha}, q). \tag{2.12}$$

Note that if $0 < \alpha < 1$ is a fixed constant, then $w = e^{-\alpha}$ is the dominant singularity of $P(b\alpha, w, q)$ (a root of $1 - N_0(b\alpha, w)$, for $j = 0$ in (2.3), cf. (2.8)), so the relation (2.12) can also be derived by standard asymptotic methods as in [6]. As a consequence, all the results found for exact m, n can easily been translated in the Poisson model.

3 A q-calculus to specify hashing random variables

All the generating functions in this paper are exponential in n and ordinary in m. As a consequence all the labelled constructions in [6] and their respective translation into EGF can be used. However, to specify the combinatorial properties related with the analysis of linear probing hashing, new constructions have to be added. These ideas have been presented by Flajolet in [4], but they do not seem to have been published in the context of hashing. As a consequence, we briefly summarize them in this section.

$\underline{\text{Adding an element}} \mapsto \int$ $\mathcal{C} = \text{Add}(\mathcal{A})$	$C_n = A_{n-1}$ $C(z) = \int_0^z A(w)dw$
$\underline{\text{Choosing a position}} \mapsto \partial$ $\mathcal{C} = \text{Pos}(\mathcal{A})$	$C_n = (n+1)A_n$ $C(z) = \frac{\partial}{\partial z}(zA(z))$
$\underline{\text{Averaging}} \mapsto \frac{1}{Z}\int$ $\mathcal{C} = \text{Ave}(\mathcal{A})$	$C_n = \frac{A_n}{n+1}$ $C(z) = \frac{1}{z}\int_0^z A(w)dw$
$\underline{\text{Adding a bucket}} \mapsto \exp$ $\mathcal{C} = \text{Bucket}(\mathcal{Z})$	$C_n = 1$ $C(z) = \exp(z)$

We present a list of combinatorial constructions used in hashing and their corresponding translation into EGF, where $\mathcal{Z}$ is an atomic class comprising a single element of size 1. Moreover, to keep track of the distribution of random variables (e.g. the displacement of a new inserted element), we need translations that belong to the area of q-calculus. Equations (3.1), (3.2) and (3.3) present some of these translations.

$$n \quad \mapsto \quad [n] = 1 + q + q^2 + \ldots + q^{n-1} = \frac{1-q^n}{1-q} \tag{3.1}$$

$$\sum (n+1) f_n z^n \quad \mapsto \quad \sum [n+1] f_n z^n \tag{3.2}$$

$$\frac{\partial}{\partial z}(zA(z)) \quad \mapsto \quad H[f(z)] = \frac{F(z) - qF(qz)}{1-q} \tag{3.3}$$

Moments result from using the operators ∂_q (differentiation w.r.t. q) and U (setting $q = 1$).

4 Probabilistic method: finite and infinite hash tables

In general, consider a hash table, with locations ("buckets") each having capacity b; we suppose that the buckets are labelled by $i \in \mathfrak{T}$, for a suitable index set $\mathfrak{T}$. Let for each bucket $i \in \mathfrak{T}$, X_i be the number of elements that have hash address i, and thus first try bucket i. Moreover, let H_i be the total number of elements that try bucket i and let Q_i be the *overflow* from bucket i, i.e., the number of elements that try bucket i but fail to find room and thus are transferred to the next bucket. We thus have the equations

$$H_i = X_i + Q_{i-1}, \qquad\qquad Q_i = (H_i - b)_+. \tag{4.1}$$

The final number of elements stored in bucket i is $Y_i := H_i \wedge b := \min(H_i, b)$; in particular, the bucket is full if and only if $H_i \geqslant b$.

Standard hashing is when the index set $\mathfrak{T}$ is the cyclic group $\mathbb{Z}_m$. Another standard case, called the *parking problem*, is when $\mathfrak{T}$ is an interval $\{1, \ldots, m\}$ for some integer m; in this case the Q_m elements that try the last bucket but fail to find room there are lost (overflow), and (4.1) uses the initial value $Q_0 := 0$.

In the analysis, we will mainly study infinite hash tables, either one-sided with $\mathfrak{T} = \mathbb{N} := \{1, 2, 3, \ldots\}$, or two-sided with $\mathfrak{T} = \mathbb{Z}$; as we shall see, these occur naturally as limits of finite hash tables. In the one-sided case, we again define $Q_0 := 0$, and then, given $(X_i)_1^\infty$, H_i and Q_i are uniquely determined recursively for all $i \geqslant 1$ by (4.1). In the doubly-infinite case, it is not obvious that the equations (4.1) really have a solution; we return to this question in Lemma 4.1 below.

In the case $\mathfrak{T} = \mathbb{Z}_m$, we allow (with a minor abuse of notation) also the index i in these quantities to be an arbitrary integer with the obvious interpretation; then X_i, H_i and so on are periodic sequences defined for $i \in \mathbb{Z}$.

We can express H_i and Q_i in X_i by the following lemma, which generalizes (and extends to infinite hashing) the case $b = 1$ treated in [10, Exercise 6.4-32], [3, Proposition 5.3], [7, Lemma 2.1].

Lemma 4.1 *Let X_i, $i \in \mathfrak{T}$, be given non-negative integers.*

(i) *If $\mathfrak{T} = \{1, \dots, m\}$ or $\mathbb{N}$, then the equations* (4.1)*, for all $i \in \mathfrak{T}$, have a unique solution given by, considering $j \geqslant 0$,*

$$H_i = \max_{j<i} \sum_{k=j+1}^{i} (X_k - b) + b, \qquad Q_i = \max_{j \leqslant i} \sum_{k=j+1}^{i} (X_k - b) \tag{4.2}$$

(ii) *If $\mathfrak{T} = \mathbb{Z}_m$, and moreover $n = \sum_1^m X_i < bm$, then the equations* (4.1)*, for all $i \in \mathfrak{T}$, have a unique solution given by* (4.2)*, now with $j \in \mathbb{Z}$. Furthermore, there exists $i_0 \in \mathfrak{T}$ such that $H_{i_0} < b$ and thus $Q_{i_0} = 0$.*

(iii) *If $\mathfrak{T} = \mathbb{Z}$, assume that*

$$\sum_{i=0}^{N-1} (b - X_{-i}) \to \infty \qquad \text{as } N \to \infty. \tag{4.3}$$

Then the equations (4.1)*, for all $i \in \mathfrak{T}$, have a solution given by* (4.2)*, with $j \in \mathbb{Z}$, and this is the minimal solution. Furthermore, for each $i \in \mathfrak{T}$ there exists $i_0 < i$ such that $H_{i_0} < b$ and thus $Q_{i_0} = 0$. Conversely, this is the only solution such that for every i there exists $i_0 < i$ with $Q_{i_0} = 0$.*

In the sequel, we will always use this solution of (4.1) for hashing on $\mathbb{Z}$ (assuming that (4.3) holds); we can regard this as a definition of hashing on $\mathbb{Z}$.

5 Convergence to an infinite hash table

We are interested in hashing on Z_m with n elements having independent uniformly random hash addresses, thus $X_1, \dots, X_m$ have a multinomial distribution with parameters n and $(1/m, \dots, 1/m)$. (We denote these X_i by $X_{m,n;i}$.) We denote the profile of this hash table by $H_{m,n;i}$, where as above $i \in Z_m$ but we also can allow $i \in \mathbb{Z}$ in the obvious way.

We consider a limit with $m, n \to \infty$ and $n/bm \to \alpha \in (0, 1)$. The appropriate limit object turns out to be an infinite hash table on $\mathbb{Z}$ with $X_i = X_{\alpha;i}$ that are independent and identically distributed (i.i.d.) with the Poisson distribution $X_i \sim \mathrm{Po}(\alpha b)$; this is the asymptotic Poisson model mentioned earlier. Note that $\mathbb{E}\, X_i = \alpha b < b$, so $\mathbb{E}(b - X_i) > 0$ and (4.3) holds almost surely by the law of large numbers; hence this infinite hash table is well-defined. We denote the profile of this hash table by $H_{\alpha;i}$.

We claim that the profile $(H_{m,n;i})_{i=-\infty}^{\infty}$, regarded as a random element of the product space $\mathbb{Z}^{\mathbb{Z}}$, converges in distribution to the $(H_{\alpha;i})_{i=-\infty}^{\infty}$. (By the definition of the product topology, this is equivalent to convergence in distribution of any finite vector $(H_{m,n;i})_{-M}^{N}$ to $(H_{\alpha;i})_{-M}^{N}$.)

Lemma 5.1 *Let $m, n \to \infty$ with $n/bm \to \alpha$ for some α with $0 < \alpha < 1$. Then $(H_{m,n;i})_{i=-\infty}^{\infty} \xrightarrow{\mathrm{d}} (H_{\alpha;i})_{i=-\infty}^{\infty}$.*

Remark 5.2 Note that the convergence of the profile implies convergence of all other quantities that we study here. Thus the theorems in the sections below for hashing on $\mathbb{Z}$ contain (and are equivalent to) limit theorems for finite hashing as $m, n \to \infty$ with $n/bm \to \alpha$.

6 The profile and overflow (parking problem)

In the combinatorial approach, let $\Omega(z, w, q)$ be the generating function for the number of elements that overflow from a hash table (i.e., the number of cars that cannot find a place in the parking problem)

$$\Omega(z, w, q) := \sum_{m\geqslant 0}\sum_{n\geqslant 0}\sum_{k\geqslant 0} N_{m,n,k} w^{bm}\frac{z^n}{n!}q^k, \tag{6.1}$$

where $N_{m,n,k}$ is the number of hash tables of length m with n elements and overflow k. (We include an empty hash table with $m = n = k = 0$ in the sum (6.1).) Thus w marks the number of places in the table, z the number of elements and q the number of elements that overflow. The following result has been independently presented by Panholzer in [11].

Theorem 6.1

$$\Omega(bz, w, q) = \frac{1}{q^b - w^b e^{qbz}} \cdot \frac{\prod_{j=0}^{b-1}\left(q - \frac{T(\omega^j zw)}{z}\right)}{\prod_{j=0}^{b-1}\left(1 - \frac{T(\omega^j zw)}{z}\right)}. \tag{6.2}$$

Proof: [Sketch] The number of elements that overflow from the table with $m \geqslant 1$ are the ones that overflow from a table of size $m - 1$ plus the number of elements that hash into position m minus b (giving the factor $\frac{w^b e^{zq}}{q^b}$, corresponding to adding a last bucket, marking the elements that hash into this last bucket, and leaving b elements in it). However, we have to include a correction factor in case that the total number of elements that probe position m is less than b. As a consequence

$$\Omega(z, w, q) = 1 + \Omega(z, w, q)\frac{w^b e^{zq}}{q^b} + \sum_{s=0}^{b-1}(1 - q^{s-b})O_s(z, w),$$

where $O_s(z, w)$ is the generating function for the number of hash tables that have s elements in bucket m.

From [13] we know that

$$O_s(z, w) = \frac{F_s(zw)w^{b-s}}{1 - N_0(z, w)},$$

and the result follows. □

For the probabilistic version, we use Lemma 5.1 and study in the sequel infinite hashing on $\mathbb{Z}$, with $X_i = X_{\alpha;i}$ i.i.d. random Poisson variables with $X_i \sim \mathrm{Po}(\alpha b)$, where $0 < \alpha < 1$. Thus X_i has the probability generating function

$$\psi_X(z) := \mathbb{E}\, z^{X_i} = e^{\alpha b(z-1)}. \tag{6.3}$$

We begin by finding the distributions of H_i and Q_i. Let $\psi_H(z) := \mathbb{E}\, z^{H_i}$ and $\psi_Q(z) := \mathbb{E}\, z^{Q_i}$ denote the probability generating functions of H_i and Q_i (which obviously do not depend on $i \in \mathbb{Z}$), defined at least for $|z| \leqslant 1$.

Theorem 6.2 *Let $0 < \alpha < 1$. The probability generating functions $\psi_H(z)$ and $\psi_Q(z)$ extend to meromorphic functions given by*

$$\psi_H(z) = \frac{b(1-\alpha)(z-1)}{z^b e^{\alpha b(1-z)} - 1} \frac{\prod_{\ell=1}^{b-1}\bigl(z - T\bigl(\omega^\ell \alpha e^{-\alpha}\bigr)/\alpha\bigr)}{\prod_{\ell=1}^{b-1}\bigl(1 - T\bigl(\omega^\ell \alpha e^{-\alpha}\bigr)/\alpha\bigr)}, \tag{6.4}$$

$$\psi_Q(z) = \frac{b(1-\alpha)(z-1)}{z^b - e^{\alpha b(z-1)}} \frac{\prod_{\ell=1}^{b-1}\bigl(z - T\bigl(\omega^\ell \alpha e^{-\alpha}\bigr)/\alpha\bigr)}{\prod_{\ell=1}^{b-1}\bigl(1 - T\bigl(\omega^\ell \alpha e^{-\alpha}\bigr)/\alpha\bigr)}. \tag{6.5}$$

The formula (6.5), which easily implies (6.4), was shown by the combinatorial method in [13, Theorem 9]. It can also be obtained from Theorem 6.1; we omit the details.

Corollary 6.3 *For $k = 0, \dots, b-1$,*

$$\Pr(Y_i = k) = \Pr(H_i = k) = -b(1-\alpha) \frac{[z^k] \prod_{\ell=0}^{b-1}\bigl(z - T\bigl(\omega^\ell \alpha e^{-\alpha}\bigr)/\alpha\bigr)}{\prod_{\ell=1}^{b-1}\bigl(1 - T\bigl(\omega^\ell \alpha e^{-\alpha}\bigr)/\alpha\bigr)}. \tag{6.6}$$

Furthermore, the probability that a bucket is not full is given by

$$\Pr(Y_i < b) = \Pr(H_i < b) = T_0(b\alpha) = \frac{b(1-\alpha)}{\prod_{\ell=1}^{b-1}\bigl(1 - T\bigl(\omega^\ell \alpha e^{-\alpha}\bigr)/\alpha\bigr)} \tag{6.7}$$

and thus

$$\Pr(Y_i = b) = \Pr(H_i \geqslant b) = 1 - T_0(b\alpha). \tag{6.8}$$

The generating functions $T_d(u)$ defined in [13] for $0 \leqslant d \leqslant b-1$ have the property [13, p. 318] that $T_d(b\alpha)$ is the limit of the probability that a given bucket contains more than d empty slots, when $m \to \infty$ and $n \sim \mathrm{Po}(\alpha b m)$. By Lemma 5.1, this limit equals the probability that a given bucket in the infinite hashing has more than d empty slots. This gives the following relation.

Theorem 6.4 *For $d = 0, \dots, b-1$,*

$$T_d(b\alpha) = \Pr(Y_i < b-d) = \Pr(H_i < b-d) = \sum_{s=0}^{b-d-1} \Pr(Y_i = s), \tag{6.9}$$

It is easy to verify that the formula (6.6) is equivalent to [13, Theorem 8].

7 Robin Hood displacement

In Robin Hood, if ties are broken in a consistent way (e.g. by hash value) then the final table is the same, independently from the sequence of insertions. As a consequence, the last inserted element, has the same distribution as any other key. Let D^{RH} be the displacement of a given element x; we may assume that x hashes to bucket 0. We first study the number C^{RH} of elements that win over x in the competition for slots in the buckets; then $D^{\mathsf{RH}} = \lfloor C^{\mathsf{RH}}/b \rfloor$. As in [13], we note that C^{RH} is the sum of the number Q_{-1} of elements that overflow into 0 plus the number V of elements that hash to 0 that win over x; if there are k other elements hashing to 0, then V is by symmetry uniformly distributed in $\{0, \dots, k\}$, and has probability generating function $\frac{1}{k+1}\sum_{r=0}^{k} q^r$.

In the combinatorial model, the generating function $\mathcal{C}^{\mathsf{RH}}(z,w,q)$ of C^{RH} thus factors as $\Omega(z,w,q)$ times the generating function for V. The latter, as presented in Section 3, is given by the specification $\mathrm{Ave}(\mathrm{Pos}(\mathrm{Bucket}))$. We then arrive at

$$\begin{aligned}\mathcal{C}^{\mathsf{RH}}(bz,w,q) &= \Omega(bz,w,q)\,\mathrm{Ave}(\mathrm{Pos}(\mathrm{Bucket}(bz,w,q)))\\ &= \Omega(bz,w,q)w^b\frac{e^{bz}-e^{qbz}}{bz(1-q)} = \frac{(we^z)^b(1-e^{bz(q-1)})}{bz(1-q)(q^b-we^{qz})}\frac{\prod_{j=0}^{b-1}\left(q-\frac{T(\omega^j zw)}{z}\right)}{\prod_{j=0}^{b-1}\left(1-\frac{T(\omega^j zw)}{z}\right)}.\end{aligned}$$

The probabilistic argument for the infinite Poisson model is very similar. Again we have $C^{\mathsf{RH}} = Q_{-1}+V$, where Q_{-1} and V are independent, and a simple calculation shows that V has probability generating function $\psi_V(q) = \bigl(1-e^{b\alpha(q-1)}\bigr)/b\alpha(1-q)$. Using (6.5), this yields

$$\psi_C(q) = \psi_Q(q)\psi_V(q) = \frac{1-\alpha}{\alpha}\,\frac{1-e^{b\alpha(q-1)}}{e^{b\alpha(q-1)}-q^b}\,\frac{\prod_{\ell=1}^{b-1}\bigl(q-T\bigl(\omega^\ell\alpha e^{-\alpha}\bigr)/\alpha\bigr)}{\prod_{\ell=1}^{b-1}\bigl(1-T\bigl(\omega^\ell\alpha e^{-\alpha}\bigr)/\alpha\bigr)}. \tag{7.1}$$

The probability generating function for the displacement $D^{\mathsf{RH}} = \lfloor C^{\mathsf{RH}}/b\rfloor$ then equals, cf. [13],

$$\psi_{\mathsf{RH}}(q) = \frac{1}{b}\sum_{j=0}^{b-1}\psi_C\bigl(\omega^j q^{1/b}\bigr)\frac{1-q^{-1}}{1-\omega^{-j}q^{-1/b}}. \tag{7.2}$$

8 Block length

In an almost full table the length of the block is marked by w in $N_0(bz,w)$. Then, in the combinatorial model, the generating function $B(z,w,q)$ for the block length is

$$B(bz,w,q) = \Lambda_0(bz,w)N_0(bz,wq^{1/b}) = \frac{1-\prod_{j=0}^{b-1}\left(1-\frac{T(\omega^j zwq^{1/b})}{z}\right)}{\prod_{j=0}^{b-1}\left(1-\frac{T(\omega^j zw)}{z}\right)}.$$

For the probabilistic version, we consider one-sided infinite hashing on $\mathfrak{T} = \mathbb{N}$, with $X_i \sim \mathrm{Po}(\alpha b)$ i.i.d. as above. Let B be the length of the first block, i.e.,

$$B := \min\{i \geqslant 1 : Y_i < b\} = \min\{i \geqslant 1 : H_i < b\}. \tag{8.1}$$

Hence, B is the first positive index i such that the number of elements $S_i = X_1+\cdots+X_i$ hashed to the i first buckets is less than the capacity bi of these buckets, i.e.,

$$B = \min\{i \geqslant 1 : S_i < bi\}. \tag{8.2}$$

(This also follows from Lemma 4.1.) In other words, if we consider the random walk

$$S'_n := S_n - bn = \sum_{i=1}^{n}(X_i - b), \tag{8.3}$$

the block length B is the first time this random walk becomes negative. Since $\mathbb{E}(X_i - b) = \alpha b - b < 0$, it follows from the law of large numbers that almost surely $S'_n \to -\infty$ as $n \to \infty$, and thus $B < \infty$.

Note also that $S'_{B-1} \geqslant 0$, and thus $0 > S'_B \geqslant -b$. In fact, the number of elements hash to the first B buckets is $S_B = S'_B + bB$, and since all buckets before B are full and thus take $(B-1)b$ elements, the number of elements in the final bucket of the block is

$$Y_B = H_B = S_B - (B-1)b = S'_B + b \in \{0, \dots, b-1\}. \tag{8.4}$$

Theorem 8.1 *The probability generating function $\psi_B(z) := \mathbb{E}\, z^B$ of B is given by*

$$\psi_B(z) = 1 - \prod_{\ell=0}^{b-1} \left(1 - T\big(\omega^\ell \alpha e^{-\alpha} z^{1/b}\big)/\alpha\right). \tag{8.5}$$

More generally,

$$\mathbb{E}\big(z^B t^{Y_B}\big) = \mathbb{E}\big(z^B t^{H_B}\big) = t^b - \prod_{\ell=0}^{b-1} \left(t - T\big(\omega^\ell \alpha e^{-\alpha} z^{1/b}\big)/\alpha\right). \tag{8.6}$$

9 Unsuccessful search

In a cluster with n keys, the number of visited buckets in a unsuccessful search, is the same as the one needed to insert the $(n+1)$st element. As a consequence, in the combinatorial model, the specification $\mathrm{Pos}(N_0)$ leads, from equation (3.3), to

$$U(bz, w, q) = \Lambda_0(bz, w) \frac{N_0(bz, w) - N_0(bz, wq^{1/b})}{1-q} = \frac{\prod_{j=0}^{b-1} \left(1 - \frac{T(\omega^j z w q^{1/b})}{z}\right) - \prod_{j=0}^{b-1} \left(1 - \frac{T(\omega^j z w)}{z}\right)}{(1-q) \prod_{j=0}^{b-1} \left(1 - \frac{T(\omega^j z w)}{z}\right)}.$$

This result is also derived in [1, Lemma 4.2].

In the probabilistic model, for an unsuccessful search for an element that does not exist in the hash table, let $U_i \geqslant 0$ denote the number of *full* buckets that we search, when we start with bucket i. Thus $U_i = k - i$ where k is the index of the bucket that ends the block containing i. In the probabilistic version, we consider again hashing on $\mathbb{Z}$, with $X_i \sim \mathrm{Po}(\alpha b)$ independent. Obviously, all U_i have the same distribution, so we may take $i = 0$.

Theorem 9.1 *The probability generating function $\psi_U(z) := \mathbb{E}\, z^{U_i}$ of U_i is given by*

$$\psi_U(z) = \frac{T_0(b\alpha)}{1-z} \prod_{\ell=0}^{b-1} \left(1 - T\big(\omega^\ell \alpha e^{-\alpha} z^{1/b}\big)/\alpha\right). \tag{9.1}$$

10 FCFS displacement

In the combinatorial model, from section 9, $U(bz, w, q) = \sum_{m \geq 1} w^{bm} \sum_{n \geq 0} \frac{(bmz)^n}{n!} P_{m,n}(q)$, where $P_{m,n}(q)$ is the probability generating function for the displacement of the $(n+1)$st inserted element. The generating function for the displacement of a random element when having $n+1$ elements in the table is $FC_{m,n}(q) := \frac{\sum_{i=0}^{n} P_{m,i}(q)}{n+1}$. We need then a transform $w^{bm} \frac{(bmz)^n}{n!} P_{m,n}(q) \mapsto w^{bm} z^n \frac{\sum_{i=0}^{n} P_{m,i}(q)}{n+1}$.

In this regard, the Laplace transform leads to the *ordinary* generating function

$$\int_0^\infty U(byt, we^{-t}, q)\, dt = \sum_{m\geq 1} \frac{w^{bm}}{bm} \sum_{n\geq 0} y^n P_{m,n}(q).$$

As a consequence we have the ordinary generating function

$$FCFS(bz, w, q) = \sum_{m\geq 1} w^{bm} \sum_{n\geq 0} FC_{m,n}(q) z^n = \frac{w\partial_w}{z} \int_0^z \left(\int_0^\infty U(byt, we^{-t}, q)\, dt \right) \frac{dy}{1-y}. \quad (10.1)$$

In the probabilistic model, when inserting a new element in the hash table with the FCFS rule, we do exactly as in an unsuccessful search, except that at the end we insert the new element. Hence the displacement of a new element has the same distribution as U_i in Section 9. However (unlike the RH rule), the elements are never moved once they are inserted, and when studying the displacement of an element already in the table, we have to consider U_i at the time the element was added.

We consider again infinite hashing on $\mathbb{Z}$, and add a time dimension by letting the elements arrive to the buckets by independent Poisson process with intensity 1. At time $t \geqslant 0$, we thus have $X_i \sim \mathrm{Po}(t)$, so at time αb we have the same model as before, but with each element given an arrival time, with the arrival times being i.i.d. and uniformly distributed on $[0, b\alpha]$. (We cannot proceed beyond time $t = b$; at this time the table becomes full and an infinite number of elements overflow to $+\infty$; however, we consider only $t < b$.)

Consider the table at time αb, containing all element with arrival times in $[0, \alpha b]$. We are interested in the FCFS displacement of a "randomly chosen element". Since there is an infinite number of elements, this is not well-defined, but we can interpret it as follows (which gives the correct limit of finite hash tables): By a basic property of Poisson processes, if we condition on the existence of an element, x say, that arrives to a given bucket i at a given time t, then all other elements form a Poisson process with the same distribution as the original process. Hence the FCFS displacement of x has the same distribution as U_i, computed with the load factor α replaced by $\beta := t/b$. Furthermore, as said above, the arrival times of the elements are uniformly distributed in $[0, \alpha b]$, so β is uniformly distributed in $[0, \alpha]$. Hence, the FCFS displacement D^{FC} of a random element is (formally by definition) a random variable with the distribution

$$\Pr(D^{\mathsf{FC}} = k) = \frac{1}{\alpha} \int_0^\alpha \Pr\big(U_i(\beta) = k\big)\, \mathrm{d}\beta, \quad (10.2)$$

where $U_i(\beta)$ means U_i with the load α replaced by β. This leads to the following, where we now write α as an explicit parameter of all quantities that depend on it.

Theorem 10.1 *The probability generating function $\psi_{\mathsf{FC}}(z) := \mathbb{E}\, z^{D_i^{\mathsf{FC}}}$ of D_i^{FC} is given by*

$$\begin{aligned} \psi_{\mathsf{FC}}(z;\alpha) &= \frac{1}{\alpha} \int_0^\alpha \psi_U(z;\beta)\, \mathrm{d}\beta = \frac{1}{\alpha} \int_0^\alpha \frac{\tau(\beta)}{1-z} \prod_{\ell=0}^{b-1} \big(1 - \zeta_\ell(z;\beta)\big)\, \mathrm{d}\beta \\ &= \frac{1}{\alpha} \int_0^\alpha \frac{b(1-\beta) \prod_{\ell=0}^{b-1} \big(1 - \zeta_\ell(z;\beta)\big)}{(1-z) \prod_{\ell=1}^{b-1} (1 - \zeta_\ell(1;\beta))}\, \mathrm{d}\beta. \end{aligned} \quad (10.3)$$

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Connectivity for a modified binomial random graph by agglomeration

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Abstract. In the classical Erdős-Rényi random graph $G(n,p)$ there are n vertices and each of the possible edges is independently present with probability p. One of the most known results for this model is the threshold for connectedness, a phenomenon which is tightly related to the nonexistence of isolated vertices.

Numerous random graphs inspired in real networks are inhomogeneous in the sense that not all vertices have the same characteristic, which may influence the connection probability between pairs of vertices. The random graph $G(n,p)$ is homogeneous in this respect. Thus, with the aim to study real networks, new random graph models have been introduced and analyzed recently.

The purpose of this paper is to contribute to this task by proposing a new inhomogeneous random graph model which is obtained in a constructive way from the classical Erdős-Rényi model. We consider an initial configuration of subsets of vertices and we call each subset a super-vertex, then the random graph model is defined by letting two super-vertices be connected if there is at least one edge between them in $G(n,p)$. Our main result concerns the threshold for connectedness.

We point out that even though our model begins from $G(n,p)$, it assumes the existence of community structure and under certain conditions it exhibits a power law degree distribution, both important properties for real applications.

Keywords: Erdős-Rényi random graph, inhomogeneous random graph, connectedness

1 Introduction

The subject of random graphs began in 1959-1960 with the papers "On random graphs I" and "On the evolution of random graphs" by Erdős and Rényi [9, 10], and since then many properties about this model have been analyzed in order to answer questions of physical and mathematical interest. In the last decades a big interest in random graphs and random graphs processes has arisen because this kind of models can

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be used to analyze real situations, since the evolution of random graphs may be considered as a model of the evolution of real nets, e.g. the electric network system of a city or the development of social relations.

The original model studied by Erdős and Rényi begins with no edges at time 0 and adds new edges, one at a time, uniformly at random among all edges not already present. The M-th stage of this process can be identified with the uniform random graph model $G(n, M)$, in which a graph is chosen with uniform probability over all graphs with n vertices and exactly M edges. It was observed that the uniform model $G(n, M)$ can be also studied by another random graph model closely related, where a set of n vertices is given, and each possible edge is present independently with probability p. This model is called the binomial model $G(n, p)$ and was introduced by Gilbert [11] at about the same time. It is well known that the models $G(n, p)$ and $G(n, M)$ are essentially equivalent for the correct choice of M and p.

One of the most famous results of Erdős and Rényi [10] is the threshold for connectedness, a phenomenon which is tightly related to the nonexistence of isolated vertices. Clearly, when there exists at least one isolated vertex the graph is disconnected, but the opposite implication is not in general true. Remarkably, it was showed that when there are no isolated vertices, the random graph is with high probability (meaning with probability tending to one as $n \to \infty$ and denoted by whp) connected (see [10, 3]).

During the last few decades, it was observed that many real-world networks are inhomogeneous, in the sense that vertices can be of different types and they are connected according to it. A general model of an inhomogeneous random graph is proposed by Bollobás, Janson and Riordan [2], which consider a conditional independence between the edges, where the number of edges is linear in the number of vertices. This model includes as special cases many models previously studied in the literature, see for instance Durret [1] and Bollobás, Janson and Riordan [8]. In the random graph model introduced in [2], it is shown that under a weak (convergence) assumption on the expected number of edges, many interesting properties can be determined, in particular the critical point of the phase transition, and the size of the giant component above the transition. Additionally other properties are also studied, including the degree distribution, the numbers of paths and cycles, and the typical distance between pairs of vertices in the giant component. More recently, van der Hofstad [12] analyzes the critical behavior of the largest component in inhomogeneous random graphs in the so called rank-1 case, where the vertices receive vertex weights, and edges are present between vertices with a probability that is approximately proportional to the product of the weights of the vertices in the edge. Such work mainly considers the Poisson random graph or Norros-Reittu random graph [15], where the degree of vertex i is close in distribution to a Poisson random variable with parameter w_i, where w_i denotes the weight of i. In [12] is showed that the critical behavior depends sensitively on the asymptotic properties of their degree sequence, i.e., the asymptotic proportion of vertices with degree k for each $k \geq 1$, futhermore the author extended these results to the model studied by Chung and Lu [5, 6] and the one studied by Britton, Deijfen and Martin-Löf [4].

This explosion of research in random graphs has been originated with the aim to find models which describe the complexity of real world networks. The purpose of this paper is to contribute to this task by proposing a new inhomogeneous random graph model which is obtained in a constructive way from the classical Erdős-Rényi model. By a constructive way, we mean an explicit scheme for constructing the graph from a given configuration of $G(n, p)$. We consider a configuration of subsets of vertices that represents the agglomeration of nodes, and we will call it a configuration of super-vertices. Then, from it an inhomogeneous random graph model is defined by letting two super-vertices be connected if there is at least one edge between them in $G(n, p)$. Note that we are not assuming that the vertices in the super-vertices should be all connected, so they are not necessarily clusters in $G(n, p)$.

As we already point out, the study of inhomogeneous random graphs and its mathematical properties is

an issue of current research and there are many recent works dealing with this kind of models. We believe that constructive models like the one proposed here are an useful contribution to addressing the modeling of real networks. Our model assumes the existence of community structure and under certain conditions it exhibits a power law degree distribution, which are both well important properties for real applications. Related constructive random graph models are analyzed for instance by Janson and Spencer [14] and by Seshadhri, Kolda and Pinar [16].

For our model we determine the precise critical point for connectedness. In order to obtain our main result, we apply Stein's method, instead of the moments method used in the original proof by Erdős and Rényi [10], and show that the number of isolated super-vertices converges in law to the Poisson distribution, similar to the alternative proof by Janson, Łuczak and Ruciński [13].

2 The model and main results

The motivation of our model comes from the construction of a random graph inspired in real networks with a community structure. In order to model such a situation we consider a random graph with a given number of "super-vertices" (the agglomerates) of given sizes where we assume that the underlying graph structure follows a $G(n,p)$ law. By a "super-vertex" of size i we mean a subset of i vertices from $G(n,p)$, not necessarily connected.

Let $N \in \mathbb{N}$, $r \in \mathbb{N}^+$, $\mathcal{K} = \{k_i : k_i \in \mathbb{N}, 1 \leq i \leq r\}$ and $p \in (0,1)$ be given. We define $G(N,\mathcal{K},p)$ to be a random graph on N super-vertices with configuration $\mathcal{K}$, where k_i denotes the number of super-vertices of size i, $i = 1,2,\ldots,r$, in which an edge between a pair of super-vertices of sizes i and j is present with probability

$$p_{ij} \quad := \quad 1-(1-p)^{ij}\,, \tag{1}$$

independently of each other, and we assume there are no loops. In words, (1) is the probability that a pair of super-vertices of sizes i and j is connected if there is at least one edge between the corresponding subsets of vertices in $G(n,p)$, see Figure 1. Note that the number of super-vertices and the number of vertices are given by $N = \sum_{i=1}^{r} k_i$ and $n = \sum_{i=1}^{r} ik_i$, respectively.

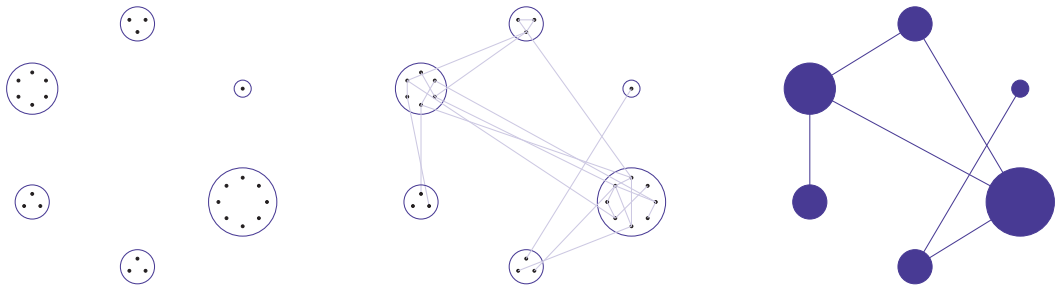
Our goal is to study properties of this random graph by considering different values of p as a function of either n or N. It seems difficult to obtain substantial asymptotic results for $G(N,\mathcal{K},p)$ without further restrictions. In this work we therefore assume that the limit of $\frac{k_i}{N}$ exists as $N \to \infty$ and denote it by μ_i. We note that, in this case, the limit of n/N exists and is given by $\sum_{i=1}^{r} \mu_i$. We further assume that

$$\mu_i > 0 \text{ for some } i \in \{1,2,\ldots,r\}, \tag{2}$$

which means there are initially many (of order N) super-vertices of size i, for some $1 \leq i \leq r$.

In this work we show that the threshold for connectedness for $G(N,\mathcal{K},p)$ is $p = \frac{\ln N + c(N)}{c'n}$, where $c(N)$ could be either a function of N or a constant, and $c' = \min\{i : \mu_i > 0\}$.

It is possible to note that our model belongs to the class of inhomogeneous random graphs studied by Bollobás, Janson and Riordan [2] and, under technical assumptions, some results about degree distribution and phase transition for the giant component can be obtained from Theorem 3.13 and Theorem 3.1 in [2], when $\lim_{N\to\infty}(n/N)$ exists. The threshold for connectedness is not studied in [2] and it is the main result of the current work.



(a) (b) (c)

Fig. 1: Construction of $G(N, \mathcal{K}, p)$. (a) Begin with a fixed configuration of N super-vertices, that is, subsets of vertices (in total there are n vertices). (b) Connect every pair of vertices independently with probability p, in other words, take a realization of $G(n, p)$. (c) A pair of super-vertices in $G(N, \mathcal{K}, p)$ is connected if there is at least one edge between the corresponding subsets of vertices in $G(n, p)$.

All our results are asymptotic, and the limits are taken as $N \to \infty$. We will use the following standard notation: for (deterministic) functions $f = f(N)$ and $g = g(N)$, we write $f = O(g)$ if f/g is bounded and $f = o(g)$ if $f/g \to 0$ as $N \to \infty$. We say that an event holds with high probability whp, if it holds with probability tending to 1 as $N \to \infty$. Formally, it is a sequence E_N of events that hold whp, but the N is often suppressed in the notation.

Our main result gives a precise location for the threshold for connectedness.

Theorem 1 *Consider the random graph $G(N, \mathcal{K}, p)$ with $r \in \mathbb{N}^+$ and let $p = \frac{\ln N + c(N)}{c' n}$, where $c' = \min\{i : \mu_i > 0\}$. Additionally, assume that the following limit exists*

$$\beta := \beta(c') = \lim_{N\to\infty} \sum_{i<c'} \frac{k_i}{N^{i/c'}}$$

if $c' > 1$ and define $\beta(1) = 0$.

(1) If either $\lim_{N\to\infty} c(N) = -\infty$ or if $c(N) \equiv c \in \mathbb{R}$ is a fixed constant and $\beta = \infty$, then

$$\lim_{N\to\infty} \mathbb{P}[G(N, \mathcal{K}, p) \text{ is connected}] = 0.$$

(2) Assume that $\beta < \infty$, then if $c(N) \equiv c \in \mathbb{R}$ is a fixed constant,

$$\lim_{N\to\infty} \mathbb{P}[G(N, \mathcal{K}, p) \text{ is connected}] = e^{-\beta - \mu_{c'} e^{-c}}.$$

In particular, if $\lim_{N\to\infty} \frac{n}{N} = 1$ then,

$$\lim_{N\to\infty} \mathbb{P}[G(N, \mathcal{K}, p) \text{ is connected}] = e^{-e^{-c}}.$$

(3) If $\lim_{N\to\infty} c(N) = +\infty$*, then*

$$\lim_{N\to\infty} \mathbb{P}[G(N,\mathcal{K},p) \text{ is connected}] = 1.$$

Remark 1 *We shall compare Theorem 1 with the threshold for connectedness in* $G(n,p)$*. Let* $p = \frac{1}{n}(\ln n + c(n))$*: If* $\lim_{n\to\infty} c(n) = -\infty$*, then* whp $G(n,p)$ *is disconnected, but if* $\lim_{n\to\infty} c(n) = +\infty$*, then* whp $G(n,p)$ *is connected. Furthermore, if* $c(n) \equiv c$ *is a fixed constant, the probability of* $G(n,p)$ *being connected is in the limit equal to* $e^{-e^{-c}}$*. Thus, Theorem 1 (2) says that if* $c(N)$ *is a fixed constant, the probability of* $G(N,\mathcal{K},p)$ *being connected is the same as that of* $G(n,p)$ *being connected provided* $\lim_{N\to\infty} \frac{n}{N} = 1$*. We observe that last condition means that* $\mu_1 = 1$ *and* $\mu_i = 0$ *for* $i > 1$*. The conclusion is natural because in this case both models have the same asymptotic number of nodes.*

Remark 2 *The property of connectedness for inhomogeneous random graphs was recently studied by Devroye and Fraiman in [7], where the authors consider an inhomogeneous random graph on a set of* n *vertices described in a similar way as the general model of [2]. In such model, each pair of vertices, say* k *and* l*, are connected independently with a probability that dependents on* x_k, x_l *and* p*, where* x_k, x_l *are associated values to the vertices* k *and* l*, respectively, and* $p = \ln n/n$*. In that paper a connectivity threshold is obtained in terms of some isolation parameter* λ_**, thus* whp *when* $\lambda_* > 1$ *the graph is connected, while if* $\lambda_* < 1$ *the graph is disconnected. Even though our model* $G(N,\mathcal{K},p)$ *is close to a discrete version of the model studied in [7] by taking* $p = \ln N/N$*, the critical point* λ_* *does not tell us when our model is not connected. For example, if* $\mu_1 > 0$ *the isolation parameter should be* $u := \lim_{N\to\infty} \frac{n}{N}$ *and if* $\mu_1 = 0$ *but* $\mu_2 > 0$*, then the isolation parameter should be* $2u$*. However* $u \geq 1$ *because* $n \geq N$*, so the isolation parameter does not tell us when* $G(N,\mathcal{K},p)$ *is disconnected. Therefore, we need to re-parametrize* p *differently in order to get the threshold for connectedness for* $G(N,\mathcal{K},p)$*.*

3 Proofs

3.1 Proof of Theorem 1

We prove the first part of the theorem by showing that with high probability isolated super-vertices exist, using the second moment method. The second part of the theorem is proved by showing that in the limit, $G(N,\mathcal{K},p)$ consists of a giant component and isolated super-vertices. Moreover, the number of isolated super-vertices follows asymptotically a Poisson law. Here we use Stein's method. Finally, the last part follows from the first moment method and by showing that in the limit, $G(N,\mathcal{K},p)$ does not contain components of order m, for $2 \leq m \leq N/2$.

In the rest of the paper we consider the random graph $G(N,\mathcal{K},p)$ with $r \in \mathbb{N}$ and

$$p = \frac{\ln N + c(N)}{c'n},$$

where $c' := \min\{i : \mu_i > 0\}$. Additionally, we denote the number of isolated super-vertices in $G(N,\mathcal{K},p)$ by X and we define the value

$$\beta := \beta(c') = \lim_{N\to\infty} \sum_{i<c'} \frac{k_i}{N^{i/c'}}$$

if $c' > 1$ and $\beta(1) = 0$.

Proof of Theorem 1 (1)

Observe that if the graph has isolated super-vertices, then it is not connected. Therefore, we shall show that whp isolated super-vertices exist on the graph.

Lemma 1 *Assume that either* $\lim_{N\to\infty} c(N) = -\infty$, $c(N) > -\ln N$, *or* $c \equiv c(N) \in \mathbb{R}$ *is a fixed constant and* $\beta = \infty$.

Then,

$$\lim_{N\to\infty} \mathbb{P}(X = 0) = 0. \tag{3}$$

Proof: Take any arbitrarily order of the super-vertices and let us write X as a sum of indicator random variables

$$X = \sum_{i=1}^{r} \sum_{k=1}^{k_i} I_k^i,$$

where $I_k^i = 1$ if the k-th super-vertex of size i is isolated and 0 otherwise. Note that $I_k^i = 1$ if the k-th super-vertex of size i is not connected with any other super-vertex of size i and neither connected with any other super-vertex of size $j \neq i$. Since the super-vertices are connected independently of each other, we have

$$\mathbb{E}(I_k^i) = (1-p_{ii})^{k_i-1} \prod_{j\neq i}^{r} (1-p_{ij})^{k_j} = (1-p)^{i^2(k_i-1)} \prod_{j\neq i}^{r} (1-p)^{ijk_j} = (1-p)^{i(n-i)},$$

and hence

$$\mathbb{E}(X) = \sum_{i=1}^{r} \sum_{k=1}^{k_i} \mathbb{E}(I_k^i) = \sum_{i=1}^{r} k_i (1-p)^{i(n-i)}. \tag{4}$$

On the other hand, we get

$$\begin{aligned} \mathbb{E}(X^2) &= \mathbb{E}\left(\left(\sum_{i=1}^{r} \sum_{k=1}^{k_i} I_k^i \right)^2 \right) \\ &= \mathbb{E}(X) - \sum_{i=1}^{r} k_i \mathbb{E}[I_1^i I_2^i] + \sum_{i,j=1}^{r} k_i k_j \mathbb{E}[I_1^i I_2^j]. \end{aligned} \tag{5}$$

For $i \neq j$, we obtain

$$\begin{aligned} \mathbb{E}[I_1^i I_2^j] &= \mathbb{P}(I_1^i = 1 \mid I_2^j = 1)\mathbb{P}(I_2^j = 1) \\ &= \left((1-p_{ii})^{k_i-1} (1-p_{ij})^{k_j-1} \prod_{l=1, l\neq i,j}^{r} (1-p_{il})^{k_l} \right) \mathbb{P}(I_2^j = 1) \\ &= (1-p)^{i(n-i)+j(n-j)-ij}, \end{aligned} \tag{6}$$

similarly for $i = j$ we get that $\mathbb{E}[I_1^i I_2^i] = (1-p)^{2i(n-i)-i^2}$. In fact, we will see that $\mathbb{E}[X] \to \infty$ and $\frac{\mathbb{E}[X^2]}{\mathbb{E}^2[X]} \to 1$ as $N \to \infty$. We will start analyzing $\mathbb{E}[X]$. Note that $1 - x = e^{-x+O(x^2/2)}$ if $|x| < 1$. For any constants $a_1, a_2 > 0$ we can write

$$\begin{aligned}(1-p)^{a_1 in - a_2 i^2} &= \exp\Big(-a_1 i\frac{(\ln N + c)}{c'} + O\Big(\frac{(\ln N + c)^2}{n}\Big)\Big) \\ &= \exp\Big(-a_1 i\frac{(\ln N + c)}{c'}\Big)\Big(1 + O\Big(\frac{(\ln N + c)^2}{n}\Big)\Big). \end{aligned} \tag{7}$$

Thus by (4) and (7) with $a_1 = a_2 = 1$, we have

$$\begin{aligned}\mathbb{E}(X) &= \Big(1 + O\Big(\frac{(\ln N + c)^2}{n}\Big)\Big)\sum_{i=1}^{r} k_i \exp\Big(-i\frac{(\ln N + c)}{c'}\Big) \\ &= \Big(1 + O\Big(\frac{(\ln N + c)^2}{n}\Big)\Big)\sum_{i=1}^{r} \frac{k_i}{N^{i/c'} e^{ic/c'}}. \end{aligned} \tag{8}$$

If $c = c(N)$ is such that $\lim_{N\to\infty} c(N) = -\infty$, $c(N) > -\ln N$, then since $c' = \min\{i : \mu_i > 0\}$, we get that (8) is greater or equal to $\Big(1 + O\Big(\frac{(\ln N+c)^2}{n}\Big)\Big)\frac{k_{c'}}{Ne^c} \to \infty$, as $N \to \infty$.

In the case that $c \in \mathbb{R}$ is a fixed constant and $\beta = \infty$, we have that there exists an $i < c'$ such that $\lim_{N\to\infty} \frac{k_i}{N^{i/c'}} = \infty$, we also get that (8) goes to infinity as N goes to infinity. Thus, we have that under the condition of this lemma, $\mathbb{E}(X) \to \infty$ as $N \to \infty$. Now observe that by (5), (6) and (7)

$$\mathbb{E}[X^2] = \mathbb{E}[X] - \Big(1 + O\Big(\frac{(\ln N + c)^2}{n}\Big)\Big)\Big(\sum_{i=1}^{r} \frac{k_i}{N^{2i/c'} e^{2ic/c'}} - \sum_{i,j=1}^{r} \frac{k_i k_j}{N^{(i+j)/c'} e^{(i+j)c/c'}}\Big),$$

and by (4) and (7) $\mathbb{E}^2[X] = \Big(1 + O\Big(\frac{(\ln N+c)^2}{n}\Big)\Big)\sum_{i,j=1}^{r} \frac{k_i k_j}{N^{(i+j)/c'} e^{(i+j)c/c'}}$, so

$$\frac{\mathbb{E}(X^2)}{\mathbb{E}^2(X)} = \frac{1}{\mathbb{E}(X)} - \frac{\Big(1 + O\Big(\frac{(\ln N+c)^2}{n}\Big)\Big)\Big(\sum_{i=1}^{r} \frac{k_i}{N^{2i/c'} e^{2ic/c'}} - \sum_{i,j=1}^{r} \frac{k_i k_j}{N^{(i+j)/c'} e^{(i+j)c/c'}}\Big)}{\Big(1 + O\Big(\frac{(\ln N+c)^2}{n}\Big)\Big)\sum_{i,j=1}^{r} \frac{k_i k_j}{N^{(i+j)/c'} e^{(i+j)c/c'}}},$$

and since $c' = \min\{i : \mu_i > 0\}$, then,

$$0 \le \frac{\sum_{i=1}^{r} \frac{k_i}{N^{2i/c'} e^{2ic/c'}}}{\sum_{i,j=1}^{r} \frac{k_i k_j}{N^{(i+j)/c'} e^{(i+j)c/c'}}} < \frac{\sum_{i<c'/2}^{r} \frac{k_i}{N^{2i/c'} e^{2ic/c'}} + \sum_{i\ge c'/2}^{r} \frac{k_i}{N^{2i/c'} e^{2ic/c'}}}{\sum_{i<c'/2}^{r} \frac{k_i^2}{N^{2i/c'} e^{2ic/c'}} + \frac{k_{c'}^2}{N^2 e^{2c}}} \to 0.$$

Thus, $\frac{\mathbb{E}(X^2)}{\mathbb{E}^2(X)} \to 1$ and

$$\mathbb{P}(X = 0) \le \frac{\mathbb{V}(X)}{\mathbb{E}^2(X)} \longrightarrow 0 \text{ as } N \to \infty$$

□

Proof of Theorem 1 (3)

Theorem 1 (3) follows by the next lemma in which we will first prove that if $c(N)$ is such that $\lim_{N\to\infty} c(N) = +\infty$, then, in the limit $G(N,\mathcal{K},p)$ does not contain isolated super-vertices, and neither components (of super-vertices) of size m, $2 \le m \le N/2$. This is clearly sufficient since if the graph is disconnected, it has a component of size between 1 and $N/2$, but if whp $G(N,\mathcal{K},p)$ does not have isolated vertices, i.e, components of size 1, then we just need to show that there is neither a connected component of size m for $2 \le m \le N/2$.

Lemma 2 *Consider the random graph $G(N,\mathcal{K},p)$ with $p = \frac{\ln N + c(N)}{c'n}$ defined as before. If $\lim_{N\to\infty} c(N) = +\infty$, then*

$$\lim_{N\to\infty} \mathbb{P}[X = 0] = 1.$$

Furthermore, whp $G(N,\mathcal{K},p)$ does not have components of order m, for $2 \le m \le N/2$.

Proof: Since $c(N) \to +\infty$, by (4) and (7) we have

$$\mathbb{E}(X) = \Big(1 + O\Big(\frac{(\ln N + c)^2}{n}\Big)\Big) \sum_{i=1}^{r} \frac{k_i}{N^{i/c'} e^{ic/c'}} \longrightarrow 0, \text{ as } N \to \infty. \tag{9}$$

Thus, by Markov's inequality we get $\lim_{N\to\infty} \mathbb{P}(X = 0) = 1$.

To prove that whp $G(N,\mathcal{K},p)$ is connected, we still need to see that whp there are no components of order m, for $2 \le m \le N/2$. Let $\mathcal{S}^m$ be the set of all subsets of m super-vertices. For each $S \in \mathcal{S}^m$, let $m_i := m_i(S)$ be the number of super-vertices of size i in S, and note that $m = m_1 + \cdots + m_r$. Note that if the super-vertices in S form a component in $G(N,\mathcal{K},p)$, the following two events should hold:

1. $A_1^S :=$ { the super-vertices in S are connected}, and
2. $A_2^S :=$ { there is not a super-vertex in S connected with a super-vertex in S^c},

where S^c denotes the complement of S. Thus,

$$\begin{aligned} \mathbb{P}(\exists \text{ a component of size } m) &= \mathbb{P}(\cup_{S\in\mathcal{S}^m} \text{the super-vertices in } S \text{ form a component in } G(N,\mathcal{K},p)) \\ &\le \sum_{\mathcal{S}^m} \mathbb{P}(A_1^S)\mathbb{P}(A_2^S). \end{aligned} \tag{10}$$

Since a component of size m contains a tree of order m and $p_{ij} \le ijp \le r^2 p$, then

$$\mathbb{P}(A_1^S) \le \mathbb{P}(S \text{ form a tree}) \le m^{m-2}(r^2 p)^{(m-1)}. \tag{11}$$

On the other hand, let $M := \sum_{i=1}^{r} i m_i$, then

$$\mathbb{P}(A_2^S) = (1-p)^{M(n-M)} < (1-p)^{M^*(n-M^{**})} < (1-p)^{nM^* - (M^{**})^2}, \tag{12}$$

where $M^* := \min_{\mathcal{S}^m}\{M\}$ and $M^{**} := \max_{\mathcal{S}^m}\{M\}$. Hence, by (10), (11) and (12),

$$\mathbb{P}(\exists \text{ a component of size } m) < \binom{N}{m} m^{m-2}(r^2 p)^{(m-1)}(1-p)^{nM^* - (M^{**})^2}. \tag{13}$$

We will work the case $m = 2$ separately. Thus by (13), when $m = 2$ we have that $M \leq 2r$, so

$$\begin{aligned}
\mathbb{P}(\exists \text{ a component of size } 2) &< \binom{N}{2}(r^2p)(1-p)^{nM^*-(M^{**})^2} \\
&< \frac{Nr^2}{2c'}(\ln N + c)\exp\Big\{\frac{-M^*}{c'}(\ln N + c) + \frac{4r^2}{c'n}(\ln N + c)\Big\} \\
&< \frac{Nr^2}{2c'}(\ln N + c)\frac{1}{N^{M^*/c'}} \\
&< \frac{r^2}{2Nc'}(\ln N + c)(1 + o(1)) + o(1), \qquad (14)
\end{aligned}$$

where the last inequality follows by observing that $M \geq 2c'$ holds whp since the probability of choosing at least one super-vertex of sizes $i < c'$ is smaller than $\sum_{i<c'} \frac{k_i}{N} \to 0$ as $N \to \infty$. In general, for $m > 2$ we have that $M \geq mc'$ holds whp.

Now we will analyze the cases $3 \leq m \leq N/2$. Again by (13) and using that $\binom{N}{m} < \frac{(2eN)^m}{m^{m+1/2}}$ and the event $M \geq mc'$ holds whp, we have that the probability of a component of size m exists is at most

$$\begin{aligned}
&\frac{(2eN)^m}{m^{m+1/2}} m^{m-2}(r^2p)^{m-1}(1-p)^{nM^*-(M^{**})^2} \\
< \;& Nm^{-5/2}\exp\Big\{m + m\ln 2r^2(\ln N + c) - \frac{M^*(\ln N + c)}{c'} + \frac{(M^{**})^2(\ln N + c)}{c'n}\Big\} \\
< \;& Nm^{-5/2}\exp\Big\{m\ln\ln N - m\ln N\Big\}(1 + o(1)) + o(1) \\
< \;& Nm^{-5/2}\exp\Big\{m\ln N^{3/5} - m\ln N\Big\}(1 + o(1)) + o(1). \qquad (15)
\end{aligned}$$

Therefore, by (14) and (15) we obtain

$$\begin{aligned}
\sum_{m=2}^{N/2}\mathbb{P}(\exists \text{ a component of size } m) &< \Big\{r^2\frac{\ln N + c}{N} + N^{-1/5}\Big\}(1 + o(1)) + o(1) \\
&= O\Big(\frac{\ln N + c}{N}\Big). \qquad (16)
\end{aligned}$$

□

Proof of Theorem 1 (2)

We will start by proving that if $c \equiv c(N) \in \mathbb{R}$ is a fixed constant, and under some extra conditions, the number of isolated super-vertices asymptotically follows a Poisson distribution. To this end we will use Stein's method, in particular Theorem 6.24 [13]. Write

$$X = \sum_{k=1}^{N} I_k,$$

where $I_k = 1$ if the k-th super-vertex is isolated and $I_k = 0$ otherwise. The random variables $\{I_k\}_k$ are said to be positively related if for each k, there exists a family of random variables J_{lk}, $l \neq k$, such that

the joint distribution of $\{J_{lk}\}_l$ equals the conditional distribution of $\{I_l\}_l$ given $I_k = 1$. Furthermore, if $J_{lk} \geq I_l$ for every $l \neq k$. Formally,

$$\mathcal{L}(\{J_{lk}\}_l) = \mathcal{L}(\{I_l\}_l \mid I_k = 1),$$

where $\mathcal{L}(\{Y_l\}_l)$ denotes the joint distribution of the random variables $\{Y_l\}_l$.

Theorem 6.24 [13] says that if the random variables $\{I_k\}_k$ are positively related, then

$$d_{TV}(X, Po(\lambda)) \leq \frac{\mathbb{V}(X)}{\mathbb{E}(X)} - 1 + 2\max_k\{\mathbb{E}(I_k)\},$$

where $\lambda = \mathbb{E}(X)$, and $d_{TV}(,)$ is the total variation distance.

Lemma 3 *Consider the random graph model $G(N, \mathcal{K}, p)$ with $p = \frac{\ln N + c(N)}{c'n}$ defined as before. Assume that $c \equiv c(N) \in \mathbb{R}$ is a fixed constant and $\beta < \infty$. Then, X has asymptotically Poisson distribution with mean $\beta + \mu_{c'} e^{-c}$.*

Proof: Let $G_k(N, \mathcal{K}, p)$ be the random graph $G(N, \mathcal{K}, p)$ with all edges from the k-th super-vertex removed, and let $J_{lk} = 1$ if the l-th super-vertex is isolated in $G_k(N, \mathcal{K}, p)$, and $J_{lk} = 0$ otherwise. Observe that

$$J_{lk} = (I_l \mid I_k = 1),$$

then,

$$\mathcal{L}(\{J_{lk}\}_l) = \mathcal{L}(\{I_l\}_l \mid I_k = 1).$$

Moreover, we can check that $J_{lk} \geq I_l$ for every $l \neq k$, thus the random variables $\{I_k\}_k$ are positively related and we can apply Theorem 6.24 [13]. To do that we need to calculate the magnitude of $\mathbb{V}(X)$ and $\mathbb{E}(X)$.

By Newton's generalized binomial theorem and since $ij \leq r^2$ for any $i, j \in \{1, \ldots, r\}$ and r is constant, we have

$$(1-p)^{-ij} = 1 + O\Big(\frac{\ln N}{n}\Big). \tag{17}$$

Thus, By (4), (5), (7) and (17) we get after some algebraic manipulations that

$$\begin{aligned}
\mathbb{V}(X) &= \mathbb{E}[X] + \sum_{i,j=1}^{r} k_i k_j (1-p)^{i(n-i)+j(n-j)}[(1-p)^{-ij} - 1] - \sum_{i=1}^{r} k_i (1-p)^{2i(n-i)-i^2} \\
&= \mathbb{E}[X] + \Big(1 + O\Big(\frac{(\ln N)^2}{n}\Big)\Big)\Big(\sum_{i,j=1}^{r} O\Big(\frac{\ln N}{n}\Big)\frac{k_i k_j}{N^{(i+j)/c'} e^{(i+j)c/c'}} - \sum_{i=1}^{r} \frac{k_i}{N^{2i/c'} e^{2ic/c'}}\Big) \\
&= \mathbb{E}[X] + \Big(1 + O\Big(\frac{(\ln N)^2}{n}\Big)\Big)\Big(O\Big(\frac{\ln N}{n}\Big) - O\Big(\frac{1}{N}\Big)\Big) \\
&= \mathbb{E}[X] + O\Big(\frac{\ln N}{n}\Big)
\end{aligned}$$

and $\mathbb{E}[X] = \Big(1 + O\Big(\frac{(\ln N)^2}{n}\Big)\Big)\Big(\sum_{i<c'} \frac{k_i e^{-ic/c'}}{N^{i/c'}} + \sum_{i \geq c'} \frac{k_i e^{-ic/c'}}{N^{i/c'}}\Big) + O\Big(\frac{\ln N}{n}\Big)$.

Furthermore,

$$\mathbb{E}(I_k) = \sum_{i=1}^{r}(1-p)^{i(n-i)} = \Big(1 + O\Big(\frac{(\ln N)^2}{n}\Big)O\Big(\frac{1}{N^{1/c'}}\Big),$$

so, $\max_{1\leq k\leq N}\{\mathbb{E}(I_k)\}$ is of magnitude $O\Big(\frac{1}{N^{1/c'}}\Big)$. Thus, we can conclude that X has asymptotically Poisson distribution with mean $\beta + \mu_{c'}e^{-c}$, where $\beta = \lim_{N\to\infty}\sum_{i<c'}\frac{k_i e^{-ic/c'}}{N^{i/c'}}$ and $0 \leq \beta < \infty$.

Additionally observe that since $n = \sum_{j=1}^{r} jk_j$ and $N = \sum_{j=1}^{r} k_j$, then $\frac{n}{N} = 1 + \frac{1}{N}\sum_{j=2}^{r}(j-1)k_j$. Thus under the condition that $\lim_{N\to\infty}\frac{n}{N} = 1$, we have that $\lim_{N\to\infty}\frac{k_j}{N} = 0$, for all $j \geq 2$, since r is fixed. Due to our assumption (2), $\mu_1 = 1$ and therefore $\beta = 0$. Then if c is a fixed constant what we have is that X has asymptotically Poisson distribution with mean e^{-c}. □

Lemma 4 *Consider the random graph model $G(N,\mathcal{K},p)$ with $p = \frac{\ln N + c(N)}{c'n}$ as before. Assume that $c \equiv c(N) \in \mathbb{R}$ is a fixed constant and $\beta < \infty$. Then,*

$$\lim_{N\to\infty}\mathbb{P}[G(N,\mathcal{K},p) \textit{ is connected}] = e^{-\beta-\mu_{c'}e^{-c}}.$$

In particular, if $\lim_{N\to\infty}\frac{n}{N} = 1$ then,

$$\lim_{N\to\infty}\mathbb{P}[G(N,\mathcal{K},p) \textit{ is connected}] = e^{-e^{-c}}.$$

Proof: By (16) we know that the probability that $G(N,\mathcal{K},p)$ has a component of order m, for $2 \leq m \leq N/2$ is smaller than $O\Big(\frac{\ln N + c}{N}\Big)$. Thus, by Lemma 3 and we conclude

$$\mathbb{P}[G(N,\mathcal{K},p) \text{ is connected}] = \mathbb{P}(X=0) + O\Big(\frac{\ln N + c}{N}\Big) \to e^{-\beta-\mu_{c'}e^{-c}}.$$

In particular, if $\lim_{N\to\infty}\frac{n}{N} = 1$, then $\mu_1 = 1$ which implies that $\beta = 0$ and

$$\lim_{N\to\infty}\mathbb{P}[G(N,\mathcal{K},p) \text{ is connected}] = e^{-e^{-c}}.$$

□

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On the Number of Multi-Base Representations of an Integer

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Abstract. In a multi-base representation of an integer (in contrast to, for example, the binary or decimal representation) the base (or radix) is replaced by products of powers of single bases. The resulting numeral system is usually redundant, which means that each integer can have multiple different digit expansions. We provide a general asymptotic formula for the number of such multi-base representations of a positive integer n. Moreover, we prove central limit theorems for the sum of digits and the Hamming weight of a random representation.

Keywords: multi-base representations, asymptotic formula, partitions

1 Introduction

A *numeral system*(i) (also called *system of numeration*) is a way to represent numbers. The most common examples are, of course, the ordinary decimal and binary systems, which represent numbers in base 10 and 2, respectively. Beside those "standard" systems, there is an immense number of other numeral systems.

For fast arithmetic, the right choice of numeral system is an important aspect. The algorithms we have in mind here are, for example, exponentiation in a finite group and the scalar multiplication on elliptic curves. Both are used in cryptography, and clearly we want to improve on the running time of those algorithms (which are often based on a Horner scheme, cf. Knuth [Knu98]).

Starting with the binary system, one can improve the performance of the aforementioned algorithms by adding more digits than needed, and thus making the numeral system *redundant*, which means that each element can have a lot of different representations. For instance, using digits 0, 1 and -1 can lead to a speed-up, cf. Morain and Olivos [MO90] for such a scalar multiplication algorithm on elliptic curves. To gain back the uniqueness, additional syntax can complement the redundant system. In the example

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(i) We use the term *numeral system* rather than *number system* as it is also called sometimes, since that name is ambiguous. For example, the system of p-adic numbers or the system of real numbers are called number systems.

using digits 0, 1 and -1, this can be the non-adjacent form, see Reitwiesner's seminal paper [Rei60]. Generalizations in that direction can be found in [BSS99, Gor98, MOC97, Sol00].

A different way to get a better running time is to use double-base and multi-base numeral systems, which usually leads to redundancy as well. In a *multi-base representation of* n (or *multi-base expansion*), a positive integer n is expressed as a finite sum

$$n = \sum_{i=1}^{I} a_i B_i, \tag{1}$$

such that the following holds.

- The a_i (called *digits*) are taken from a fixed finite *digit set* (here, we will be using the canonical digit set $\{0, 1, \dots, d-1\}$ for some fixed integer $d \geq 2$).
- The B_i are in increasing order (i.e., $B_1 < B_2 < \cdots < B_I$) and taken from the set

$$\mathcal{S} = \{p_1^{\alpha_1} p_2^{\alpha_2} \dots p_m^{\alpha_m} : \alpha_i \in \mathbb{N} \cup \{0\}\}.$$

  The $p_1, \dots, p_m$ are called the *bases* (in our setting, these are fixed coprime positive integers).

Double-base numeral systems are used for cryptographic applications, see for example [ADDS06, DIM08, DJM99]. The typical bases are 2 and 3. With these bases (and digits at least 0 and 1), each positive integer has a double-base representation, cf. Berthé and Imbert [BI09]. When using general bases, less is known on the existence, cf. Krenn, Thuswaldner and Ziegler [KTZ13] for some results using small symmetric digit sets. However, choosing the digit set large enough (so that the numeral system with only one of the bases can already represent all positive integers), existence can always be guaranteed. Thus, when each positive integer has a multi-base representation, a natural next question to ask is: How many representations does each integer have?

This question has also already been studied for redundant single-base representations; see Protasov [Pro00, Pro04] for recent results involving non-negative digits. When negative digits are used as well (for example in elliptic curve cryptography), there are usually infinitely many representations of a number, so counting these does not make sense. In this case, expansions with a minimum number of non-zero digits are of interest, since they lead to fast evaluation schemes. See Grabner and Heuberger [GH06] for a result counting minimal representations (one minimal representation is the non-adjacent form mentioned above, cf. also [HK13a, HK13b, Rei60]).

In the following, we will study the number of representations of n in a given multi-base system, which we denote by $P(n)$ (we suppress the dependence on $p_1, p_2, \dots, p_m$ and d).

Let us start with the double-base system with bases 2 and p, where $p > 1$ is an odd integer, and digits 0 and 1. We can group terms involving the same powers of p and use the uniqueness of the binary expansion to show that double-base representations with bases 2 and p are in bijection with partitions into powers p, i.e., representations of the form

$$n = n_0 + n_1 p + n_2 p^2 + n_3 p^3 + \cdots$$

with non-negative integers n_i. More generally, the same is true for double-base representations with bases q and p and digit set $\{0, 1, \dots, q-1\}$. It seems that the first non-trivial approximation of $P(n)$ in this

special case is due to Mahler [Mah40]. By studying Mordell's functional equation, he obtained

$$\log P(pn) \approx (\log n)^2/(2\log p).$$

The much more precise result

$$\log P(pn) = \frac{1}{2\log p}\left(\log\frac{n}{\log n}\right)^2 + \left(\frac{1}{2} + \frac{1}{\log p} + \frac{\log\log p}{\log p}\right)\log n - \left(1 + \frac{\log\log p}{\log p}\right)\log\log n + \mathcal{O}(1)$$

was derived by Pennington [Pen53]. The error term in the previous asymptotic formula exhibits a periodic fluctuation.

For further reference, see A005704 in the On-Line Encyclopedia of Integer Sequences [OEI14] for more information and see also [DIM08, MD08] for the connection to double-base systems.

The aim of this work is to give an asymptotic formula in a more general set-up. Throughout this paper, $d \geq 2$ and $m \geq 2$ are fixed integers, and $p_1, p_2, \ldots, p_m$ are integers such that $1 < p_1 < p_2 < \cdots < p_m$ and $(p_i, p_j) = 1$ for $i \neq j$. As our first main theorem, we prove an asymptotic formula for the number of representations of n of the form (1). It will be convenient to use the abbreviation

$$\kappa = \frac{\log d}{m!}\prod_{i=1}^{m}\frac{1}{\log p_i}.$$

Theorem 1. *If $m \geq 3$, then the number $P(n)$ of distinct multi-base representations of n of the form* (1) *satisfies the asymptotic formula*

$$\log P(n) = C_0(\log n)^m + C_1(\log n)^{m-1}\log\log n + C_2(\log n)^{m-1} + \mathcal{O}\Big((\log n)^{m-2}\log\log n\Big)$$

for $n \to \infty$, where

$$\begin{aligned} C_0 &= \kappa,\\ C_1 &= -m(m-1)\kappa,\\ C_2 &= \kappa m\Big(1 + \tfrac{1}{2}\sum_{i=1}^{m}\log p_i - \tfrac{1}{2}\log d - \log(\kappa m)\Big). \end{aligned}$$

In the case that there are precisely two bases, we have the following more precise asymptotic result:

Theorem 2. *If $m = 2$, then the number $P(n)$ of distinct multi-base representations of n of the form* (1) *satisfies the asymptotic formula*

$$P(n) = K(n)(\log n)^{K_0} n^{K_1}\exp\left(\kappa\log^2\left(\frac{n}{\log n}\right)\right),$$

for $n \to \infty$, where $K(n)$ is a fluctuating function of n that is bounded above and below by positive numbers, and

$$\begin{aligned} K_0 &= \tfrac{1}{2} + 2\kappa\big(\log(2\kappa) - \tfrac{1}{2}(\log p_1 + \log p_2 - \log d)\big),\\ K_1 &= 2\kappa\big(1 - \log(2\kappa) + \tfrac{1}{2}(\log p_1 + \log p_2 - \log d)\big) - 1. \end{aligned}$$

Moreover, we study the distribution of two natural parameters in random multi-base representations, namely the sum of digits, i.e. $a_1 + a_2 + \cdots + a_I$ in the notation of (1), and the Hamming weight (the number of non-zero coefficients a_i):

Theorem 3. *The sum of digits in a random multi-base representation of n of the form* (1) *asymptotically follows a Gaussian distribution with mean and variance equal to*

$$\mu_n = \frac{\kappa(d-1)}{2\log d}(\log n)^m + \mathcal{O}\Big((\log n)^{m-1}\log\log n\Big)$$

and

$$\sigma_n^2 = \frac{\kappa(d-1)(d+1)}{12\log d}(\log n)^m + \mathcal{O}\Big((\log n)^{m-1}\log\log n\Big)$$

respectively.

Theorem 4. *The Hamming weight of a random multi-base representation of n of the form* (1) *asymptotically follows a Gaussian distribution with mean and variance equal to*

$$\mu_n = \frac{\kappa(d-1)}{d\log d}(\log n)^m + \mathcal{O}\Big((\log n)^{m-1}\log\log n\Big)$$

and

$$\sigma_n^2 = \frac{\kappa(d-1)}{d^2\log d}(\log n)^m + \mathcal{O}\Big((\log n)^{m-1}\log\log n\Big)$$

respectively.

The proofs of all these theorems are based on a saddle-point analysis of the associated generating functions. As it turns out, the tail estimates are most challenging, especially in the case $m = 2$ (see Section 3 for details). For the asymptotic analysis of the various harmonic sums that occur, we apply the classical Mellin transform technique, see [FGD95]. We remark that our approach would also allow us to prove central limit theorems for other parameters as, for instance, the number of occurrences of a fixed digit.

2 The Generating Function

We start with a generating function for our problem. Consider the set

$$\mathcal{S} = \{p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_m^{\alpha_m} : \alpha_i \in \mathbb{N} \cup \{0\}\},$$

which is exactly the monoid that is freely generated by $p_1, p_2, \ldots, p_m$. Note that the representations of n correspond exactly to partitions of n into elements of $\mathcal{S}$ where each term has multiplicity at most $d-1$. The generating function for such partitions, where the first variable z marks the size n and the second variable u marks the sum of digits, can be written as

$$F(z,u) = \prod_{h\in\mathcal{S}} \Big(1 + uz^h + u^2 z^{2h} + \cdots + u^{d-1} z^{(d-1)h}\Big) = \prod_{h\in\mathcal{S}} \frac{1-(uz^h)^d}{1-uz^h}. \tag{2}$$

Likewise, we have the following generating function where the second variable marks the Hamming weight (number of non-zero digits, or equivalently number of distinct parts in a partition):

$$G(z,u)=\prod_{h\in\mathcal{S}}\left(1+uz^h+uz^{2h}+\cdots+uz^{(d-1)h}\right)=\prod_{h\in\mathcal{S}}\left(1+uz^h\frac{1-z^{(d-1)h}}{1-z^h}\right). \tag{3}$$

Obviously, $F(z,1)=G(z,1)$. We would like to apply the saddle point method to these generating functions. The trickiest part in this regard are the rather technical tail estimates, especially when $m=2$, which will be discussed in the following section. We will also need an asymptotic expansion in the central region. To this end, we define the two functions

$$f(t,u)=\log F(e^{-t},u)=\sum_{h\in\mathcal{S}}\log\left(1+ue^{-ht}+u^2e^{-2ht}+\cdots+u^{d-1}e^{-(d-1)ht}\right)$$

and

$$g(t,u)=\log G(e^{-t},u)=\sum_{h\in\mathcal{S}}\log\left(1+ue^{-ht}+ue^{-2ht}+\cdots+ue^{-(d-1)ht}\right).$$

Lemma 5. *Suppose that u lies in a fixed bounded, positive interval around 1, e.g. $u\in[1/2,2]$.*

1. *For certain (real-)analytic functions $a_1(u)$, $a_2(u)$, …, $a_m(u)$ with*

$$a_m(u)=\log(1+u+\cdots+u^{d-1})\prod_{k=1}^{m}\frac{1}{\log p_k},$$

we have the following asymptotic formula as $t\to 0^+$ (t positive and real), uniformly in u:

$$f(t,u)=\frac{a_m(u)}{m!}(\log 1/t)^m+\frac{a_{m-1}(u)}{(m-1)!}(\log 1/t)^{m-1}+\cdots+a_1(u)(\log 1/t)+\mathcal{O}(1).$$

Moreover,

$$\frac{\partial}{\partial t}f(t,u)=-\frac{a_m(u)}{(m-1)!t}(\log 1/t)^{m-1}+\mathcal{O}\big(t^{-1}(\log 1/t)^{m-2}\big)$$

and

$$\frac{\partial^2}{\partial t^2}f(t,u)=\frac{a_m(u)}{(m-1)!t^2}(\log 1/t)^{m-1}+\mathcal{O}\big(t^{-2}(\log 1/t)^{m-2}\big).$$

Finally, there exists an $\eta>0$ such that for complex t with $|\operatorname{Im} t|\le\eta$, we have

$$\frac{\partial^3}{\partial t^3}f(t,u)=\mathcal{O}\left((\operatorname{Re} t)^{-3}(\log 1/(\operatorname{Re} t))^{m-1}\right)$$

as $\operatorname{Re} t\to 0^+$, again uniformly in u.

2. *Likewise, there exist (real-)analytic functions $b_1(u),b_2(u),\dots,b_m(u)$ with*

$$b_m(u)=\log(1+(d-1)u)\prod_{k=1}^{m}\frac{1}{\log p_k},$$

such that the following asymptotic formula holds as $t \to 0^+$ (t positive and real), uniformly in u:

$$g(t,u) = b_m(u)(\log 1/t)^m + b_{m-1}(u)(\log 1/t)^{m-1} + \cdots + b_1(u)(\log 1/t) + \mathcal{O}(1).$$

Moreover,

$$\frac{\partial}{\partial t} g(t,u) = -\frac{m b_m(u)}{t}(\log 1/t)^{m-1} + \mathcal{O}\big(t^{-1}(\log 1/t)^{m-2}\big)$$

and

$$\frac{\partial^2}{\partial t^2} g(t,u) = \frac{m b_m(u)}{t^2}(\log 1/t)^{m-1} + \mathcal{O}\big(t^{-2}(\log 1/t)^{m-2}\big).$$

Finally, there exists an $\eta > 0$ such that for complex t with $|\operatorname{Im} t| \le \eta$, we have

$$\frac{\partial^3}{\partial t^3} g(t,u) = \mathcal{O}\left((\operatorname{Re} t)^{-3}(\log 1/(\operatorname{Re} t))^{m-1}\right),$$

as $\operatorname{Re} t \to 0^+$, again uniformly in u.

Proof (Sketch): We apply the classical Mellin transform technique, see the paper of Flajolet, Gourdon and Dumas [FGD95]. The Mellin transform

$$Y(s,u) = \int_0^\infty \log\big(1 + ue^{-t} + u^2e^{-2t} + \cdots + u^{d-1}e^{-(d-1)t}\big)t^{s-1}\,dt$$

can be meromorphically continued, with poles at $0, -1, -2, \ldots$. The residue at 0 is $\log(1+u+u^2+\cdots+u^{d-1})$. Moreover, $Y(s,u)$ decays exponentially as $\operatorname{Im} s \to \pm\infty$, uniformly in u. Second, the Dirichlet series associated with the set $\mathcal{S}$, i.e., $D(s) = \sum_{h\in\mathcal{S}} h^{-s}$, can be written as a product of elementary functions:

$$D(s) = \prod_{i=1}^{m} \frac{1}{1 - p_i^{-s}}.$$

Now the Mellin transform of $f(t,u)$ is given by $Y(s,u)D(s)$. We apply the Mellin inversion formula to get

$$f(t,u) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} Y(s,u)D(s)t^{-s}\,ds$$

for any $c > 0$. Following Flajolet, Gourdon and Dumas [FGD95], we shift the line of integration, picking up residues at the poles to obtain the terms in the asymptotic expansion. The derivatives of f as well as those of g (and g itself) are treated in a similar fashion. □

3 Estimating the Tails

For our application of the saddle point method, we need to estimate the tails (i.e., the parts where z is away from the positive real axis) of the generating functions given in (2) and (3), which is done in the following sequence of lemmas. First of all, let us introduce some notation: for $x > 0$, we write $\mathcal{S}(x)$ for $\mathcal{S} \cap [1, 1/x] = \{h \in \mathcal{S}, hx \le 1\}$. It is straightforward to prove that

$$|\mathcal{S}(x)| = \frac{(\log 1/x)^m}{m!\prod_{j=1}^m \log p_j} + \mathcal{O}\big((\log 1/x)^{m-1}\big). \tag{4}$$

as $x \to 0^+$.

Lemma 6. *Let u be in the interval $[\frac{1}{2}, 2]$, and let $z = e^{-x+2\pi iy}$ with $x > 0$ and $y \in [-\frac{1}{2}, \frac{1}{2}]$. There exists an absolute constant C such that*

$$\frac{F(z,u)}{F(|z|,u)} \le \exp\Big(- C \sum_{h \in \mathcal{S}(x)} \|hy\|^2 \Big)$$

and

$$\frac{G(z,u)}{G(|z|,u)} \le \exp\Big(- C \sum_{h \in \mathcal{S}(x)} \|hy\|^2 \Big),$$

where $\|\cdot\|$ denotes the distance to the nearest integer.

Proof (Sketch): It is not hard to show that

$$\frac{|1+aw|^2}{(1+a|w|)^2} \le \exp\big(- C_1(|w| - \operatorname{Re} w)\big)$$

for $a \in [\frac{1}{2}, 2]$ and $|w| \le 2$, where C_1 is an absolute constant. An analogous inequality also holds for $|1 + aw + aw^2|/(1 + a|w| + a|w|^2)$. The factors in $F(z,u)$ are of the form

$$1 + uz^h + u^2w^2 + \cdots + u^{d-1}z^{(d-1)h}.$$

We group the terms in pairs (and possibly one triple) and apply the aforementioned estimate to each of these pairs to get an inequality for each factor in the product that defines $F(z,u)$. Multiplying over all h then yields the desired result. The proof for $G(z,u)$ is completely analogous. □

Next we estimate the sum that occurs in the previous lemma. When $m > 2$, relatively simple estimates suffice for our purposes, while we need an additional auxiliary result in the case that $m = 2$. The following lemma provides the necessary estimates. Since the proof (especially in the case $m = 2$) is rather technical, it is skipped here.

Lemma 7. *Let $x > 0$ and $y \in [-\frac{1}{2}, \frac{1}{2}]$, and set*

$$\Sigma = \Sigma(x,y) = \sum_{h \in \mathcal{S}(x)} \|hy\|^2.$$

For sufficiently small x, we have the following estimates for Σ:

(a) If $|y| \le x/2$, then $\Sigma \ge A_1(y/x)^2(\log(1/x))^{m-1}$ for some constant A_1 (that only depends on m and the set of bases $\{p_1, p_2, \ldots, p_m\}$),

(b) If $|y| \ge x/2$, then $\Sigma \ge A_2(\log(1/x))^{m-1}$ for some constant A_2 (that also only depends on m and the set of bases $\{p_1, p_2, \ldots, p_m\}$).

Now let $m = 2$. For any constant $K > 0$ and any $\delta > 0$, there exists a constant $B > 0$ depending on p_1, p_2, K and δ such that the following holds for sufficiently small x:

(c) $\Sigma \ge K \log(1/x)$, except when y lies in a certain set $E(K,x)$ of Lebesgue measure at most $Bx^{1-\delta}$.

4 Application of the Saddle Point Method

We are now ready to apply the saddle point method (see Chapter VIII of [FS09] for an excellent introduction), which gives us asymptotic formulas for the coefficients of the generating functions $F(z,u)$ and $G(z,u)$. In the following, we use the notations $f_t(t,u)$, $f_{tt}(t,u)$, ... for the derivatives of f with respect to the first coordinate.

Lemma 8. *Let $u \in [\frac{1}{2}, 2]$, and define $r > 0$ implicitly by the saddle-point equation*

$$n = -f_t(r,u).$$

The coefficients of $F(z,u)$ satisfy the asymptotic formula

$$[z^n]F(z,u) = \frac{1}{\sqrt{2\pi f_{tt}(r,u)}} e^{nr+f(r,u)} \left(1 + \mathcal{O}((\log n)^{-(m-1)/5})\right),$$

uniformly in u. Likewise, if we define $r > 0$ by

$$n = -g_t(r,u),$$

then the coefficients of $G(z,u)$ satisfy the asymptotic formula

$$[z^n]G(z,u) = \frac{1}{\sqrt{2\pi g_{tt}(r,u)}} e^{nr+g(r,u)} \left(1 + \mathcal{O}((\log n)^{-(m-1)/5})\right),$$

uniformly in u.

Proof (Sketch): Cauchy's integral formula gives us

$$[z^n]F(z,u) = \frac{1}{2\pi i} \oint_{\mathcal{C}} F(z,u) \frac{dz}{z^{n+1}},$$

where $\mathcal{C}$ is a circle around 0 with radius less than 1. Let $r > 0$ and perform the change of variables $z = e^{-t} = e^{-(r+i\tau)}$, so that this becomes

$$[z^n]F(z,u) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp\big(nr + f(r+i\tau,u) + in\tau\big) d\tau.$$

Now we choose r to be the saddle point, as in the statement of the lemma, so that the Taylor expansion in the central region becomes

$$nr + f(r+i\tau,u) + in\tau = nr + f(r,u) - f_{tt}(r,u)\frac{\tau^2}{2} + \mathcal{O}\Big(|\tau|^3 \sup_{|y|\le\tau} |f_{ttt}(r+iy,u)|\Big). \tag{5}$$

Lemma 5 shows that r is of order $(\log n)^{m-1}/n$. Now we split the integral into the central part, where $|\tau| \le r(\log 1/r)^{-2(m-1)/5}$, and the rest. In the central region, the error term in (5) is $\mathcal{O}(\log(1/r)^{-(m-1)/5})$ by Lemma 5, and we can complete the tails to get a Gaussian integral. The remaining parts of the integral

are estimated by means of Lemmas 6 and 7. If $m > 2$, parts (a) and (b) of Lemma 7 already give sufficiently strong bounds. In the case that $m = 2$, we have to divide the tails further into a small "exceptional part", where we apply (b), and the rest, where the stronger bound from (c) holds.

Putting everything together, one arrives at

$$\begin{aligned}[z^n]F(z,u) &= \frac{e^{nr+f(r,u)}}{2\pi}\int_{-\infty}^{\infty}\exp\left(-f_{tt}(r,u)\frac{\tau^2}{2}\right)d\tau\left(1+\mathcal{O}((\log n)^{-(m-1)/5})\right)\\ &= \frac{1}{\sqrt{2\pi f_{tt}(r,u)}}e^{nr+f(r,u)}\left(1+\mathcal{O}((\log n)^{-(m-1)/5})\right),\end{aligned}$$

and the proof for $G(z,u)$ is analogous. □

5 The Number of Representations

It is straightforward now to prove Theorem 1 and Theorem 2 by specialising $u = 1$ in Lemma 8, which gives us

$$P(n) = [z^n]F(z,1) \sim \frac{1}{\sqrt{2\pi f_{tt}(r,1)}}e^{nr+f(r,1)},$$

where r is given by the saddle point equation $n = -f_t(r,1)$. Making use of Lemma 5, we get

$$n = \frac{a_m(1)}{(m-1)!}(\log 1/r)^{m-1} + \mathcal{O}\left((\log 1/r)^{m-2}\right),$$

which readily gives us

$$\log 1/r = \log n - (m-1)\log\log n - \log\frac{a_m(1)}{(m-1)!} + \mathcal{O}\left(\frac{\log\log n}{\log n}\right)$$

for $n \to \infty$. Now it follows that

$$nr = \frac{a_m(1)}{(m-1)!}(\log n)^{m-1}\left(1+\mathcal{O}\left(\frac{\log\log n}{\log n}\right)\right),$$

and Lemma 5 also yields

$$\begin{aligned}f(r,1) &= \frac{a_m(1)}{m!}(\log 1/r)^m + \frac{a_{m-1}(1)}{(m-1)!}(\log 1/r)^{m-1} + \mathcal{O}\left((\log n)^{m-2}\right)\\ &= \frac{a_m(1)}{m!}(\log n)^m\left(1-\frac{m(m-1)}{\log n}\log\log n - \frac{m}{\log n}\log\frac{a_m(1)}{(m-1)!} + \mathcal{O}\left(\frac{\log\log n}{(\log n)^2}\right)\right)\\ &\quad + \frac{a_{m-1}(1)}{(m-1)!}(\log n)^{m-1} + \mathcal{O}\left((\log n)^{m-2}\log\log n\right).\end{aligned}$$

Since $a_m(1)/m! = \kappa$ and $a_{m-1}(1)/(m-1)! = \kappa m(\sum_{i=1}^m \log p_i - \log d)/2$, this readily proves Theorem 1 (note that the factor $f_{tt}(r,1)$ only contributes $\mathcal{O}(\log n)$ to $\log P(n)$). To get the more precise formula (Theorem 2) in the case $m = 2$, we only need to expand a little further. In principle, it would be possible to obtain similar, more precise asymptotic formulas (in terms of $\log n$ and $\log\log n$) for all $m \geq 2$, but the expressions become very lengthy.

6 Sum of Digits and Hamming Weight

The central limit theorems for the sum of digits and the Hamming weight (Theorems 3 and 4) now follow from a general version of the quasi-power theorem (see [FS09, Theorem IX.13]); we only explain how the asymptotic formulas for mean and variance are obtained. We restrict ourselves to the case of the sum of digits, since the situation for the Hamming weight is similar. Recall the bivariate generating function

$$F(z,u) = \prod_{h \in \mathcal{S}} \frac{1-(uz^h)^d}{1-uz^h}.$$

In order to obtain the average sum of digits in a random representation of n, we differentiate with respect to u and set $u=1$ as usual: This yields

$$\mu_n = \frac{1}{P(n)}[z^n]\frac{\partial}{\partial u}F(z,u)\Big|_{u=1} = \frac{1}{P(n)}[z^n]F(z,1)\sum_{h\in S}\left(\frac{z^h}{1-z^h} - \frac{dz^{dh}}{1-z^{dh}}\right),$$

which gives us the integral representation

$$\mu_n = \frac{1}{2\pi i P(n)}\oint_{\mathcal{C}} F(z,1)\sum_{h\in S}\left(\frac{z^h}{1-z^h} - \frac{dz^{dh}}{1-z^{dh}}\right)\frac{dz}{z^{n+1}}.$$

Again it is convenient to define a function

$$J(t) = \sum_{h\in S}\left(\frac{e^{-ht}}{1-e^{-ht}} - \frac{de^{-dht}}{1-e^{-dht}}\right).$$

We use the saddle point method as in Section 4 to estimate $P(n)\Big(\mu_n - J(r)\Big)$, where r is defined as in the statement of Lemma 8 for $u=1$. We have

$$P(n)\Big(\mu_n - J(r)\Big) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \exp\Big(nr + f(r+i\tau,1) + in\tau\Big)\Big(J(r+i\tau) - J(r)\Big)d\tau.$$

As in Section 4, we can approximate this integral by an integral over a small interval around zero, with an error term that is smaller than any power of $\log 1/r$. Making use of the same Mellin transform approach as in the proof of Lemma 5, one verifies easily that the term $J(r+i\tau)-J(r)$ is of order at most $(\log 1/r)^m$, and this estimate holds uniformly for $|\tau| \le \pi$.

Let now $c>0$ be a constant satisfying the inequalities $3(m-1)/7 < c < (m-1)/2$. For $|\tau| \le r(\log 1/r)^{-c}$, by using more terms in the Taylor approximation of $f(r+i\tau,1)$ we get

$$e^{f(r+i\tau,1)-f(r,1)+in\tau} = e^{-f_{tt}(r,1)\frac{\tau^2}{2}}\left(1 - if_{ttt}(r,1)\frac{\tau^3}{6} + \mathcal{O}\Big((\log 1/r)^{2(m-1)-6c}\Big)\right).$$

Similarly,

$$J(r+i\tau) = J(r) + iJ_t(r)\tau - J_{tt}(r)\frac{t^2}{2} + \mathcal{O}\Big((\log 1/r)^{m-1-3c}\Big).$$

We multiply the two expansions and complete the tails of the integral as we did in the proof of Lemma 8. Evaluating the resulting integrals yields

$$P(n)\Big(\mu_n - J(r)\Big) = P(n)\left(\frac{f_{ttt}(r,1)J_t(r) - f_{tt}(r,1)J_{tt}(r)}{2(f_{tt}(r,1))^2} + \mathcal{O}\Big((\log 1/r)^{3(m-1)-7c}\Big)\right),$$

which in turn implies

$$\mu_n = J(r) + \frac{f_{ttt}(r,1)J_t(r) - f_{tt}(r,1)J_{tt}(r)}{2(f_{tt}(r,1))^2} + \mathcal{O}\Big((\log 1/r)^{3(m-1)-7c}\Big). \tag{6}$$

Here, we are also using the asymptotic formula for $P(n)$ from Lemma 8. Similarly, we also have

$$P(n)\sigma_n^2 = [z^n]\frac{\partial^2}{\partial u^2}F(z,u)\Big|_{u=1} + P(n)\mu_n(1-\mu_n).$$

If we set

$$L(t) = \sum_{h\in S}\left(\frac{e^{-ht}}{(1-e^{-ht})^2} - \frac{d^2e^{-dht}}{(1-e^{-dht})^2}\right),$$

then, using the estimate (6), we get the asymptotic formula

$$\sigma_n^2 = L(r) + \mathcal{O}\Big((\log 1/r)^{m-1} + (\log 1/r)^{4m-7c-3}\Big) \tag{7}$$

for the variance.

Finally, asymptotics for $J(r)$ and $L(r)$ in (6) and (7) are obtained by the same Mellin transform approach as in Lemma 5 again to obtain the formulas for mean and variance in Theorem 3.

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The Number of Compositions into Powers of b

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Abstract.

For a fixed integer base $b \geq 2$, we consider the number of compositions of 1 into a given number of powers of b and, related, the maximum number of representations a positive integer can have as an ordered sum of powers of b.

We study the asymptotic growth of those numbers and give precise asymptotic formulae for them, thereby improving on earlier results of Molteni. Our approach uses generating functions, which we obtain from infinite transfer matrices.

Keywords: compositions, powers of 2, infinite transfer matrices, asymptotic enumeration

1 Introduction

Representations of integers as sums of powers of 2 occur in various contexts, most notably of course in the usual binary representation. *Partitions* of integers into powers of 2, i.e., representations of the form

$$\ell = 2^{a_1} + 2^{a_2} + \cdots + 2^{a_n} \tag{1.1}$$

with nonnegative integers $a_1 \geq a_2 \geq \cdots \geq a_n$ (not necessarily distinct!) are also known as *Mahler partitions* (see [2, 11, 14, 18]).

The number of such partitions exhibits interesting periodic fluctuations. The situation changes, however, when *compositions* into powers of 2 are considered, i.e., when the summands are arranged in an order. In other words, we consider representations of the form (1.1) without further restrictions on the exponents $a_1, a_2, \ldots, a_n$ other than being nonnegative.

Motivated by the study of the exponential sum

$$s(\xi) = \sum_{r=1}^{\tau} \xi^{2^r},$$

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where ξ is a primitive qth root of unity and τ is the order of 2 modulo q (see [15]), Molteni [16] recently studied the maximum number of representations a positive integer can have as an ordered sum of n powers of 2. More generally, fix an integer $b \geq 2$, let

$$\mathcal{U}_b(\ell, n) = \#\{(a_1, a_2, \ldots, a_n) \in \mathbb{N}_0^n \mid b^{a_1} + b^{a_2} + \cdots + b^{a_n} = \ell\} \tag{1.2}$$

be the number of representations of ℓ as an ordered sum of n powers of b, and let $\mathcal{W}_b(s, n)$ be the maximum of $\mathcal{U}_b(\ell, n)$ over all positive integers ℓ with b-ary sum of digits equal to s. It was shown in [15] that

$$\frac{\mathcal{W}_2(s,n)}{n!} = \sum_{\substack{k_1,k_2,\ldots,k_r \geq 1 \\ k_1+k_2+\cdots+k_r=n}} \prod_{j=1}^{r} \frac{\mathcal{W}_2(1,k_j)}{k_j!}, \tag{1.3}$$

which generalizes in a straightforward fashion to arbitrary bases b. So knowledge of $\mathcal{W}_b(1, n)$ is the key to understanding $\mathcal{W}_b(s, n)$ for arbitrary s.

For the moment, let us consider the case $b = 2$. There is an equivalent characterisation of $\mathcal{W}_2(1, n)$ in terms of compositions of 1. To this end, note that the number of representations of $2^h\ell$ as a sum of powers of 2 is the same as the number of representations of ℓ for all integers h if negative exponents are allowed as well (simply multiply/divide everything by 2^h). Therefore, $\mathcal{W}_2(1, n)$ is also the number of solutions to the Diophantine equation

$$2^{-k_1} + 2^{-k_2} + \cdots + 2^{-k_n} = 1 \tag{1.4}$$

with nonnegative integers $k_1, k_2, \ldots, k_n$, i.e., the number of *compositions* of 1 into powers of 2. This sequence starts with

$$1, 1, 3, 13, 75, 525, 4347, 41245, 441675, 5259885, 68958747, \ldots$$

and is A007178 in the On-Line Encyclopedia of Integer Sequences [17].

The main goal of this paper is to determine precise asymptotics for the number of such binary compositions as $n \to \infty$. Lehr, Shallit and Tromp [13] encountered these compositions in their work on automatic sequences and gave a first bound, namely

$$\mathcal{W}_2(1, n)/n! \leq K \cdot 1.8^n$$

for some constant K. It was mainly based on an asymptotic formula for the number of *partitions* of 1 into powers of 2, which was derived independently in different contexts, cf. [1, 7, 12] for example (or see the recent paper of Elsholtz, Heuberger and Prodinger [5] for a detailed survey). This bound was further improved by Molteni, who gave the inequalities

$$0.3316 \cdot (1.1305)^n \leq \mathcal{W}_2(1, n)/n! \leq (1.71186)^{n-1} \cdot n^{-1.6}$$

in [15]. Giorgilli and Molteni [9] provided an efficient recursive formula for $\mathcal{W}_2(1, n)$ and used it to prove an intriguing congruence property. In his recent paper [16], Molteni succeeded in proving the following result, thus also disproving a conjecture of Knuth on the asymptotic behaviour of $\mathcal{W}_2(1, n)$.

Theorem I (Molteni [16])**.** *The limit*

$$\gamma = \lim_{n\to\infty} (\mathcal{W}_2(1, n)/n!)^{1/n} = 1.19267434121346603222128898252875 5\ldots$$

exists.

Molteni's argument is quite sophisticated and involves the study of the spectral radii of certain matrices. The aim of this paper will be to present a different approach to the asymptotics of $\mathcal{W}_2(1,n)$ (and more generally, $\mathcal{W}_2(s,n)$) by means of generating functions that allows us to obtain more precise information. Our main theorem reads as follows.

Theorem II. *There exist constants* $\alpha = 0.2963720490\ldots$, $\gamma = 1.1926743412\ldots$ *(as in Theorem I) and* $\kappa = 2/(3\gamma) < 1$ *such that*

$$\frac{\mathcal{W}_2(1,n)}{n!} = \alpha\gamma^n(1+O(\kappa^n)).$$

More generally, for every fixed s, there exists a polynomial $P_s(n)$ *with leading term* $\alpha^s n^{s-1}/(s-1)!$ *such that*

$$\frac{\mathcal{W}_2(s,n)}{n!} = P_s(n)\,\gamma^n(1+O(\kappa^n)).$$

We also prove a more general result for arbitrary bases instead of 2. Consider the Diophantine equation

$$b^{-k_1} + b^{-k_2} + \cdots + b^{-k_n} = 1. \tag{1.5}$$

Multiplying by the common denominator and taking the equation modulo $b-1$, we see that there can only be solutions if $n \equiv 1 \bmod b-1$, i.e., $n = (b-1)m+1$ for some nonnegative integer m. We write $q_b(m)$ for the number of solutions (n-tuples of nonnegative integers satisfying (1.5)) in this case. Note that $q_b(m)$ is also the maximum number of representations of an arbitrary power of b as an ordered sum of $n = (b-1)m+1$ powers of b. We have the following general asymptotic formula.

Theorem III. *For every positive integer* $b \geq 2$*, there exist constants* $\alpha = \alpha_b$*,* $\gamma = \gamma_b$ *and* $\kappa = \kappa_b < 1$ *such that the number* $q_b(m)$ *of compositions of* 1 *into* $n = (b-1)m+1$ *powers of b, which is also the maximum number* $\mathcal{W}_b(1,n)$ *of representations of a power of b as an ordered sum of n powers of b, satisfies*

$$\frac{\mathcal{W}_b(1,n)}{n!} = \frac{q_b(m)}{n!} = \alpha\gamma^m(1+O(\kappa^m)).$$

More generally, the maximum number $\mathcal{W}_b(s,n)$ *of representations of a positive integer with b-ary sum of digits s as an ordered sum of* $n = (b-1)m+s$ *powers of b is asymptotically given by*

$$\frac{\mathcal{W}_b(s,n)}{n!} = P_{b,s}(m)\,\gamma^m(1+O(\kappa^m)),$$

where $P_{b,s}(m)$ *is a polynomial with leading term* $\alpha^s m^{s-1}/(s-1)!$.

The key idea is to equip every *partition* of 1 into powers of 2 (or generally b) with a weight that essentially gives the number of ways it can be permuted to a composition, and to apply the recursive approach that was used to count partitions of 1: if $p_2(n)$ denotes the number of such partitions into n summands, then the remarkable generating function identity

$$\sum_{n=1}^{\infty} p_2(n)x^n = \frac{\sum_{j=0}^{\infty}(-1)^j x^{2^j-1}\prod_{i=1}^{j}\frac{x^{2^i-1}}{1-x^{2^i-1}}}{\sum_{j=0}^{\infty}(-1)^j\prod_{i=1}^{j}\frac{x^{2^i-1}}{1-x^{2^i-1}}} \tag{1.6}$$

holds, and this can be generalised to arbitrary bases b, see the recent paper of Elsholtz, Heuberger and Prodinger [5]. In our case, we do not succeed to obtain a similarly explicit formula for the generating

function, but we can write it as the quotient of two determinants of infinite matrices and infer analytic information from it. The paper is organised as follows: we first describe the combinatorial argument that yields the generating function, a priori only within the ring of formal power series. We then study the expression obtained for the generating function in more detail to show that it can actually be written as the quotient of two entire functions. The rest of the proof is a straightforward application of residue calculus (using the classical Flajolet–Odlyzko singularity analysis [6]).

Finally, we consider the maximum of $\mathcal{U}_b(\ell, n)$ over all ℓ, for which we write

$$M_b(n) = \max_{\ell \geq 1} \mathcal{U}_b(\ell, n) = \max_{s \geq 1} \mathcal{W}_b(s, n)\,.$$

This means that $M_b(n)$ is the maximum possible number of representations of a positive integer as a sum of exactly n powers of b. Equivalently, it is the largest coefficient in the power series expansion of

$$\left(x + x^b + x^{b^2} + \cdots\right)^n.$$

When $b = 2$, Molteni [16] obtained the following bounds for this quantity:

$$(1.75218)^n \ll M_2(n)\,/n! \leq (1.75772)^n.$$

The gap between the two estimates is already very small; we improve this a little further by providing the precise constant of exponential growth.

Theorem IV. *For a certain constant $\nu = 1.7521819\ldots$ (defined precisely in Section 5), we have*

$$M_2(n)\,/n! \leq \nu^n$$

for all $n \geq 1$, and the constant is optimal: we have the more precise asymptotic formula

$$M_2(n)\,/n! \sim \lambda n^{-1/2} \nu^n$$

with $\lambda = 0.2769343\ldots$.

Again, Theorem IV holds for arbitrary integer bases $b \geq 2$ for some constants $\nu = \nu_b$ and $\lambda = \lambda_b$ (it will be explained precisely how they are obtained). This is formulated as Theorem V in Section 5.

2 The recursive approach

For our purposes, it will be most convenient to work in the setting of compositions of 1, i.e., we are interested in the number $q_b(m)$ of (ordered) solutions to the Diophantine equation (1.5), where $n = (b-1)m + 1$, as explained in the introduction. Our first goal is to derive a recursion for $q_b(m)$ and some related quantities, which leads to a system of functional equations for the associated generating functions.

Let $\mathbf{k} = (k_1, k_2, \ldots, k_n)$ be a solution to the Diophantine equation (1.5) with $k_1 \geq k_2 \geq \cdots \geq k_n$. We will refer to such an n-tuple as a "partition" (although technically the k_i are only the exponents in a partition). We denote by $\mathsf{c}(\mathbf{k})$ the number of ways to turn it into a composition. If a_0 is the number of zeros, a_1 the number of ones, etc. in $\mathbf{k}$, then we clearly have

$$\mathsf{c}(\mathbf{k}) = \frac{n!}{\prod_{j \geq 0} a_j!}.$$

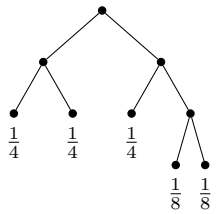

Fig. 2.1: The canonical tree associated with the partition $1 = 3 \cdot 2^{-2} + 2 \cdot 2^{-3}$ of 1 into powers of 2. This partition has weight $\frac{1}{12}$ and corresponds to 10 distinct compositions.

The *weight* of a partition $\mathbf{k}$, denoted by $\mathsf{w}(\mathbf{k})$, is now simply defined as

$$\mathsf{w}(\mathbf{k}) = \frac{1}{\prod_{j\geq 0} a_j!} = \frac{\mathsf{c}(\mathbf{k})}{n!}.$$

Now let

$$\mathcal{P}_m = \left\{\mathbf{k} = (k_1, k_2, \ldots, k_n) \,\middle|\, n = (b-1)m+1,\, b^{-k_1} + b^{-k_2} + \cdots + b^{-k_n} = 1,\, k_1 \geq k_2 \geq \cdots \geq k_n\right\}$$

be the set of all partitions of 1 with $n = (b-1)m+1$ terms and, likewise,

$$\mathcal{C}_m = \left\{\mathbf{k} = (k_1, k_2, \ldots, k_n) \,\middle|\, n = (b-1)m+1,\, b^{-k_1} + b^{-k_2} + \cdots + b^{-k_n} = 1\right\}$$

the set of compositions. We obtain the formula

$$q_b(m) = \#\mathcal{C}_m = \sum_{\mathbf{k}\in\mathcal{P}_m} \mathsf{c}(\mathbf{k}) = n! \sum_{\mathbf{k}\in\mathcal{P}_m} \mathsf{w}(\mathbf{k})$$

for their number.

Our next step involves an important observation that is also used to obtain (1.6). Consider an element $\mathbf{k}$ of $\mathcal{P}_m$, and let r be the number of times the greatest element k_1 occurs (i.e., $k_1 = k_2 = \cdots = k_r > k_{r+1}$). This number must be divisible by b (as can be seen by multiplying (1.5) by b^{k_n}) unless $\mathbf{k}$ is the trivial partition, so we can replace them by r/b fractions with denominator b^{k_n-1}.

This process can be reversed. Given a partition $\mathbf{k}$ in which the largest element occurs r times, we can replace s, $1 \leq s \leq r$, of these fractions by bs fractions with denominator b^{k_n+1}. This recursive construction can be illustrated nicely by a tree structure, as in Figure 2.1 in the case $b = 2$. Each partition corresponds to a so-called canonical tree (see [5]), and vice versa. Note that if $\mathbf{k} \in P_m$, then the resulting partition $\mathbf{k}'$ lies in P_{m+s}, and we clearly have

$$\mathsf{w}(\mathbf{k}') = \mathsf{w}(\mathbf{k}) \cdot \frac{r!}{(r-s)!\,(bs)!}. \tag{2.1}$$

Now we can turn to generating functions. Let $\mathcal{P}_{m,r}$ be the subset of $\mathcal{P}_m$ that only contains partitions for which $k_1 = k_2 = \cdots = k_r > k_{r+1}$ (i.e., in (1.5), the largest exponent occurs exactly r times), and

let $\mathcal{C}_{m,r}$ be the set of compositions obtained by permuting the terms of an element of $\mathcal{P}_{m,r}$. We define a generating function by

$$Q_r(x) = \sum_{m\geq 0} \frac{\#\mathcal{C}_{m,r}}{((b-1)m+1)!}x^m = \sum_{m\geq 0}\sum_{\mathbf{k}\in\mathcal{P}_{m,r}} \frac{\mathsf{c}(\mathbf{k})}{((b-1)m+1)!}x^m = \sum_{m\geq 0}\sum_{\mathbf{k}\in\mathcal{P}_{m,r}} \mathsf{w}(\mathbf{k})x^m.$$

In view of the recursive relation described above and in particular (2.1), we have $Q_1(x) = 1$ and $Q_r(x) = 0$ for all other r not divisible by b, and for all $s \geq 1$ we obtain

$$\begin{aligned} Q_{bs}(x) &= \sum_{m\geq 0}\sum_{\mathbf{k}\in\mathcal{P}_{m,bs}} \mathsf{w}(\mathbf{k})x^m = \sum_{r\geq s}\sum_{m\geq s}\sum_{\mathbf{k}\in\mathcal{P}_{m-s,r}} \mathsf{w}(\mathbf{k})\frac{r!}{(r-s)!\,(bs)!}x^m \\ &= x^s\sum_{r\geq s}\frac{r!}{(r-s)!\,(bs)!}\sum_{m\geq s}\sum_{\mathbf{k}\in\mathcal{P}_{m-s,r}} \mathsf{w}(\mathbf{k})x^{m-s} = x^s\sum_{r\geq s}\frac{r!}{(r-s)!\,(bs)!}\,Q_r(x)\,. \end{aligned} \tag{2.2}$$

This can be seen as an infinite system of linear equations. Define the infinite (column-)vector $\mathbf{V}(x) = (Q_b(x)\,, Q_{2b}(x)\,, Q_{3b}(x)\,, \ldots)^T$, and the infinite matrix $\mathbf{M}(x)$ by its entries

$$m_{ij} = \begin{cases} \frac{(bj)!\,x^i}{(bj-i)!\,(bi)!} & \text{if } i \leq bj, \\ 0 & \text{otherwise.} \end{cases}$$

Then the identity (2.2) above turns into the matrix identity

$$\mathbf{V}(x) = \mathbf{M}(x)\mathbf{V}(x) + \frac{x}{b!}\mathbf{e}_1, \tag{2.3}$$

where $\mathbf{e}_1 = (1, 0, 0, \ldots)^T$ denotes the first unit vector. Within the ring of formal power series, this readily yields

$$\mathbf{V}(x) = \frac{x}{b!}(\mathbf{I} - \mathbf{M}(x))^{-1}\mathbf{e}_1, \tag{2.4}$$

and the generating function

$$Q(x) = \sum_{r\geq 1} Q_r(x) = \sum_{m\geq 0}\frac{q_b(m)}{((b-1)m+1)!}x^m$$

(recall that $q_b(m)$ is the number of compositions of 1 into $n = (b-1)m+1$ powers of b) is given by

$$Q(x) = 1 + \mathbf{1}^T\mathbf{V}(x) = 1 + \frac{x}{b!}\mathbf{1}^T(\mathbf{I} - \mathbf{M}(x))^{-1}\mathbf{e}_1.$$

For our asymptotic result, we will need the dominant singularity of $Q(x)$, i.e., the zero of $\det(\mathbf{I} - \mathbf{M}(x))$ that is closest to 0. It is not even completely obvious that this determinant is well-defined, but the reasoning is similar to a number of comparable problems.

As mentioned earlier, the determinant $T(x) = \det(\mathbf{I} - \mathbf{M}(x))$ exists a priori within the ring of formal power series, as the limit of the principal minor determinants. We can write it as

$$\det(\mathbf{I} - \mathbf{M}(x)) = \sum_{h\geq 0}(-1)^h \sum_{\substack{1\leq i_1<i_2<\cdots<i_h \\ i_1,\ldots,i_h\in\mathbb{N}}} x^{i_1+i_2+\cdots+i_h}\sum_{\sigma}(\operatorname{sgn}\sigma)\prod_{k=1}^{h}\frac{(b\,\sigma(i_k))!}{(b\,\sigma(i_k)-i_k)!\,(bi_k)!}, \tag{2.5}$$

where the inner sum is over all permutations of $\{i_1, i_2, \ldots, i_h\}$. Using Eaves' sufficient condition, cf. [4], we get at least convergence for $|x| < 1$.

We can even show that the formal power series given by (2.5) defines an entire function. Write $n = i_1 + i_2 + \cdots + i_h$ for the exponent of x, and note that

$$\prod_{k=1}^{h} \frac{(b\,\sigma(i_k))!}{(bi_k)!} = 1,$$

which is independent of σ. We also have $\sum_{k=1}^{h}(b\,\sigma(i_k) - i_k) = (b-1)n$. This, combined with the inequality $a! \geq \exp(a(\log a - 1))$ and the fact that $f(x) = x(\log x - 1)$ is a convex function, gives us

$$\prod_{k=1}^{h}(b\,\sigma(i_k) - i_k)! \geq \exp\left(\frac{b-1}{2} n \log n + O(n)\right).$$

On the other hand, the number of choices for $i_1, i_2, \ldots, i_h$ given n is equal to the number of partitions $q(n)$ of n into distinct parts, which is well known to be $\exp\left(\pi\sqrt{n/3} + O(\log n)\right)$. Finally, since $h \leq \sqrt{2n} + 1$ because $i_1, i_2, \ldots, i_h$ are all distinct, Stirling's formula tells us that the number of permutations σ of $i_1, i_2, \ldots, i_h$ is at most $\exp\left(\sqrt{n/2}\log n + O(\sqrt{n})\right)$. It follows that the coefficient of x^n in (2.5) is at most

$$\exp\left(-\frac{b-1}{2} n \log n + O(n)\right).$$

Since this bound decays superexponentially, the determinant $T(x) = \det(\mathbf{I} - \mathbf{M}(x))$ is an entire function. The same is true (by the same argument) for

$$S(x) = \mathbf{1}^T \operatorname{adj}(\mathbf{I} - \mathbf{M}(x))\mathbf{e}_1 = \det(\mathbf{M}^*(x)),$$

where $\mathbf{M}^*$ is obtained from $\mathbf{I} - \mathbf{M}(x)$ by replacing the first row by $\mathbf{1}$. Hence we can write the generating function $Q(x)$ as

$$Q(x) = 1 + \frac{x}{b!}\frac{S(x)}{T(x)}, \tag{2.6}$$

where $S(x)$ and $T(x)$ are both entire functions. The singularities of $Q(x)$ are thus all poles, and it remains to determine the dominant singularity, i.e., the zero of $T(x) = \det(\mathbf{I} - \mathbf{M}(x))$ with smallest modulus.

3 Analysing the generating function

Infinite systems of functional equations appear quite frequently in the analysis of combinatorial problems, see for example the recent work of Drmota, Gittenberger and Morgenbesser [3]. Alas, their very general theorems are not applicable to our situation as the infinite matrix $\mathbf{M}$ does not represent an ℓ_p-operator (one of their main requirements), due to the fact that its entries increase (and tend to ∞) along rows. However, we can adapt some of their ideas to our setting.

The main result of this section is the following lemma, whose proof we only sketch.

Lemma 3.1. *For every $b \geq 2$, the generating function $Q(x)$ has a simple pole at a positive real point ρ_b and no other poles with modulus $< \rho_b + \epsilon_b$ for some $\epsilon_b > 0$.*

b	α	γ
2	0.296372	1.19268
3	0.279852	0.534502
4	0.236824	0.170268
5	0.196844	0.0419317
6	0.165917	0.00834837
7	0.142679	0.00138959
8	0.1249575	0.000198440

Tab. 4.1: Values (numerical approximations) for the constants of Theorem III.

Proof (Sketch): By considering compositions of 1 consisting of $b-1$ copies of b^{-1}, b^{-2}, ..., b^{1-m} and b copies of b^{-m}, we see that

$$q_b(m) \geq \frac{((b-1)m+1)!}{((b-1)!)^{m-1}b!},$$

which allows us to conclude that the radius of convergence of $Q(x)$ is at most $(b-1)!$. Since all coefficients are positive, Pringsheim's theorem guarantees that the radius of convergence, which we denote by ρ_b, is also a singularity (a pole since $Q(x)$ is meromorphic).

Next we consider $w_r = \lim_{x\to\rho_b^-}(x-\rho_b)^p\, Q_r(x)$, where p is the pole order of ρ_b. Multiplying the matrix equation (2.3) by $(x-\rho_b)^p$ and taking the limit, we see that $\mathbf{w} = (w_1, w_2, \ldots)^T$ is a right eigenvector of $\mathbf{M}(\rho_b)$, and because this matrix has positive entries on and above the main diagonal, all w_r are positive. It follows that all functions $Q_r(x)$ have the same pole order (as $Q(x)$).

Now we split the identity (2.3) appropriately to obtain an equation for $Q_1(x)$ only, whose solution takes the form

$$Q_1(x) = \frac{x}{b!}\left(1 - R(x)\right)^{-1}$$

for some function $R(x)$ which has only positive coefficients. Thus, $R(x) = 1$ has a unique positive real solution, which must be ρ_b (and is a simple zero). Moreover, by the triangle inequality there are no complex solutions of $R(x) = 1$ with the same modulus, which means that there are no further singularities of $Q_1(x)$ (and thus $Q(x)$) in a circle of radius $\rho_b + \epsilon_b$ around 0 for suitable $\epsilon_b > 0$. □

4 Getting the Asymptotics

In this section, we prove Theorems II and III, which give us constants α_b, γ_b and $\kappa_b < 1$ such that for $n = (b-1)m + 1$

$$\frac{\mathcal{W}_b(s,n)}{n!} = P_{b,s}(m)\,\gamma_b^m(1 + O(\kappa_b^m))$$

holds, where $P_{b,s}(m)$ is a polynomial with leading term $\alpha_b^s m^{s-1}/(s-1)!$. Numerical values of the α_b and γ_b can be found in Table 4.1.

For easier reading, we skip the index b again, i.e., we set $\alpha = \alpha_b$, $\gamma = \gamma_b$ and so on. The proof is the same for all b, except for the fact that different constants occur. Thus, we restrict ourselves here to $b = 2$, where we also give explicit estimates for all the constants involved.

Proof of Theorem II: By now, we know that the function $Q(x)$ can be written as the quotient of two entire functions. More specifically,

$$Q(x) = 1 + \frac{xS(x)}{2T(x)},$$

and the first few terms of these power series are given by

$$S(x) = \mathbf{1}^T \operatorname{adj}(I - \mathbf{M}(x))\mathbf{e}_1 = \det(M^*(x)) = 1 - \tfrac{5}{12}x^2 - \tfrac{1}{6}x^3 - \tfrac{1}{24}x^4 + \tfrac{1}{45}x^5 + \cdots$$

and

$$T(x) = \det(I - \mathbf{M}(x)) = 1 - x - \tfrac{1}{2}x^2 + \tfrac{1}{6}x^3 + \tfrac{1}{8}x^4 + \tfrac{3}{40}x^5 + \cdots .$$

One can show that $T(x)$ has exactly one zero x_0 (which is a simple zero) inside a disk of radius $\frac{3}{2}$ around 0. This is then a simple pole of $Q(x)$, as one checks that $S(x_0) \neq 0$. Thus we can directly apply singularity analysis [6] in the meromorphic setting (cf. Theorem IV.10 of [8]) to obtain

$$\frac{q_2(n)}{(n+1)!} = [x^n]Q(x) = -\frac{S(x_0)}{2\,T'(x_0)}x_0^{-n} + O((2/3)^n)\,.$$

In the general case (arbitrary s), we use the relation

$$\sum_{n=1}^{\infty} \frac{\mathcal{W}_b(s,n)}{n!}x^n = \Big(\sum_{n=1}^{\infty} \frac{\mathcal{W}_b(1,n)}{n!}x^n\Big)^s,$$

which follows from Equation (1.3). Once again, we make use of the fact here that the (exponential) generating function is meromorphic, cf. Section 2. The singular expansion at $x = 1/\gamma$ is given by

$$\sum_{n=1}^{\infty} \frac{\mathcal{W}_b(s,n)}{n!}x^n = \Big(\frac{\alpha}{1-\gamma x} + O(1)\Big)^s,$$

which has $\alpha^s/(1-\gamma x)^s$ as a main term. Once again, singularity analysis [6] yields the desired asymptotic formula with main term as indicated in the statement of the theorem. □

We close this section with a remark concerning numerical calculations.

Remark 4.1. We can calculate numerical values (by using interval arithmetic) of all the constants involved in the statement of our theorems.

Denote the polynomials consisting of the first N terms of $S(x)$ and $T(x)$, by $S_N(x)$ and $T_N(x)$, respectively. We get, for instance, that $|T'(x) - T'_{60}(x)| \le B_{T'_{60}}$ with $B_{T'_{60}} = 8.397 \cdot 10^{-12}$. We also have $|S(x) - S_{60}(x)| \le B_{S_{60}}$ with $B_{S_{60}} = 1.848 \cdot 10^{-13}$ for the function in the numerator of $Q(x)$. We plug x_0 into the approximations S_{60} and T'_{60} and use these bounds to obtain precise values (with guaranteed error estimates) for all the constants that occur in our formula.

If one does not insist on such explicit error bounds for the numerical approximations, one can get more precise results. Here, specifically, the first three terms in the asymptotic expansion are as follows (although the numerical approximations lack the "certifiability" of e.g. those in Table 4.1):

$$\begin{aligned}\mathcal{W}_2(1,n)\,/n! = {} & 0.29637204905352907558864864213 3 \cdot 1.19267434121346603222128898252 9^n \\ & + 0.11973633538363165349506855424 5 \cdot 0.64342741814950007012057031850 9^n \\ & + 0.01747836352103880070513843818 33 \cdot (-0.51839777389933777286272735707 10)^n \\ & + \cdots .\end{aligned}$$

b	λ	θ	$\nu = 1/\theta$	μ	σ^2
2	0.27693430	0.57071698	1.75218196	0.44867215	0.41775807
3	0.70656285	0.84340237	1.18567368	0.66924459	0.57114748
4	1.70314663	0.95872521	1.04305174	0.87318716	0.37650717
5	4.20099030	0.99167231	1.00839763	0.96645454	0.13477198
6	10.61691472	0.99861115	1.00139078	0.99304650	0.03480989
7	28.28286119	0.99980159	1.00019845	0.99880929	0.00714564
8	80.09108610	0.99997520	1.00002480	0.99982638	0.00121534

Tab. 5.1: Values (numerical approximations) for the constants of Theorem V.

5 Maximum Number of Representations

Let $\mathcal{U}_b(\ell, n)$ and $\mathcal{W}_b(s, n)$ be as defined in (1.2) in the introduction. In this section we analyze the function $M(n) = M_b(n)$, which equals the maximum of $\mathcal{U}_b(\ell, n)$ over all ℓ, i.e., we have

$$M(n) = \max_{\ell \geq 1} \mathcal{U}_b(\ell, n) = \max_{s \geq 1} \mathcal{W}_b(s, n)\,.$$

This gives the maximum number of representations any positive integer can have as the sum of exactly n powers of b. We get the following result.

Theorem V. *Let $W(x)$ be the generating function*

$$W(x) = \sum_{n=1}^{\infty} \frac{\mathcal{W}_b(1, n)}{n!} x^n.$$

Let θ be the unique positive real solution of the equation $W(\theta) = 1$, and set $\nu = 1/\theta$. Then we have

$$M(n)\,/n! \leq \nu^n \tag{5.1}$$

for all $n \geq 1$, and the constant is optimal: We have the more precise asymptotic formula

$$M(n)\,/n! = \lambda n^{-1/2} \nu^n \big(1 + O\big(n^{-1/2}\big)\big)$$

with $\lambda = (b-1)\left(\theta\, W'(\theta)\, \sigma \sqrt{2\pi}\right)^{-1}$, where $\sigma > 0$ is defined by

$$\sigma^2 = \frac{W''(\theta)}{\theta\, W'(\theta)^3} - \frac{1}{\theta\, W'(\theta)} + \frac{1}{\theta^2\, W'(\theta)^2}.$$

Moreover, the maximum $M(n) = \max_{s \geq 1} \mathcal{W}_b(s, n)$ is attained at $s = \mu n + O(1)$ with the constant $\mu = (\theta\, W'(\theta))^{-1}$.

In Table 5.1, we are listing numerical values for the constants of Theorem V.

We start with the upper bound (5.1) of Theorem V, which is easy to obtain. Recall that Equation (1.3) gives us

$$\sum_{n=1}^{\infty} \frac{\mathcal{W}_b(s, n)}{n!} x^n = \left(\sum_{n=1}^{\infty} \frac{\mathcal{W}_b(1, n)}{n!} x^n \right)^s = W(x)^s\,.$$

Since $\theta > 0$ was chosen such that $W(\theta) = 1$, it clearly follows that

$$\sum_{n=1}^{\infty} \frac{\mathcal{W}_b(s,n)}{n!}\theta^n = 1,$$

hence $\mathcal{W}_b(s,n)/n! \le \theta^{-n}$ for all s and n, and taking the maximum over all $s \ge 1$ yields

$$M(n)/n! = \max_{s\ge 1} \mathcal{W}_b(s,n)/n! \le \theta^{-n} = \nu^n,$$

which is what we wanted to show. It remains to prove the asymptotic formula for $M(n)$. To this end, we consider the bivariate generating function

$$G(x,u) = 1 + \sum_{n=1}^{\infty}\sum_{s=1}^{\infty} \frac{\mathcal{W}_b(s,n)}{n!}x^n u^s = \sum_{s=0}^{\infty} W(x)^s\, u^s = \frac{1}{1-u\,W(x)}.$$

In order to get $\max_{s\ge 1} \mathcal{W}_b(s,n)$, we show that the coefficients varying with s fulfil a local limit law (as n tends to ∞). The maximum is then attained at its mean.

Proof of Theorem V (Sketch): Set

$$g_n(u) = \sum_{s=1}^{\infty} \frac{\mathcal{W}_b(s,n)}{n!}u^s.$$

We extract g_n from the bivariate generating function $G(x,u)$, and we would like to determine its largest coefficient. Note that the coefficient of u^k in $g_n(u)$ can only be nonzero if $k \equiv n \mod (b-1)$. Now we proceed as in Theorem IX.9 (singularity perturbation for meromorphic functions) of Flajolet and Sedgewick [8]. Note that the function $G(x,1)$ has a dominant simple pole at $x = \theta$. There exists a nonconstant function $\theta(u)$ with the following properties: it is analytic at $u = 1$, it fulfils $\theta(1) = \theta$, and we have $W(\theta(u)) = 1/u$. Moreover, for some $\epsilon > 0$ and u in a suitable neighbourhood of 1, there is no $x \ne \theta(u)$ with $W(x) = 1/u$ and $|x| \le \theta + \epsilon$. Finally, $\left|\theta(e^{i\phi})\right|$ attains its minimum at $\phi = 2a\pi/(b-1)$ ($a \in \{0,1,\ldots,b-2\}$) and nowhere else.

By Cauchy's integral formula and the residue theorem, we obtain

$$g_n(u) = \frac{1}{u\,\theta(u)\,W'(\theta(u))}\left(\frac{1}{\theta(u)}\right)^n + O\big((\theta+\epsilon)^{-n}\big)$$

for u in a suitable neighbourhood of 1.

The get the statement of Theorem V, we use the local version of the quasi-power theorem, see Theorem IX.14 of [8] or Hwang's original paper [10], in a suitably modified version to account for the fact that only every $(b-1)$-th coefficient is nonzero. □

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Analysis of Radix Selection on Markov Sources

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Abstract. The complexity of the algorithm Radix Selection is considered for independent data generated from a Markov source. The complexity is measured by the number of bucket operations required and studied as a stochastic process indexed by the ranks; also the case of a uniformly chosen rank is considered. The orders of mean and variance of the complexity and limit theorems are derived. We find weak convergence of the appropriately normalized complexity towards a Gaussian process with explicit mean and covariance functions (in the space $\mathrm{D}[0,1]$ of càdlàg functions on $[0,1]$ with the Skorokhod metric) for uniform data and the asymmetric Bernoulli model. For uniformly chosen ranks and uniformly distributed data the normalized complexity was known to be asymptotically normal. For a general Markov source (excluding the uniform case) we find that this complexity is less concentrated and admits a limit law with non-normal limit distribution.

Keywords: Radix Selection, Markov source model, complexity, weak convergence, Gaussian process.

1 Introduction

Radix Selection is an algorithm to select an order statistic from a set of data in $[0,1]$ as follows. An integer $b \geq 2$ is fixed. In the first step the unit interval is decomposed into the intervals, also called *buckets*, $[0,1/b), [1/b,2/b), \ldots, [(b-2)/b,(b-1)/b)$ and $[(b-1)/b,1]$ and the data are assigned to these buckets according to their value. If the bucket containing the datum with rank to be selected contains further data the algorithm is recursively applied by again decomposing this bucket equidistantly and recursing. The algorithm stops once the bucket containing the rank to be selected contains no other data. Assigning a datum to a bucket is called a *bucket operation* and the algorithm's complexity is measured by the total number of bucket operations required.

Radix Selection is especially suitable when data are stored as expansions in base (radix) b, the case $b = 2$ being the most common on the level of machine data. For such expansions a bucket operation breaks down to access a digit (or bit).

In this extended abstract we study the complexity of Radix Selection in a probabilistic model. We assume that n data are modeled independently with b-ary expansions generated from a Markov chain on

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the alphabet $\{0, \dots, b-1\}$. For the ranks to be selected we use two models. First, we consider the complexity of a random rank uniformly distributed over $\{1, \dots, n\}$ and independent from the data. This is the model proposed and studied (for independent, uniformly over $[0,1]$ distributed data) in Mahmoud, Flajolet, Jacquet and Régnier [15]. The complexities of all ranks are averaged in this model and, in accordance with the literature, we call it the model of *grand averages*. Second, all possible ranks are considered simultaneously. Hence, we study the stochastic process of the complexities indexed by the ranks $1, \dots, n$. We choose a scaling in time and space which asymptotically gives access to the complexity to select quantiles from the data, i.e., ranks of the size tn with $t \in [0,1]$. We call this model for the ranks the *quantile-model*.

The main results of this extended abstract are on the asymptotic orders of mean and variance and limit laws for the complexity of Radix Selection for our Markov source model both for grand averages and for the quantile-model. For the quantile-model we find Gaussian limit processes for the uniform model (defined below) for the data as well as for the asymmetric Bernoulli model (defined below). For the general Markov source model with $b = 2$ we identify the first asymptotic term of the mean complexity. For grand averages and uniform data it was shown in Mahmoud et al. [15] that the normalized complexity is asymptotically normal. We find that for Markov sources (with $b = 2$) other than uniform the limit distribution is no longer normal and the complexity is less concentrated. An explanation of this behavior is given at the end of section 3.2.

We present our analysis separately for uniform data in section 2 and for Markov sources different from the uniform model in section 3, where the quantile-model is discussed in section 3.1, the grand averages in section 3.2.

A general reference on bucket algorithms is Devroye [5]. A large body of probabilistic analysis of digital structures is based on methods from analytic combinatorics, see Flajolet and Sedgewick [7], Knuth [13] and Szpankowski [18]. For an approach based on renewal theory see Janson [10] and the references given there. Our Markov source model is a special case of the model of dynamical sources, see Clément, Flajolet and Vallée [4].

We close this introduction defining the Markov source model explicitly, fixing some standard notation and stating corresponding results for the related Radix Sorting algorithm.

The Markov source model: We model data strings over the alphabet $\Sigma = \{0, \dots, b-1\}$ with a fixed integer $b \geq 2$ generated by a homogeneous Markov chain. The data strings $s = (s_i)_{i \geq 1}$ are also interpreted as b-ary expansions of a real number $s \in [0,1]$ via the identification

$$s = \sum_{i=1}^{\infty} s_i b^{-i}.$$

Conversely, if to $s \in [0,1)$ a b-ary expansion $s = (s_i)_{i \geq 1}$ is associated, to avoid ambiguity, we chose the expansion such that we have $s_i < b-1$ for infinitely many $i \in \mathbb{N}$. (For $s = 1$ we use the expansion where $s_i = b-1$ for all $i \in \mathbb{N}$.) The most important case is $b = 2$ where the data are binary strings.

In general, a homogeneous Markov chain on Σ is given by its initial distribution $\mu = \sum_{\ell=0}^{b-1} \mu_\ell \delta_\ell$ on Σ and the transition matrix $(p_{ij})_{i,j \in \Sigma}$. Here, δ_x denotes the Dirac measure in $x \in \mathbb{R}$. Hence, the initial state is ℓ with probability μ_ℓ for $\ell = 0, \dots, b-1$. We have $\mu_\ell \in [0,1]$ and $\sum_{\ell=0}^{b-1} \mu_\ell = 1$. A transition from state i to j happens with probability p_{ij}, $i, j \in \Sigma$. Now, a data string is generated as the sequence of

states taken by the Markov chain. In our Markov source model assumed subsequently all data strings are independent and identically distributed according to the given Markov chain.

We always assume that $p_{ij} < 1$ for all $i, j \in \Sigma$. Note that we do not necessarily assume the Markov chain to converge to a stationary distribution nor that it starts in a stationary distribution.

The case $p_{ij} = \mu_i = 1/b$ for all $i, j \in \Sigma$ is the case where all symbols within all data are independent and uniformly distributed over Σ. Then the associated numbers are independent and uniformly distributed over $[0, 1]$. We call this the *uniform model*. For $b = 2$ the uniform model is also called *symmetric Bernoulli model*. The *asymmetric Bernoulli model* for $b = 2$ is the case where $p_{i1} = \mu_1 = p$ for $i = 0, 1$ and a $p \in (0, 1)$ with $p \neq \frac{1}{2}$.

Notation. We write $\xrightarrow{d}$ for convergence in distribution and $\stackrel{d}{=}$ for equality in distribution. By $\mathrm{B}(n, p)$ with $n \in \mathbb{N}$ and $p \in [0, 1]$ the binomial distribution is denoted, by $\mathrm{B}(p)$ the Bernoulli distribution with success probability p, by $\mathcal{N}(\mu, \sigma^2)$ the normal distribution with mean $\mu \in \mathbb{R}$ and variance $\sigma^2 > 0$. The Bachmann–Landau symbols are used.

Radix Sorting. The Radix Sorting algorithm consists of assigning all data to the buckets as for Radix Selection. Then the algorithm recurses on all buckets containing more than one datum. Clearly, this leads to a sorting algorithm. The complexity of Radix Sorting is also measured by the number of bucket operations. It has thoroughly been analyzed in the uniform model with refined expansions for mean and variance involving periodic functions and a central limit law for the normalized complexity, see Knuth [13], Jacquet and Régnier [9], Kirschenhofer, Prodinger and Szpankowski [11] and Mahmoud et al. [15].

For the Markov source model (with $b = 2$ and $0 < p_{ij} < 1$ for all $i, j = 1, 2$) the orders of mean and variance and a central limit theorem for the complexity of Radix Sorting were derived in Leckey, Neininger and Szpankowski [14].

2 The uniform model — selection of quantiles

In this section our model consists of independent data, identically and uniformly distributed over $[0, 1]$. We fix $b \geq 2$ and consider bucket selection using b buckets in each step. The number $Y_n(\ell)$ of bucket operations needed by bucket selection to select rank $\ell \in \{1, \dots, n\}$ in a set of n such data is studied as a process in $1 \leq \ell \leq n$. We write $Y_n := (Y_n(\ell))_{1 \leq \ell \leq n}$. For a refined asymptotic analysis we normalize the process in space and time and consider $X_n = (X_n(t))_{0 \leq t \leq 1}$ defined for $n \geq 1$ and $t \in [0, 1]$ by

$$X_n(t) := \frac{Y_n(\lfloor tn \rfloor + 1) - \frac{b}{b-1} n}{\sqrt{n}}, \tag{1}$$

where we set $Y_n(n + 1) := Y_n(n)$. The process X_n has càdlàg paths and is considered as a random variable in $\mathrm{D}[0, 1]$ endowed with the Skorokhod metric d_{sk}, see Billingsley [2, Chapter 3].

Subsequently, we use prefixes of b-ary expansions. For $s, t \in [0, 1]$ based on their b-ary expansions $s = \sum_{i=1}^{\infty} s_i \cdot b^{-i}$, $t = \sum_{i=1}^{\infty} t_i \cdot b^{-i}$ with $s_i, t_i \in \{0, \dots, b - 1\}$ with the conventions stated in the introduction we denote the length of the longest common prefix by

$$j(s, t) := \max\{i \in \mathbb{N} \,|\, (s_1, \dots, s_i) = (t_1, \dots, t_i)\} \tag{2}$$

with the conventions $\max \emptyset := 0$ and $\max \mathbb{N} := \infty$.

Theorem 2.1 *Let $b \in \mathbb{N}$ with $b \geq 2$. Consider bucket selection using b buckets on a set of independent data uniformly distributed on $[0,1]$. For the process $X_n = (X_n(t))_{0\leq t\leq 1}$ of the normalized number of bucket operations $Y_n(\ell)$ as defined in (1) we have weak convergence, as $n \to \infty$, in $(\mathrm{D}[0,1], d_{sk})$:*

$$X_n \xrightarrow{d} G.$$

Here, $G = (G(t))_{t\in[0,1]}$ is a centered Gaussian process (depending on b) with covariance function

$$\mathbb{E}[G(s)G(t)] = \frac{b}{(b-1)^2} - \frac{b+1}{(b-1)^2} b^{-j(s,t)}, \quad s,t \in [0,1],$$

where $j(s,t)$ is the length of the longest common prefix defined in (2) and $b^{-\infty} := 0$.

Theorem 2.1 implies the asymptotic behavior of the worst case complexity $\max_{\ell=1,\dots,n} Y_n(\ell)$ of Radix Selection:

Corollary 2.2 *For the worst case complexity of Radix Selection in the model and notation of Theorem 2.1 we have, as $n \to \infty$, that*

$$\frac{1}{\sqrt{n}} \left(\sup_{1\leq \ell \leq n} Y_n(\ell) - \frac{b}{b-1} n \right) \xrightarrow{d} \sup_{t\in[0,1]} G(t).$$

For the Gaussian process G in Theorem 2.1 we have the following results on the tails of its supremum and regarding the continuity of its paths.

Theorem 2.3 *For the supremum $S = \sup_{t\in[0,1]} G(t)$ of the Gaussian process G in Theorem 2.1 we have for any $t > 0$ that*

$$\mathbb{P}(|S - \mathbb{E}[S]| \geq t) \leq 2 \exp\left(-\frac{(b-1)^2}{2b} t^2 \right).$$

In the Euclidean topology on $[0,1]$ (induced by absolute value) the Gaussian process G in Theorem 2.1 does not have continuous paths. Typically, in the study of Gaussian processes a metric on the index set is derived from the covariance function. We consider

$$d(s,t) := \sqrt{\mathbb{E}[(G(t) - G(s))^2]} = \frac{\sqrt{2(b+1)}}{b-1} \cdot b^{-j(s,t)/2}, \quad s,t \in [0,1].$$

The subsequent results in this section are stated with respect to the (topologically) equivalent metric

$$d_b(s,t) := b^{-j(s,t)}, \quad s,t \in [0,1].$$

Theorem 2.4 (Modulus of continuity) *For the Gaussian process $G = (G(t))_{t\in[0,1]}$ in Theorem 2.1 we have, almost surely,*

$$2\frac{\sqrt{\log b}}{\sqrt{b-1}} \leq \limsup_{n\to\infty} \sup_{\substack{s,t\in[0,1],\\ d_b(s,t)=b^{-n}}} \frac{|G(t) - G(s)|}{\sqrt{nb^{-n}}} \leq 2\frac{\sqrt{2\log b}}{\sqrt{b-1}(1-b^{-1/2})}.$$

Theorem 2.5 (Hölder continuity) *For any $\beta < 1/2$, almost surely, the paths of the Gaussian process $G = (G(t))_{t\in[0,1]}$ in Theorem 2.1 are Hölder continuous with exponent β with respect to d_b. For any $\beta > 1/2$, almost surely, the paths of G are nowhere pointwise Hölder continuous with exponent β with respect to d_b.*

Outline of the analysis: We outline the analysis leading to Theorems 2.1–2.5. To set up a recurrence for the process $Y_n := (Y_n(\ell))_{1\le\ell\le n}$ we denote by $I^n = (I_1^n, \ldots, I_b^n)$ the numbers of elements in the b buckets after distribution of all n elements in the first partitioning stage. We abbreviate $F_0^n := 0$ and

$$F_r^n := \sum_{j=1}^{r} I_j^n, \qquad 1 \le r \le b.$$

Note that we have $F_b^n = n$. Then, after the first partitioning phase, the element of rank ℓ is in bucket r if and only if $F_{r-1}^n < \ell \le F_r^n$. This implies the recurrence

$$Y_n \stackrel{d}{=} \left(\sum_{r=1}^{b} \mathbf{1}_{\{F_{r-1}^n < \ell \le F_r^n\}} Y_{I_r^n}^r \left(\ell - F_{r-1}^n\right) + n \right)_{1\le\ell\le n}, \tag{3}$$

where $(Y_j^1), \ldots, (Y_j^b), I^n$ are independent and the Y_j^r have the same distribution as Y_j for all $j \ge 0$ and $r = 1, \ldots, b$.

By the model of independent and uniformly distributed data we have that the vector I^n has the multinomial $M(n; \frac{1}{b}, \ldots, \frac{1}{b})$ distribution. Hence, we have $\frac{1}{n} I^n \to (\frac{1}{b}, \ldots, \frac{1}{b})$ almost surely as $n \to \infty$ and

$$\frac{I^n - \frac{1}{b}(n, \ldots, n)}{\sqrt{n}} \to (N_1, \ldots, N_b),$$

where $(N_1, \ldots, N_b)$ is a multivariate normal distribution $\mathcal{N}(0, \Omega)$ with mean zero and covariance matrix Ω given by $\Omega_{ij} = \frac{b-1}{b^2}$ if $i = j$ and $\Omega_{ij} = -\frac{1}{b^2}$ if $i \ne j$. Note that for $b = 2$ we have $N_2 = -N_1$. Below, we denote by

$$\mathcal{N} = (\mathcal{N}_1, \ldots, \mathcal{N}_b)$$

a vector with distribution $\frac{b}{b-1}(N_1, \ldots, N_b)$. Hence $(\mathcal{N}_1, \ldots, \mathcal{N}_b)$ has a multivariate normal distribution with mean zero and covariance matrix $\Upsilon = (\Upsilon_{ij})_{i,j\in\Sigma}$ given by

$$\Upsilon_{ij} = \begin{cases} \frac{1}{b-1}, & \text{if } i = j, \\ -\frac{1}{(b-1)^2}, & \text{if } i \ne j. \end{cases} \tag{4}$$

For the normalized processes X_n in (1) we thus obtain

$$X_n \stackrel{d}{=} \left(\sum_{r=1}^{b} \mathbf{1}_{\{F_{r-1}^n < \lfloor tn \rfloor + 1 \le F_r^n\}} \sqrt{\frac{I_r^n}{n}} X_{I_r^n}^r \left(\frac{nt - F_{r-1}^n}{I_r^n} \right) + \sum_{r=1}^{b} \mathbf{1}_{\{F_{r-1}^n < \lfloor tn \rfloor + 1 \le F_r^n\}} \frac{b}{b-1} \frac{I_r^n - \frac{1}{b}n}{\sqrt{n}} \right)_{0\le t\le 1}, \tag{5}$$

with conditions on independence and identical distributions as in (3).

To associate to recurrence (5) a limit equation in the spirit of the contraction method we introduce the indicator functions

$$\mathbf{I}_r(x) := \mathbf{1}_{[r-1,r)}(x) \text{ for } r = 1, \dots, b-1, \qquad \mathbf{I}_b(x) := \mathbf{1}_{[b-1,b]}(x)$$

and the sawtooth function $s_b : [0,1] \to [0,1]$

$$s_b(t) := \begin{cases} bt - \lfloor bt \rfloor, & 0 \le t < 1, \\ 1, & t = 1. \end{cases}$$

Moreover, we use the transformations $\mathfrak{A}_r : \mathrm{D}[0,1] \to \mathrm{D}[0,1]$ for $r = 1, \dots, b$ with

$$f \mapsto \mathfrak{A}_r(f), \quad \mathfrak{A}_r(f)(t) = \mathbf{I}_r(tb) f(s_b(t)) \text{ for } t \in [0,1],$$

and $\mathfrak{B} : \mathbb{R}^b \to \mathrm{D}[0,1]$ with (for $v = (v_1, \dots, v_b)$)

$$v \mapsto \mathfrak{B}(v), \quad \mathfrak{B}(v)(t) = \sum_{r=1}^{b} \mathbf{I}_r(tb) v_r \text{ for } t \in [0,1].$$

Then we associate the limit equation

$$X \stackrel{d}{=} \sum_{r=1}^{b} \frac{1}{\sqrt{b}} \mathfrak{A}_r(X^r) + \mathfrak{B}(\mathcal{N}), \tag{6}$$

where $X^1, \dots, X^b, \mathcal{N}$ are independent, the X^r are identically distributed $(\mathrm{D}[0,1], d_{sk})$-valued random variables with the distribution of X, and $\mathcal{N}$ has the centered multivariate normal distribution with covariance matrix Υ given in (4).

A distributional fixed-point equation related to (6) appeared in Sulzbach et al. [17], see the map T in equation (2.5) of [17]. The proof of our Theorem 2.1 can be carried out analogously to the proof in sections 2.1, 2.2 and 3.3 of [17]. Note that in analogy to Lemma 2.3 in [17] our fixed-point equation (6) characterizes the Gaussian limit process G in Theorem 2.1 as the unique fixed-point of (6) subject to the constraint $\mathbb{E}[\|X\|_\infty^{2+\varepsilon}] < \infty$ for any $\varepsilon > 0$ and, hence, in the analysis one has to adapt exponents appropriately. The proofs of our Theorems 2.3–2.5 can be carried out as the corresponding results in section 4 of [17] which are related to and partly based on fundamental work on Gaussian processes, see Dudley [6], Talagrand [19], Adler [1] and Boucheron, Lugosi and Massart [3].

3 The Markov source model

Now the Markov source model is considered for the data. For the rank to be selected the quantile-model is studied in section 3.1, the model of grand averages in section 3.2. We restrict ourselves to the study of Radix Selection using $b = 2$ buckets.

3.1 Selection of quantiles

We consider the complexity of Radix Selection with $b = 2$ buckets assuming the Markov source model for the data and the quantile-model for the rank to be selected. We first define functions $m_\mu : [0,1] \to (0,\infty)$ which appear in the average complexity. For $n \geq 1$ and $i = 0,1$ we recursively define sets $\mathcal{D}_n^i = \{s_{n,k}^i \,|\, k = 0,\ldots,2^n\}$ as follows: For $n = 1$ we set $(s_{1,0}^i, s_{1,1}^i, s_{1,2}^i) := (0, p_{i0}, 1)$ for $i = 0,1$. Further, for all $n \geq 1$, $i = 0,1$ and $0 \leq k \leq 2^n$ we set

$$s_{n+1,k}^i := \begin{cases} s_{n,k/2}^i, & \text{if } k \bmod 4 \in \{0,2\}, \\ p_{00} s_{n,(k+1)/2}^i + p_{01} s_{n,(k-1)/2}^i, & \text{if } k \bmod 4 = 1. \\ p_{10} s_{n,(k+1)/2}^i + p_{11} s_{n,(k-1)/2}^i, & \text{if } k \bmod 4 = 3, \end{cases}$$

We further define $\mathcal{D}_\infty^i := \cup_{n=1}^\infty \mathcal{D}_n^i$. Note that for each $n \geq 1$ the set $\mathcal{D}_n^i$ decomposes the unit interval into 2^n sub-intervals. For $t \in [0,1] \setminus \mathcal{D}_\infty^i$ we denote by $\lambda_n^i(t)$ the length of the (unique) sub-interval of this decomposition that contains t. Then, for $i = 0,1$ and $t \in [0,1] \setminus \mathcal{D}_\infty^i$ we set

$$m_i(t) := 1 + \sum_{n=1}^\infty \lambda_n^i(t).$$

Further, for an initial distribution $\mu = \mu_0\delta_0 + \mu_1\delta_1$ with $\mu_0 \in [0,1]$ we denote

$$\mathcal{D}_\infty^\mu := \mu_0 \mathcal{D}_\infty^0 \cup \left(\mu_0 + \mu_1 \mathcal{D}_\infty^1\right)$$

and, for $t \in [0,1] \setminus \mathcal{D}_\infty^\mu$,

$$m_\mu(t) := \begin{cases} \mu_0 m_0\left(\frac{t}{\mu_0}\right) + 1, & \text{if } t < \mu_0, \\ (1-\mu_0) m_1\left(\frac{t-\mu_0}{1-\mu_0}\right) + 1, & \text{if } t > \mu_0. \end{cases}$$

We have the following asymptotic behavior of the average complexity:

Theorem 3.1 *Let $Y_n^\mu(\ell)$ denote the number of bucket operations of Radix Selection with $b = 2$ selecting a rank $1 \leq \ell \leq n$ among n independent data generated from the Markov source model with initial distribution $\mu = \mu_0\delta_0 + \mu_1\delta_1$ where $\mu_0 \in [0,1]$ and transition matrix $(p_{ij})_{i,j\in\{0,1\}}$ with $p_{ij} < 1$ for all $i,j = 0,1$. Then, for all $t \in [0,1] \setminus D_\infty^\mu$ as $n \to \infty$, we have*

$$\mathbb{E}[Y_n^\mu(\lfloor tn \rfloor + 1)] = m_\mu(t) n + o(n). \tag{7}$$

Outline of the analysis: We denote by $Y_n^0 = (Y_n^0(\ell))_{1\leq\ell\leq n}$ and $Y_n^1 = (Y_n^1(\ell))_{1\leq\ell\leq n}$ the number of bucket operations for a Markov source model as in Theorem 3.1 for initial distributions $p_{00}\delta_0 + p_{01}\delta_1$ and $p_{10}\delta_0 + p_{11}\delta_1$ respectively. Then we have the system of recursive distributional equations, for $n \geq 2$,

$$Y_n^i \stackrel{d}{=} \left(\mathbf{1}_{\{\ell\leq J_n^i\}} Y_{J_n^i}^0(\ell) + \mathbf{1}_{\{\ell > J_n^i\}} Y_{n-J_n^i}^1(\ell - J_n^i) + n\right)_{1\leq\ell\leq n}, \quad i = 0,1, \tag{8}$$

where $Y_0^0, \ldots, Y_n^0, Y_0^1, \ldots, Y_n^1, J_n^0, J_n^1$ are independent (the independence between J_n^0 and J_n^1 is not required) and we have that J_n^i is $\mathrm{B}(n, p_{i0})$ distributed for $i = 0,1$. Moreover, for general initial distribution μ we further have

$$Y_n^\mu \stackrel{d}{=} \left(\mathbf{1}_{\{\ell\leq K_n\}} Y_{K_n}^0(\ell) + \mathbf{1}_{\{\ell > K_n\}} Y_{n-K_n}^1(\ell - K_n) + n\right)_{1\leq\ell\leq n}, \tag{9}$$

where $Y_0^0, \dots, Y_n^0, Y_0^1, \dots, Y_n^1, K_n$ are independent and K_n has the binomial $\mathrm{B}(n, \mu_0)$ distribution.

The proof of Theorem 3.1 is based on k times iterating the system (8) with $k = k(n) = \Theta(\log n)$ chosen appropriately. The contributions of the toll functions within these k iterations yield the main contribution, the other terms are asymptotically negligible.

A distributional analysis of the quantile-model is left for the full paper version of this extended abstract as well as the behavior at the $t \in \mathcal{D}_\infty^\mu$. For these t the expansion (7) still holds when defining $m_\mu(t)$ as the average of the left-hand and right-hand limit of m_μ at t.

A special case where the analysis is simplified considerably is the asymmetric Bernoulli model discussed next where we obtain a functional limit law as for the uniform model in Theorem 2.1.

The asymmetric Bernoulli model: The data model called *asymmetric Bernoulli model* consists of all data being independent and having independent bits all identically distributed over $\Sigma = \{0, 1\}$ with Bernoulli $\mathrm{B}(p)$ distribution for a fixed $p \in (0, 1)$ with $p \neq \frac{1}{2}$. Note that this can also be considered as a special case of the Markov source model by choosing $\mu_0 = p_{00} = p_{10} = 1 - p$ and $\mu_1 = p_{01} = p_{11} = p$. Here, the analysis simplifies considerably compared to the general Markov source model due to the fact that the mean function m corresponding to m_0, m_1, m_μ in Theorem 3.1 becomes an affine function. We have the following results:

Theorem 3.2 *Consider bucket selection using $b = 2$ buckets on a set of n independent data generated from the asymmetric Bernoulli model with success probability $p \in (0, 1) \setminus \{\frac{1}{2}\}$. For the process $X_n^{\mathrm{asyB}} = (X_n^{\mathrm{asyB}}(t))_{0 \le t \le 1}$ of the normalized number of bucket operations $Y_n^{\mathrm{asyB}}(\ell)$ defined by*

$$X_n^{\mathrm{asyB}}(t) := \frac{Y_n^{\mathrm{asyB}}(\lfloor tn \rfloor + 1) - m(t)n}{\sqrt{n}}, \quad t \in [0, 1],$$

with $Y_n^{\mathrm{asyB}}(n + 1) := Y_n^{\mathrm{asyB}}(n)$ and

$$m(t) = \frac{2p - 1}{p(1 - p)} t + \frac{1}{p}, \quad t \in [0, 1],$$

we have weak convergence, as $n \to \infty$, in $(\mathrm{D}[0, 1], d_{sk})$:

$$X_n^{\mathrm{asyB}} \xrightarrow{d} G^{\mathrm{asyB}}.$$

Here, $G^{\mathrm{asyB}} = (G^{\mathrm{asyB}}(t))_{t \in [0,1]}$ is a centered Gaussian process (depending on p) with covariance function given, for $s, t \in [0, 1]$, by

$$\mathbb{E}[G^{\mathrm{asyB}}(s) G^{\mathrm{asyB}}(t)] = -\prod_{k=1}^{r(s,t)} p[g(t, k)] + \sum_{k=1}^{r(s,t)} \frac{\prod_{j=1}^{k} p[g(t, j)]}{p[1 - g(t, k)]},$$

where $p[0] := 1 - p$, $p[1] := p$ and the functions $r : [0, 1]^2 \to \mathbb{N}_0 \cup \{\infty\}$ and $g : [0, 1] \times \mathbb{N}_0 \to \{0, 1\}$ are defined as follows:

$$r(s, t) = \max\{n \in \mathbb{N}_0 | g(s, \ell) = g(t, \ell),\ 1 \le \ell \le n\}$$

and g and $h : [0,1] \times \mathbb{N}_0 \to [0,1]$ are recursively defined by $g(t,0) = 0$, $h(t,0) = t$ for $t \in [0,1]$ and for $k \geq 1$ by

$$g(t,k) = \begin{cases} 0, & \text{if } h(t,k-1) < 1-p, \\ 1, & \text{if } h(t,k-1) \geq 1-p, \end{cases} \qquad h(t,k) = \begin{cases} \frac{h(t,k-1)}{1-p}, & \text{if } h(t,k-1) < 1-p, \\ \frac{h(t,k-1)-(1-p)}{p}, & \text{if } h(t,k-1) \geq 1-p. \end{cases}$$

For the maximum of the complexities we obtain the following corollary:

Corollary 3.3 *In the model and notation of Theorem 3.2 we have, as $n \to \infty$, that*

$$\frac{1}{\sqrt{n}} \left(\sup_{1 \leq \ell \leq n} \left(Y_n^{\mathrm{asyB}}(\ell) - m\left(\frac{\ell}{n}\right) n \right) \right) \xrightarrow{d} \sup_{t \in [0,1]} G^{\mathrm{asyB}}(t).$$

Theorem 3.4 *For the supremum $S' = \sup_{t \in [0,1]} G^{\mathrm{asyB}}(t)$ of the Gaussian process G^{asyB} in Theorem 3.2 we have for any $t > 0$ with $p_\vee := \max\{p, 1-p\}$ that*

$$\mathbb{P}(|S' - \mathbb{E}[S']| \geq t) \leq 2 \exp\left(-\frac{(1-p_\vee)^2}{2p_\vee} t^2 \right).$$

3.2 Selection of a uniform rank

We now consider the complexity of Radix Selection with $b = 2$ buckets assuming the Markov source model for the data and the model of grand averages for the rank. We have the following asymptotic behavior:

Theorem 3.5 *Let W_n denote the number of bucket operations of Radix Selection with $b = 2$ selecting a uniformly distributed rank independent from n independent data generated from the Markov source model with initial distribution $\mu = \mu_0 \delta_0 + \mu_1 \delta_1$ where $\mu_0 \in [0,1]$ and transition matrix $(p_{ij})_{i,j \in \{0,1\}}$ with $p_{ij} < 1$ for all $i, j = 0, 1$. Then, as $n \to \infty$, we have*

$$\mathbb{E}[W_n] = \kappa_\mu n + o(n)$$

with $\kappa_\mu > 0$ given in (15) and

$$\frac{W_n}{n} \xrightarrow{d} Z_\mu,$$

where the convergence also holds with all moments. The distribution of Z_μ is given by

$$Z_\mu \stackrel{d}{=} B_{\mu_0} \mu_0 Z^0 + (1 - B_{\mu_0})(1 - \mu_0) Z^1 + 1, \tag{10}$$

where B_{μ_0}, Z^0, Z^1 are independent and B_{μ_0} has the Bernoulli distribution $\mathrm{B}(\mu_0)$. The distributions of Z^0 and Z^1 are the unique integrable solutions of the system (12).

Outline of the analysis: We denote by $W_n^\mu := W_n$ the complexity as stated in Theorem 3.5 and, for initial distributions $p_{i0}\delta_0 + p_{i1}\delta_1$, write $W_n^i := W_n^{p_{i0}\delta_0 + p_{i1}\delta_1}$ for $i = 0, 1$. We have the system of distributional recurrences, for $n \geq 2$,

$$W_n^i \stackrel{d}{=} B_{ii} W_{J_n^i}^0 + (1 - B_{ii}) W_{n-J_n^i}^1 + n, \quad i = 0, 1, \tag{11}$$

where $W_1^0, \dots, W_n^0, W_1^1, \dots, W_n^1$ and $(J_n^0, J_n^1, B_{00}, B_{11})$ are independent and we have that J_n^i is Binomial $\mathrm{B}(n, p_{i0})$ distributed and B_{ii} is mixed Bernoulli distributed with distribution $\mathrm{B}(J_n^i/n)$ for $i = 0, 1$. We normalize

$$Z_n^i := \frac{W^i}{n}, \quad n \geq 1,\ i = 0, 1$$

and obtain, for all $n \geq 2$ that

$$Z_n^i \stackrel{d}{=} B_{ii} \frac{J_n^i}{n} Z_{J_n^i}^0 + (1 - B_{ii}) \frac{n - J_n^i}{n} Z_{n-J_n^i}^1 + 1, \quad i = 0, 1,$$

with independence relations as in (11). This leads to the limit system

$$Z^i \stackrel{d}{=} B_{p_{i0}} p_{i0} Z^0 + (1 - B_{p_{i0}})(1 - p_{i0}) Z^1 + 1, \quad i = 0, 1, \tag{12}$$

where Z^0, Z^1 and $B_{p_{i0}}$ are independent and $B_{p_{i0}}$ has the Bernoulli $\mathrm{B}(p_{i0})$ distribution for $i = 0, 1$. It is easy to show that subject to $\mathbb{E}[|Z^i|] < \infty$ the limit system (12) has a unique solution; cf. Knape and Neininger [12, section 5]. Also, the convergences $Z_n^i \to Z^i$ can be shown by a contraction argument in any Wasserstein ℓ_p metric with $p \geq 1$. From the limit system (12) we obtain for the expectations $\kappa_i := \mathbb{E}[Z^i]$ for $i = 0, 1$ that

$$\kappa_0 = \frac{1 + p_{01}^2 - p_{11}^2}{2(p_{00} + p_{11})(1 + p_{00} p_{11}) - 2(p_{00} + p_{11})^2} > 0, \tag{13}$$

$$\kappa_1 = \frac{1 + p_{10}^2 - p_{00}^2}{2(p_{00} + p_{11})(1 + p_{00} p_{11}) - 2(p_{00} + p_{11})^2} > 0. \tag{14}$$

Now, for a general initial distribution μ we have

$$W_n^\mu \stackrel{d}{=} B_{\mu\mu} W_{K_n}^0 + (1 - B_{\mu\mu}) W_{n-K_n}^1 + n,$$

where $W_1^0, \dots, W_n^0, W_1^1, \dots, W_n^1, (K_n, B_{\mu\mu})$ are independent, K_n has the binomial $\mathrm{B}(n, \mu_0)$ distribution and $B_{\mu\mu}$ has the mixed Bernoulli $\mathrm{B}(K_n/n)$ distribution. This implies for the limit Z_μ of W_n^μ/n the representation

$$Z_\mu \stackrel{d}{=} B_{\mu_0} \mu_0 Z^0 + (1 - B_{\mu_0})(1 - \mu_0) Z^1 + 1,$$

where B_{μ_0}, Z^0, Z^1 are independent and B_{μ_0} has the Bernoulli distribution $\mathrm{B}(\mu_0)$. Hence, we obtain for $\kappa_\mu := \mathbb{E}[Z_\mu]$ the representation

$$\kappa_\mu = \mu_0^2 \kappa_0 + (1 - \mu_0)^2 \kappa_1 + 1, \tag{15}$$

with κ_0, κ_1 given in (13) and (14). The claims of Theorem 3.5 follow from this outline by an application of the contraction method within the Wasserstein metrics.

A remark on concentration for grand averages: Note that for the special case $p_{ij} = \mu_i = \frac{1}{2}$ for $i = 0, 1$ the Markov source model reduces to the uniform model. In this case it was shown (together with more refined results) in Mahmoud et al. [15] that the complexity W_n in Theorem 3.5 as $n \to \infty$ satisfies

$$\frac{W_n - 2n}{\sqrt{2n}} \xrightarrow{d} \mathcal{N}(0, 1). \tag{16}$$

Our Theorem 3.5 also applies: We find that for the uniform model system (12) is solved deterministically by $Z^i = 2$ almost surely for $i = 0, 1$, hence plugging in into (10) we also obtain $Z_\mu = 2$ and thus $W_n/n \to 2$, which is, although only a law of large numbers, consistent with (16). (The full limit law in (16) is a corollary to our Theorem 2.1.)

However, for $(p_{00}, p_{01}, p_{10}, p_{11}) \neq (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ the system (12) does no longer solve deterministically, so that W_n/n then has a nondeterministic limit and is less concentrated, typical fluctuations are of linear order compared to $\sqrt{n}$ for the uniform model. This behavior becomes transparent when looking at the quantile-model: In the uniform model we have the same leading linear term $2n$ in the expansion of the means of all quantiles, which implies that a uniformly chosen rank conditional on its size will always lead to a complexity of the same linear order $2n$. This does no longer hold for a non-uniform Markov model. The constant $m_\mu(t)$ in the linear growth $m_\mu(t)n$ of the complexity depends on the quantiles $t \in [0, 1]$, see Theorem 3.1. This implies that the complexity can no longer remain concentrated: The fluctuations are now forced to be at least of linear order since different choices of the ranks lead to different linear orders. This is consistent with the fact that in Theorem 3.5 we then find a non-deterministic limit for W_n/n and a variance of the order $\Theta(n^2)$. Further note, that this also implies a simple representation of the limit distribution of Z_μ in Theorem 3.5 as

$$Z_\mu \stackrel{d}{=} m_\mu(U),$$

with m_μ as in Theorem 3.1 und U uniformly distributed on $[0, 1]$.

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The k-th Total Path Length and the Total Steiner k-Distance for Digital Search Trees

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Abstract. The total Steiner k-distance and the k-th total path length are the sum of the size of Steiner trees and ancestor-trees over sets of k nodes of a given tree, respectively. They are useful statistics with many applications. Consequently, they have been analyzed for many different random trees, including increasing trees, binary search trees, generalized m-ary search trees and simply generated trees.

In this paper, we investigate the two parameters for digital search trees, which are fundamental data structures in computer science with wide applications. We derive the means, covariances and variances for the total Steiner k-distances and the k-th total path lengths by the "Poisson-Laplace-Mellin Method". Moreover, results about the limiting distributions are obtained as well.

Keywords: internal path length, Wiener index, total Steiner k-distance, digital search trees, Steiner tree

1 Introduction

Digital search trees (DSTs) are fundamental data structure in computer science first introduced by Coffman and Eve [CJE70]. They have attracted considerable attention due to their wide applications, especially their close connection to the famous Lempel-Ziv compression scheme [JS95]. In a DST, strings are stored in the nodes of a binary tree under the following rules. Given a series of binary strings, we place the first string in the root and the other strings are distributed to the right or the left subtree of the root depending on whether their first symbol is "0" (left) or "1" (right). This process will be recursively applied to the subtrees but with the removal of the first bits when comparison is completed. The resulting tree will be called a DST. See Figure 1 hereafter as an illustration.

Many parameters of DSTs, including depth, height, total path length, peripheral path length, Wiener index, fillup level and expected profile, have been analyzed, see [DS11], [FHZ10] and [FL] for details and many references. In this paper, we are interested in two parameters, the k-th total path length and the total Steiner k-distance, which have not been analyzed yet. We equip DSTs with the so-called Bernoulli model which assumes that every bit of the string is independent and admits a Bernoulli distribution with the probability p of being 0. In order to make the analysis more brief and simpler, we consider in this paper only the symmetric case. In other words, the probability p for the Bernoulli model will be $1/2$ for the entire paper.

For a given tree T with vertex set V and a subset $M \subset V$, the smallest spanning tree containing M is called the *Steiner tree* for M in T while the smallest subtree containing M and the root is the so-called

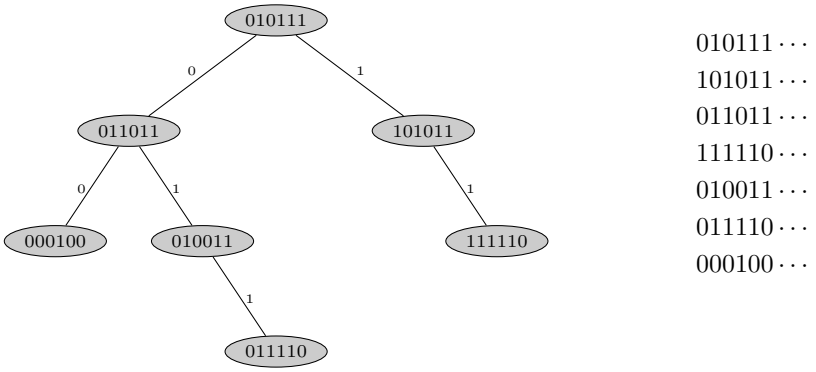

Fig. 1: A DST built from 7 keys.

ancestor-tree for M in T. The size of the Steiner tree for M in T (denoted by $S_M(T)$) and the size of the ancestor-tree for M in T (denoted by $D_M(T)$) are called the Steiner distance and the $|M|$-th path length, respectively. Furthermore, for the given tree T and integer $k \in \mathbb{N}$, the k-th total path length $P_k(T)$ and the Steiner k-distance $W_k(T)$ are defined as

$$P_k(T) = \sum_{|M|=k} D_M(T) \quad \text{and} \quad W_k(T) = \sum_{|M|=k} S_M(T).$$

Steiner trees and ancestor trees have many real-life applications, e.g. in transportation and multiprocessor networks [PP04], circuit layouts, internet communication [PS02] and many others. Consequently, the Steiner distance and the $|M|$-th path length are useful statistics. For example, when comparing the efficiency of communication potential of different networks, the Steiner distance can be used [DOS96]. Moreover, the Steiner distance and k-th total path length have also applications to Multiple Quickselect algorithm [PP04] and the efficiency of certain traceroute algorithms [GR09].

In the last decade, several papers dedicated to the analysis of the two parameters in various random trees, including random increasing tree [PP04], random binary search tree [MPP04], generalized random m-ary search tree [Pan04b], recursive trees [Mun10, Pan04a] and random simply generated trees [Mun10, Pan04a] have been published. As mentioned in [Mun10], the size of a Steiner tree is related to the communication potential of its nodes. Thus, it is of interest to study the Steiner k-distance of different data structures, such as DSTs. In this paper, we use the "Laplace-Mellin Method" which was first proposed in [FHZ10] to obtain the means, variances and covariances of the k-th total path length and the total Steiner k-distance for DSTs under the Poisson model. With the help of the JS-admissibility language from [FHZ10] and then analytical depoissonization, which was first proposed by P. Jacquet and W. Szpankowski, we can get the means, variances and covariances under the above Bernoulli model directly from the results under the Poisson model. Limit laws for the two parameter are derived as well. In the rest of the paper, we use $P_n^{[k]}$ and $S_n^{[k]}$ to denote the k-th total path length and total k-th Steiner distance of random digital search trees built on n strings, respectively. Also, we use the common notation for the constant $Q_m = \prod_{j=1}^{m} \left(1 - 2^{-j}\right)$ and $Q_\infty = \lim_{m\to\infty} Q_m$. The main results of this paper are:

Theorem 1 *We have that for $k \geq 2$,*

$$\mathbb{E}\left(P_n^{[k]}\right) \sim \mathbb{E}\left(S_n^{[k]}\right) \sim \frac{n^k \log_2 n}{(k-1)!}.$$

Moreover, the variance and covariance of $P_n^{[k]}$ and $S_n^{[k]}$ are given by

$$\begin{aligned}
\mathrm{Var}\left(P_n^{[k]}\right) \sim \mathrm{Var}\left(S_n^{[k]}\right) &\sim n^{2k-1} \frac{2^{2-2k}}{Q_{k-1}^2} \left(C_{kps} + \varpi_{kps}(\log_2 n)\right), \\
\mathrm{Cov}\left(P_n^{[k_1]}, P_n^{[k_2]}\right) \sim \mathrm{Cov}\left(S_n^{[k_1]}, P_n^{[k_2]}\right) &\sim n^{k_1+k_2-1} \frac{2^{2-k_1-k_2}}{Q_{k_1-1}Q_{k_2-1}} \left(C_{kps} + \varpi_{kps}(\log_2 n)\right).
\end{aligned}$$

where C_{kps} and ϖ_{kps} are defined in Theorem 2.1 of [FHZ10].

Theorem 2 *Let*

$$X_n^{[k]} = \frac{P_n^{[k]} - \mathbb{E}(P_n^{[k]})}{\sqrt{\mathrm{Var}(P_n^{[k]})}} \quad \textit{and} \quad Y_n^{[k]} = \frac{S_n^{[k]} - \mathbb{E}(S_n^{[k]})}{\sqrt{\mathrm{Var}(S_n^{[k]})}}.$$

We have that for any $k \geq 2$,

$$\left(X_n^{[1]}, \ldots, X_n^{[k-1]}, Y_n^{[k]}\right) \xrightarrow{d} (X, \ldots, X),$$

where X is the standard normal distributed random variable and $\xrightarrow{d}$ denotes weak convergence.

Remark 1 The asymptotics of $S_n^{[k]}$ can be explained intuitively. It is well-known that the expected value of the depth of a node is of order $\log_2 n$. For a Steiner tree, the size will be more or less the sum of the depth of the k chosen nodes. Thus, for k chosen nodes, the expected size of the Steiner tree will be of order $k \log_2 n$. Since there are $\binom{n}{k}$ ways to choose the k nodes, the mean of the total Steiner k-distance will be roughly $\binom{n}{k} k \log_2 n \sim \frac{n^k \log_2 n}{(k-1)!}$.

Remark 2 As we have seen, the leading terms for the asymptotics of k-th total path length and Steiner k-distance are the same. This is not surprising, intuitively speaking, because the k-subsets which are most relevant are those contain vertices from both subtrees for which the ancestor tree and the Steiner tree will be the same. This is similar to the distance between two random nodes (see [ALM05, ALM06]) which is also twice the depth, because the most relevant cases are again those include the root.

Remark 3 In fact, we can find more terms in the asymptotic of the means, variances and covariances for $P_n^{[k]}$ and $S_n^{[k]}$ by the same method applied in the following sections. For example, let $\chi_m = 2m\pi i/\log 2$, we have that

$$\mathbb{E}\left(P_n^{[k]}\right) \sim \mathbb{E}\left(S_n^{[k]}\right) + D^{[k]} n^k \sim \frac{n^k \log n}{(k-1)!} + \frac{n^k}{(k-1)!}\left(c_k + \frac{e_k}{k} + \frac{1}{\log 2} \sum_{m \in \mathbb{Z}\setminus\{0\}} \frac{G_k(\chi_m) n^{\chi_m}}{\Gamma(k+1+\chi_m)}\right).$$

where

$$G_k(\chi_m) = \Gamma(k+1-\chi_m)\Gamma(-1-\chi_m), \quad D^{[k]} = \frac{1}{k!(2^{k-1}-1)}$$

and the constant c_k is given by

$$c_k = \frac{\gamma - 1}{\log 2} + \frac{1}{2} - \sum_{j \geq 1} \frac{(k-1)!}{2^j - 1} + \frac{(k-1)! d_k}{\log 2}.$$

In the expression, d_k is defined recursively as $d_1 = 0$ and

$$d_k = \frac{1}{2^{k-1} - 1} \sum_{r=1}^{k-1} \frac{d_{k-r}}{r!} - \frac{2^{k-1}}{2^{k-1} - 1} \frac{\log 2}{(k-1)!}.$$

Also, the sequence $\{e_k\}_{k \geq 1}$ is defined recursively as $e_1 = 0$ and

$$e_k = \frac{1}{2^{k-1} - 1} \sum_{r=1}^{k-2} \frac{k!}{r!} e_{k-r} + \frac{2^k - 1}{2^{k-1} - 1}, \quad \text{for } k \geq 2.$$

We state the main result in the form of Theorem 1 because the leading term is the most interesting part and it would be enough for proving the central limit theorem. Also, computing more terms can be extremely complicated. As we see from the above statements, the difference between the asymptotics of the two shape parameters is $\frac{n^k}{k!(2^{k-1}-1)}$. This can be explained heuristically. Let $d_n^{[k]}$ be the difference of the two shape parameters, then $d_n^{[k]} \sim 2d_{n/2}^{[k]} + 2\binom{\frac{n}{2}}{k}$ since the size of both subtrees will be roughly $n/2$ under the Bernoulli model. Iterating it, we get $d_n^{[k]} = \Theta(n^k)$, which matches the difference above.

Remark 4 Note that the Steiner k-distance is a generalization of the Wiener index, namely, for $k = 2$ we obtain the Wiener index. Thus, Theorem 2 of [FL] is actually a special case of Theorem 2 of this paper with $k = 2$.

The paper is organized as follows. In Section 2, we derive the means, covariances and variance of the k-th total path length for DSTs. In Section 3, we give the asymptotics of the means, covariances and variances of the total Steiner k-distance. We also explain how to prove Theorem 2 in Section 3.

Notation 1 For a given function f, we use $\mathscr{L}[f; s]$ and $\mathscr{M}[f; \omega]$ to denote the Laplace transform and Mellin transform of f, respectively. Moreover, ϵ is an arbitrarily small positive number.

2 k-th Total Path Length

In this section, we start with the recurrence under the Bernoulli model and then use it to get the differential-functional equation of the Poisson model. The rest of the analysis will focus on the Poisson model, since the depoissonization is standard, see [FHZ10]. The method we use in the analysis of the Poisson model is the "Laplace-Mellin Method" which uses a combination of the Laplace and Mellin transform; see [FL] for a summary of the method and [FGD95] for a comprehensive introduction to the Mellin transform and its properties.

2.1 Mean of the k-th Total Path Length of DSTs

First, we start with deriving a distributional recurrence relation for the k-th total path length. Recall the notation $P_n^{[k]}$ for the k-th total path length from the introduction. Moreover, we will use the notation $B_n \stackrel{d}{=} \text{Binom}(n, \frac{1}{2})$. Let a DST with $n+1$ nodes given. Depending on how the k nodes are chosen, there are 4 cases:

1. All k nodes are from one subtree.
The contribution to the k-th total path length will be

$$P_{B_n}^{[k]} + P_{n-B_n}^{[k]*} + \binom{B_n}{k} + \binom{n-B_n}{k},$$

where $P_{B_n}^{[k]}$ is independent of $P_{n-B_n}^{[k]*}$ and $P_{B_n}^{[k]} \stackrel{d}{=} P_{n-B_n}^{[k]*}$.

2. The k nodes are chosen from both subtrees and the root is not chosen.
We will have the contribution

$$\sum_{r=1}^{k-1} \left(\binom{n-B_n}{k-r} P_{B_n}^{[r]} + \binom{B_n}{r} P_{n-B_n}^{[k-r]*} + 2\binom{B_n}{r}\binom{n-B_n}{k-r} \right).$$

3. The root is chosen, the other $k-1$ nodes are all from one subtree.
It will contribute

$$P_{B_n}^{[k-1]} + P_{n-B_n}^{[k-1]*} + \binom{n-B_n}{k-1} + \binom{B_n}{k-1}.$$

4. The root is chosen, the other $k-1$ nodes are from both subtrees.
The contribution will be

$$\sum_{r=1}^{k-2} \left(\binom{n-B_n}{k-r-1} P_{B_n}^{[r]} + \binom{B_n}{r} P_{n-B_n}^{[k-r-1]*} + 2\binom{B_n}{r}\binom{n-B_n}{k-r-1} \right).$$

Combining all four cases, we get that for $n+1 \geq k \geq 1$:

$$\begin{aligned} P_{n+1}^{[k]} \stackrel{d}{=} & P_{B_n}^{[k]} + P_{n-B_n}^{[k]*} + P_{B_n}^{[k-1]} + P_{n-B_n}^{[k-1]*} + \sum_{r=1}^{k-1} \left(\binom{n-B_n}{k-r} P_{B_n}^{[r]} + \binom{B_n}{r} P_{n-B_n}^{[k-r]*} \right) \\ & + 2\binom{n}{k} + 2\binom{n}{k-1} + \sum_{r=1}^{k-2} \left(\binom{n-B_n}{k-r-1} P_{B_n}^{[r]} + \binom{B_n}{r} P_{n-B_n}^{[k-r-1]*} \right) \\ & - \binom{n-B_n}{k} - \binom{B_n}{k} - \binom{n-B_n}{k-1} - \binom{B_n}{k-1}. \end{aligned}$$

Note that from the above equation, we see that the k-th total path length depends on the 1-st, 2-nd,..., $(k-1)$-th total path length. Thus, we actually have a system of recurrences. The initial conditions are $P_n^{[0]} = 0$ for all n and $P_n^{[k]} = 0$ for all $k > n$.

Let $\tilde{f}^{[k]}(z) = e^{-z}\sum_{n\geq 0}\mathbb{E}(P_n^{[k]})\frac{z^n}{n!}$ which is the mean in the Poisson model. Then, from the recurrence relation above, we get

$$\begin{aligned}\tilde{f}^{[k]}(z) + \tilde{f}^{[k]'}(z) =& 2\tilde{f}^{[k]}\left(\frac{z}{2}\right) + 2\tilde{f}^{[k-1]}\left(\frac{z}{2}\right) + 2\sum_{r=1}^{k-1}\frac{\left(\frac{z}{2}\right)^r}{r!}\tilde{f}^{[k-r]}\left(\frac{z}{2}\right) + 2\sum_{r=1}^{k-2}\frac{\left(\frac{z}{2}\right)^r}{r!}\tilde{f}^{[k-r-1]}\left(\frac{z}{2}\right)\\ &+ 2\left(\frac{z^k - (\frac{z}{2})^k}{k!} + \frac{z^{k-1} - (\frac{z}{2})^{k-1}}{(k-1)!}\right).\end{aligned}$$

Note that when $k = 1$, the above equation will be exactly the same as the one derived in [FHZ10] and hence the order of $\tilde{f}^{[1]}(z)$ is known. Thus, by induction and the closure properties of JS-admissibility from [FHZ10], we get that

$$\tilde{f}^{[k]}(z) = \begin{cases} \mathcal{O}(z^{k+\epsilon}), & \text{as } z \to \infty;\\ \mathcal{O}(z^k), & \text{as } z \to 0^+\end{cases}$$

uniformly for z with $|\arg z| \leq \frac{\pi}{2} - \epsilon$, where $\epsilon > 0$ is an arbitrary small constant. Applying Laplace transform, we get the differential-functional equation

$$\begin{aligned}(1+s)\mathscr{L}[\tilde{f}^{[k]}; s] =& 4\mathscr{L}[\tilde{f}^{[k]}; 2s] + 4\mathscr{L}[\tilde{f}^{[k-1]}; 2s] + 4\sum_{l=1}^{k-1}\frac{(-1)^l}{l!}\mathscr{L}^{(l)}[\tilde{f}^{[k-l]}; 2s]\\ &+ 4\sum_{l=1}^{k-2}\frac{(-1)^l}{l!}\mathscr{L}^{(l)}[\tilde{f}^{[k-l-1]}; 2s] + 2\left(\frac{1+s}{s^{k+1}} - \frac{1+2s}{2^k s^{k+1}}\right),\end{aligned}$$

where $\mathscr{L}^{(l)}[\tilde{f}^{[k-l]}; s]$ is the l-th differentiation of $\mathscr{L}[\tilde{f}^{[k-l]}; s]$. Let

$$Q(-s) = \prod_{j\geq 1}\left(1 - \frac{s}{2^j}\right) \quad \text{and} \quad \bar{\mathscr{L}}[\tilde{f}^{[k]}; s] = \frac{\mathscr{L}[\tilde{f}^{[k]}; s]}{Q(-s)}$$

and divide both sides of above equation by $Q(-2s)$. This yields

$$\begin{aligned}\bar{\mathscr{L}}[\tilde{f}^{[k]}; s] =& 4\bar{\mathscr{L}}[\tilde{f}^{[k]}; 2s] + 4\bar{\mathscr{L}}[\tilde{f}^{[k-1]}; 2s] + 4\sum_{l=1}^{k-1}\frac{(-1)^l}{l!}\bar{\mathscr{L}}^{(l)}[\tilde{f}^{[k-l]}; 2s] + 4\sum_{l=1}^{k-2}\frac{(-1)^l}{l!}\bar{\mathscr{L}}^{(l)}[\tilde{f}^{[k-l-1]}; 2s]\\ &+ 2\left(\frac{1}{s^{k+1}Q(-s)} - \frac{1+2s}{2^k s^{k+1}Q(-2s)}\right) - 4\sum_{l=1}^{k-1}\sum_{r=0}^{l-1}\frac{(-1)^l}{r!(l-r)!}2^{r-l}\mathscr{L}^{(r)}[\tilde{f}^{[k-l]}; 2s]h^{(l-r)}(s)\\ &- 4\sum_{l=1}^{k-2}\sum_{r=0}^{l-1}\frac{(-1)^l}{r!(l-r)!}2^{r-l}\mathscr{L}^{(r)}[\tilde{f}^{[k-l-1]}; 2s]h^{(l-r)}(s),\end{aligned}$$

where $h(s) = \frac{1}{Q(-2s)}$ and $h^{(n)}(s)$ is the n-th derivative of $h(s)$. From the bound for $1/Q(-2s)$ obtained in [FHZ10]

$$\frac{1}{Q(-2s)} = \begin{cases} \mathcal{O}(s^{-b}), & \text{as } s \to \infty;\\ \mathcal{O}(1), & \text{as } s \to 0,\end{cases}$$

where b can be arbitrarily large, we obtain the bounds

$$\bar{\mathscr{L}}[\tilde{f}^{[k]};s] = \begin{cases} \mathcal{O}(|s|^{-b}), & \text{as } s \to \infty; \\ \mathcal{O}(|s|^{-(k+1+\epsilon)}), & \text{as } s \to 0^+ \end{cases} \quad \text{and} \quad h^{(n)}(s) = \begin{cases} \mathcal{O}(|s|^{-b}), & \text{as } s \to \infty; \\ \mathcal{O}(1), & \text{as } s \to 0^+ \end{cases}$$

uniformly for s with $|\arg(s)| \leq \pi - \epsilon$. We let

$$\begin{aligned} R^{[k]}(s) = &-4\sum_{l=1}^{k-1}\sum_{r=0}^{l-1}\frac{(-1)^l}{r!(l-r)!}2^{r-l}\mathscr{L}^{(r)}[\tilde{f}^{[k-l]};2s]h^{(l-r)}(s) \\ &-4\sum_{l=1}^{k-2}\sum_{r=0}^{l-1}\frac{(-1)^l}{r!(l-r)!}2^{r-l}\mathscr{L}^{(r)}[\tilde{f}^{[k-l-1]};2s]h^{(l-r)}(s). \end{aligned}$$

Then, by Ritt's Theorem (Theorem 4.2 of [Olv74]), we derive the bounds

$$R^{[k]}(s) = \begin{cases} \mathcal{O}(|s|^{-b}), & \text{as } s \to \infty; \\ \mathcal{O}(|s|^{-(k+\epsilon)}), & \text{as } s \to 0^+ \end{cases}$$

uniformly for s with $|\arg z| \leq \pi - \epsilon$. Thus, we may apply the Mellin transform:

$$\begin{aligned} \mathscr{M}[\bar{\mathscr{L}}^{[k]};\omega] =& \frac{2^{2-\omega}}{1-2^{2-\omega}}\mathscr{M}[\bar{\mathscr{L}}^{[k-1]};\omega] + \frac{2^{2-\omega}}{1-2^{2-\omega}}\sum_{l=1}^{k-1}\frac{\prod_{i=1}^{l}(\omega-i)}{l!}\mathscr{M}[\bar{\mathscr{L}}^{[k-l]};\omega-l] \\ &+ \frac{2^{2-\omega}}{1-2^{2-\omega}}\sum_{l=1}^{k-2}\frac{\prod_{i=1}^{l}(\omega-i)}{l!}\mathscr{M}[\bar{\mathscr{L}}^{[k-l-1]};\omega-l] \\ &+ \frac{2}{1-2^{2-\omega}}\frac{Q(2^{\omega-k-1})}{Q(1)}\Gamma(k-\omega)\Gamma(\omega-k+1)(1-2^{-k}) \\ &+ \frac{2}{1-2^{2-\omega}}\frac{Q(2^{\omega-k})}{Q(1)}\Gamma(k+1-\omega)\Gamma(\omega-k)(1-2^{1-k}) + \frac{\mathscr{M}[R^{[k]};\omega]}{1-2^{2-\omega}}, \end{aligned}$$

where for convenience, we use the notation $\mathscr{M}[\bar{\mathscr{L}}^{[k]};\omega]$ for $\mathscr{M}[\bar{\mathscr{L}}[\tilde{f}^{[k]};s];\omega]$. The fundamental strip of the above expression will be the half plane $\Re(\omega) > k+1$. To apply the inverse Mellin transform, we need to figure out all the singularities of the above expression. Since the case $k = 1$ is already solved in [FHZ10] and the general case k will be determined by $1, \ldots, k-1$, we get that for $k \geq 2$ the expression can be simplified as

$$\begin{aligned} \mathscr{M}[\bar{\mathscr{L}}^{[k]};\omega] =& \frac{2^{2-\omega}}{1-2^{2-\omega}}\sum_{r=1}^{k-1}\frac{\prod_{i=1}^{r}(\omega-i)}{r!}\mathscr{M}[\bar{\mathscr{L}}^{[k-r]};\omega-r] \\ &+ \frac{1}{1-2^{2-\omega}}\frac{Q(2^{\omega-k-1})}{Q(1)}\Gamma(k-\omega)\Gamma(\omega-k+1)(2-2^{1-k}) + \bar{g}_k(\omega) \end{aligned}$$

where $\bar{g}_k(\omega)$ is the sum of all the remaining terms in the expression. From the bound we derived for $R^{[k]}(s)$ and $\bar{\mathscr{L}}[\tilde{f}^{[k]};s]$ and the properties of the Mellin transform [FGD95], we get that if α is a singularity

of $\bar{g}_k(\omega)$, then $\Re(\alpha) \leq k$. From [FHZ10], we have that

$$\mathscr{M}[\bar{\mathscr{L}}^{[1]};\omega] = \frac{G_1(\omega)}{1-2^{2-\omega}},$$

where

$$G_1(\omega) = \frac{Q(2^{\omega-2})}{Q(1)}\Gamma(\omega)\Gamma(1-\omega).$$

Plugging this into the recurrence and iterating, we get that for $k \geq 2$

$$\mathscr{M}[\bar{\mathscr{L}}^{[k]};\omega] = \frac{\prod_{i=1}^{k-1}(\omega-i)}{1-2^{k+1-\omega}}G_1(\omega-k+1)A_k(\omega) + T_k(\omega)G_1(\omega-k+1) + g_k(\omega)$$

where $g_k(\omega)$ is defined recursively by $g_1(\omega) = 0$, $g_2(\omega) = \bar{g}_2(\omega)$ and

$$g_k(\omega) = \frac{2^{2-\omega}}{1-2^{2-\omega}}\sum_{r=1}^{k-1}\frac{\prod_{i=1}^{r}(\omega-i)}{r!}g_{k-r}(\omega-r) + \bar{g}_k(\omega).$$

Again, by similar argument as above, we have that if α is a singularity of $g_k(\omega)$, then $\Re(\alpha) \leq k$. The function $A_k(\omega)$ is defined recursively as $A_1(\omega) = 1$, $A_2(\omega) = \dfrac{1}{2^{\omega-2}-1}$ and

$$A_k(\omega) = \frac{2^{2-\omega}}{1-2^{2-\omega}}\sum_{r=1}^{k-1}\frac{A_{k-r}(\omega-r)}{r!}.$$

Also, $T_k(\omega)$ is defined recursively as $T_1(\omega) = 0$, $T_2(\omega) = \frac{6}{4(1-2^{2-\omega})}$ and

$$T_k(\omega) = \frac{2^{2-\omega}}{1-2^{2-\omega}}\sum_{r=1}^{k-1}\frac{\prod_{i=1}^{k-1}(\omega-i)}{r!}T_{k-r}(\omega-r) + \frac{2(1-2^{-k})}{1-2^{2-\omega}}.$$

Note that one can easily prove that

$$A_k(k+1+\chi_m) = A_k(k+1) = \frac{1}{(k-1)!}$$

for $\chi_m = \dfrac{2i\pi m}{\log 2}$, $m \in \mathbb{Z}$ by induction. Moreover, the Laurent series of $A_k(\omega)$ at $\omega = k+1+\chi_r$ is given as

$$A_k(\omega) = \frac{1}{(k-1)!} + d_k(\omega-k-1) + \mathcal{O}((\omega-k-1)^2),$$

where $\{d_k\}_{k\geq 1}$ is a sequence which is defined recursively as $d_1 = 0$ and

$$d_k = \frac{1}{2^{k-1}-1}\sum_{r=1}^{k-1}\frac{d_{k-r}}{r!} - \frac{2^{k-1}}{2^{k-1}-1}\frac{\log 2}{(k-1)!}.$$

Because we have the explicit form of $G_1(\omega)$, we rewrite the expression as

$$\mathscr{M}[\bar{\mathscr{L}}^{[k]};\omega] = \frac{Q(2^{\omega-k-1})}{(1-2^{k+1-\omega})Q(1)}\Gamma(\omega)\Gamma(k-\omega)A_k(\omega) + g_k(\omega).$$

Finally, applying the inverse Mellin transform and collecting residues, we get that

$$\bar{\mathscr{L}}[\tilde{f}^{[k]};s] = ks^{-(k+1)}\log_2\frac{1}{s} + s^{-(k+1)}\left(c'_k + e_k + \frac{1}{\log 2}\sum_{m\in\mathbb{Z}\setminus\{0\}}\frac{G_k(\chi_m)}{(k-1)!}s^{-\chi_m}\right) + \mathcal{O}(|s|^{-k-\epsilon})$$

where $G_k(\chi_m)$ is introduced in previous section, $e_k = T_k(k+1)$ and

$$c'_k = k\left(\frac{H_k-1}{\log 2} + \frac{1}{2} - \sum_{j\geq 1}\frac{(k-1)!}{2^j-1} + \frac{(k-1)!d_k}{\log 2}\right).$$

Note that the asymptotic hold uniformly as $|s|\to 0$ with $|\arg(s)|\leq \pi-\epsilon$. Finally, we apply Proposition 1 of [FHZ10] and obtain that, as $z\to\infty$,

$$\tilde{f}^{[k]}(z) = \frac{z^k\log z}{(k-1)!} + \frac{z^k}{(k-1)!}\left(c_k + \frac{e_k}{k} + \frac{1}{\log 2}\sum_{m\in\mathbb{Z}\setminus\{0\}}\frac{G_k(\chi_m)z^{\chi_m}}{\Gamma(k+1+\chi_m)}\right) + \mathcal{O}(z^{k-1+\epsilon}).$$

2.2 Variance and Covariance of the k-th Total Path Length

Next, let us consider the variance. Here we introduce the poissonized variance and covariance as

$$\begin{aligned}\tilde{V}^{[k]}(z) =& \tilde{f}_2^{[k]}(z) - \tilde{f}^{[k]}(z)^2 - z\tilde{f}^{[k]'}(z)^2,\\ \tilde{C}^{[k_1,k_2]}(z) =& \tilde{f}_2^{[k_1,k_2]}(z) - \tilde{f}^{[k_1]}(z)\tilde{f}^{[k_2]}(z) - z\tilde{f}^{[k_1]'}(z)\tilde{f}^{[k_2]'}(z),\end{aligned}$$

where

$$\tilde{f}_2^{[k]}(z) = e^{-z}\sum_{n\geq 0}\mathbb{E}\left(P_n^{[k]2}\right)\frac{z^n}{n!} \quad\text{and}\quad \tilde{f}_2^{[k_1,k_2]}(z) = e^{-z}\sum_{n\geq 0}\mathbb{E}\left(P_n^{[k_1]}P_n^{[k_2]}\right)\frac{z^n}{n!}.$$

For detailed explanation of why we choose them this way, see [FHZ10]. Note that when $k_1 = k_2 = k$, $\tilde{V}^{[k]}(z) = \tilde{C}^{[k_1,k_2]}(z)$. Thus, we will consider only $\tilde{C}^{[k_1,k_2]}(z)$ in this section.

With the help of computer algebra systems, we get that

$$\tilde{C}^{[k_1,k_2]}(z) + \tilde{C}^{[k_1,k_2]'}(z) = 2\sum_{r_1=1}^{k_1}\sum_{r_2=1}^{k_2}\left(\frac{z}{2}\right)^{k_1+k_2-r_1-r_2}\tilde{C}^{[k_1,k_2]}\left(\frac{z}{2}\right) + \tilde{g}^{[k_1,k_2]}(z).$$

Because the exact expression of $\tilde{g}_2^{[k_1,k_2]}(z)$ is way too complicated, we do not list the whole expression here. To apply the Poisson-Laplace-Mellin method, we only need the property that $\tilde{g}_2^{[k_1,k_2]}(z) = \mathcal{O}(z^{k_1+k_2-2})$ as $z\to\infty$. Since the process of using the Poisson-Laplace-Mellin method is already shown

and the computations for the variance and covariance will be more or less the same as for the mean, we will not show the details of computation here. Note that in the previous section, we used the well-known expression of $\mathscr{M}[\bar{\mathscr{L}}[\tilde{f}^{[1]};s];\omega]$ in the recurrence. For variance and covariance, we also use the expression of $\mathscr{M}[\bar{\mathscr{L}}[\tilde{C}^{[1,1]};s];\omega]$ from [FHZ10].

Similar computation will eventually yield that

$$\tilde{C}^{[k_1,k_2]}(z) = z^{k_1+k_2-1}C_{k_1,k_2}\left(C_{kps}+\varpi_{kps}(\log_2 n)\right)+\mathcal{O}(|z|^{k_1+k_2-2+\epsilon}),$$

where $C_{k_1,k_2}=\frac{2^{2-k_1-k_2}}{Q_{k_1-1}Q_{k_2-1}}$. In particular,

$$\tilde{V}^{[k]}(z) = \frac{z^{2k-1}}{\log 2}C_{k,k}\left(C_{kps}+\varpi_{kps}(\log_2 n)\right)+\mathcal{O}(|z|^{2k-2+\epsilon})$$

as $z\to\infty$.

Remark 5 Note that from the expression of C_{k_1,k_2}, we have $C_{k_1,k_2}^2 = C_{k_1,k_1}C_{k_2,k_2}$. Thus,

$$\rho(P_n^{[k_1]},P_n^{[k_2]}) = \frac{\mathrm{Cov}(P_n^{[k_1]},P_n^{[k_2]})}{\sqrt{\mathrm{Var}(P_n^{[k_1]})\mathrm{Var}(P_n^{[k_2]})}} \overset{n\to\infty}{\longrightarrow} 1.$$

Remark 6 Since we already know that $P_n^{[1]}$ satisfies a central limit theorem [JS95], together with the result in the above remark and applying similar argument as of [FL], we obtain that

$$\left(\frac{P_n^{[1]}-\mathbb{E}(P_n^{[1]})}{\sqrt{\mathrm{Var}(P_n^{[1]})}},\ldots,\frac{P_n^{[k]}-\mathbb{E}(P_n^{[k]})}{\sqrt{\mathrm{Var}(P_n^{[k]})}}\right)\xrightarrow{d}(X,\ldots,X),$$

where X is a standard normal distributed random variable and $\xrightarrow{d}$ denotes weak convergence.

3 Total Steiner k-distance

Let $S_n^{[k]}$ be the Steiner k-distance. Then, using the same idea as for the k-th total path length, we consider four cases:

1. All k nodes are from one subtree.
$S_{B_n}^{[k]}+S_{n-B_n}^{[k]*}$.

2. The k nodes are chosen from both subtrees and the root is not chosen.
$$\sum_{l=1}^{k-1}\left(\binom{n-B_n}{k-l}P_{B_n}^{[l]}+\binom{B_n}{l}P_{n-B_n}^{[k-l]*}+2\binom{B_n}{l}\binom{n-B_n}{k-l}\right).$$

3. The root is chosen, the other $k-1$ nodes are all from one subtree.
$$P_{B_n}^{[k-1]}+P_{n-B_n}^{[k-1]*}+\binom{n-B_n}{k-1}+\binom{B_n}{k-1}.$$

4. The root is chosen, the other $k-1$ nodes are from both subtrees.
$$\sum_{l=1}^{k-2}\left(\binom{n-B_n}{k-l-1}P_{B_n}^{[l]}+\binom{B_n}{l}P_{n-B_n}^{[k-l-1]*}+2\binom{B_n}{l}\binom{n-B_n}{k-l-1}\right).$$

Note that as for the k-th total path length, here we have a system of recurrences for the Steiner k-distance. Similar to the analysis of the k-th total path length, we let $\tilde{g}^{[k]}(z)$ be the Poisson generating function of the mean of the total Steiner k-distance, $\tilde{W}^{[k_1,k_2]}(z)$ be the Poissonized covariance of the total k_1-th Steiner distance and the total k_2-th total path length and $\tilde{V}_S^{[k]}(z)$ be the variance of the k-th Steiner distance. With the help from computer algebra systems, we get the differential-functional equations

$$\begin{aligned}\tilde{g}^{[k]}(z)+\tilde{g}^{[k]'}(z)=&2\tilde{g}^{[k]}\left(\frac{z}{2}\right)+2\tilde{f}^{[k-1]}\left(\frac{z}{2}\right)+2\sum_{r=1}^{k-1}\frac{(\frac{z}{2})^r}{r!}\tilde{f}^{[k-r]}\left(\frac{z}{2}\right)\\&+2\sum_{r=1}^{k-2}\frac{(\frac{z}{2})^r}{r!}\tilde{f}^{[k-r-1]}\left(\frac{z}{2}\right)+\frac{2z^k-4(\frac{z}{2})^k}{k!}+\frac{2z^{k-1}-2(\frac{z}{2})^{k-1}}{(k-1)!},\\ \tilde{W}^{[k_1,k_2]}(z)+\tilde{W}^{[k_1,k_2]'}(z)=&2\sum_{r=1}^{k_2}\left(\frac{z}{2}\right)^{k_2-r}\tilde{W}^{[k_1,r]}\left(\frac{z}{2}\right)+2\sum_{r_1=1}^{k_1-1}\sum_{r_2=1}^{k_2}\left(\frac{z}{2}\right)^{k'-r_1-r_2}\tilde{C}^{[r_1,r_2]}\left(\frac{z}{2}\right)\\&+\tilde{h}_2^{[k_1,k_2]}(z)\end{aligned}$$

and

$$\begin{aligned}\tilde{V}_S^{[k]}(z)+\tilde{V}_S^{[k]'}(z)=&2\tilde{V}_S^{[k]}\left(\frac{z}{2}\right)+4\sum_{r=1}^{k-1}\left(\frac{z}{2}\right)^{k-r}\tilde{W}^{[k,r]}\left(\frac{z}{2}\right)+4\sum_{r=1}^{k-1}\left(\frac{z}{2}\right)^{k-r}\tilde{W}^{[k,r]}\left(\frac{z}{2}\right)\\&+2\sum_{r_1=1}^{k-1}\sum_{r_2=1}^{k-1}\left(\frac{z}{2}\right)^{2k-r_1-r_2}\tilde{C}^{[r_1,r_2]}\left(\frac{z}{2}\right)+\tilde{h}_S^{[k]}(z).\end{aligned}$$

We use $\tilde{h}_2^{[k_1,k_2]}(z)$ and $\tilde{h}_S^{[k]}(z)$ to denote the lower order terms. Because the rest of the analysis will be very similar to the one with the k-th total path length, we skip the details and list only the results

$$\begin{aligned}\mathbb{E}\left(S_n^{[k]}\right)=&\frac{n^k\log n}{(k-1)!}+\frac{n^k}{(k-1)!}\left(c_k+\frac{e_k}{k}-D^{[k]}+\frac{1}{\log 2}\sum_{r\in\mathbb{Z}\setminus\{0\}}\frac{G_k(\chi_r)n^{\chi_r}}{\Gamma(k+1+\chi_r)}\right)\\&+\mathcal{O}(n^{k-1+\epsilon}),\\ \mathrm{Cov}\left(S_n^{[k_1]},P_n^{[k_2]}\right)=&\frac{n^{k_1+k_2-1}}{\log 2}C_{k_1,k_2}\left(C_{kps}+\varpi_{kps}(\log_2 n)\right)+\mathcal{O}(n^{k_1+k_2-2}),\\ \mathrm{Var}\left(S_n^{[k]}\right)=&\frac{n^{2k-1}}{\log 2}C_{k,k}\left(C_{kps}+\varpi_{kps}(\log_2 n)\right)+\mathcal{O}(n^{2k-2}).\end{aligned}$$

Since the leading terms are exactly the same as for the k-th total path length, the same arguments as for $P_n^{[k]}$ gives us the results stated in Theorem 2.

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On Symmetry of Uniform and Preferential Attachment Graphs

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Abstract. Motivated by the problem of graph structure compression under realistic source models, we study the symmetry behavior of preferential and uniform attachment graphs. These are two dynamic models of network growth in which new nodes attach to a constant number m of existing ones according to some attachment scheme. We prove symmetry results for $m = 1$ and 2, and we conjecture that for $m \geq 3$, both models yield asymmetry with high probability. We provide new empirical evidence in terms of graph defect. We also prove that vertex defects in the uniform attachment model grow at most logarithmically with graph size, then use this to prove a weak asymmetry result for all values of m in the uniform attachment model. Finally, we introduce a natural variation of the two models that incorporates preference of new nodes for nodes of a similar age, and we show that the change introduces symmetry for all values of m.

Keywords: preferential attachment, symmetry, automorphism, random graphs

1 Introduction

Study of the asymptotic behavior of the symmetries of random graphs, originally motivated by combinatorial problems, has relatively recently found a new application in the problem of compression of graph structures. The basic problem can be formulated as follows: given a probability distribution on labeled graphs, determine an encoding of graph structures (that is, *unlabeled* graphs) so as to minimize expected description length.

[CS12] studied this problem in the setting of Erdős-Rényi graphs. They showed that, under any distribution giving equal probability to isomorphic graphs, the entropy of the induced distribution on graph structures (i.e., isomorphism classes of graphs) is less than the entropy of the original distribution by an amount proportional to the expected logarithm of the number of automorphisms. Thus the solution to the

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above problem is intimately connected with the symmetries of the random graph model under consideration.

Study of symmetries is further motivated by their connection to various measures of information contained in a graph structure. For instance, the *topological entropy* of a random graph, studied by [Ras55] and [Tru56], measures the uncertainty in the orbit class (i.e., the set of nodes having the same long-term neighborhood structure) of a node chosen uniformly at random from the node set of the graph. If the graph is asymmetric with high probability, then the topological entropy is maximized: if n is the size of the graph, then the topological entropy is, to leading order, $\log n$. In general, if the symmetries of the graph can be characterized precisely, then so can the topological entropy. Furthermore, tools developed here will allow us to study and compare topological information of nodes (i.e., by how many bits a graph view of one node differs from another).

The present paper is a first step toward the goal of extending graph structure compression results to other random graph models. In particular, many real-world graphs, such as biological and social networks, exhibit a power law degree distribution (see [Dur06]). To explain this phenomenon, [AB02] proposed the *preferential attachment* mechanism, in which a graph is built one vertex at a time, and each new vertex t attaches to a given old vertex v with probability proportional to the current degree of v. Thus, we study a variant of a preferential attachment model. The primary problem appears to be difficult, so we also study a closely related model in which attachment is uniform, in the hope that the proof techniques used there may be generalized. In both uniform and preferential attachment models, we prove that when each new vertex chooses only one previous vertex as a neighbor, there is symmetry with high probability, and when each new vertex makes two choices, there is a positive probability of symmetry. In addition, we determine the asymptotic behavior of a quantity known as the *defect* of a vertex, introduced by [KSV02], which measures the extent to which the neighborhood of the vertex contributes to asymmetry of the graph. We then use this to prove a weak asymmetry result for the uniform attachment case.

We also introduce the *sliding window* model, a dynamic model in which new vertices choose neighbors from within windows of expected size uniformly bounded above by a constant, the purpose being to exhibit a "natural" mechanism that, coupled with a quite general attachment scheme that includes preferential and uniform attachment as special cases, results in symmetry with asymptotically positive probability.

Study of the asymptotic behavior of the automorphism group of a random graph started with [ER63], wherein Erdős-Rényi graphs with constant connection probability were shown to be asymmetric with high probability, a result motivated by the combinatorial question of determining the asymptotics of the number of unlabeled graphs on n vertices for $n \to \infty$. A similar question motivated the investigation of symmetry properties of random regular graphs by [Bol82] and [KSV02]. In the latter paper, the authors precisely characterized the range for which Erdős-Rényi graphs are asymmetric by proving concentration results for random variables defined in terms of vertex defect. They then proved an asymmetry result for random regular graphs using the previous result.

For general models, symmetry and asymmetry results can be nontrivial to prove, due to the nonmonotonicity of the properties considered. Furthermore, the particular models considered here present more difficulties not seen in the Erdős-Rényi case: there is significant dependence between edge events, and graph sparseness makes derivation of concentration results difficult.

The rest of the paper is organized as follows: in Section 2, we formally state the models and the main problem; we then state the main results, along with a discussion of their significance. We also present some empirical validation of the symmetry results, as well as evidence in support of the asymmetry conjecture.

Finally, in Section 3, we give sketches of some proofs.

2 Main Results

In this section, we state the main problems, introduce the models that we consider, and formulate the main results. First, we introduce some standard graph-theoretic terminology and notation. We start with the notion of structure-preserving transformations between labeled graphs: given two graphs G_1 and G_2 with vertex sets $V(G_1)$ and $V(G_2)$, a mapping $\phi : V(G_1) \to V(G_2)$ is said to be an *isomorphism* if it is bijective and preserves edge relations; that is, for any $x, y \in V(G_1)$, there is an edge between x and y if and only if there is an edge in G_2 between $\phi(x)$ and $\phi(y)$. When such a ϕ exists, G_1 and G_2 are said to be *isomorphic*; that is, they have the same structure.

An isomorphism from the vertices of a graph G to itself is called an *automorphism* or *symmetry*. The set of automorphisms of G, together with the operation of function composition, forms a group, which is called the *automorphism group* of G, denoted by $\mathrm{Aut}(G)$. Note that the image of G under any of its symmetries is G, the same labeled graph.

We then say that G is *symmetric* if it has at least one *nontrivial symmetry* and that G is *asymmetric* if the only symmetry of G is the identity permutation. Intuitively, G is symmetric if and only if there are at least two vertices whose graph perspectives are the same; that is, their neighborhoods at any distance have the same structure.

The main problem can then be stated as follows: given a random graph process $\{G_n\}_{n\geq 1}$, characterize the behavior of its automorphism group for $n \to \infty$.

2.1 Definitions of Models

In what follows, vertices of an n-vertex graph are the elements of the set $[n] := \{1, 2, \ldots, n\}$.

A preferential attachment model is a dynamic model of network growth in which new vertices, when they choose vertices already in the graph as neighbors, have a preference for a given vertex that is proportional to its current degree, see [AB02]. Thus, nodes with high degree tend to be preferred for new connections. The following definition formalizes this. (A slightly different formalization of the Barabási–Albert model is given by [BR04].)

Definition 1 (Preferential attachment model) *A preferential attachment graph $\mathcal{P}(n, m)$ on n vertices, with parameter m, is constructed as follows: at time $t = 1$, a single vertex with name 1 and attractiveness $\mathrm{att}_1(1) = 0$ is added. For each time $1 < t \leq n$, a vertex with name t is added, and m vertices $c_{t1}, \ldots, c_{tm}$ in $[t-1]$ are chosen with replacement such that*

$$\Pr[c_{tj} = v] = \frac{\mathrm{att}_v(t-1)}{\sum_{w=1}^{t-1} \mathrm{att}_w(t-1)} = \frac{\mathrm{att}_v(t-1)}{2m(t-2)}.$$

(Here we adopt the convention that $0/0 = 1$.) An edge between t and v is added if and only if $c_{ti} = v$ for some i. For each $v \in [t-1]$, we set $\mathrm{att}_v(t) = \mathrm{att}_v(t-1) + |\{j | c_{tj} = v\}|$. Finally, we set $\mathrm{att}_t(t) = m$.

Another way to express this is to first construct a growing multigraph, where we at each step add one new vertex and m edges from it, with the other endpoints chosen at random with replacement as above; then $\mathrm{att}_v(t)$ equals the degree of v at time t. We then reduce any set of multiple edges to a single edge to obtain the simple graph $\mathcal{P}(n, m)$.

We will also consider a variation, which we call the *uniform attachment* model, with the only change being that vertex choices are now equiprobable; that is, we now fix $\mathrm{att}_v(t-1) = 1$ for all t and $v \in [t-1]$. (For $m = 1$ this yields the well-known *random recursive tree* (see [SM95]).) The rationale for studying this simpler model is that solving our symmetry problems poses many of the same challenges for both models: both, for example, generate sparse graphs, which seems to rule out an approach to proving asymmetry based on defect (discussed below); furthermore, in both models, in considering a neighborhood of a vertex, one must distinguish between incoming and outgoing vertices, which complicates other possible approaches to asymmetry proofs. On the other hand, the uniform attachment model is advantageous, in that we need not deal with the dependence resulting from the preferential attachment mechanism.

We also study another practical variant of the attachment model called the sliding window model that we define next.

Definition 2 (Sliding window model) *The sliding window model with random window size works as follows: at time* 1*, vertex* 1 *is added. At time* $t > 1$*, vertex* t *is added, and a window size* W_t*, taking values in* $\{2, \ldots, t-1\}$*, is chosen according to the distribution function* F_t*, independent of anything else. Then,* m *vertices are chosen with replacement from the set* $[t - W_t, t - 1]$ *(which we call the* window *of vertex* t*), with the distribution of each choice* c_{tj} *determined by the ratio of the attractiveness of any node in the window to the total attractiveness of the window. That is,*

$$\Pr[c_{tj} = v | W_t = w] = \frac{\mathrm{att}_v(t-1)}{\sum_{k=t-w}^{t-1} \mathrm{att}_k(t-1)}.$$

Here, $\mathrm{att}_v(x)$ *denotes the attractiveness of vertex* v *at time* x*. In the preferential attachment sliding window model,* $\mathrm{att}_v(x)$ *is given by*

$$\mathrm{att}_v(x) = m + \sum_{k=1}^{x-1} \sum_{j=1}^{m} [c_{kj} = v].$$

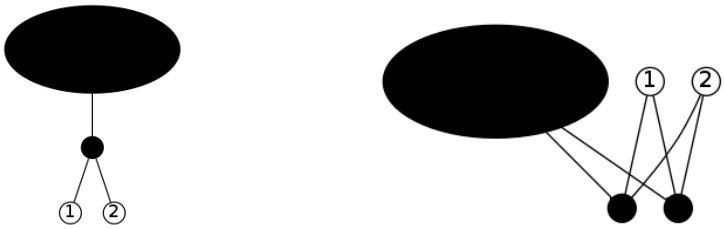
In the uniform attachment version, $\mathrm{att}_v(x) = 1$.

2.2 Statement of Results

The first result characterizes the expected vertex defect for the uniform attachment model. Vertex, permutation, and graph defect were introduced by [KSV02] in order to prove asymmetry for Erdős-Rényi graphs. The definitions are as follows.

Definition 3 (Defect) *Fix a graph* G *on* n *vertices. Given a permutation* $\pi \in S_n$ *and* $u \in [n]$*, we define the defect of* u *with respect to* π *to be* $D_\pi(u) = |N(\pi(u)) \triangle \pi(N(u))|$*, where* $N(x)$ *denotes the set of neighbors of vertex* x*, and* $\triangle$ *denotes the symmetric difference of two sets. We define the defect of* π *to be* $D_\pi(G) = \max_{u \in [n]} D_\pi(u)$*. Finally, we define the defect of* G *to be* $D(G) = \min_{\pi \neq \mathrm{ID}} D(\pi)$.

Some simple consequences of these definitions are as follows: for a graph G on n vertices and a permutation $\pi \in [n]$, π is an automorphism of G if and only if $D_\pi(G) = 0$, which is equivalent to nonexistence of a vertex $u \in [n]$ such that $D_\pi(u) \neq 0$; G has nontrivial symmetries if and only if $D(G) = 0$. Thus, vertex defect measures the extent to which a given vertex's neighborhood structure breaks the symmetry of π, permutation defect measures the number of edges adjacent to any particular vertex that



(a) (b)

Fig. 1: The shapes on which we focus for the proof of Theorem 3.

need to be modified in order to make π a symmetry of G, and graph defect measures the number of edges adjacent to any vertex that need to be modified in order to introduce a nontrivial symmetry into G.

For a nontrivial permutation $\pi \in S_n$ and any $u \in [n]$, define $\omega(\pi, u) = \min\{u, \pi(u)\}$. We also define $\omega(\pi)$ to be the minimum vertex not fixed by π (where we say that π *fixes* a vertex w if $\pi(w) = w$).

Theorem 1 (Expected defect for a vertex) *Fix $m \in \mathbb{N}$ in the uniform attachment model. For any n sufficiently large, $\pi \neq \mathrm{ID}, \pi \in S_n$, and $u \in [n]$ not fixed by π,*

$$\log\left(\frac{n}{\max\{\omega(\pi,u)+2,(2m+2)\}}\right) \leq \mathbb{E}[D_\pi(u)] \leq 1 + 4m\left(2 + \log\left(\frac{n}{\omega(\pi,u)}\right)\right).$$

This theorem is significant for two reasons: it plays a central role in the proof of Theorem 2, and it gives an indication that an approach to an asymmetry proof via defects, as used in the setting of Erdős-Rényi graphs (see [KSV02]), may not be fruitful. A key difference between the Erdős-Rényi model and the uniform and preferential attachment ones is that the expected defect in the former is $\Theta(np(1-p))$ for $p, 1-p \gg \frac{\log n}{n}$, which is essential for the proof technique used for that model to work.

The previous theorem can be used to derive a *weak asymmetry* result for the uniform attachment model as follows: for a given sequence of permutations $\pi_n \neq \mathrm{ID}$, to show that $\pi_n \notin \mathrm{Aut}(G_n)$ with high probability, it is sufficient to exhibit a sequence of vertices u_n such that $\lim_{n\to\infty} \Pr[D_{\pi_n}(u_n) = 0] = 1$. In particular, we can choose $u_n = \omega(\pi_n)$, the minimum non-fixed vertex of π_n. We prove the following result.

Theorem 2 (Probability of vertex defect being 0) *Fix $m \geq 1$ and consider a sequence of graphs in the uniform attachment model $G_n \sim \mathcal{U}(n, m)$. Let $\{\pi_n\}_{n=1}^{\infty}, \pi_n \in S_n - \{\mathrm{ID}\}$, and, for each n, let $u_n = \omega(\pi_n)$. Then*

$$\Pr[D_{\pi_n}(u_n) = 0] \xrightarrow{n\to\infty} 0,$$

so that the asymptotic probability that $\pi_n \in \mathrm{Aut}(G_n)$ is 0.

We remark that we call this a weak asymmetry result because it is a statement about which permutations are *not* in the automorphism group of G_n: any given sequence of permutations (or small sets of permutations) is asymptotically not likely to be in the automorphism group of a growing uniform attachment graph. Thus, this result has the flavor of an asymmetry result.

Observe that Theorem 2 does not prove asymmetry of a uniform attachment model. For this we would need to prove that the *graph defect* $D(G) > 0$ whp. However, we are able to make some statements about symmetry/asymmetry of this model. We discuss it next.

In the case $m = 1$, both the uniform and preferential attachment process yield trees. In such trees, we find $\Theta(n)$ leaves with high probability, so that the probability of vertex n choosing a parent of a leaf, thereby forming a pair of sibling leaves which may be swapped (which some authors have called a *cherry* as shown in Figure 1(a)), is positive. Results on random recursive trees allow this argument to be strengthened to symmetry with high probability in the uniform attachment case.

The case $m = 2$ is midway between the high-probability symmetry of the $m = 1$ case and the conjectured asymmetry of the $m \geq 3$ case. Examining the asymptotic probability of two vertices making the same choices and being unchosen by subsequent vertices yields the following results as shown in Figure 1(b).

Theorem 3 (Symmetry results for $m = 1, 2$) *Fix $m = 1, 2$, and let $G_n \sim \mathcal{U}(n, m)$ or $G_n \sim \mathcal{P}(n, m)$. Then there exists a constant $C > 0$ such that, for n sufficiently large,*

$$\Pr[|\mathrm{Aut}(G_n)| > 1] > C.$$

For both models, in the result for $m = 1$, we can strengthen the statement to symmetry with high probability (that is, the statement is true for all $C < 1$).

We conjecture that for $m = 2$, in both models, $\Pr[|\mathrm{Aut}(G_n)| > 1]$ converges to a constant strictly less than 1.

The result for $m = 2$ is particularly interesting in light of the fact that empirical investigations of the symmetries of $\mathcal{U}(n, 2)$ graphs with insufficiently many samples may lead to the incorrect conclusion that there is asymmetry with high probability in this case.

For fixed $m \geq 3$, we propose the following conjecture.

Conjecture 1 (Asymmetry conjecture) *Fix $m \geq 3$ and let $G_n \sim \mathcal{U}(n, m)$ or $G_n \sim \mathcal{P}(n, m)$. Then*

$$\Pr[|\mathrm{Aut}(G_n)| > 1] \xrightarrow{n\to\infty} 0.$$

That is, graphs drawn according to the specified distributions are asymmetric with high probability.

Empirical evidence in support of this conjecture abounds. For instance, [MA06] give plots of number of automorphisms as n increases for sampled graphs, which show initial increase and then swift decay to 1. We contribute defect-based evidence here.

Figure 2 shows growth of a graph defect estimate as n, the number of vertices of the sampled graphs, grows large, for a few values of m. As only a small subset of permutations could be sampled due to time and space constraints, the pictured defect estimates only give upper bounds on the true defects. For $m = 1$, the estimate quickly drops to 0, due to the presence of automorphisms that are swaps of two vertices, as the proof of Theorem 3 indicates. For $m = 2$, the estimate grows away from 0, but this does not give a complete picture of the situation in this case: it fails to capture the phenomenon of symmetry with asymptotically nonzero (but quite small) probability predicted by Theorem 3. For $m \geq 3$, the graph defect exhibits logarithmic growth, which is in keeping with the statement of Theorem 1. Furthermore, since the defect grows away from 0, the evidence is in keeping with the asymmetry conjecture (though the small permutation sample size prevents us from claiming it as strong evidence of the conjecture).

We also give some weak supporting evidence in the form of a theorem about probability of automorphism group membership for sequences of permutations, that of Theorem 2.

Finally, we discuss the sliding window model, that could naturally capture the behavior of dynamic networks in which new nodes are very unlikely to attach to old ones, but whose attachment policy is

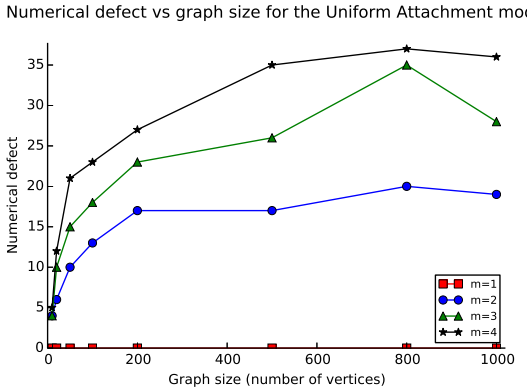


Fig. 2: Plots showing minimum/maximum vertex defects for certain classes of permutations.

otherwise quite general. (For example, one may think of a social network whose nodes are people admitted to a university and whose edges represent friendships formed after admission, and then, except with small probability, nodes will choose neighbors in a window of bounded size.) The next result deals with symmetry in the sliding window model. If windows are restricted to be of expected length less than a constant bound, then considering the event that nodes $n-1$ and n form a cherry shows that symmetry results with nonzero probability.

Theorem 4 (Symmetry results for sliding window model) *In the sliding window model with random window size, for any m, if there exists a constant w such that $\mathbb{E}[W_i] \leq w$ for all i, then the probability of symmetry is asymptotically positive. If there exists w such that, for all i, $W_i \leq w$ with probability 1, then a graph drawn according to this distribution is symmetric with high probability.*

3 Some Proofs

In this section, we fix some useful notation, then give proofs only of Theorems 1 and 3 leaving the other proofs to the full version of the paper. Given two vertices u and v, we write $E[u,v]$ for the event that there is an (undirected) edge between u and v. For vertex $u \in [n]$ and permutation π, we can write the defect $D_\pi(u)$ as:

$$D_\pi(u) = \sum_{v=1}^{n} B_{u,\pi}(v),$$

where we define $B_{u,\pi}(v)$ to be 1 if $v \in N(\pi(u)) \triangle \pi(N(u))$ and 0 otherwise. We can express each such indicator in terms of edge events:

$$B_{u,\pi}(v) = (E[v,\pi(u)] \cap \neg E[\pi^{-1}(v),u]) \cup (\neg E[v,\pi(u)] \cap E[\pi^{-1}(v),u]).$$

Note that the two conjunctions are disjoint.

3.1 Proof of Theorem 1

We now assume uniform attachment model. First, we state some useful lemmas about probabilities of edge events. We omit the simple proofs.

Lemma 1 *For all i, q, j, r such that $i < j$ and $q < r$, if $j < r$, then* $\Pr[E[i,j]] > \Pr[E[q,r]]$.

Lemma 2 *For all $i < j$,*

$$\frac{1}{j} \le \Pr[E[i,j]] \le \frac{2m}{j}.$$

Lemma 3 *For all i, q, j, r such that $i < j$, $q < r$, $r \ge 2m+1$, and either $i \ne q$ or $j \ne r$,*

$$\Pr[E[i,j] \cap \neg E[q,r]] \ge \Pr[E[i,j] \cap E[q,r]].$$

Lemma 4 *For all $x \ge 1$, $\sum_{i=1}^{x} \Pr[E[i,x]] \le 2m$.*

Lemma 5 (Harmonic Sum Log Sandwich) *For all n and $j \in \mathbb{Z}$ such that $1 \le j \le n$,*

$$\log \frac{n}{j} \le \sum_{i=j}^{n} \frac{1}{i} \le \frac{1}{j} + \log \frac{n}{j}.$$

Now we move on to the proof of the main result. Throughout, we assume that $u < \pi(u)$; the case $u > \pi(u)$ follows from this by noting that $D_{\pi^{-1}}(\pi(u)) = D_\pi(u)$. First, we derive the lower bound. We start by lower bounding the probability of event $B_{u,\pi}(i)$ by the probability of an edge. For any vertex i such that $\pi^{-1}(i) \ge 2m+1$ and $i \ne u, \pi(u)$ (so all but a constant number of them), we have

$$\begin{aligned}
\Pr[B_{u,\pi}(i)] &= \Pr[E[i,\pi(u)] \cap \neg E[\pi^{-1}(i),u]] + \Pr[\neg E[i,\pi(u)] \cap E[\pi^{-1}(i),u]] \\
&\overset{(a)}{\ge} \Pr[E[i,\pi(u)] \cap E[\pi^{-1}(i),u]] + \Pr[E[\pi^{-1}(i),u] \cap \neg E[i,\pi(u)]] \\
&= \Pr[E[\pi^{-1}(i),u]].
\end{aligned}$$

Here, (a) is a result of Lemma 3 since $\max\{\pi^{-1}(i),u\} \ge 2m+1$. Hence,

$$\begin{aligned}
\sum_{i=1}^{n} \Pr[B_{u,\pi}(i)] &\ge \sum_{\pi^{-1}(i)=\max\{\omega(\pi,u)+1,(2m+1)\}}^{n} \Pr[B_{u,\pi}(i)] \\
&\overset{(a)}{\ge} \sum_{\pi^{-1}(u)\ne\pi^{-1}(i)=\max\{\omega(\pi,u)+1,(2m+1)\}}^{n} \Pr[E[\pi^{-1}(i),u]] \\
&\overset{(b)}{\ge} \sum_{\pi^{-1}(u)\ne\pi^{-1}(i)=\max\{\omega(\pi,u)+1,(2m+1)\}}^{n} \frac{1}{\pi^{-1}(i)} \\
&\overset{(c)}{\ge} \log\left(\frac{n}{\max\{\omega(\pi,u)+2,(2m+2)\}}\right),
\end{aligned}$$

where (a) is a consequence of the previous inequality, (b) is an invocation of Lemma 2, and (c) is a result of Lemma 5 and the observation that, if $\pi^{-1}(u) \ge \max\{\omega(\pi,u)+1, 2m+1\}$, then its contribution to the sum is $\frac{1}{\pi^{-1}(u)} \le \frac{1}{\max\{\omega(\pi,u)+1,2m+1)\}}$. This completes the proof of the lower bound.

Now we prove the upper bound. We start by upper bounding the probability of $B_{u,\pi}(i)$:

$$\begin{aligned}\Pr[B_{u,\pi}(i)] &= \Pr[E[i,\pi(u)] \cap \neg E[\pi^{-1}(i),u]] + \Pr[\neg E[i,\pi(u)] \cap E[\pi^{-1}(i),u]] \\ &\overset{(a)}{\leq} \Pr[E[i,\pi(u)]] + \Pr[E[\pi^{-1}(i),u]],\end{aligned}$$

where (a) is a consequence of two applications of monotonicity of probabilities. Hence

$$\begin{aligned}\sum_{i=1}^{n} \Pr[B_{u,\pi}(i)] &\overset{(a)}{\leq} \sum_{i=1}^{n} \Pr[E[i,\pi(u)]] + \sum_{\pi^{-1}(i)=1}^{n} \Pr[E[\pi^{-1}(i),u]] \\ &\overset{(b)}{\leq} 1 + 2 \sum_{\pi^{-1}(i)=1}^{n} \Pr[E[\pi^{-1}(i),u]] \\ &\leq 1 + 2 \sum_{\pi^{-1}(i)=1}^{\omega(\pi,u)} \Pr[E[\pi^{-1}(i),u]] + 2 \sum_{\pi^{-1}(i)=\omega(\pi,u)}^{n} \Pr[E[\pi^{-1}(i),u]] \\ &\overset{(c)}{\leq} 1 + 4m + 2 \sum_{\pi^{-1}(i)=\omega(\pi,u)}^{n} \Pr[E[\pi^{-1}(i),u]],\end{aligned}$$

where (a) follows from the previous inequality, (b) from Lemma 1, and (c) from Lemma 4. The justification for (b) is slightly more complicated: it follows from the fact that,

$$\Pr[E[i,\pi(u)]] \leq \Pr[E[i,u]], \quad i \neq u,$$

which can be seen as follows: for $u \neq i < \pi(u)$, it follows from Lemma 1. If $i = \pi(u)$, then the left-hand side is 0, so the inequality holds. Finally, if $i > \pi(u) > u$, then the two probabilities are equal, due to the uniformity of the attachment process. For the case $i = u$, the inequality fails, and we instead upper bound that term by 1.

Thus, we can upper bound some more:

$$\sum_{\pi^{-1}(i)=\omega(\pi,u)}^{n} \Pr[E[\pi^{-1}(i),u]] \overset{(a)}{\leq} 2m \sum_{\pi^{-1}(i)=\omega(\pi,u)}^{n} \frac{1}{\pi^{-1}(i)} \overset{(b)}{\leq} 2m \left(1 + \log \frac{n}{\omega(\pi,u)}\right),$$

where (a) follows from Lemma 2 and (b) from Lemma 5. This completes the proof.

3.2 Proof of Theorem 3

CASE $m = 1$.

Though we are able to prove symmetry with high probability in both models, we leave it for the journal version of this paper. Here, for simplicity, we shall only prove asymptotically positive probability of symmetry. In order to do so, we examine the probability of the nth node resulting in at least one cherry after making its choice of parent. To bound this probability below, we start by conditioning on the event that, after node $n-1$ has been added and its choice is made, there are at least Cn leaves, for an appropriately chosen constant C. This happens with high probability in both the uniform and preferential attachment

model. Now, we split into three cases: there are no cherries, there is exactly one cherry, and there are at least two cherries.

In the case of no cherries, there are exactly as many parents of leaves as there are leaves, so that there are at least Cn leaf parents. In order to form a cherry, node n must choose a parent of a leaf, which happens with asymptotically positive probability: each leaf parent has degree exactly 2, so that the probability that n chooses such a node is at least

$$\frac{2Cn}{2(n-1)} \sim C$$

in the case of preferential attachment and

$$\frac{Cn}{n-1} \sim C$$

in the case of uniform attachment. In the case where there is exactly one cherry, the only way in which G_n can contain no cherries is by n choosing one of the leaves of the cherry. These leaves have total attractiveness 2 (in either model), so that the conditional probability that n destroys the cherry is at most $\frac{2}{(n-1)}$, which implies that G_n contains a cherry with conditional probability at least $1 - \frac{2}{n-1}$. In the final case, in which there are at least two cherries, the addition of node n cannot destroy more than one cherry, so that, with conditional probability 1, a cherry exists after n makes its choice. Putting everything together proves the positive probability claim.

In the uniform attachment case (i.e., for a random recursive tree), it follows from Example 3.2 of [Ald91], see also Theorem 1 of [FM10], that the number of cherries with high probability is linear in n; in particular, with high probability there is at least one cherry and thus a symmetry.

CASE $m = 2$

We will show that, with positive probability, in both models, there is at least one *diamond* (i.e., a pair of nodes that choose the same parents and that are not chosen by any subsequent nodes) as shown in Figure 1(b). The details are technically more intricate than in the $m = 1$ case, and the argument there does not work in this case, because node n must choose, from a set of size $\Theta(n^2)$ (pairs of vertices), one of $O(n)$ elements (previously chosen pairs). We thus rely on a birthday paradox-style argument to show that there is a positive probability of two vertices making the same choices, then condition on the lexicographically smallest such pair to complete the proof.

Let $A(u, v)$ be the event that vertices u and v choose the same pair of parents, and let $B(u, v)$ be the event that u and v are both unchosen. Now, define $N(k)$ to be the number of pairs u, v of vertices such that $k < u < v$ and $A(u, v)$ and $B(u, v)$ simultaneously hold. Define $N_A(k)$ and $N_B(k)$ analogously for pairs for which events A and B hold, respectively. Finally, denote by $S_{>x}$ the set $\{k \in [n] | k > x\}$. We then aim to prove that $\Pr[N(0) > 0] > C > 0$ for some constant C and n large enough. For any x, we have

$$\Pr[N(x) > 0] = \Pr[N(x) > 0 \cap N_A(x) > 0] = \Pr[N(x) > 0 | N_A(x) > 0] \cdot \Pr[N_A(x) > 0],$$

where the first equality is from the fact that $[N(x) > 0] \subseteq [N(x)_A > 0]$. The goal now is bound the remaining probabilities below by positive constants. We do this in the next two lemmas, which hold for both uniform and preferential attachment graphs. We will prove them in the uniform case, then explain the modifications needed to extend them to the preferential case.

Lemma 6 (Probability of two vertices picking the same pair) *There exists a positive constant C such that*

$$\Pr[N_A(n/2) > 0] > C$$

for all n sufficiently large.

Proof: To show this, we will instead compute $\Pr[N_A(n/2) = 0]$ and bound it above by a constant less than 1. The condition $N_A(n/2) = 0$ means that all vertices $> n/2$ choose distinct pairs. This is given by

$$\begin{aligned}\Pr[N_A(n/2) = 0] &= \prod_{k=1}^{n/2} \left(1 - \frac{k-1}{(\frac{n}{2}+k-1)^2}\right) \\ &\leq \prod_{k=1}^{n/2} \left(1 - \frac{k-1}{n^2}\right) \leq \prod_{k=n/4+1}^{n/2} \left(1 - \frac{k-1}{n^2}\right) \\ &\leq \prod_{k=n/4+1}^{n/2} \left(1 - \frac{n}{4n^2}\right) = \left(1 - \frac{(1/4)}{n}\right)^{\frac{n}{4}} \xrightarrow{n\to\infty} e^{-\frac{1}{16}} < 1.\end{aligned}$$

In the preferential attachment case, the proof is similar, except that we apply the fact that the attractiveness of any vertex $v < t$ at time t is at least $\frac{m}{2m(t-2)} = \frac{1}{2(t-2)}$. □

Lemma 7 (Conditional probability of two vertices with the same neighborhood) *There exists a positive constant C such that*

$$\Pr[N(n/2) > 0 | N_A(n/2) > 0] > C$$

for all n sufficiently large.

Proof: We condition on the lexicographically smallest pair X from $S_{>n/2}$ such that $A(X)$ holds. Let $D(u, v)$ be the event that the pair (u, v) is the smallest pair from $S_{>n/2}$ for which A holds. Then

$$\begin{aligned}\Pr[N(n/2) > 0 | N_A(n/2) > 0] &= \sum_{u<v\in S_{>n/2}} \Pr[N(n/2) > 0 | D(u,v)] \Pr[D(u,v) | N_A(n/2) > 0] \\ &\geq \sum_{u<v\in S_{>n/2}} \Pr[B(u,v) | D(u,v)] \Pr[D(u,v) | N_A(n/2) > 0] \\ &\geq C \sum_{u<v\in S_{>n/2}} \Pr[D(u,v) | N_A(n/2) > 0] = C.\end{aligned}$$

Here, the equalities are simply due to the law of total probability, and the first inequality is because the event $B(u, v)$ is a subset of the event $N(n/2) > 0$. The second inequality is by direct computation. Note first that $D(u, v)$ means that all lexicographically smaller pairs choose distinct pairs, and u and v choose

the same pair (so that v cannot choose u). So

$$\begin{aligned}\Pr[B(u,v)|D(u,v)] &= \prod_{j=u+1}^{v} \Pr[j \text{ avoids } u|D(u,v)] \prod_{j=v+1}^{n} \Pr[j \text{ avoids } v,u|D(u,v)] \\ &\geq \prod_{j=u+1}^{v-1} \left(\frac{(j-1)^2-2j-u}{(j-1)^2}\right) \cdot 1 \cdot \prod_{j=v+1}^{n} \left(\frac{(j-1)^2-4j-2u}{(j-1)^2}\right) \\ &\geq \prod_{j=u+1}^{v-1} \left(1-\frac{c}{n}\right) \prod_{j=v+1}^{n} \left(1-\frac{c}{n}\right) \geq \left(1-\frac{c}{n}\right)^n,\end{aligned}$$

where $c > 0$ is some constant. Here, the first inequality results from bounding the numerators below by giving upper bounds for the number of pairs that vertex j must avoid in order to avoid u and v and for the number of pairs that j must avoid in order to pick a pair that is distinct from the choices of all vertices x such that (x, j) is lexicographically smaller than (u, v). The 1 between the products is from the fact that v avoids u with probability 1, due to the conditioning by $D(u, v)$. The second inequality holds for all n sufficiently large, since $j > \frac{n}{2}$. The last inequality is because all factors are bounded above by 1. Finally, by taking n sufficiently large, the last value can be made arbitrarily close to e^{-c}. The proof in the preferential case is again similar, relying on the previously stated lower bound on vertex attractiveness. □

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Choices and Intervals

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Abstract. We consider a random interval splitting process, in which the splitting rule depends on the empirical distribution of interval lengths. We show that this empirical distribution converges to a limit almost surely as the number of intervals goes to infinity. We give a characterization of this limit as a solution of an ODE and use this to derive precise tail estimates. The convergence is established by showing that the size-biased empirical distribution evolves in the limit according to a certain deterministic evolution equation. Although this equation involves a non-local, non-linear operator, it can be studied thanks to a carefully chosen norm with respect to which this operator is contractive.

In finite-dimensional settings, convergence results like this usually go under the name of *stochastic approximation* and can be approached by a general method of Kushner and Clark. An important technical contribution of our work is the extension of this method to an infinite-dimensional setting.

Keywords: Stochastic approximation, interval fragmentation, empirical distribution function, Kakutani model

1 Introduction

Consider the following stochastic process on the unit circle. At its initiation, finitely many distinct points are placed on the circle in any arbitrary configuration. This configuration of points subdivides the circle into a finite number of intervals. At each time step, two points are sampled uniformly from the circle. Each of these points lands within some pair of intervals formed by the previous configuration. Add the point that falls in the larger interval to the existing configuration of points, and discard the other. If there is a tie, break it by flipping a fair coin, and continue adding points to the circle ad infinitum. We call this process the *max*-2 *process*. If instead of keeping the points that fall in the larger intervals, we keep the points that fall in the smaller intervals, we call this process the *min*-2 *process*. If we simply choose between the two points uniformly at random, then we recover standard i.i.d. sampling of points from the circle, which we call the *uniform process*.

Heuristically, the effect of having the two choices in the max-2 process should be to more evenly distribute the points around the circle than the uniform process. In effect, the points repulse each other, as short intervals will be subdivided less frequently and large intervals will be subdivided more frequently. In the min-2 process, on the other hand, points should have some tendency to clump together, so as to cause abnormally dense regions on the circle. Nevertheless, we conjecture that in all cases, the limiting distribution of points is uniform on the circle (see paragraph "Open problems" below).

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Main result

In this article, we focus on the evolution of the law of a typical interval length. We first formalize the dynamics of the process. Let $I_1^{(n)}, I_2^{(n)}, \dots, I_{n+n_0}^{(n)}$ denote the lengths of the intervals after n steps of the process (started with n_0 intervals). Define the size-biased empirical distribution function by

$$\widetilde{D}_n(x) = \sum_{i=1}^{n+n_0} I_i^{(n)} \mathbf{1}\left\{I_i^{(n)} \leq x\right\}.$$

This function is now defined to evolve according to Markovian dynamics as follows. Given $\widetilde{D}_n$, at the $(n+1)$-st step we choose an interval at random, with length $\ell_n = \widetilde{D}_n^{-1}(u)$, where u is sampled from a law on $(0,1]$ whose cumulative distribution function we denote by Ψ. This randomly chosen interval is now subdivided into two pieces at a point chosen uniformly inside the interval. This produces a new sequence of interval lengths $I_1^{(n+1)}, I_2^{(n+1)}, \dots, I_{n+n_0+1}^{(n+1)}$ and the process is repeated. We call the resulting process the Ψ-process. Note that the max-2, uniform and min-2 processes are Ψ-processes with $\Psi(u) = u^2$, u and $1-(1-u)^2$, respectively.

For $n \geq 0$, denote by μ_n the empirical distribution of the rescaled interval lengths, i.e.

$$\mu_n = \frac{1}{n+n_0} \sum_{i=1}^{n+n_0} \delta_{(n+n_0)I_i^{(n)}}.$$

Set $D_n(x) = \widetilde{D}_n(x/(n+n_0))$ for $n \geq 0$, $x \geq 0$, so that $D_n(x) = \int_0^{x+} y\, \mu_n(dy)$. Our main theorem is the following:

Theorem 1.1 *Assume that Ψ is continuous and satisfies $1-\Psi(u) \geq c(1-u)^{\kappa_\Psi}$ for some $c > 0$ and $\kappa_\Psi \in [1,\infty)$, for all $u \in (0,1)$. Then there is an absolutely continuous probability measure μ^Ψ on $(0,\infty)$ with mean 1, independent of the initial configuration, such that D_n converges pointwise to the function $F^\Psi(x) = \int_0^x y\, \mu^\Psi(dy)$, almost surely as $n \to \infty$. In particular, μ_n (weakly) converges to μ^Ψ, almost surely as $n \to \infty$. The function F^Ψ is the same as in Lemma 2.2.*

A remark on the assumptions in Theorem 1.1: we believe that continuity of Ψ is not necessary for the theorem to hold. It is probably possible to extend our proof to cover the cases of discontinuous Ψ, at the expense of greater technicalities. However, we have not worked out the details. As for the second assumption, we first remark that a necessary condition for the theorem to hold is $\Psi(x) < 1$ for all $x < 1$. Under this condition, however, the entropy bounds (see below) would fail to hold, so some more restrictive estimates are fundamental for the current proof to work. The theorem might still be true with only the above condition, although the almost sure convergence might have to be replaced by convergence in probability.

Theorem 1.1 implies in particular that the max-2 process and the min-2 process have empirical interval distributions that converge, regardless the starting configuration, to a limit after rescaling (see Figure 1). This theorem also covers the analogous max-k processes and min-k processes for natural numbers k, defined by first choosing k points and then selecting the point in the largest or smallest interval respectively.

We also study properties of the the limiting distribution $F = F^\Psi$. It is shown to be characterized by the following integro-differential equation

$$F'(x) = x \int_x^\infty \frac{1}{z}\, d\Psi(F(z)),$$

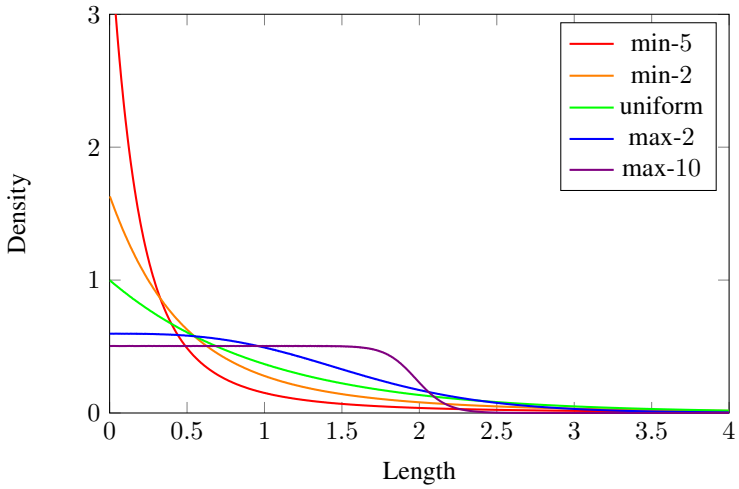

Fig. 1: Empirical density of interval lengths in simulation of max-10, max-2, uniform, min-2 and min-5 processes with 10^9 points. For the plot, the x-axis has been discretized into 1024 equally sized bins.

which allows us to derive tail estimates for many choices of Ψ. Note that $f^{\Psi}(x) = F'(x)/x$ is the density of the (non-size-biased) empirical distribution. For the max-k process, it is shown that $f^{\Psi}(x) \sim C_k e^{-kx}$ as $x \to \infty$ for some (implicit) C_k, while for the min-k process the tail satisfies $f^{\Psi}(x) \sim (c_k/(k-1))x^{-2-1/(k-1)}$ for some explicit c_k which satisfies $c_k \to 1$ as $k \to \infty$. See Propositions 3.2 and 3.4 for more precise statements. For comparison, in the uniform process, it is a a classical theorem of [Wei55] that the limiting interval distribution is the exponential distribution of parameter 1. Theorem 1.1 gives a new, complete proof of this fact. Many other precise results exist for the uniform splitting model, see for example [Dev81, Dev82, Deh82].

Additionally, this theorem should be compared to results for the *Kakutani interval splitting procedure* (see [Loo77], [vZ78] and [Slu78] for results and further background on this process; note the correction [Slu82] to the latter paper). In its simplest form, this can be described by always taking ℓ_n to be the largest interval and then subdividing this interval by a uniformly chosen point. Alternatively, it can be defined by letting $\Psi(u) = \mathbf{1}\{u \geq 1\}$ in the above definition (this case is not covered by Theorem 1.1, but the proof could be adapted). By a theorem of [Pyk80], the interval distribution of the Kakutani procedure converges to a $\mathrm{Unif}[0,2]$ variable. Indeed, we can see that the max-k process for large k resembles the Kakutani process more and more, and in fact F^{u^k} converges as $k \to \infty$ to the function $F^U(x) = x^2/4 \wedge 1$, which is the size-biased distribution function of a $\mathrm{Unif}[0,2]$ variable (see Proposition 3.5).

Methodology

We begin by embedding the discrete-time process $D_n(x)$ into a continuous time process $A_t(x)$ in such a way that $n \approx e^t$. This continuous time process A_t essentially evolves according to a stochastic evolution

equation

$$\partial_t A_t(x) = -x\partial_x A_t(x) + x^2 \int_x^\infty \frac{1}{y} d\Psi(A_t(y)) + \dot{M}_t(x) \tag{1}$$

for some centered noise $M_t(x)$. This equation is both nonlinear and nonlocal, and thus it requires very specialized analysis. First off, we transform the problem to studying an integrated form of the evolution, given by

$$A_t(x) = A_0(e^{-t}x) + \int_0^t (e^{s-t}x)^2 \left[\int_{e^{s-t}x}^\infty \frac{1}{z} d\Psi(A_s(z))\right] ds + M_t(x).$$

This allows to us to write $\boldsymbol{A} = \mathscr{S}^\Psi(\boldsymbol{A}) + \boldsymbol{M}$, with $\mathscr{S}^\Psi$ an operator acting on time-indexed distributions (here and throughout, we use boldface letters to denote function-valued processes indexed by time). Fixed points of $\mathscr{S}^\Psi$ solve the following deterministic evolution equation:

$$F_t(x) = F_0(e^{-t}x) + \int_0^t (e^{s-t}x)^2 \left[\int_{e^{s-t}x}^\infty \frac{1}{z} d\Psi(F_s(z))\right] ds. \tag{2}$$

Second, we show that (2) has strong ergodicity properties. The key to this is the following carefully selected norm,

$$\|f\|_{x^{-2}} = \int_0^\infty x^{-2}|f(x)|\, dx,$$

with respect to which the evolution operator associated to (2) quite surprisingly turns out to be a contraction (see Proposition 2.1). This assures that there is a unique distribution F^Ψ so that for any starting distribution, the large-time limit of the evolution is F^Ψ (Lemma 2.2).

Third, we show how for any Ψ satisfying the hypotheses of Theorem 1.1, we can control the entropy of the size-biased empirical interval distribution. The aim of bounding the entropy is to establish tightness of the family of distribution functions $\{A_t\}_{t\geq 0}$. One ingredient for this is an estimate for the size of the largest interval, which is shown to be smaller than $n^{-\alpha}$ for large n, for every $\alpha < (\kappa_\Psi + 1)^{-1}$ (and under more restrictive conditions on Ψ, for every $\alpha < \kappa_\Psi^{-1}$). We obtain these estimates by comparing the Ψ-process with the Kakutani process or the uniform process.

Finally, in order to show that A_t converges to F^Ψ despite the presence of noise, we adapt the Kushner–Clark method (see [KC78]), which was developed for the study of stochastic approximation algorithms. To do so, we show that the sequence of shifted evolutions $A_t^{(n)} = A_{t+n}$ is almost surely precompact in a suitable topology, using the previously established tightness of the family $\{A_t\}_{t\geq 0}$ together with an equicontinuity result. We then show that the limit points of this sequence are fixed points of the operator $\mathscr{S}^\Psi$, from which we can conclude that the unique limit is the stationary evolution $\boldsymbol{F}^* \equiv F^\Psi$. This yields almost sure convergence of the stochastic evolution $\boldsymbol{A}$.

We remark that there exists a fairly extensive literature dealing with stochastic approximation in infinite-dimensional spaces (see e.g. [Wal77, Yin92, CCZ13] and the references therein). However, the results obtained there seem to be substantially too restrictive to apply to our setting. The most serious difficulty arises from the fact that the norm $\|\cdot\|_{x^{-2}}$, which is our only tool to study convergence of the (deterministic) evolution, is very sensitive to perturbations, due to the absolute value appearing inside the integral. As a consequence, we are not able to directly control the stochastic evolution $\boldsymbol{A}$ or the noise $\boldsymbol{M}$ in terms of this norm. For this reason, our proof of Theorem 1.1 does not yield any bounds on the rate of convergence of D_n to F^Ψ, although simulations indicate that this convergence is quite fast, possibly polynomial in n (see Figure 1, in which the noise is completely invisible despite the high resolution of the data).

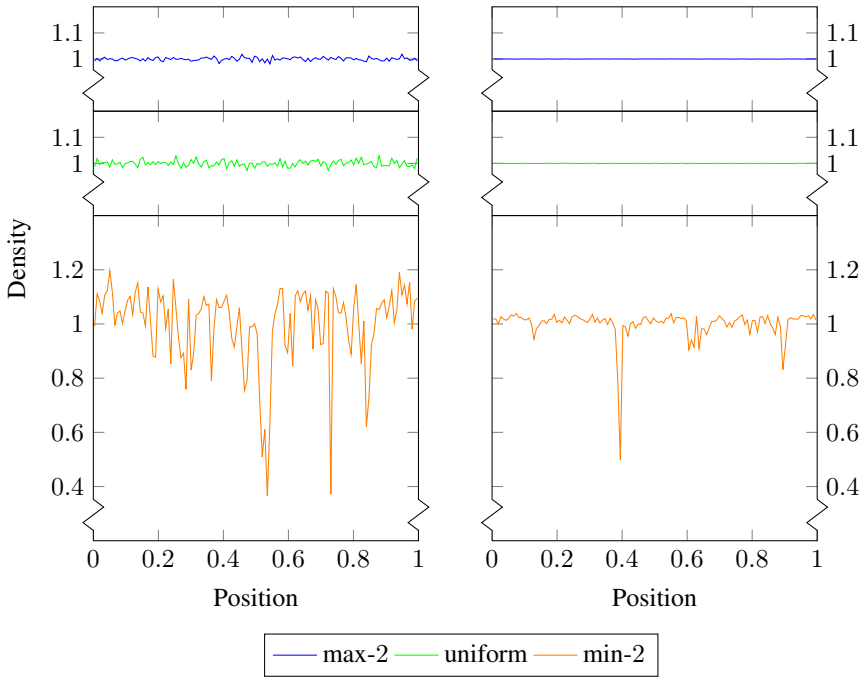

Fig. 2: Empirical density of points in the unit interval in simulation of max-2, uniform and min-2 processes with 10^6 points (left) and 10^9 points (right). For the plot, the x-axis has been discretized into 128 equally sized bins.

Discussion

The max-k choice and min-k choice models are inspired by the general paradigm known as the "power of 2 choices," which has seen considerable attention in the computer science and random graph literature (see [ABKU99, ADS09, RW12]). Suppose one throws n balls into n bins, each uniformly at random, it is a simple exercise to see the maximum load (i.e. the number of balls in the fullest bin) is about $\log n / \log \log n$. In [ABKU99], n balls are thrown into n bins, but for each ball, two bins are selected uniformly at random and the ball is placed in the bin with fewer balls. This is seen to reduce the maximal number of balls in a bin to $\log_2 \log n$, a considerable decrease from the same model without the two choices (if one instead chooses the bin with the larger load, one can easily see heuristically that the maximum load still is about $\log n / \log \log n$). Similar considerations by [MP13] show that the same conclusions hold in the min-choice case if the bins are sampled in a size-biased manner. For another model, similar in spirit, see [DKM07].

It is not clear to us whether there is a direct correspondence between the balls-and-bins model and our interval splitting process. However, in both models, the evolution of the large objects (the bins with high load/the large intervals) is simply accelerated by a factor of 2 in the max-version, whereas it is substantially slowed down in the min-version. To wit, in the uniform splitting model, the size of the largest interval is $\approx \log n/n$ (see [Dar53] and [Whi97]). In the max-2 process, the tail of the interval distribution is of order

e^{-2x}, which suggests that the size of the largest interval is $\approx \frac{1}{2}\log n/n$. In the min-2 process on the other hand, the size of the largest interval is $n^{-1/2+o(1)}$ and thus on a completely different scale, mirroring what occurs in the balls-and-bins model (without size biasing).

There are many other interval subdivision models that are related directly or indirectly to the Ψ-process. [BD87] study a model where each interval evolves independently, and an interval of length L is subdivided with rate L^α. This is exactly the uniform process in the case $\alpha = 1$, and they show that the empirical interval distribution converges to a distribution with density proportional to e^{-y^α}. This work in turns sits within the larger class of fragmentation processes, see [Ber06] for a comprehensive account. Another, fairly different, interval split-merge model arises in the study of compositions of random transpositions, see [DMWZZ04, Sch05].

Open questions

As mentioned above, Theorem 1.1 does not yield any information about the rate of convergence to the limiting interval distribution which therefore remains an open question. One could even expect a central limit theorem to hold.

The size of the largest interval in the process is a natural object to study. Here, we only have very crude estimates. One might expect that its magnitude can be deduced from the limiting interval distribution: it should be of the order of $\overline{F}^{-1}(1/n)/n$, where $\overline{F}$ is the tail of the (non-size-biased) limiting interval distribution.

Another interesting open problem is to study the spatial positions of the points in the Ψ-process. We believe that the limiting empirical distribution is always uniform (although the min-k choice process displays extremely slow convergence, see Figure 1). This is indeed the case for the above-mentioned Kakutani process ([Loo77, vZ78, Slu78]), but the methods do not carry over. One of the motivations for proving Theorem 1.1 is that it could help resolve that question. We are actively working on this problem.

The problem of the spatial positions of the points originates with a problem posed to us by I. Benjamini about a similar, albeit technically quite different problem. Once again, consider throwing pairs of points on the circle. Now, keep the point that is *farthest* from other points and discard the point which is closest. One can similarly define a process that does the reverse. The evolution of the interval distribution in this case now becomes substantially more complicated, and simulations give very strong evidence that the limiting interval distributions are different. Nevertheless, we expect that the points are almost surely equidistributed on the circle. This problem can be naturally generalized to other classes of homogeneous spaces.

Structure of this document

The remainder of this extended abstract consists of two sections. Section 2 contains the proof of the geometric ergodicity of the deterministic evolution equation, which is based on an algebraic "miracle" due to the choice of the norm $\|\cdot\|_{x^{-2}}$. Section 3 on the other hand contains statements of the results on the limiting empirical distribution in Theorem 1.1.

A full version of this article with complete proofs has been submitted elsewhere and is available on the arXiv, see [MP14].

Acknowledgements

We are grateful to Itai Benjamini, who asked us a question which motivated this research.

2 Proof of ergodicity of the deterministic evolution equation

In this section, we prove the geometric ergodicity of the deterministic evolution equation mentioned in the introduction. We consider functions from $[0,\infty)$ to the space of distribution functions satisfying the following equation for every $t \geq 0$:

$$F_t(x) = F_0(e^{-t}x) + \int_0^t (e^{s-t}x)^2 \left[\int_{e^{s-t}x}^{\infty} \frac{1}{z} d\Psi(F_{s-}(z))\right] ds. \tag{3}$$

We have the following proposition:

Proposition 2.1 *Let $\boldsymbol{F}, \boldsymbol{G}$ satisfy* (3)*. For every $t \geq 0$, we have*

$$\|F_t - G_t\|_{x^{-2}} \leq e^{-t} \|F_0 - G_0\|_{x^{-2}}.$$

The most central consequence of this proposition is that all solutions to (3) share a common large t limit.

Lemma 2.2 *Suppose there exists a solution $\boldsymbol{F} = (F_t)_{t\geq 0}$ to* (3)*, such that $\|F_0\|_{x^{-2}} = 1$. Then there is a unique distribution function F^Ψ so that for any solution $\boldsymbol{F}$ to* (3)*,*

$$\left\|F^\Psi - F_t\right\|_{x^{-2}} \leq 2e^{-t}, \quad \forall t \geq 0.$$

Furthermore, setting $\boldsymbol{F}^* \equiv F^\Psi$, then $\boldsymbol{F}^*$ solves (3)*. Finally, F^Ψ is continuous.*

In order to prove Proposition 2.1, we first define $\widetilde{F}_t(x) = F_t(e^t x)$ and $\widetilde{G}_t(x) = G_t(e^t x)$. Then $\widetilde{\boldsymbol{F}} = \widetilde{\mathscr{S}}^\Psi(\widetilde{\boldsymbol{F}})$ and $\widetilde{\boldsymbol{G}} = \widetilde{\mathscr{S}}^\Psi(\widetilde{\boldsymbol{G}})$, where the operator $\widetilde{\mathscr{S}}^\Psi$ is defined through

$$\widetilde{\mathscr{S}}^\Psi(\widetilde{\boldsymbol{F}})_t(x) = \widetilde{F}_0(x) + \int_0^t e^s x^2 \left[\int_x^{\infty} \frac{1}{z} d\Psi(\widetilde{F}_{s-}(z))\right] ds.$$

In particular, for every $x \geq 0$, the map $t \mapsto \widetilde{\mathscr{S}}^\Psi(\widetilde{\boldsymbol{F}})_t(x)$ is differentiable and its derivative is given by

$$\partial_t \widetilde{\mathscr{S}}^\Psi(\widetilde{\boldsymbol{F}})_t(x) = e^t x^2 \int_x^{\infty} \frac{1}{z} d\Psi(\widetilde{F}_{t-}(z)). \tag{4}$$

We now claim the following:

Lemma 2.3 *For every $t \geq 0$, we have*

$$\left\|\widetilde{F}_t - \widetilde{G}_t\right\|_{x^{-2}} \leq \left\|\widetilde{F}_0 - \widetilde{G}_0\right\|_{x^{-2}}.$$

Proof: It is enough to show that

$$\partial_t \left\|\widetilde{F}_t - \widetilde{G}_t\right\|_{x^{-2}} = \int_0^{\infty} x^{-2} \partial_t |\widetilde{F}_t(x) - \widetilde{G}_t(x)|\, dx \leq 0, \quad \forall t \geq 0. \tag{5}$$

We start from (4) and write for each $x \geq 0$ the dynamics for the difference $\widetilde{F}_t(x) - \widetilde{G}_t(x)$ as

$$\partial_t(\widetilde{F}_t(x) - \widetilde{G}_t(x)) = e^t x^2 I_t(x),$$

where

$$I_t(x) = \int_x^\infty \frac{\partial_z(\Psi(\widetilde{F}_t(z)) - \Psi(\widetilde{G}_t(z)))}{z}\, dz.$$

Multiply through both sides by $\operatorname{sgn}(\widetilde{F}_t - \widetilde{G}_t)$ to get

$$e^{-t}\partial_t|\widetilde{F}_t(x) - \widetilde{G}_t(x)| = x^2 \begin{cases} \operatorname{sgn}(\widetilde{F}_t(x) - \widetilde{G}_t(x))I_t(x) & \text{if } \widetilde{F}_t(x) \neq \widetilde{G}_t(x) \\ |I_t(x)| & \text{if } \widetilde{F}_t(x) = \widetilde{G}_t(x). \end{cases}$$

Apply integration by parts to the integral, so that

$$I_t(x) = -x^{-1}(\Psi(\widetilde{F}_t(x)) - \Psi(\widetilde{G}_t(x))) + \int_x^\infty \frac{(\Psi(\widetilde{F}_t(z)) - \Psi(\widetilde{G}_t(z)))}{z^2}\, dz.$$

Now note that Ψ is a non-decreasing function, so that $\widetilde{F}_t(x) - \widetilde{G}_t(x)$ and $\Psi(\widetilde{F}_t(x)) - \Psi(\widetilde{G}_t(x))$ have the same sign as long as $\Psi(\widetilde{F}_t(x)) \neq \Psi(\widetilde{G}_t(x))$. The previous two equations therefore yield

$$e^{-t}\partial_t|\widetilde{F}_t(x) - \widetilde{G}_t(x)| \leq -x|\Psi(\widetilde{F}_t(x)) - \Psi(\widetilde{G}_t(x))| + x^2 \int_x^\infty \frac{|\Psi(\widetilde{F}_t(z)) - \Psi(\widetilde{G}_t(z))|}{z^2}\, dz.$$

Multiply both sides by x^{-2} and integrate in x from 0 to infinity:

$$e^{-t}\int_0^\infty x^{-2}\partial_t|\widetilde{F}_t(x) - \widetilde{G}_t(x)|\, dx \leq -\int_0^\infty \frac{|\Psi(\widetilde{F}_t(x)) - \Psi(\widetilde{G}_t(x))|}{x}\, dx + \int_0^\infty \int_x^\infty \frac{|\Psi(\widetilde{F}_t(z)) - \Psi(\widetilde{G}_t(z))|}{z^2}\, dz\, dx.$$

The magic is that the last two integrals are actually equal. By the Fubini–Tonelli theorem,

$$\begin{aligned} \int_0^\infty \int_x^\infty \frac{|\Psi(\widetilde{F}_t(z)) - \Psi(\widetilde{G}_t(z))|}{z^2}\, dz\, dx &= \int_0^\infty \frac{|\Psi(\widetilde{F}_t(z)) - \Psi(\widetilde{G}_t(z))|}{z^2}\left[\int_0^z 1\, dx\right] dz \\ &= \int_0^\infty \frac{|\Psi(\widetilde{F}_t(z)) - \Psi(\widetilde{G}_t(z))|}{z}\, dz. \end{aligned}$$

This implies (5) which concludes the proof of the lemma. □

Proof of Proposition 2.1: Recall that we have $F_t(x) = \widetilde{F}_t(e^{-t}x)$ and $G_t(x) = \widetilde{G}_t(e^{-t}x)$ for every $t \geq 0$ and $x \geq 0$. This gives for every $t \geq 0$,

$$\|F_t - G_t\|_{x^{-2}} = \int_0^\infty x^{-2}|\widetilde{F}_t(e^{-t}x) - \widetilde{G}_t(e^{-t}x)|\, dx = e^{-t}\left\|\widetilde{F}_t - \widetilde{G}_t\right\|_{x^{-2}}.$$

The statement then follows from Lemma 2.3. □

3 Properties of limiting profile

In this section, we study properties of the distribution function $F = F^{\Psi}$ from Lemma 2.2, i.e. the distribution function of the size-biased empirical measure of interval lengths in the limit as the number of intervals goes to infinity. We have the following lemma:

Lemma 3.1 *Let $F = F^{\Psi}$ be the limiting distribution function from Lemma 2.2. Then $F \in C^1(\mathbb{R}_+, [0,1])$ and satisfies the equation*

$$F'(x) = x \int_x^{\infty} \frac{1}{z}\, d\Psi(F(z)). \tag{6}$$

If furthermore the function Ψ is continuously differentiable with derivative ψ, then $F \in C^2(\mathbb{R}_+, [0,1])$ and satisfies the following ordinary differential equation:

$$xF''(x) - F'(x) + xF'(x)\psi(F(x)) = 0. \tag{7}$$

Furthermore, these two equations have unique increasing solutions subject to the boundary conditions $F(0) = 0$ and $F(+\infty) = 1$.

In what follows, we write $F = F^{\Psi}$ to denote the distribution function from Lemma 2.2. We first study its right tail.

Proposition 3.2 *Assume that Ψ is absolutely continuous with derivative ψ satisfying $\lim_{u\to 1} \psi(u) = \psi(1) > 0$.*

1. *For every $a < \psi(1)$, we have $F'(x) \le e^{-ax}$ for large x.*
2. *If furthermore there exists $\beta > 1/\psi(1)$, such that $|\psi(1) - \psi(1-u)| \le |\log u|^{-\beta}$ for small enough u, then as $x \to \infty$,*
$$F'(x) \sim Cx \exp(-\psi(1)x),$$
for some $C > 0$.

Corollary 3.3 *In the max-k process (i.e. $\Psi(u) = u^k$), there exists $C > 0$, such that $F'(x) \sim Cx\exp(-kx)$ as $x \to \infty$.*

In contrast to the case treated in Proposition 3.2, the case $\lim_{u\to 1} \psi(u) = \psi(1) = 0$ is more delicate. Here we were only able to give a satisfying answer for the min-k process, i.e. $\psi(u) = k(1-u)^{k-1}$ for $k > 1$. In this case, we are able to transform equation (7) into the following *autonomous* differential equation by setting $F(x) = 1 - G(\log x^{1/(k-1)})/x^{1/(k-1)}$:

$$G'' - G' - (2k - 1 - k(k-1)G^{k-1})(G' - G) = 0. \tag{8}$$

This equation can then be studied by standard phase plane analysis (see e.g. [Arn92]), yielding the following result:

Proposition 3.4 *Assume $\Psi(u) = 1 - (1-u)^k$ for some $k > 1$. Then, as $x \to \infty$,*

$$1 - F(x) \sim \frac{c_k}{x^{1/(k-1)}} \text{ and } F'(x) \sim \frac{c_k}{(k-1)x^{1+1/(k-1)}},$$

where $c_k = ((2k-1)/k(k-1))^{1/(k-1)}$.

Lastly, we study the asymptotics when the measure $d\Psi$ converges weakly to δ_1 (which corresponds to the *Kakutani process* as mentioned in the introduction). Formally, the function F satisfies in this case the equation

$$xF'' - F' + xF'(x-)\delta_1(F(x)) = 0,$$

which implies that F is of the form $F(x) = Cx^2 \wedge 1$ for some $C > 0$. Since $F'(x)/x$ is the density of the interval distribution, we have with $x_0 = 1/\sqrt{C}$,

$$1 = \int_0^\infty F'(x)/x\, dx = 2Cx_0 = 2\sqrt{C} \Rightarrow C = 1/4.$$

The following proposition makes this argument rigorous and is proved by compactness methods.

Proposition 3.5 *Let $(\Psi_n)_{n\geq 0}$ be a sequence of distribution functions of measures on $(0,1]$ with $\Psi_n(x) \to 0$ for all $x \in (0,1)$. Assume that for all these Ψ_n, there are distribution functions F_n satisfying*

$$F_n(x) = \int_0^x y \int_y^\infty \frac{1}{z} d\Psi_n(F_n(z))\, dy \tag{9}$$

for all $x \geq 0$. Then $F_n(x) \to x^2/4 \wedge 1$ pointwise as $n \to \infty$.

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On variance of an additive function with respect to a generalized Ewens probability

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Abstract. An additive function defined on the symmetric group is a sum of dependent random variables when a permutation is taken according to a generalized Ewens probability. We establish an upper bound of its variance via a sum of variances of the summands. The idea of our approach goes back to a paper by A. Biró and T. Szamuely generalizing the Turán-Kubilius inequality for number-theoretic functions.

Keywords: Random permutation, cycle structure, Ewens Sampling Formula, separable statistics

1 Introduction

Let $\mathbf{S}_n$ be the symmetric group of permutations of order $n \in \mathbf{N}$. If the canonical representation of $\sigma \in \mathbf{S}_n$ into a product of independent cycles has $k_j(\sigma) \in \mathbf{N}_0 := \mathbf{N} \cup \{0\}$ cycles of length $1 \le j \le n$, then we define the so-called cycle vector $\bar{k}(\sigma) = \big(k_1(\sigma), \dots, k_n(\sigma)\big)$ satisfying a relation $\ell(\bar{k}(\sigma)) = n$ for each $\sigma \in \mathbf{S}_n$. Here and afterwards

$$\ell(\bar{s}) := 1s_1 + \cdots + ns_n,$$

where $\bar{s} = (s_1, \dots, s_n) \in {\mathbf{N}_0}^n$; moreover, always $i, j, k, l, r \in \mathbf{N}$ while $s \in \mathbf{N}_0$. Further, given a real two-dimensional array $\{h_j(s)\}$, where $1 \le j \le n$ and $s \ge 0$, such that $h_j(0) = 0$ for all $j \le n$, we define an additive function $h : \mathbf{S}_n \to \mathbf{R}$ by setting

$$h(\sigma) = \sum_{j \le n} h_j\big(k_j(\sigma)\big). \tag{1}$$

Apart from the most popular example of the number-of-cycles function $w(\sigma) = k_1(\sigma) + \cdots + k_n(\sigma)$, they appear in many algebraic and combinatorial problems. In the so-called Erdős-Turán problem they are used to approximate the logarithm of group theoretical order of $\sigma \in \mathbf{S}_n$ (see [22], [10] and the references therein). Particular additive functions appear in physical models as a part of Hamiltonians in the Bose gas theory (see, *e.g.*, [3]). Moreover, one may mention additive functions related to a permutation matrix

$$M(\sigma) := \big(m_{ij}(\sigma)\big), \quad 1 \le i, j \le n, \ \sigma \in \mathbf{S}_n.$$

Here $m_{ij}(\sigma) = 1$ if $i = \sigma(j)$ and $m_{ij}(\sigma) = 0$ otherwise. It is known (see, *e.g.*, [23]) that the characteristic polynomial is

$$Z_n(x;\sigma) := \det\big(I - xM(\sigma)\big) = \prod_{j\le n}(1-x^j)^{k_j(\sigma)}.$$

Let $\mathrm{e}^{2\pi i\varphi_j(\sigma)}$, where $\varphi_j(\sigma) \in [0,1)$ and $j \le n$, be its eigenvalues. A lot of work has been done on $\log|Z_n(x;\sigma)|$, $\Im\log Z_n(x;\sigma)$ or the trace-related mappings

$$\sum_{j\le n} f\big(\varphi_j(\sigma)\big) = \sum_{j\le n} k_j(\sigma) \sum_{0\le s\le j-1} f\Big(\frac{s}{j}\Big), \tag{2}$$

where $f : [0,1] \to \mathbf{R}$ is an arbitrary function. We just mention [1], [21], [23], and [8] to name but a few. The papers confirm a need to examine the value distribution of general additive functions (*separable statistics*, as the authors of [10] propose) as $n \to \infty$ if σ is taken at random. One can also observe the recent trend to do this with respect to a generalized Ewens probability measure endowed in $\mathbf{S}_n$ (see, *e.g.*, [4], [19], [18], [8], [6]). The measure has been introduced in 2002 [13] where some limit theorems for additive functions have been proved. Later this line of research was continued in a few of the first author's papers.

Let $\theta_j \ge 0$, $1 \le j \le n$, be an arbitrary, maybe, dependent on n, and not identical to zero sequence, then the generalized Ewens probability measure is defined by

$$\nu_n^{(\bar\theta)}(\{\sigma\}) = (n!Q(n))^{-1}\prod_{j\le n}\theta_j^{k_j(\sigma)}, \qquad Q(n) := \sum_{\ell(\bar s)=n}\prod_{j\le n}\Big(\frac{\theta_j}{j}\Big)^{s_j}\frac{1}{s_j!}, \qquad \sigma\in\mathbf{S}_n.$$

If $\theta_j \equiv \theta > 0$, some fixed constant, then $\nu_n^{(\bar\theta)} =: \nu_n^{(\theta)}$ is the classical Ewens measure on $\mathbf{S}_n$. In this case

$$Q(n) = \Theta(n) := \binom{\theta+n-1}{n}$$

and the cycle vector has a distribution

$$\nu_n^{(\theta)}(\bar k(\sigma) = \bar s) = \mathbf{1}\{\ell(\bar s) = n\}\Theta(n)^{-1}\prod_{j\le n}\frac{1}{s_j!}\Big(\frac{\theta}{j}\Big)^{s_j} = P_n(\{\bar s\}), \tag{3}$$

where $\bar s \in \Omega_n := \big\{\bar s \in {\mathbf{N}_0}^n : \ \ell(\bar s) = n\big\}$. The expression of probabilities $P_n(\{\bar s\})$ ascribed to $\bar s \in \Omega_n$ is well known as the Ewens Sampling Formula (see [9]).

Expressions of power moments of an additive function $\mathbf{E}_n^{(\bar\theta)}h(\sigma)^r$, $r > 0$, with respect to $\nu_n^{(\bar\theta)}$, except the mean value presented below in formula (11), are fairly complicated (see, for example, [2]). Upper and lower bounds can shed some light on their behaviour. In the present note, we focus on the estimates of the variance which we denote by $\mathbf{V}_n^{(\bar\theta)}h(\sigma)$. This seemingly simple problem concerns a sum of dependent random variables (r.vs); therefore, an estimate of its variance in terms of a sum of variances of the summands is not that easy if general weights θ_j, $j \le n$, are involved. Even for the Ewens measure, if $\theta_j \equiv \theta < 1$, we had not any result so far. The simpler case with $\theta \ge 1$ has been dealt with in [12]. As the corollary of Theorem 3 shows, variance estimates imply the law of large numbers (see also [12]).

Together with the total variation approximation of the distribution of the first cycle vector coordinates by independent r.vs (see [16]), they comprise an instrument allowing to estimate the error appearing by truncating sums over long cycles (see, *e..g.*, [7]).

Our first theorem is for simplicity stated for a completely additive function defined via $h_j(s) = sa_j$ with arbitrary $a_j \in \mathbf{R}$, where $j \le n$ and $s \ge 0$, and for the Ewens probability. Let $\mathbf{E}_n^{(\theta)} g(\sigma)$ and $\mathbf{V}_n^{(\theta)} g(\sigma)$ be the mean value and the variance with respect to $\nu_n^{(\theta)}$ of a r.v. $g : \mathbf{S}_n \to \mathbf{R}$ and

$$B_n^2 := B_n^2(h) := \theta \sum_{j \le n} \frac{a_j^2}{j} \frac{\Theta(n-j)}{\Theta(n)}.$$

We will establish in Section 2 that

$$R_n := \sum_{j \le n} \mathbf{V}_n^{(\theta)}\big(a_j k_j(\sigma)\big) - B_n^2 = O\big(n^{-\min\{1,\theta\}} B_n^2\big) \tag{4}$$

if $n \to \infty$. This motivates the application of B_n in the inequalities below and its use as a scaling sequence in limit theorems for $h(\sigma)$ as well. As it has been shown in [1], for a particular class of additive functions $h(\sigma)$, the relation $\mathbf{V}_n^{(\theta)} h(\sigma) \sim B_n^2(h)$ as $n \to \infty$ holds but this is not the case in general. A complete characterization of the additive functions $h(\sigma)$ satisfying the latter relation for variances seems to be an uneasy problem.

Theorem 1 *There exists an absolute constant $C > 1$ such that, for any completely additive function $h(\sigma)$, $\theta > 0$, and for any $n \ge 1$,*

$$\mathbf{V}_n^{(\theta)} h(\sigma) \le C B_n^2. \tag{5}$$

If $\theta \ge 1$, one can take $C = 2$. For large n, even smaller constants can be obtained. Indeed, if

$$\tau_n(\theta) := \sup\Big\{ \mathbf{V}_n^{(\theta)} h(\sigma) B_n(h)^{-2} : \ h \ne 0 \Big\},$$

then $\tau_n(1) = 3/2 + O(n^{-1})$ and $\tau_n(2) = 4/3 + O(n^{-1})$ (see [14] and [17]).

Problem. Find the remaining asymptotical values for $\tau_n(\theta)$ as $n \to \infty$.

To simplify B_n^2, one can apply the asymptotic formula

$$\Theta(n-j)/\Theta(n) = (1 - j/n)^{\theta-1}\Big(1 + O_T\big((n-j)^{-1}\big)\Big), \quad 1 \le j \le n-1, \tag{6}$$

following from the well known Darboux type estimate

$$\Theta(m) = [z^m](1-z)^{-\theta} = \frac{m^{\theta-1}}{\Gamma(\theta)}\left(1 + O_T\Big(\frac{1}{m}\Big)\right)$$

where $\Gamma(z)$ denotes the Euler gamma-function, $0 < \theta \le T$ and $m \ge 1$. This is implemented in the next inequality valid in a more general case. However, now the dependence on θ of the appearing constant is more involved.

Theorem 2 *For an arbitrary real additive function given in* (1) *and all* $n \ge 1$*, there exists a constant* $C(\theta) > 0$ *depending on* θ *only and such that*

$$\mathbf{V}_n^{(\theta)} h(\sigma) \le C(\theta) \sum_{jk \le n} \Big(\frac{\theta}{j}\Big)^k \frac{h_j(k)^2}{k!} \Big(1 - \frac{jk}{n+1}\Big)^{\theta-1}.$$

The variance $\mathbf{V}_n^{(\bar\theta)} h(\sigma)$ with respect to the generalized Ewens probability measure will be estimated in terms of the quantity

$$D_n^2 := D_n^2(h) := \sum_{jk \le n} \Big(\frac{\theta_j}{j}\Big)^k \frac{h_j(k)^2}{k!} \frac{Q(n-jk)}{Q(n)}.$$

By virtue of (6), Theorem 2 will follow from the next result.

Theorem 3 *Assume that* $0 < \alpha \le \theta_j \le \beta < \infty$ *for all* $j \le n$*. Then, for an arbitrary real additive function given in* (1) *and all* $n \ge 1$*, there exists a positive constant* C_1 *depending only on* α *and* β *such that*

$$\mathbf{V}_n^{(\bar\theta)} h(\sigma) \le C_1 D_n^2(h). \tag{7}$$

Corollary 1 *If the conditions of Theorem 3 are satisfied, then*

$$\nu_n^{(\bar\theta)} \Big(\big| h(\sigma) - \mathbf{E}_n^{(\bar\theta)} h(\sigma) \big| \ge u D_n(h) \Big) \le C_1 u^{-2}$$

for an arbitrary $u > 0$*.*

As it has been shown in Lemma 1 of [13], under conditions of Theorem 3, we have

$$Q(n) \asymp \exp\Big\{ \sum_{i \le n} \frac{\theta_i - 1}{i} \Big\}, \tag{8}$$

where $a \asymp b$ means that $a = O(b)$ and $b = O(a)$ with constants depending on α and β. This allows to change the ratio $Q(n-jk)/Q(n)$ in D_n^2 by other quantities.

Do the obtained inequalities give the right order of the variance? Yes, except for functions proportional to the completely additive function $L(\sigma) := \ell\big(\bar k(\sigma)\big) \equiv n$. Evidently, $\mathbf{V}_n^{(\bar\theta)} L(\sigma) = 0$ but $D_n^2(L) \ne 0$. So, the estimate

$$\mathbf{V}_n^{(\bar\theta)} h(\sigma) = \min_{\lambda \in \mathbf{R}} \mathbf{V}_n^{(\bar\theta)} \big(h(\sigma) - \lambda L(\sigma) \big) \le C_1 \min_{\lambda \in \mathbf{R}} D_n(h - \lambda L)$$

is better in the cases when the eliminating of the deterministic part is available. In particular, if $\theta = 1$, then the latter can be rewritten as

$$\mathbf{V}_n^{(1)} h(\sigma) \le C_1 \min_{\lambda \in \mathbf{R}} \sum_{jk \le n} \frac{\big(h_j(k) - \lambda jk\big)^2}{j^k k!}.$$

On the other hand, we have the following lower estimate

$$\mathbf{V}_n^{(1)} h(\sigma) \ge c \min_{\lambda \in \mathbf{R}} \sum_{jk \le n - n_0} \frac{\big(h_j(k) - \lambda jk\big)^2}{j^k k!}$$

obtained in [15]. Here $c > 0$ is a constant, $n \geq n_0$, and n_0 is a sufficiently large number. Here omitting of the summands over $n - n_0 < jk \leq n$ is essential. For example, the values like $h_1(n-1)$ never appear in any moment expression because of $\ell\big(\bar{k}(\sigma)\big) = n$ and there is no a permutation with $k_1(\sigma) = n-1$. In other words, the variance can not be a bound for a sum of such values.

The deterministic component appears for the function mentioned in (2). Let $h_\alpha(\sigma)$ count the eigenvalues of the permutation matrix $M(\sigma)$ on the arc of the unit circumference between the points 1 and $\mathrm{e}^{2\pi\alpha i}$ where $0 < \alpha < 1$ is fixed. Then (see [21])

$$h_\alpha(\sigma) = \alpha n - \sum_{j \leq n} \{\alpha j\} k_j(\sigma).$$

Here $\{u\}$ denotes the fractional part of $u \in \mathbf{R}$. Consequently,

$$\mathbf{E}_n^{(1)} h_\alpha(\sigma) = \alpha n - c_1 \log n + o(\log n)$$

and

$$\mathbf{V}_n^{(1)} h_\alpha(\sigma) = B_n^2(h_\alpha - \alpha L) + O(1) = c_2 \log n + o(\log n),$$

where

$$c_r = \lim_{n\to\infty} \frac{1}{n} \sum_{j \leq n} \{\alpha j\}^r, \quad r = 1, 2.$$

So, $c_1 = 1/2$ and $c_2 = 1/3$ for an irrational number α and $c_1 = (q-1)/2q$ and $c_2 = (q-1)(2q-1)/(6q^2)$ for a rational number $\alpha = p/q$ where p and q are co-prime natural numbers. Theorem 1 gives the exact order of growth of $\mathbf{V}_n^{(1)} h_\alpha(\sigma)$ as $n \to \infty$.

Proofs of Theorem 1 and 2 are presented in the two subsequent sections. The existing analogy between additive functions defined on natural numbers and permutations has been very helpful for us. We have gained an idea of the proof of Theorem 3 from paper [5] by A. Biró and T. Szamuely.

2 Proof of Theorem 1

We will use the following particular cases of Watterson's formula [20]:

$$\mathbf{E}_n^{(\theta)} k_j(\sigma) = \frac{\theta}{j} \frac{\Theta(n-j)}{\Theta(n)}, \quad j \leq n;$$

$$\mathbf{E}_n^{(\theta)} k_j(\sigma)\big(k_j(\sigma) - 1\big) = \frac{\theta^2}{j^2} \frac{\Theta(n-2j)}{\Theta(n)}, \quad j \leq n/2;$$

and

$$\mathbf{E}_n^{(\theta)} k_i(\sigma) k_j(\sigma) = \mathbf{1}\{i + j \leq n\} \frac{\theta^2}{ij} \frac{\Theta(n-i-j)}{\Theta(n)}, \quad i \neq j,\ i, j \leq n.$$

Now, to verify the already mentioned relation (4), we have

$$R_n = \theta^2 \sum_{j \leq n/2} \frac{a_j^2}{j^2} \left[\frac{\Theta(n-2j)}{\Theta(n)} - \frac{\Theta(n-j)^2}{\Theta(n)^2} \right] - \theta^2 \sum_{n/2 < j \leq n} \frac{a_j^2}{j^2} \frac{\Theta(n-j)^2}{\Theta(n)^2}.$$

Applying a rough form of (6), we can evaluate the last sum by

$$\frac{1}{n}\sum_{n/2<j\le n}\frac{a_j^2}{j}\frac{\Theta(n-j)}{\Theta(n)}\Big(1-\frac{j}{n+1}\Big)^{\theta-1}=O\big(n^{-\min\{1,\theta\}}B_n^2\big).$$

The same estimate holds for the partial sum in R_n over $n/4<j\le n/2$. Finally, combining $(1-x)^u=1-ux+O(x^2)$ where $0\le x\le 1/2$ and $u=\theta-1$, with the asymptotical formula (6), we obtain

$$\sum_{j\le n/4}\frac{a_j^2}{j^2}\left[\frac{\Theta(n-2j)}{\Theta(n)}-\frac{\Theta(n-j)^2}{\Theta(n)^2}\right]=O\big(n^{-1}B_n^2\big).$$

Collecting the above estimates we obtain (4).

Returning to the moments of $h(\sigma)$, we have

$$\mathbf{E}_n^{(\theta)}h(\sigma)=\theta\sum_{j\le n}\frac{a_j}{j}\frac{\Theta(n-j)}{\Theta(n)},$$

and

$$\mathbf{E}_n^{(\theta)}h(\sigma)^2=B_n^2+\theta^2\sum_{i+j\le n}\frac{a_ia_j}{ij}\frac{\Theta(n-i-j)}{\Theta(n)}.$$

Hence

$$\begin{aligned}\mathbf{V}_n^{(\theta)}h(\sigma) &= \mathbf{E}_n^{(\theta)}h(\sigma)^2-\big(\mathbf{E}_n^{(\theta)}h(\sigma)\big)^2\\ &= B_n^2-\theta^2\sum_{\substack{i,j\le n\\ i+j>n}}\frac{a_ia_j}{ij}\frac{\Theta(n-i)\Theta(n-j)}{\Theta(n)^2}\\ &\quad+\theta^2\sum_{i+j\le n}\frac{a_ia_j}{ij}\left[\frac{\Theta(n-i-j)}{\Theta(n)}-\frac{\Theta(n-i)\Theta(n-j)}{\Theta(n)^2}\right].\end{aligned}\tag{9}$$

It is worth to point out that an analysis of the maximal eigenvalues of matrices of the last two quadratic forms with respect to a_j, $j\le n$, as $n\to\infty$ yielded the above mentioned asymptotical formulas for $\tau_n(\theta)$ if $\theta=1$ or 2.

Proving upper estimates we firstly observe that it suffices to deal with $a_j\ge 0$, $j\le n$, only and later apply the result for positive and negative parts of $h(\sigma)$ separately. Secondly, we may omit the non-positive terms on the right-hand side of (9). If $\theta\ge 1$, the difference in brackets of the last sum is non-positive. So we can get rid of the last two sums in (9). This yields the desired inequality if $\theta\ge 1$ as has been also observed in [12].

Let us examine the more delicate case $\theta<1$. We now have

$$\begin{aligned}\mathbf{V}_n^{(\theta)}h(\sigma) &\le B_n^2+\theta^2\sum_{i+j\le n}\frac{a_ia_j}{ij}\left[\frac{\Theta(n-i-j)}{\Theta(n)}-\frac{\Theta(n-i)\Theta(n-j)}{\Theta(n)^2}\right]^+\\ &\le B_n^2+\theta^2\sum_{j<n}\frac{a_j^2}{j}\sum_{i\le n-j}\frac{1}{i}\left[\frac{\Theta(n-i-j)}{\Theta(n)}-\frac{\Theta(n-i)\Theta(n-j)}{\Theta(n)^2}\right]^+\end{aligned}$$

by the inequality $xy \le (x^2+y^2)/2$ for $x, y \in \mathbf{R}$. Here x^+ denotes the positive part of $x \in \mathbf{R}$. We now see that an inequality

$$\begin{aligned}\Delta(m) &:= \Big(\sum_{i\le m/2} + \sum_{m/2<i\le m}\Big)\frac{1}{i}\Big[\Theta(n)\Theta(m-i) - \Theta(n-i)\Theta(m)\Big]^+ \\ &=: \Delta_1(m) + \Delta_2(m) \le (C_2/\theta)\Theta(n)\Theta(m), \end{aligned} \tag{10}$$

where $m := n - j \ge 1$ and $C_2 > 0$ is an absolute constant, suffices to complete the proof. We have

$$\theta\Delta_2(m) \le \frac{2\theta\Theta(n)}{m}\sum_{k=0}^{m}\Theta(k) = \frac{2\theta\Theta(n)}{m}\binom{\theta+m}{m} = \frac{2(\theta+m)}{m}\Theta(n)\Theta(m) \le 4\Theta(n)\Theta(m).$$

The sum $\Delta_1(m)$ over $i \le m/2$ can be estimated by the use of asymptotic formula (6) which is valid with an absolute constant in the symbol $O(\cdot)$ if $\theta \le 1$. Indeed, applying it twice, we have

$$\begin{aligned}\Delta_1(m) &= \sum_{i\le m/2}\frac{1}{i}\Big[\Theta(n)\Theta(m-i) - \Theta(n-i)\Theta(m)\Big]^+ \\ &\le \Theta(n)\Theta(m)\sum_{i\le m/2}\frac{1}{i}\Big[\Big(1-\frac{i}{m}\Big)^{\theta-1}\Big(1+O\Big(\frac{1}{m}\Big)\Big) - \Big(1-\frac{i}{n}\Big)^{\theta-1}\Big(1+O\Big(\frac{1}{n}\Big)\Big)\Big]^+ \\ &= \Theta(n)\Theta(m)\sum_{i\le m/2}\frac{1}{i}O\Big(\frac{i}{m}\Big) \le C_3\Theta(n)\Theta(m),\end{aligned}$$

where $C_3 > 0$ is an absolute constant. In the step we have applied the inequality $(1-x)^{-u} - 1 \le 2x$ if $0 < u < 1$ and $0 \le x \le 1/2$. Adding the estimates of $\Delta_1(m)$ and $\Delta_2(m)$ we obtain (10) with $C_2 = 4 + C_3$.

Theorem 1 is proved.

3 Proof of Theorem 3

The idea is to reduce the problem to the key inequality (12) concerning only the weight which defines probability measure $\nu_n^{(\bar\theta)}$. Let

$$Q^{(j)}(n) := \sum_{\substack{\ell(\bar s)=n\\ s_j=0}}\prod_{i\le n}\Big(\frac{\theta_i}{i}\Big)^{s_i}\frac{1}{s_i!}, \qquad Q^{(i,j)}(n) := \sum_{\substack{\ell(\bar s)=n\\ s_i=s_j=0}}\prod_{r\le n}\Big(\frac{\theta_r}{r}\Big)^{s_r}\frac{1}{s_r!},$$

where $i \ne j$.

We begin with the mean value

$$\mathbf{E}_n^{(\bar\theta)}h(\sigma) = \frac{1}{Q(n)n!}\sum_{\sigma\in\mathbf{S}_n}h(\sigma)\prod_{r\le n}\theta_r^{k_r(\sigma)}.$$

There are $n!\prod_{r\le n}\left(r^{s_r}s_r!\right)^{-1}$ permutations in a class corresponding to the vector $\bar{s}\in\Omega_n$. Therefore grouping over the classes, we obtain

$$\begin{aligned}\mathbf{E}_n^{(\bar\theta)}h(\sigma) &= \frac{1}{Q(n)}\sum_{\ell(\bar{s})=n}\sum_{j\le n}h_j(s_j)\prod_{r\le n}\Big(\frac{\theta_r}{r}\Big)^{s_r}\frac{1}{s_r!}\\ &= \frac{1}{Q(n)}\sum_{jk\le n}\frac{\theta_j^k h_j(k)}{j^k k!}\sum_{\substack{\ell(\bar{s})=n-jk\\ s_j=0}}\prod_{r\le n-jk}\Big(\frac{\theta_r}{r}\Big)^{s_r}\frac{1}{s_r!}\\ &=: \sum_{jk\le n}\frac{\theta_j^k h_j(k)}{j^k k!}\frac{Q^{(j)}(n-jk)}{Q(n)}. \end{aligned}\tag{11}$$

Here we have changed the order of summation taking sums firstly over natural numbers j and $s_j =: k$ and used the property $js_j = jk \le n$.

Similarly,

$$\begin{aligned}Q(n)\mathbf{E}_n^{(\bar\theta)}h^2(\sigma) &= \sum_{\ell(\bar{s})=n}\sum_{j\le n}h_j(s_j)\sum_{i\le n}h_i(s_i)\prod_{r\le n}\Big(\frac{\theta_r}{r}\Big)^{s_r}\frac{1}{s_r!}\\ &= \sum_{jk\le n}\frac{\theta_j^k h_j^2(k)}{j^k k!}\sum_{\substack{\ell(\bar{s})=n-jk\\ s_j=0}}\prod_{r\le n-jk}\Big(\frac{\theta_r}{r}\Big)^{s_r}\frac{1}{s_r!}\\ &\quad+\sum_{\substack{jk+il\le n\\ i\ne j}}\frac{\theta_j^k\theta_i^l h_j(k)h_i(l)}{j^k k!i^l l!}\sum_{\substack{\ell(\bar{s})=n-il-jk\\ s_i=s_j=0}}\prod_{r\le n-il-jk}\Big(\frac{\theta_r}{r}\Big)^{s_r}\frac{1}{s_r!}\\ &= \sum_{jk\le n}\frac{\theta_j^k h_j^2(k)}{j^k k!}Q^{(j)}(n-jk)+\sum_{\substack{jk+il\le n\\ i\ne j}}\frac{\theta_j^k\theta_i^l h_j(k)h_i(l)}{j^k k!i^l l!}Q^{(i,j)}(n-jk-il).\end{aligned}$$

As in the proof of Theorem 1, it suffices to deal with the nonnegative $h(\sigma)$ only. Omitting a part of summands we have

$$\Big(\mathbf{E}_n^{(\bar\theta)}h(\sigma)\Big)^2 \ge \sum_{jk+il\le n}\frac{\theta_j^k h_j(k)}{j^k k!}\,\frac{Q^{(j)}(n-jk)}{Q(n)}\,\frac{\theta_i^l h_i(l)}{i^l l!}\,\frac{Q^{(i)}(n-il)}{Q(n)}.$$

Hence

$$\begin{aligned}\mathbf{V}_n^{\bar\theta}h(\sigma) &\le D_n^2+\sum_{jk+il\le n}\frac{\theta_j^k h_j(k)\theta_i^l h_i(l)}{j^k k!i^l l!}\\ &\qquad\times\Big(\frac{Q^{(i,j)}(n-il-jk)}{Q(n)}-\frac{Q^{(j)}(n-jk)Q^{(i)}(n-il)}{Q(n)^2}\Big)^+.\end{aligned}$$

By virtue of $ab \le (1/2)(a^2+b^2)$, this implies

$$\mathbf{V}_n^{\bar\theta} h(\sigma) \le D_n^2 + \sum_{jk<n} \frac{\theta_j^k h_j^2(k)}{j^k k!} \sum_{il \le n-jk} \frac{\theta_i^l}{i^l l!} \Big(\frac{Q^{(i,j)}(n-il-jk)}{Q(n)} - \frac{Q^{(j)}(n-jk)Q^{(i)}(n-il)}{Q(n)^2} \Big)^+.$$

It remains to estimate the inner sum, namely, we have to prove that

$$\sum_{il \le m} \frac{\theta_i^l}{i^l l!} \Big(Q(n)Q^{(i,j)}(m-il) - Q^{(j)}(m)Q^{(i)}(n-il) \Big)^+ \le C_4 Q(n)Q(m), \tag{12}$$

where $1 \le m := n - jk < n$ and $C_4 = C_4(\alpha,\beta) > 0$ is a constant.

It is easy to get rid of the sum over $m/2 < il \le m$ on the left-hand side. Indeed,

$$\begin{aligned} &\sum_{m/2<il\le m} \frac{\theta_i^l}{i^l l!} \Big(Q(n)Q^{(i,j)}(m-il) - Q^{(j)}(m)Q^{(i)}(n-il) \Big)^+ \\ \le\ & Q(n) \sum_{m/2<il\le m} \frac{\theta_i^l}{i^l l!} Q^{(i)}(m-il) = Q(n) \sum_{m/2<il\le m} \frac{\theta_i^l}{i^l l!} \sum_{\substack{\ell(\bar t)=m-il \\ t_i=0}} \prod_{r \le m-il} \Big(\frac{\theta_r}{r}\Big)^{t_r} \frac{1}{t_r!} \\ \le\ & Q(n)Q(m). \end{aligned}$$

In the last step, we observed that the double summation is over the vectors $\bar s$ satisfying $\ell(\bar s) = m$ and having a unique decomposition $\bar s = \bar t + l\bar e_i \in {\mathbf{N}_0}^m$ with $\bar t \perp \bar e_i$, where $\bar e_i := (0,\dots,1,\dots,0) \in {\mathbf{N}_0}^m$ with the only 1 at the ith place and $m/2 < il \le m$, while $Q(m)$ sums up the summands over all $\bar s \in {\mathbf{N}_0}^m$ satisfying the condition $\ell(\bar s) = m$.

Observe that $Q^{(i,j)}(m-il) \le Q(m-il) \asymp Q(m)$ for $il \le m/2$ by estimate (8). Consequently, if $0 < \delta < 1/2$ is an arbitrary fixed number, then

$$\begin{aligned} &\sum_{\delta m<il\le m/2} \frac{\theta_i^l}{i^l l!} \Big(Q(n)Q^{(i,j)}(m-il) - Q^{(j)}(m)Q^{(i)}(n-il) \Big)^+ \\ \le\ & C_5 Q(n)Q(m) \sum_{\delta m<il\le m/2} \frac{\theta_i^l}{i^l l!} \le C_6(\delta) Q(n)Q(m), \end{aligned}$$

where $C_5 = C_5(\alpha,\beta)$ and $C_6(\delta) = C_6(\delta,\alpha,\beta)$ are positive constants.

To estimate the remaining sum in (12) over $il \le \delta m$, we analyze the quantities involved in

$$R(i,l) := Q(n)Q^{(i,j)}(m-il) - Q^{(j)}(m)Q^{(i)}(n-il).$$

In contrast to the proof of Theorem 1, $Q(n)$ can be irregular as $n \to \infty$ if only the condition $\alpha < \theta_j < \beta$, $j \le n$, is assumed; therefore, we apply the comparative analysis of the Taylor coefficients of two power series proposed in [13]. In this way, we derive the following relations:

$$Q^{(j)}(m) = \exp\Big\{ -\frac{\theta_j}{j} \Big\} Q(m) \Big(1 + O\Big(\frac{1}{m^\varepsilon} \Big) \Big),$$

$$Q^{(i)}(n-il)=\exp\Big\{-\frac{\theta_i}{i}\Big\}Q(n)\Big(1+O\Big(\Big(\frac{il}{n}\Big)^{\varepsilon}\Big)\Big),$$

and

$$Q^{(i,j)}(m-il)=\exp\Big\{-\frac{\theta_i}{i}-\frac{\theta_j}{j}\Big\}Q(m)\Big(1+O\Big(\Big(\frac{il}{m}\Big)^{\varepsilon}\Big)\Big),$$

where $0<\varepsilon<1$ is a constant depending at most on α and β, provided that $il\le\delta m$ and δ is a sufficiently small constant depending at most on α and β. Actually, the first of the relations is a corollary of Proposition 1 in [13]. The other two have been proved in a similar way. We omit a bit lengthy details. Fixing further such a δ, we also achieve that the previous estimate with $C_6(\delta)$ depends only on α and β.

The relations imply $R(i,l)=O\big(Q(n)Q(m)(il/m)^{\varepsilon}\big)$ and further

$$\begin{aligned}\sum_{il\le\delta m}\frac{\theta_i^l}{i^l l!}R(i,l) &\le C_7Q(n)Q(m)\sum_{i\le\delta m}\Big(\frac{i}{m}\Big)^{\varepsilon}\sum_{l\ge1}\Big(\frac{\beta}{i}\Big)^{l}\frac{l^{\varepsilon}}{l!}\\ &\le C_8Q(n)Q(m)\frac{1}{m}\sum_{i\le\delta m}\Big(\frac{i}{m}\Big)^{\varepsilon-1}\\ &\le C_9Q(n)Q(m),\end{aligned}$$

where the constants C_7, C_8 and C_9 depend at most on α and β.

The obtained estimates of partial sums show that (12) holds. Theorem 3 is proved.

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Asymptotic lattice path enumeration using diagonals

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Abstract. This work considers restricted lattice path models in any dimension such that the defining step set is highly symmetric. Combining the kernel method with multivariate generating function analysis, we determine general formulas for the dominant asymptotics of counting sequences of walks restricted to the first orthant. The step sets under consideration are symmetric with respect to each axis, which is a strong condition, however the resulting formulas are very straightforward. The exponential growth of each model is given by the number of steps, while the sub-exponential growth depends only on the dimension of the underlying lattice and the number of steps moving forward in each coordinate. These expressions are derived by analyzing the singular variety of a multivariate rational function whose diagonal counts the lattice paths in question.

Keywords: Lattice path enumeration, D-finite, diagonal, analytic combinatorics in several variables

1 Introduction

Lattice path models in restricted regions, having been studied in many contexts since the nineteenth century, are currently an active area of research. The recent interest has been driven by novel applications of algebra and analysis, along with new computational techniques, and has focused on exact and asymptotic enumeration. Furthermore, there seems to be a correlation between combinatorial properties of a given model and the nature of the corresponding generating function; in particular whether it is: rational, algebraic, or transcendental D-finite[(i)], or none of these. These connections are intriguing, and not wholly understood.

The specific context of lattice paths classes which restrict walks to the positive quadrant and take only "small" steps forms a little universe which demonstrates many interesting phenomena. One key predictor of the nature of the generating function is the order of a group that is associated to each model. This group has its origins in the probabilistic study random walks (see Fayolle et al. (1999)) and can, in many cases when it is finite, be used to determine explicit expressions for generating functions as the positive part of a multivariate rational Laurent series. This group was explored in a combinatorial context by Bousquet-Mélou and Mishna (2010), and also appears to be correlated to properties of the asymptotic number of walks returning to the origin (see Bostan et al. (2014)). We give a d-dimensional analogue in this case.

[(i)] satisfies a linear differential equation with polynomial coefficients

Indeed, here we give an appropriate group for models of higher dimensions whose set of allowable directions (the defining step set) are *highly symmetric*, that is they are symmetric with respect to each axis. We then perform an asymptotic analysis of the coefficients of counting generating functions using techniques from the study of analytic combinatorics in several variables, and consequently link some of the combinatorial symmetries in a walk model to both analytic properties of the generating function and geometric properties of an associated variety.

More precisely, the lattice path models we consider are restricted as follows. For a fixed dimension d, we define a model by its step set $\mathcal{S} \subseteq \{\pm 1, 0\}^d \setminus \{\mathbf{0}\}$ and say that $\mathcal{S}$ is *symmetric about the x_k axis* if $(i_1, \ldots, i_k, \ldots, i_d) \in \mathcal{S}$ implies $(i_1, \ldots, -i_k, \ldots, i_d) \in \mathcal{S}$. We further impose a non-triviality condition: for each coordinate there is at least one step in $\mathcal{S}$ which moves in the positive direction of that coordinate (this implies that for each coordinate there is a walk in the model which moves in that coordinate).

The number of walks taking steps in $\mathcal{S}$ which are restricted to the positive orthant $\mathbb{Z}^d_{\geq 0}$ are studied by expressing the counting generating functions of such models as positive parts of multivariate rational Laurent series, which are then converted to diagonals of rational functions in $d+1$ variables. A first consequence is that all of these models have D-finite generating functions (since D-finite functions are closed under the diagonal operation, and rational functions are D-finite). This result is not particularly surprising in view of an analysis of symmetric two dimensional models by Bousquet-Mélou (2002). In fact, following her reasoning may allow for more general results on the D-finiteness of symmetric functions with larger steps in higher dimensions; we address the difficulties in dealing with larger steps in the conclusion.

After the above manipulations, these models are very well suited to the asymptotic enumeration methods for diagonals of rational functions outlined in Pemantle and Wilson (2013), in particular the cases which were developed in Pemantle and Wilson (2002) and Raichev and Wilson (2008). Following these methods, we study the singular variety of the denominator of this rational function to determine related asymptotics. The condition of having a symmetry across each axis ensures that the variety is smooth and allows us to calculate the leading asymptotic term explicitly. This is not generally the case, in our experience, and hence we focus on this particular kind of restriction.

Our main result is the following theorem, which appears as Theorem 2.

Main Theorem. Let $\mathcal{S} \subseteq \{-1, 0, 1\}^d \setminus \{\mathbf{0}\}$ be a set of unit steps in dimension d. If $\mathcal{S}$ is symmetric with respect to each axis, and $\mathcal{S}$ takes a positive step in each direction, then the number of walks of length n taking steps in $\mathcal{S}$, beginning at the origin, and never leaving the positive orthant has asymptotic expansion

$$s_n \sim \left[\left(s^{(1)} \cdots s^{(d)} \right)^{-1/2} \pi^{-d/2} |\mathcal{S}|^{d/2} \right] \cdot n^{-d/2} \cdot |\mathcal{S}|^n,$$

where $s^{(k)}$ denotes the number of steps in $\mathcal{S}$ which have k^{th} coordinate 1.

This formula is easy to compute explicitly for any given model, and for certain infinite families as well.

Example 1 *Let $\mathcal{S} = \{-1, 0, 1\}^d \setminus \{\mathbf{0}\}$, the full set of possible steps. This is symmetric across each axis. We compute that $|\mathcal{S}| = 3^d - 1$, and $s^{(j)} = 3^{d-1}$ for all j and so*

$$s_n \sim \left(\frac{(3^d - 1)^{d/2}}{3^{d(d-1)/2} \cdot \pi^{d/2}} \right) \cdot n^{-d/2} \cdot (3^d - 1)^n.$$

Example 2 *Let $e_k = (0, \ldots, 0, 1, 0, \ldots, 0)$ be the k^{th} standard basis vector in $\mathbb{R}^d$, and consider the set of steps $\mathcal{S} = \{e_1, -e_1, \ldots, e_d, -e_d\}$. Then the number of walks of length n taking steps from $\mathcal{S}$ and never leaving the positive orthant has asymptotic expansion*

$$s_n \sim \left(\frac{2d}{\pi}\right)^{d/2} n^{-d/2} (2d)^n.$$

The results are organized as follows. Section 2 illustrates to how apply the orbit sum method described in Bousquet-Mélou and Mishna (2010) to find expressions for the generating functions of walks in the positive orthant. Specifically, Equation (6) describes the generating function as the diagonal of a rational power series in multiple variables. Section 3 justifies why the work of Pemantle and Wilson (2013) is applicable, with the asymptotic results computed in Section 3.3. The reader is directed to Melczer (2014) for additional details and examples.

2 Deriving an expression for the generating function

Fix a dimension d and a highly symmetric set of steps $\mathcal{S} \subseteq \{\pm 1, 0\}^d \setminus \{\mathbf{0}\}$. Recall this means that $(i_1, \ldots, i_k, \ldots, i_d) \in \mathcal{S}$ implies $(i_1, \ldots, -i_k, \ldots, i_d) \in \mathcal{S}$. In this section we derive a functional equation for a multivariate generating function, apply the orbit sum method to derive a closed expression related to this generating function, and conclude by writing the univariate counting generating function for the number of walks as the complete diagonal of a rational function.

The following notation is used throughout: $\overline{x}_i = x_i^{-1}$; $\mathbf{x} = (x_1, \ldots, x_d)$; and $\mathbf{i} = (i_1, i_2, \ldots, i_d) \in \mathbb{Z}^d$.

2.1 A functional equation

To begin, we define the generating function:

$$F(\mathbf{x}, t) = \sum_{\mathbf{i}; n \geq 0} s_{\mathbf{i}}(n) x_1^{i_1} \cdots x_d^{i_d} t^n,$$

where $s_{\mathbf{i}}(n)$ counts the number of walks of length n taking steps from $\mathcal{S}$ which stay in the positive orthant and end at lattice point $\mathbf{i}$. Note that the series $F(\mathbf{1}, t)$ is the generating function for the total number of walks in the orthant, and we can recover the series for walks ending on the hyperplane $x_k = 0$ by setting $x_k = 0$ in the series $F(\mathbf{x}, t)$ (the variables $x_1, \ldots, x_d$ are referred to as *catalytic* variables in the literature, as they are present during the analysis and removed at the end of the 'reaction' via specialization to 1). We also define the function (known as either the *characteristic polynomial* or the *inventory* of $\mathcal{S}$) by

$$S(\mathbf{x}) = \sum_{(s_1, s_2, \ldots, s_d) \in \mathcal{S}} x_1^{s_1} \cdots x_d^{s_d} \in \mathbb{Q}\left[x_1, \overline{x}_1, \ldots, x_d, \overline{x}_d\right].$$

In many recent analyses of lattice walks, functional equations are derived by translating the following description of a walk into a generating function equation: a walk is either an empty walk, or a shorter walk followed by a single step. To ensure the condition that the walks remain in the positive orthant, we must not count walks that add a step with a negative k-th component to a walk ending on the hyperplane $x_k = 0$. To account for this, it is sufficient to subtract an appropriate multiple of F from the functional equation: $t\overline{x}_k F(x_1, \ldots, x_{k-1}, 0, x_{k+1}, \ldots, x_d, t)$, however if a given step has several negative components we must use inclusion and exclusion to prevent over compensation.

This can be made explicit. Let $\mathcal{S} \subseteq \{1, 0, -1\}^d$ define a d-dimensional lattice model restricted to the first orthant, and let $F(\mathbf{x}, t)$ be the generating function for this model, counting the number of walks of length n with marked endpoint. Let $V = \{1, \ldots, d\}$ be the set of coordinates j for which there is at least one step in $\mathcal{S}$ with -1 in the j-th coordinate (here it is the full set of indices by non-triviality). Then, by translating the combinatorial recurrence described above, we see that F satisfies the following functional equation:

$$(x_1 \cdots x_d)F(\mathbf{x}) = (x_1 \cdots x_d) + (x_1 \cdots x_d)S(\mathbf{x})F(\mathbf{x}) \\ - \sum_{V' \subseteq V} (-1)^{|V'|} \left[(x_1 \cdots x_d)S(\mathbf{x})F(\mathbf{x})\right]_{\{x_j = 0 : j \in V'\}}. \tag{1}$$

We can manipulate this into an equation of the form:

$$(x_1 \cdots x_d)\left(1 - tS(\mathbf{x})\right)F(\mathbf{x}, t) = (x_1 \cdots x_d) + \sum_{k=1}^{d} A_k(x_1, \ldots, x_{k-1}, x_{k+1} \ldots, x_d, t), \tag{2}$$

where each $A_k \in \mathbb{Q}[x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_d][[t]]$.

Example 3 *Set $\mathcal{S} = \{e_1, -e_1, \ldots, e_d, -e_d\}$. In this case $S(\mathbf{x}) = \sum_{j=1}^{d}(x_j + \overline{x}_j)$, so $(x_1 \cdots x_d)S(\mathbf{x})$ vanishes when at least two of the x_j are zero, and the generating function satisfies*

$$F(\mathbf{x}) = 1 + tS(\mathbf{x})F(\mathbf{x}) - \sum_{j=1}^{d} \overline{x}_j t F(x_1, \ldots, x_{j-1}, 0, x_{j+1} \ldots, x_d).$$

2.2 The Orbit Sum Method

The orbit sum method, when it applies, has three main steps: find a suitable group $\mathcal{G}$ of rational maps; apply the elements of the group to the functional equation and form a telescoping sum; and (ultimately) represent the generating function of a model as the positive series extraction of an explicit rational function. Bousquet-Mélou and Mishna (2010) illustrate the applicability in the case of lattice walks, and it has been adapted to several dimensions by Bousquet-Mélou et al. (2014).

1. The group $\mathcal{G}$ For any d-dimensional model, we define the group $\mathcal{G}$ of 2^d rational maps by

$$\mathcal{G} := \left\{(x_1, \ldots, x_d) \mapsto (x_1^{i_1}, \ldots, x_d^{i_d}) : (i_1, \ldots, i_d) \in \{-1, 1\}^d\right\}. \tag{3}$$

Given $\sigma \in \mathcal{G}$, we can consider σ as a map on $\mathbb{Q}[x_1, \overline{x}_1, \ldots, x_d, \overline{x}_d][[t]]$ through the group action defined by $\sigma\left(A(\mathbf{x}, t)\right) := A\left(\sigma(\mathbf{x}), t\right)$. Due to the symmetry of the step set across each axis, one can verify that $\sigma(S(\mathbf{x})) = S(\sigma(\mathbf{x})) = S(\mathbf{x})$ always holds. The fact that this group does not depend on the step set of the model – only on the dimension d – is crucial to obtaining the general results here. When d equals two, the group $\mathcal{G}$ matches the group used by Bousquet-Mélou and Mishna (2010).

2. A telescoping sum Next we apply each of the 2^d elements of $\mathcal{G}$ to Equation (2), and take a weighted sum by defining $\operatorname{sgn}(\sigma) = (-1)^r$ for $r = \#\{k : \sigma(x_k) = \overline{x}_k\}$.

Lemma 1 *Let $F(\mathbf{x}, t)$ be the generating function counting the number of walks of length n with marked endpoint. Then, as elements of the ring $\mathbb{Q}[x_1, \overline{x}_1, \ldots, x_d, \overline{x}_d][[t]]$,*

$$\sum_{\sigma \in \mathcal{G}} \operatorname{sgn}(\sigma) \cdot \sigma(x_1 \cdots x_d)\sigma(F(\mathbf{x}, t)) = \frac{\sum_{\sigma \in \mathcal{G}} \operatorname{sgn}(\sigma) \cdot \sigma(x_1 \cdots x_d)}{1 - tS(\mathbf{x})}. \tag{4}$$

Proof: For each $\sigma \in \mathcal{G}$ we have $\operatorname{sgn}(\sigma) = -\operatorname{sgn}(\sigma_k \sigma)$ and, since A_k has no x_k term,

$$\sigma(A_k(x_1, \ldots, x_{k-1}, x_{k+1} \ldots, x_d, t)) = (\sigma_k \sigma)(A_k(x_1, \ldots, x_{k-1}, x_{k+1} \ldots, x_d, t)).$$

Thus, we can apply each $\sigma \in \mathcal{G}$ to Equation (2) and sum the results, weighted by $\operatorname{sgn}(\sigma)$, to cancel all the A_k terms. Minor algebraic manipulation, along with the fact that the group elements fix $S(x_1, \ldots, x_d)$, then gives Equation (4). □

3. Positive series extraction Considering the expression $-(\overline{x}_1 x_2 \cdots x_d)F(\overline{x}_1, x_2, \ldots, x_d, t)$ in the left hand side of Equation (4) as an element of $\mathbb{Q}[x_1, \overline{x}_1, \ldots, x_d, \overline{x}_d][[t]]$, we see that each term in its expansion has a negative power of x_1. Similarly, except for the case when σ is the identity any term in $\sigma(x_1 \cdots x_d)\sigma(F(\mathbf{x}, t))$ contains a negative power of at least one variable. Let $[x_k^{\geq}]A(x_1, \ldots, x_d, t)$ denote the sum of all terms of $A(x_1, \ldots, x_d, t)$ which contain only non-negative powers of x_k; Lemma 2 then follows directly from the identity

$$\sum_{\sigma \in \mathcal{G}} \operatorname{sgn}(\sigma) \cdot \sigma(x_1 \cdots x_d) = (x_1 - \overline{x}_1) \cdots (x_d - \overline{x}_d),$$

which can be proven by induction.

Lemma 2 *Let $F(\mathbf{x}, t)$ be the generating function counting the number of walks of length n with marked endpoint. Then*

$$F(\mathbf{x}, t) = [x_1^{\geq}] \cdots [x_d^{\geq}] R(\mathbf{x}, t), \tag{5}$$

where

$$R(\mathbf{x}, t) = \frac{(x_1 - \overline{x}_1) \cdots (x_d - \overline{x}_d)}{(x_1 \cdots x_d)(1 - tS(\mathbf{x}))}.$$

Since the class of D-finite functions are closed under positive series extraction by a result of Lipshitz (1989), an immediate consequence is the following.

Corollary 1 *Under the above conditions on $\mathcal{S}$, the generating function $F(\mathbf{x}, t)$ and thus also $F(\mathbf{1}, t)$ are D-finite functions.*

2.3 The generating function as a diagonal

Given an element

$$A(\mathbf{y}, t) = \sum_{n \geq 0} \left(\sum_{i_1, \ldots, i_d} a_{i_1, \ldots, i_d, n} y_1^{i_1} \cdots y_d^{i_d} \right) t^n \in \mathbb{Q}[y_1, \overline{y}_1, \ldots, y_d, \overline{y}_d][[t]],$$

we let Δ denote the (complete) diagonal operator

$$\Delta A(\mathbf{y}, t) = \sum_{n \geq 0} a_{n,\dots,n} t^n.$$

The series extraction, combined with the evaluation can be expressed as a diagonal of rational functions.

Proposition 1 *Let $B(\mathbf{x}, t)$ be an element of $\mathbb{Q}[x_1, \overline{x}_1, \dots, x_d, \overline{x}_d][[t]]$. Then*

$$[x_1^{\geq}] \cdots [x_d^{\geq}] B(\mathbf{x}, t) \Big|_{x_1 = 1, \dots, x_d = 1} = \Delta \left(\frac{B\left(\overline{y}_1, \dots, \overline{y}_d, y_1 \cdots y_d \cdot t\right)}{(1 - y_1) \cdots (1 - y_d)} \right)$$

The proof results from direct manipulations.

We note also that in our context of lattice walk generating functions, $F\left(\overline{x}_1, \dots, \overline{x}_d, x_1 \cdots x_d \cdot t\right)$ is actually a power series in the variables $x_1, \dots, x_d, t$. Combining Lemma 2 and Proposition 1 implies that the generating function for the number of walks can be represented as $F(\mathbf{1}, t) = \Delta \left(\frac{G(\mathbf{y}, t)}{H(\mathbf{y}, t)} \right)$, where

$$\begin{aligned} \frac{G(\mathbf{y}, t)}{H(\mathbf{y}, t)} &= \frac{(1 - y_1^2) \cdots (1 - y_d^2)}{1 - t(y_1 \cdots y_d) S(\mathbf{y})} \cdot \frac{1}{(1 - y_1) \cdots (1 - y_d)} \\ &= \frac{(1 + y_1) \cdots (1 + y_d)}{1 - t(y_1 \cdots y_d) S(\mathbf{y})}. \end{aligned} \tag{6}$$

To be precise, $G(\mathbf{y}, t)$ and $H(\mathbf{y}, t)$ are defined as the numerator and denominator of Equation (6).

Example 4 *For the walks defined by $\mathcal{S} = \{e_1, -e_1, \dots, e_d, -e_d\}$, we have*

$$\frac{G(\mathbf{y}, t)}{H(\mathbf{y}, t)} = \frac{(1 + y_1) \cdots (1 + y_d)}{1 - t \sum_{k=1}^{n} (1 + y_k^2)(y_1 \cdots y_{k-1} y_{k+1} \cdots y_d)}.$$

Note that this rational function is not unique, in the sense that there are other rational functions whose diagonals yield the same counting sequence.

2.4 The singular variety associated to the kernel

Here, we pause to note that the *combinatorial* symmetries of the step sets that we consider affect the *geometry* of the variety of $H(\mathbf{y}, t)$ – called the *singular variety*. This has a direct impact on both the asymptotics of the counting sequence under consideration and the ease with which its asymptotics are computed. In particular, any factors of the form $(1 - y_k)$ present in the denominator of this rational function before simplification would have made the singular variety non-smooth. Although non-smooth varieties can be handled in many cases – see Pemantle and Wilson (2013) – having a smooth singular variety is the easiest situation in which one can work in the multivariate setting. Understanding the interplay between the step set symmetry and the singular variety geometry, and in the process dealing with the non-smooth cases, is promising future work.

3 Analytic combinatorics in several variables

Following the work of Pemantle and Wilson (2002) and Raichev and Wilson (2008), we can determine the dominant asymptotics for the diagonal of the multivariate power series $\frac{G(\mathbf{y},t)}{H(\mathbf{y},t)}$ by studying the variety (complex set of zeroes) $\mathcal{V} \subseteq \mathbb{C}^{d+1}$ of the denominator

$$H(\mathbf{y},t) = 1 - t \cdot (y_1 \cdots y_d) S(\mathbf{y}).$$

In this situation, a particular set of singular points – called the *critical points* – which could affect the asymptotics of $\Delta(G/H)$ are first computed in Section 3.1. The set of critical points is then refined to those which determine the dominant asymptotics up to an exponential decay in Section 3.2; this refined set is called the set of *minimal points* as they are the critical points which are 'closest' to the origin in a sense made precise below. The enumerative results come from calculating a Cauchy residue type integral, and after determining the minimal points we find determine asymptotics in Section 3.3 using pre-computed formulas for such integrals which can be found in Pemantle and Wilson (2013).

To begin, we verify our claim in the previous section that the variety is smooth (that is, at every point on $\mathcal{V}$ one of the partial derivatives H_{y_k} or H_t does not vanish). Indeed, any non-smooth point on $\mathcal{V}$ would have to satisfy both

$$\begin{aligned} 1 - t(y_1 \cdots y_d) S(\mathbf{y}) &= H = 0 \\ \text{and} \quad -(y_1 \cdots y_d) S(\mathbf{y}) &= H_t = 0, \end{aligned}$$

which can never occur. Equivalently, this shows that at each point in $\mathcal{V}$ there exists a neighbourhood $N \subseteq \mathbb{C}^{d+1}$ such that $\mathcal{V} \cap N$ is a complex submanifold of N.

3.1 Critical points

The next step is to determine the critical points. For a smooth variety, the critical points are those which satisfy the following *critical point equations*:

$$H = 0, \quad tH_t = y_1 H_{y_1}, \quad tH_t = y_2 H_{y_2}, \quad \ldots \quad tH_t = y_d H_{y_d}.$$

That these are all the critical points is justified by Morse Theory laid out in the theory. Given $\mathbf{y} = (y_1, \ldots, y_d) \in \mathbb{C}^d$, we define $\mathbf{y}_{\overline{k}} := (y_1, \ldots, y_{k-1}, y_{k+1}, \ldots, y_d) \in \mathbb{C}^{d-1}$. As each step in $\mathcal{S}$ has coordinates taking values in $\{-1, 0, 1\}$, we may collect the coefficients of the k^{th} variable, and use the symmetries present to write

$$S(\mathbf{y}) = (\overline{y}_k + y_k) S_1^{(k)}(\mathbf{y}_{\overline{k}}) + S_0^{(k)}(\mathbf{y}_{\overline{k}}), \tag{7}$$

which uniquely defines the Laurent polynomials $S_1^{(k)}(\mathbf{y}_{\overline{k}})$ and $S_0^{(k)}(\mathbf{y}_{\overline{k}})$. With this notation the equation $tH_t = y_k H_{y_k}$ becomes

$$t(y_1 \cdots y_d) S(\mathbf{y}) = t(y_1 \cdots y_d) S(\mathbf{y}) + t(y_1 \cdots y_d)(y_k S_{y_k}(\mathbf{y})),$$

which implies

$$0 = t(y_1 \cdots y_d) \cdot y_k S_{y_k}(\mathbf{y}) = t\left(y_k^2 - 1\right)(y_1 \cdots y_{k-1} y_{k+1} \cdots y_d) S_1^{(k)}(\mathbf{y}_{\overline{k}}). \tag{8}$$

Note that while $(y_1 \cdots y_{k-1} y_{k+1} \cdots y_d) S_1^{(k)}$ is a polynomial, $S_1^{(k)}(\mathbf{y}_{\overline{k}})$ itself is a Laurent polynomial, so one must be careful when specializing variables to 0 in the expression. This calculation characterizes the critical points of $\mathcal{V}$.

Proposition 2 *The point $(\mathbf{z}, t) = (z_1, \ldots, z_d, t) \in \mathcal{V}$ is a critical point of $\mathcal{V}$ if and only if for each $1 \leq k \leq d$ either:*

1. *$z_k = \pm 1$ or,*
2. *the polynomial $(y_1 \cdots y_{k-1} y_{k+1} \cdots y_d) S_1^{(k)}(\mathbf{y}_{\overline{k}})$ has a root at $\mathbf{z}$.*

Proof: We have shown above that the critical point equations reduce to Equation (8). Furthermore, if t were zero at a point on $\mathcal{V}$ then $0 = H(z_1, \ldots, z_n, 0) = 1$, a contradiction. □

3.2 Minimal points

Among the critical points, only those which are 'closest' to the origin will contribute to the asymptotics, up to an exponentially decaying error. This is analogous to the single variable case, where the singularities of minimum modulus are those which contribute to the dominant asymptotic term. To be precise, for any point $(\mathbf{z}, t) \in \mathbb{C}^{d+1}$ we define the torus

$$T(\mathbf{z}, t) := \{(\mathbf{w}, t') \in \mathbb{C}^{d+1} : |t'| \leq |t| \text{ and } |w_j| \leq |z_j| \text{ for } j = 1, \ldots, d\}.$$

The critical point $(\mathbf{z}, t)$ is called *strictly minimal* if $T(\mathbf{z}, t) \cap \mathcal{V} = \{(\mathbf{z}, t)\}$, and *finitely minimal* if the intersection contains only a finite number of points, all of which are on the boundary of $T(\mathbf{z}, t)$. Finally, we call a critical point *isolated* if there exists a neighbourhood of $\mathbb{C}^{d+1}$ where it is the only critical point. In our case, we need only be concerned with isolated finitely minimal points.

Proposition 3 *The point $\boldsymbol{\rho} = (\mathbf{1}, 1/|\mathcal{S}|)$ is a finitely minimal point of the variety $\mathcal{V}$. Furthermore, any point in $T(\boldsymbol{\rho}) \cap \mathcal{V}$ is an isolated critical point.*

Proof: The point $\boldsymbol{\rho}$ is critical as it lies on $\mathcal{V}$ and its first d coordinates are all one. Suppose $(\mathbf{w}, t_{\mathbf{w}})$ lies in $\mathcal{V} \cap T(\boldsymbol{\rho})$, where we note that any choice of $\mathbf{w}$ uniquely determines $t_{\mathbf{w}}$ on $\mathcal{V}$. Then, as $t_{\mathbf{w}} \neq 0$,

$$\left| \sum_{(i_1, \ldots, i_d) \in \mathcal{S}} w_1^{i_1+1} \cdots w_d^{i_d+1} \right| = \left| (w_1 \cdots w_d) S(\mathbf{w}) \right| = \left| \frac{1}{t_{\mathbf{w}}} \right| \geq |\mathcal{S}|.$$

But $(\mathbf{w}, t_{\mathbf{w}}) \in T(\boldsymbol{\rho})$ implies $|w_j| \leq 1$ for each $1 \leq j \leq d$. Thus, the above inequality states that the sum of $|\mathcal{S}|$ complex numbers of modulus at most one has modulus $|\mathcal{S}|$. The only way this can occur is if each term in the sum has modulus one, and all terms point in the same direction in the complex plane. By symmetry, and the assumption that we take a positive step in each direction, there are two terms of the form $w_2^{i_2+1} \cdots w_d^{i_d+1}$ and $w_1^2 w_2^{i_2+1} \cdots w_d^{i_d+1}$ in the sum, so that w_1^2 must be 1 in order for them to point in the same direction. This shows $w_1 = \pm 1$, and the same argument applies to each w_k, so there are at most 2^d points in $\mathcal{V} \cap T(\boldsymbol{\rho})$.

By Proposition 2 every such point $(\mathbf{w}, t_{\mathbf{w}}) \in \mathcal{V} \cap T(\boldsymbol{\rho})$ is critical, and to show it is isolated it is sufficient to prove $S_1^{(k)}(\mathbf{w}_{\overline{k}}) \neq 0$ for all $1 \leq k \leq d$. Indeed, if $S_1^{(k)}(\mathbf{w}_{\overline{k}}) = 0$ then $\mathbf{w} \in \mathcal{V}$ implies

$$|t_{\mathbf{w}}| = \frac{1}{\left| w_1 \cdots w_d S_0^{(k)}(\mathbf{w}_{\overline{k}}) \right|} \geq \frac{1}{\left| S_0^{(k)}(\mathbf{w}_{\overline{k}}) \right|} \geq \frac{1}{S_0^{(k)}(\mathbf{1})} > \frac{1}{|\mathcal{S}|},$$

by our assumption that $\mathcal{S}$ contains a step which moves forward in the k^{th} coordinate. This contradicts $(\mathbf{w}, t_{\mathbf{w}}) \in T(\boldsymbol{\rho})$. □

3.3 Asymptotics Results

To apply the formulas of Pemantle and Wilson (2002) we need to define a few quantities. On all of $\mathcal{V}$ we may parametrize the coordinate t as

$$t(\mathbf{y}) = \frac{1}{y_1 \cdots y_d S(\mathbf{y})}.$$

For each point $(\mathbf{w}, t_{\mathbf{w}}) \in \mathcal{V} \cap T(\boldsymbol{\rho})$, the analysis of Pemantle and Wilson (2002) shows that the asymptotics of such an integral depends on the function

$$\begin{aligned} \tilde{f}^{(\mathbf{w})}(\boldsymbol{\theta}) &= \log\left(\frac{t(w_1 e^{i\theta_1}, \ldots, w_d e^{i\theta_d})}{t_{\mathbf{w}}} \right) + i \sum_{k=1}^{d} \theta_k \\ &= \log\left(\frac{S(\mathbf{w})}{e^{i(\theta_1 + \cdots + \theta_d)} S(w_1 e^{i\theta_1}, \ldots, w_d e^{i\theta_d})} \right) + i(\theta_1 + \cdots + \theta_d) \\ &= \log S(\mathbf{w}) - \log S(w_1 e^{i\theta_1}, \ldots, w_d e^{i\theta_d}). \end{aligned} \tag{9}$$

Let $\mathcal{H}_{\mathbf{w}}$ denote the determinant of the Hessian of $\tilde{f}^{(\mathbf{w})}(\boldsymbol{\theta})$ at $\mathbf{0}$. If $\mathcal{H}_{\mathbf{w}} \neq 0$, then we say $(\mathbf{w}, t_{\mathbf{w}})$ is *non-degenerate*. The main asymptotic result of smooth multivaritate analytic combinatorics, in this restricted context, is the following (the original result allows for asymptotic expansions of coefficient sequences more generally defined from multivariate functions than the diagonal sequence).

Theorem 1 (Adapted from Theorem 3.5 of Pemantle and Wilson (2002)) *Suppose that the meromorphic function $F(\mathbf{y}, t) = G(\mathbf{y}, t)/H(\mathbf{y}, t)$ has an isolated strictly minimal simple pole at $(\mathbf{z}, t_{\mathbf{z}})$. If tH_t does not vanish at $(\mathbf{z}, t_{\mathbf{z}})$ then there is an asymptotic expansion*

$$c_n \sim (z_1 \cdots z_d \cdot t)^{-n} \sum_{l \geq l_0} C_l n^{-(d+l)/2} \tag{10}$$

for constants C_l, where l_0 is the degree to which G vanishes near $(\mathbf{z}, t_{\mathbf{z}})$. When G does not vanish at $(\mathbf{z}, t_{\mathbf{z}})$ then $l_0 = 0$ and the leading term of this expansion is

$$C_0 = (2\pi)^{-d/2} \mathcal{H}_{\mathbf{z}}^{-1/2} \cdot \frac{G(\mathbf{z}, t_{\mathbf{z}})}{t H_t(\mathbf{z}, t_{\mathbf{z}})}. \tag{11}$$

In fact, Corollary 3.7 of Pemantle and Wilson (2002) shows that in the case of a finitely minimal point one can simply sum the contributions of each point. Combining this with the above calculations gives our main result.

Theorem 2 *Let $\mathcal{S} \subseteq \{-1,0,1\}^d \setminus \{\mathbf{0}\}$ be a set of unit steps in dimension d. If $\mathcal{S}$ is symmetric with respect to each axis, and $\mathcal{S}$ takes a positive step in each direction, then the number of walks of length n taking steps in $\mathcal{S}$, beginning at the origin, and never leaving the positive orthant has asymptotic expansion*

$$s_n \sim \left[\left(s^{(1)} \cdots s^{(d)}\right)^{-1/2} \pi^{-d/2} |\mathcal{S}|^{d/2}\right] \cdot n^{-d/2} \cdot |\mathcal{S}|^n, \tag{12}$$

where $s^{(k)}$ denotes the number of steps in $\mathcal{S}$ which have k^{th} coordinate 1.

Proof: We begin by verifying that each point $(\mathbf{w}, t_{\mathbf{w}}) \in \mathcal{V} \cap T(\boldsymbol{\rho})$ satisfies the conditions of Theorem 1:

1. $(\mathbf{w}, t_{\mathbf{w}})$ **is a simple pole** As $\mathcal{V}$ is smooth, the point $(\mathbf{w}, t_{\mathbf{w}})$ is a simple pole.

2. $(\mathbf{w}, t_{\mathbf{w}})$ **is isolated** This is proven in Proposition 3.

3. tH_t **does not vanish at** $(\mathbf{w}, t_{\mathbf{w}})$ This follows from $t_{\mathbf{w}} H_t(\mathbf{w}, t_{\mathbf{w}}) = 1/(w_1 \cdots w_d) \neq 0$.

4. $(\mathbf{w}, t_{\mathbf{w}})$ **is non-degenerate** Directly taking partial derivatives in Equation (9) implies

$$\tilde{f}^{(\mathbf{w})}_{\theta_j \theta_k}(\mathbf{0}) = \begin{cases} w_j w_k \dfrac{S_{y_j y_k}(\mathbf{w}) S(\mathbf{w}) - S_{y_j}(\mathbf{w}) S_{y_k}(\mathbf{w})}{S(\mathbf{w})^2} & : j \neq k \\ \dfrac{S_{y_j y_j}(\mathbf{w}) S(\mathbf{w}) + w_j S_{y_j}(\mathbf{w}) S(\mathbf{w}) - S_{y_j}(\mathbf{w})^2}{S(\mathbf{w})^2} & : j = k \end{cases}.$$

Since $S_{y_j}(\mathbf{y}) = (1 - y_j^{-2}) S_1^{(j)}(\mathbf{y}_{\bar{j}})$ we see that $S_{y_j}(\mathbf{w}) = 0$. Furthermore, one can calculate that $S_{y_j y_j}(\mathbf{w}) = 2S_1^{(j)}(\mathbf{w})$ and $S_{y_j y_k}(\mathbf{w}) = 0$ for $j \neq k$, so that the Hessian of $\tilde{f}^{(\mathbf{w})}(\boldsymbol{\theta})$ at $\mathbf{0}$ is a diagonal matrix and

$$\mathcal{H}_{\mathbf{w}} = \frac{2^d}{S(\mathbf{w})^d} S_1^{(1)}(\mathbf{w}) \cdots S_1^{(d)}(\mathbf{w}). \tag{13}$$

The proof of Proposition 3 implies that $S_1^{(k)}(\mathbf{w}) \neq 0$ for any $1 \leq k \leq d$, so each $(\mathbf{w}, t_{\mathbf{w}})$ is non-degenerate.

Thus, we can apply Corollary 3.7 of Pemantle and Wilson (2002) and sum the expansions (10) at each point in $\mathcal{V} \cap T(\boldsymbol{\rho})$ to obtain the asymptotic expansion

$$s_n \sim |\mathcal{S}|^n \sum_{\mathbf{w} \in \mathcal{V} \cap T(\boldsymbol{\rho})} \left(\sum_{l \geq l_{\mathbf{w}}} C_l^{\mathbf{w}} n^{-(d+l)/2} \right) \tag{14}$$

for constants $C_l^{\mathbf{w}}$, where $l_{\mathbf{w}}$ is the degree to which $G(\mathbf{y}, t)$ vanishes near $(\mathbf{w}, t_{\mathbf{w}})$. Since the numerator $G(\mathbf{y}, t) = (1 + y_1) \cdots (1 + y_d)$ vanishes at all points of $\mathbf{w} \in \mathcal{V} \cap T(\boldsymbol{\rho})$ except for $\boldsymbol{\rho} = (\mathbf{1}, 1/|\mathcal{S}|)$, the dominant term of (14) is determined only by the contribution of $\mathbf{w} = \boldsymbol{\rho}$. Substituting the value for $\mathcal{H}_{\boldsymbol{\rho}}$ given by Equation (13) into Equation (11) gives the desired asymptotic result. □

4 Conclusion

The purpose of this article, aside from the specific combinatorial results it contains, is to enforce the notion that there are many possibilities for studying lattice walks in restricted regions through the use of diagonals and analytic combinatorics in several variables. As shown above, walks with symmetry across each axis all have a smooth singular variety, making them the perfect entry point.

It also seems that the remarkable symmetries could be exploited another way if the generating functions could be described directly by symmetric functions. Diagonals first appear in the study of D-finite symmetric functions in the work of Gessel (1990).

4.1 Generalizations: less symmetry

A major goal moving forward is to deal with step sets missing some symmetries. For general (unit) step sets there is the notion of the group of a walk, which can help write the generating function for the number of walks as a diagonal of a rational function in many cases, however this is not always possible. First of all, such diagonals are always D-finite, and as shown by Bousquet-Mélou and Petkovšek (2003) there are already walks in two dimensions restricted to the positive quadrant which have non D-finite generating functions. Indeed, in the two dimensional case for walks with unit steps there is strong evidence in the work of Bostan and Kauers (2009) and Bostan et al. (2014) that all walks which are non D-finite have their related group being infinite, although it has only been proven for the univariate counting function in 5 of 56 cases Melczer and Mishna (2014).

For walks with longer steps, the difficulty lies in determining an analogue to the group $\mathcal{G}$ which would allow one to write the counting generating function as a diagonal. If the step sets still contain symmetry across each axis, the elements of the group defined here will still fix the step set $\mathcal{S}$, but new types of terms appearing in the functional Equation (2) require additional group elements to get a result analogous to Equation (4).

4.2 Are all D-finite models diagonals?

Even in when this group is finite, trying to sum the functional equation using group elements to get a result as in Theorem 2 does not always work (including some cases where the generating functions are algebraic and thus *can* be written as a diagonal of some rational function). A conjecture of Christol (1990) states that any globally bounded D-finite function (which includes power series convergent at the origin with integer coefficients) can be written as the diagonal of a multivariate rational function. Determining an automatic method of writing known D-finite functions as diagonals, even if only in the case of lattice walks, would have great use.

4.3 The singular variety

Finally, assuming one can get the generating function for the number of walks in a more general setting as a rational diagonal, results on asymptotics can be reduced to an analysis of this rational function. Both Pemantle and Wilson (2013) and Raichev and Wilson (2011) give results for singular varieties which are non-smooth, but whose critical points are *multiple points*. Due to the constraints on the rational functions arising from the combinatorial nature of lattice paths in restricted regions, there is hope for a more general treatment which allows for some non symmetries.

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Pivot Sampling in Dual-Pivot Quicksort: † *Exploiting Asymmetries in Yaroslavskiy's Partitioning Scheme*

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Abstract. The new dual-pivot Quicksort by Vladimir Yaroslavskiy — used in Oracle's Java runtime library since version 7 — features intriguing asymmetries in its behavior. They were shown to cause a basic variant of this algorithm to use less comparisons than classic single-pivot Quicksort implementations. In this paper, we extend the analysis to the case where the two pivots are chosen as fixed order statistics of a random sample and give the precise leading term of the average number of comparisons, swaps and executed Java Bytecode instructions. It turns out that — unlike for classic Quicksort, where it is optimal to choose the pivot as median of the sample — the asymmetries in Yaroslavskiy's algorithm render pivots with a systematic skew more efficient than the symmetric choice. Moreover, the optimal skew heavily depends on the employed cost measure; most strikingly, abstract costs like the number of swaps and comparisons yield a very different result than counting Java Bytecode instructions, which can be assumed most closely related to actual running time.

Keywords: Quicksort, dual-pivot, Yaroslavskiy's partitioning method, median of three, average case analysis

1 Introduction

Quicksort is one of the most efficient comparison-based sorting algorithms and is thus widely used in practice, for example in the sort implementations of the C++ standard library and Oracle's Java runtime library. Almost all practical implementations are based on the highly tuned version of Bentley and McIlroy (1993), often equipped with the strategy of Musser (1997) to avoid quadratic worst case behavior. The Java runtime environment was no exception to this — up to version 6. With version 7 released in 2009, however, Oracle broke with this tradition and replaced its tried and tested implementation by a dual-pivot Quicksort with a new partitioning method proposed by Vladimir Yaroslavskiy.

The decision was based on extensive running time experiments that clearly favored the new algorithm. This was particularly remarkable as earlier analyzed dual-pivot variants had not shown any potential for performance gains over classic single-pivot Quicksort (Sedgewick, 1975; Hennequin, 1991). However, we

† An extended version with proof details in the appendix is available at `http://arxiv.org/abs/1403.6602`.

could show for pivots from fixed array positions (*i.e.* no sampling) that Yaroslavskiy's asymmetric partitioning method beats classic Quicksort in the comparison model: asymptotically $1.9\,n \ln n$ vs. $2\,n \ln n$ comparisons on average (Wild and Nebel, 2012). As these savings are opposed by a large increase in the number of swaps, the overall competition still remained open. To settle it, we compared two Java implementations of the Quicksort variants and found that Yaroslavskiy's method actually executes *more* Java Bytecode instructions on average (Wild et al., 2013b). A possible explanation why it still shows better running times was recently given by Kushagra et al. (2014): Yaroslavskiy's algorithm needs fewer scans over the array than classic Quicksort, and is thus more efficient in the *external memory model*.

Our analyses cited above ignore a very effective strategy in Quicksort: for decades, practical implementations choose their pivots as *median of a random sample* of the input to be more efficient (both in terms of average performance and in making worst cases less likely). Oracle's Java 7 implementation also employs this optimization: it chooses its two pivots as the *tertiles of five* sample elements. This equidistant choice is a plausible generalization, since selecting the pivot as median is known to be optimal for classic Quicksort (Sedgewick, 1975; Martínez and Roura, 2001).

However, the classic partitioning methods treat elements smaller and larger than the pivot in symmetric ways — unlike Yaroslavskiy's partitioning algorithm: depending on how elements relate to the two pivots, one of *five* different execution paths is taken in the partitioning loop, and these can have highly different costs! How often each of these five paths is taken depends on the *ranks* of the two pivots, which we can push in a certain direction by selecting *other* order statistics of a sample than the tertiles. The partitioning costs alone are then minimized if the cheapest execution path is taken all the time. This however leads to very unbalanced distributions of sizes for the recursive calls, such that a *trade-off* between partitioning costs and balance of subproblem sizes results.

We have demonstrated experimentally that there is potential to tune dual-pivot Quicksort using skewed pivots (Wild et al., 2013c), but only considered a small part of the parameter space. **It will be the purpose of this paper to identify the optimal way to sample pivots by means of a precise analysis of the resulting overall costs,** and to validate (and extend) the empirical findings that way.

Related work. Single-pivot Quicksort with pivot sampling has been intensively studied over the last decades (Emden, 1970; Sedgewick, 1975, 1977; Hennequin, 1991; Martínez and Roura, 2001; Neininger, 2001; Chern and Hwang, 2001; Durand, 2003). We heavily profit from the mathematical foundations laid by these authors. There are scenarios where, even for the symmetric, classic Quicksort, a skewed pivot can yield benefits over median of k (Martínez and Roura, 2001; Kaligosi and Sanders, 2006). An important difference to Yaroslavskiy's algorithm is, however, that the situation remains symmetric: a relative pivot rank $\alpha < \frac{1}{2}$ has the same effect as one with rank $1 - \alpha$. For dual-pivot Quicksort with an *arbitrary* partitioning method, Aumüller and Dietzfelbinger (2013) establish a lower bound of asymptotically $1.8\,n \ln n$ comparisons and they also propose a partitioning method that attains this bound.

Outline. After listing some general notation, Section 3 introduces the subject of study. Section 4 collects the main analytical results of this paper, whose proof is divided into Sections 5, 6 and 7. Arguments are kept concise here, but the interested reader is provided with details in the extended version on the arXiv. The algorithmic consequences of our analysis are discussed in Section 8. Section 9 concludes the paper.

2 Notation and Preliminaries

We write vectors in bold font, for example $\mathbf{t} = (t_1, t_2, t_3)$. For concise notation, we use expressions like $\mathbf{t} + 1$ to mean *element-wise* application, *i.e.*, $\mathbf{t} + 1 = (t_1 + 1, t_2 + 1, t_3 + 1)$. By $\mathrm{Dir}(\boldsymbol{\alpha})$, we denote a random variable with *Dirichlet distribution* and shape parameter $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_d) \in \mathbb{R}^d_{>0}$. Likewise for parameters $n \in \mathbb{N}$ and $\mathbf{p} = (p_1, \dots, p_d) \in [0,1]^d$ with $p_1 + \cdots + p_d = 1$, we write $\mathrm{Mult}(n, \mathbf{p})$ for a random variable with *multinomial distribution* with n trials. $\mathrm{HypG}(k, r, n)$ is a random variable with *hypergeometric distribution*, *i.e.*, the number of red balls when drawing k times without replacement from an urn of $n \in \mathbb{N}$ balls, r of which are red, (where $k, r \in \{1, \dots, n\}$). Finally, $\mathcal{U}(a, b)$ is a random variable uniformly distributed in the interval (a, b), and $\mathrm{B}(p)$ is a Bernoulli variable with probability p to be 1. We use "$\overset{\mathcal{D}}{=}$" to denote equality in distribution. As usual for the average case analysis of sorting algorithms, we assume the *random permutation model*, *i.e.*, all elements are different and every ordering of them is equally likely. The input is given as array $\mathtt{A}$ of length n and we denote the initial entries of $\mathtt{A}$ by $U_1, \dots, U_n$. We further assume that $U_1, \dots, U_n$ are i. i. d. uniformly $\mathcal{U}(0,1)$ distributed; as their ordering forms a random permutation (Mahmoud, 2000), this assumption is without loss of generality.

A comprehensive list of notations is given in Appendix A of the extended version.

3 Generalized Yaroslavskiy Quicksort

In this section, we review Yaroslavskiy's partitioning method and combine it with the pivot sampling optimization to obtain what we call the *Generalized Yaroslavskiy Quicksort* algorithm. We leave some parts of the algorithm unspecified here that are not important for the analysis. A full-detail implementation is provided in Appendix B of the extended version of the paper.

3.1 Generalized Pivot Sampling

Our pivot selection process is declaratively specified as follows, where $\mathbf{t} = (t_1, t_2, t_3) \in \mathbb{N}^3$ is a fixed parameter: choose a random sample $\mathbf{V} = (V_1, \dots, V_k)$ of size $k = k(\mathbf{t}) := t_1 + t_2 + t_3 + 2$ from the elements and denote by $(V_{(1)}, \dots, V_{(k)})$ the *sorted*[(i)] sample, *i.e.*, $V_{(1)} \le V_{(2)} \le \cdots \le V_{(k)}$. Then choose the two pivots $P := V_{(t_1+1)}$ and $Q := V_{(t_1+t_2+2)}$ such that they divide the sorted sample into three regions of respective sizes t_1, t_2 and t_3:

$$\underbrace{V_{(1)} \dots V_{(t_1)}}_{t_1 \text{ elements}} \le \underbrace{V_{(t_1+1)}}_{=P} \le \underbrace{V_{(t_1+2)} \dots V_{(t_1+t_2+1)}}_{t_2 \text{ elements}} \le \underbrace{V_{(t_1+t_2+2)}}_{=Q} \le \underbrace{V_{(t_1+t_2+3)} \dots V_{(k)}}_{t_3 \text{ elements}} . \quad (3.1)$$

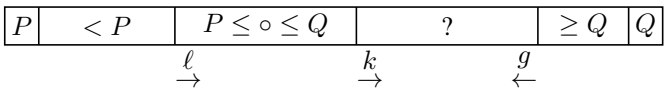
Note that by definition, P is the small(er) pivot and Q is the large(r) one. We refer to the $k-2$ elements of the sample that are not chosen as pivot as *"sampled-out"*; P and Q are the chosen *pivots*. All other elements — those which have not been part of the sample — are referred to as *ordinary* elements. Pivots and ordinary elements together form the set of *partitioning elements*, (because we exclude sampled-out elements from partitioning).

3.2 Yaroslavskiy's Dual Partitioning Method

In bird's-eye view, Yaroslavskiy's partitioning method consists of two indices, k and g, that start at the left resp. right end of $\mathtt{A}$ and scan the array until they meet. Elements left of k are smaller or equal than Q,

[(i)] In case of equal elements any possible ordering will do. However in this paper, we assume distinct elements.

elements right of g are larger. Additionally, a third index ℓ lags behind k and separates elements smaller than P from those between both pivots. Graphically speaking, the invariant of the algorithm is as follows:



We write $\mathcal{K}$ and $\mathcal{G}$ for the sets of all indices that k resp. g attain in the course of the partitioning process. Moreover, we call an element *small*, *medium*, or *large* if it is smaller than P, between P and Q, or larger than Q, respectively. The following properties of the algorithm are needed for the analysis, (see Wild and Nebel (2012); Wild et al. (2013b) for details):

(Y1) Elements U_i, $i \in \mathcal{K}$, are first compared with P. Only if U_i is not small, it is also compared to Q.

(Y2) Elements U_i, $i \in \mathcal{G}$, are first compared with Q. If they are not large, they are also compared to P.

(Y3) Every small element eventually causes one swap to put it behind ℓ.

(Y4) The large elements located in $\mathcal{K}$ and the non-large elements in $\mathcal{G}$ are always swapped in pairs.

For the number of comparisons we will thus need to count the large elements U_i with $i \in \mathcal{K}$; we abbreviate their number by "$l@\mathcal{K}$". Similarly, $s@\mathcal{K}$ and $s@\mathcal{G}$ denote the number of small elements in k's resp. g's range.

When partitioning is finished, k and g have met and thus ℓ and g divide the array into three ranges, containing the small, medium resp. large (ordinary) elements, which are then sorted recursively. For subarrays with at most w elements, we switch to Insertionsort, (where w is constant and at least k). The resulting algorithm, Generalized Yaroslavskiy Quicksort with pivot sampling parameter $\mathbf{t} = (t_1, t_2, t_3)$ and Insertionsort threshold w, is henceforth called $Y^w_{\mathbf{t}}$.

4 Results

For $\mathbf{t} \in \mathbb{N}^3$ and $\mathcal{H}_n$ the nth harmonic number, we define the *discrete entropy* $\mathrm{H}(\mathbf{t})$ of $\mathbf{t}$ as

$$\mathrm{H}(\mathbf{t}) \;=\; \sum_{l=1}^{3} \frac{t_l + 1}{k+1} (\mathcal{H}_{k+1} - \mathcal{H}_{t_l+1}) \,. \tag{4.1}$$

The name is justified by the following connection between $\mathrm{H}(\mathbf{t})$ and the *entropy function* H^* of information theory: for the sake of analysis, let $k \to \infty$, such that ratios t_l/k converge to constants τ_l. Then

$$\mathrm{H}(\mathbf{t}) \;\sim\; -\sum_{l=1}^{3} \tau_l \big(\ln(t_l+1) - \ln(k+1)\big) \;\sim\; -\sum_{l=1}^{3} \tau_l \ln(\tau_l) \;=:\; \mathrm{H}^*(\boldsymbol{\tau}) \,. \tag{4.2}$$

The first step follows from the asymptotic equivalence $\mathcal{H}_n \sim \ln(n)$ as $n \to \infty$. (4.2) shows that for large $\mathbf{t}$, the maximum of $\mathrm{H}(\mathbf{t})$ is attained for $\tau_1 = \tau_2 = \tau_3 = \frac{1}{3}$. Now we state our main result:

Theorem 4.1 (Main theorem): *Generalized Yaroslavskiy Quicksort with pivot sampling parameter* $\mathbf{t} = (t_1, t_2, t_3)$ *performs on average* $C_n \sim \frac{a_C}{\mathrm{H}(\mathbf{t})}\, n \ln n$ *comparisons and* $S_n \sim \frac{a_S}{\mathrm{H}(\mathbf{t})}\, n \ln n$ *swaps to sort a random permutation of* n *elements, where*

$$a_C \;=\; 1 + \frac{t_2+1}{k+1} + \frac{(2t_1+t_2+3)(t_3+1)}{(k+1)(k+2)} \quad \textit{and} \quad a_S \;=\; \frac{t_1+1}{k+1} + \frac{(t_1+t_2+2)(t_3+1)}{(k+1)(k+2)}\,. \tag{4.3}$$

Moreover, if the partitioning loop is implemented as in Appendix C of (Wild et al., 2013b), it executes on average $BC_n \sim \frac{a_{BC}}{\mathrm{H}(\mathbf{t})}\, n \ln n$ *Java Bytecode instructions to sort a random permutation of size* n *with*

$$a_{BC} \;=\; 10 \;+\; 13\frac{t_1+1}{k+1} \;+\; 5\frac{t_2+1}{k+1} \;+\; 11\frac{(t_1+t_2+2)(t_3+1)}{(k+1)(k+2)} \;+\; \frac{(t_1+1)(t_1+t_2+3)}{(k+1)(k+2)}\,. \tag{4.4}$$

The following sections are devoted to the proof of Theorem 4.1. Section 5 sets up a recurrence of costs and characterizes the distribution of costs of one partitioning step. The expected values of the latter are computed in Section 6. Finally, Section 7 provides a generic solution to the recurrence of the expected costs; in combination with the expected partitioning costs, this concludes our proof.

5 Distributional Analysis

5.1 Recurrence Equations of Costs

Let us denote by C_n the *costs* of $Y_{\mathbf{t}}^w$ on a random permutation of size n — where different "cost measures", like the number of comparisons, will take the place of C_n later. C_n is a non-negative *random* variable whose distribution depends on n. The total costs decompose into those for the first partitioning step plus the costs for recursively solving subproblems. As Yaroslavskiy's partitioning method preserves randomness (see Appendix B of the extended version), we can express the total costs C_n recursively in terms of the same cost function with smaller arguments: for sizes J_1, J_2 and J_3 of the three subproblems, the costs of corresponding recursive calls are distributed like C_{J_1}, C_{J_2} and C_{J_3}, and conditioned on $\mathbf{J} = (J_1, J_2, J_3)$, these random variables are independent. Note, however, that the subproblem sizes are themselves random and inter-dependent. Denoting by T_n the costs of the first partitioning step, we obtain the following *distributional recurrence* for the family $(C_n)_{n\in\mathbb{N}}$ of random variables:

$$C_n \;\overset{\mathcal{D}}{=}\; \begin{cases} T_n \;+\; C_{J_1} + C'_{J_2} + C''_{J_3}, & \text{for } n > w; \\ W_n, & \text{for } n \le w. \end{cases} \tag{5.1}$$

Here W_n denotes the cost of Insertionsorting a random permutation of size n. $(C'_j)_{j\in\mathbb{N}}$ and $(C''_j)_{j\in\mathbb{N}}$ are independent copies of $(C_j)_{j\in\mathbb{N}}$, *i.e.*, for all j, the variables C_j, C'_j and C''_j are identically distributed and for all $\mathbf{j} \in \mathbb{N}^3$, C_{j_1}, C'_{j_2} and C''_{j_3} are totally independent, and they are also independent of T_n. We call T_n the *toll function* of the recurrence, as it quantifies the "toll" we have to pay for unfolding the recurrence once. Different cost measures only differ in the toll functions, such that we can treat them all in a uniform fashion by studying (5.1). Taking expectations on both sides, we find a recurrence equation for the *expected* costs $\mathbb{E}[C_n]$:

$$\mathbb{E}[C_n] \;=\; \begin{cases} \mathbb{E}[T_n] \;+\; \sum\limits_{\substack{\mathbf{j}=(j_1,j_2,j_3)\\ j_1+j_2+j_3=n-2}} \mathbb{P}(\mathbf{J}=\mathbf{j})\big(\mathbb{E}[C_{j_1}] + \mathbb{E}[C_{j_2}] + \mathbb{E}[C_{j_3}]\big), & \text{for } n > w; \\ \mathbb{E}[W_n], & \text{for } n \le w. \end{cases} \tag{5.2}$$

A simple combinatorial argument gives access to $\mathbb{P}(\mathbf{J} = \mathbf{j})$, the probability of $\mathbf{J} = \mathbf{j}$: of the $\binom{n}{k}$ different size k samples of n elements, those contribute to the probability of $\{\mathbf{J} = \mathbf{j}\}$, in which exactly t_1 of the sample elements are chosen from the overall j_1 small elements; and likewise t_2 of the j_2 medium elements and t_3 of the j_3 large ones are contained in the sample. We thus have

$$\mathbb{P}(\mathbf{J} = \mathbf{j}) \;=\; \binom{j_1}{t_1}\binom{j_2}{t_2}\binom{j_3}{t_3} \Big/ \binom{n}{k} \,. \tag{5.3}$$

5.2 Distribution of Partitioning Costs

Let us denote by I_1, I_2 and I_3 the number of small, medium and large elements among the ordinary elements, (*i.e.*, $I_1 + I_2 + I_3 = n - k$) — or equivalently stated, $\mathbf{I} = (I_1, I_2, I_3)$ is the (vector of) sizes of the three partitions (excluding sampled-out elements). Moreover, we define the indicator variable $\delta = \mathbb{1}_{\{U_\chi > Q\}}$ to account for an idiosyncrasy of Yaroslavskiy's algorithm (see the proof of Lemma 5.1), where χ is the point where indices k and g first meet. As we will see, we can characterize the distribution of partitioning costs *conditional* on $\mathbf{I}$, *i.e.*, when considering $\mathbf{I}$ *fixed*.

5.2.1 Comparisons

For constant size samples, only the comparisons during the partitioning process contribute to the linearithmic leading term of the asymptotic average costs, as the number of partitioning steps remains linear. We can therefore ignore comparisons needed for sorting the sample. As w is constant, the same is true for subproblems of size at most w that are sorted with Insertionsort. It remains to count the comparisons during the first partitioning step.

Lemma 5.1: *Conditional on the partition sizes* $\mathbf{I}$*, the number of comparisons* $T_C = T_C(n)$ *in the first partitioning step of* $Y_{\mathbf{t}}^w$ *on a random permutation of size* $n > w$ *fulfills*

$$T_C(n) \;=\; (n-k) \;+\; I_2 \;+\; (l@\mathcal{K}) \;+\; (s@\mathcal{G}) \;+\; 2\delta \tag{5.4}$$

$$\overset{\mathcal{D}}{=}\; (n-k) \;+\; I_2 \;+\; \mathrm{HypG}(I_1 + I_2, I_3, n-k) \;+\; \mathrm{HypG}(I_3, I_1, n-k) \;+\; 3\mathrm{B}\big(\tfrac{I_3}{n-k}\big) \,. \tag{5.5}$$

Proof: Every ordinary element is compared to at least one of the pivots, which makes $n-k$ comparisons. Additionally, for all medium elements, the second comparison is inevitably needed to recognize them as "medium", and there are I_2 such elements. Large elements only cause a second comparison if they are first compared with P, which happens if and only if they are located in k's range, see (Y1). We abbreviated the (random) number of large elements in $\mathcal{K}$ as $l@\mathcal{K}$. Similarly, $s@\mathcal{G}$ counts the second comparison for all small elements found in g's range, see (Y2).

The last summand 2δ accounts for a technicality in Yaroslavskiy's algorithm. If U_χ, the element where k and g meet, is large, then index k overshoots g by one, which causes two additional (superfluous) comparisons with this element. $\delta = \mathbb{1}_{\{U_\chi > Q\}}$ is the indicator variable of this event. This proves (5.4).

For the equality in distribution, recall that I_1, I_2 and I_3 are the number of small, medium and large elements, respectively. Then we need the cardinalities of $\mathcal{K}$ and $\mathcal{G}$. Since the elements right of g after partitioning are exactly all large elements, we have $|\mathcal{G}| = I_3$ and $|\mathcal{K}| = I_1 + I_2 + \delta$; (again, δ accounts for the overshoot, see Wild et al. (2013b) for detailed arguments). The distribution of $s@\mathcal{G}$, conditional on $\mathbf{I}$, is now given by the following urn model: we put all $n-k$ ordinary elements in an urn and draw their

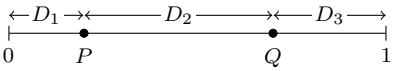


Figure 1: Graphical representation of the relation between $\mathbf{D}$ and the pivot values P and Q on the unit interval.

positions in $\mathtt{A}$. I_1 of the elements are colored red (namely the small ones), the rest is black (non-small). Now we draw the $|\mathcal{G}| = I_3$ elements in g's range from the urn without replacement. Then $s@\mathcal{G}$ is exactly the number of red (small) elements drawn and thus $s@\mathcal{G} \overset{\mathcal{D}}{=} \mathrm{HypG}(I_3, I_1, n-k)$.

The arguments for $l@\mathcal{K}$ are similar, however the additional δ in $|\mathcal{K}|$ needs special care. As shown in the proof of Lemma 3.7 of Wild et al. (2013b), the additional element in k's range for the case $\delta = 1$ is U_χ, which then is large by definition of δ. It thus simply contributes as additional summand: $l@\mathcal{K} \overset{\mathcal{D}}{=} \mathrm{HypG}(I_1 + I_2, I_3, n-k) + \delta$. Finally, the distribution of δ is Bernoulli $\mathrm{B}\big(\frac{I_3}{n-k}\big)$, since conditional on $\mathbf{I}$, the probability of an ordinary element to be large is $I_3/(n-k)$. □

5.2.2 Swaps

As for comparisons, only the swaps in the partitioning step contribute to the leading term asymptotics.

Lemma 5.2: *Conditional on the partition sizes* $\mathbf{I}$*, the number of swaps* $T_S = T_S(n)$ *in the first partitioning step of* $Y_{\mathbf{t}}^w$ *on a random permutation of size* $n > w$ *fulfills*

$$T_S(n) \;=\; I_1 \;+\; (l@\mathcal{K}) \;\overset{\mathcal{D}}{=}\; I_1 \;+\; \mathrm{HypG}(I_1 + I_2, I_3, n-k) \;+\; \mathrm{B}\big(\tfrac{I_3}{n-k}\big)\,. \tag{5.6}$$

Proof: No matter where a small element is located initially, it will eventually incur one swap that puts it at its final place (for this partitioning step) to the left of ℓ, see (Y3); this gives a contribution of I_1. The remaining swaps come from the "crossing pointer" scheme, where k stops on the first large and g on the first non-large element, which are then exchanged in one swap (Y4). For their contribution, it thus suffices to count the large elements in k's range, that is $l@\mathcal{K}$. The distribution of $l@\mathcal{K}$ has already been discussed in the proof of Lemma 5.1. □

5.2.3 Bytecode Instructions

A closer investigation of the partitioning method reveals the number of executions for every single Bytecode instruction in the algorithm. Details are omitted here; the analysis is very similar to the case without pivot sampling that is presented in detail in (Wild et al., 2013b).

Lemma 5.3: *Conditional on the partition sizes* $\mathbf{I}$*, the number of executed Java Bytecode instructions* $T_{BC} = T_{BC}(n)$ *of the first partitioning step of* $Y_{\mathbf{t}}^w$ *— implemented as in Appendix C of (Wild et al., 2013b) — fulfills on a random permutation of size* $n > w$

$$T_{BC}(n) \;\overset{\mathcal{D}}{=}\; 10n + 13I_1 + 5I_2 + 11\,\mathrm{HypG}(I_1 + I_2, I_3, n-k) + \mathrm{HypG}(I_1, I_1 + I_2, n-k) \;+\; O(1)\,. \tag{5.7}$$

□

Other cost measures can be analyzed similarly, *e. g.*, the analysis of Kushagra et al. (2014) for I/Os in the *external memory model* is easily generalized to pivot sampling. We omit it here due to space constraints.

5.2.4 Distribution of Partition Sizes

There is a close relation between $\mathbf{I}$, the number of small, medium and large ordinary elements, and $\mathbf{J}$, the size of subproblems; we only have to add the sampled-out elements again before the recursive calls. So

we have $\mathbf{J} = \mathbf{I} + \mathbf{t}$ and $\mathbb{P}(\mathbf{I} = \mathbf{i}) = \binom{i_1+t_1}{t_1}\binom{i_2+t_2}{t_2}\binom{i_3+t_3}{t_3}\big/\binom{n}{k}$ by (5.3). Albeit valid, this form results in nasty sums with three binomials when we try to compute expectations involving $\mathbf{I}$.

An alternative characterization of the distribution of $\mathbf{I}$ that is better suited for our needs exploits that we have i. i. d. $\mathcal{U}(0,1)$ variables. If we condition on the pivot *values*, *i.e.*, consider P and Q fixed, an ordinary element U is small, if $U \in (0,P)$, medium if $U \in (P,Q)$ and large if $U \in (Q,1)$. The lengths $\mathbf{D} = (D_1, D_2, D_3)$ of these three intervals (see Figure 1), thus are the *probabilities* for an element to be small, medium or large, respectively. Note that this holds *independently* of all other ordinary elements! The partition sizes $\mathbf{I}$ are then obtained as the collective outcome of $n-k$ independent drawings from this distribution, so conditional on $\mathbf{D}$, $\mathbf{I}$ is multinomially $\mathrm{Mult}(n-k, \mathbf{D})$ distributed.

With this alternative characterization, we have *decoupled* the pivot *ranks* (determined by $\mathbf{I}$) from the pivot *values*, which allows for a more elegant computation of expected values. This decoupling trick has (implicitly) been applied to the analysis of classic Quicksort earlier, *e. g.*, by Neininger (2001).

5.2.5 Distribution of Pivot Values

The input array is initially filled with n i. i. d. $\mathcal{U}(0,1)$ random variables from which we choose a sample $\{V_1, \dots, V_k\} \subset \{U_1, \dots, U_n\}$ of size k. The pivot values are then selected as order statistics of the sample: $P := V_{(t_1+1)}$ and $Q := V_{(t_1+t_2+2)}$ (cf. Section 3.1). In other words, $\mathbf{D}$ is the vector of *spacings* induced by the order statistics $V_{(t_1+1)}$ and $V_{(t_1+t_2+2)}$ of k i. i. d. $\mathcal{U}(0,1)$ variables $V_1, \dots, V_k$, which is known to have a *Dirichlet* $\mathrm{Dir}(\mathbf{t}+1)$ distribution (Proposition C.1 of the extended version).

6 Expected Partitioning Costs

In Section 5, we characterized the full distribution of the costs of the first partitioning step. However, since those distributions are *conditional* on other random variables, we have to apply the *law of total expectation*. By linearity of the expectation, it suffices to consider the following summands:

Lemma 6.1: *For pivot sampling parameter $\mathbf{t} \in \mathbb{N}^3$ and partition sizes $\mathbf{I} \stackrel{\mathcal{D}}{=} \mathrm{Mult}(n-k, \mathbf{D})$, based on random spacings $\mathbf{D} \stackrel{\mathcal{D}}{=} \mathrm{Dir}(\mathbf{t}+1)$, the following (unconditional) expectations hold:*

$$\mathbb{E}[I_j] = \frac{t_j+1}{k+1}(n-k)\,, \qquad (j=1,2,3), \tag{6.1}$$

$$\mathbb{E}\big[\mathrm{B}\big(\tfrac{I_3}{n-k}\big)\big] = \frac{t_3+1}{k+1} = \Theta(1)\,, \qquad (n \to \infty), \tag{6.2}$$

$$\mathbb{E}\big[\mathrm{HypG}(I_3, I_1, n-k)\big] = \frac{(t_1+1)(t_3+1)}{(k+1)(k+2)}(n-k-1)\,, \tag{6.3}$$

$$\mathbb{E}\big[\mathrm{HypG}(I_1+I_2, I_3, n-k)\big] = \frac{(t_1+t_2+2)(t_3+1)}{(k+1)(k+2)}(n-k-1)\,. \tag{6.4}$$

Using known properties of the involved distributions, the proof is elementary (see Appendix D of the extended version for detailed computations).

7 Solution of the Recurrence

Theorem 7.1: *Let $\mathbb{E}[C_n]$ be a sequence of numbers satisfying recurrence* (5.2) *on page 329 for a constant $w \geq k$ and let the toll function $\mathbb{E}[T_n]$ be of the form $\mathbb{E}[T_n] = an + O(1)$ for a constant a. Then we have $\mathbb{E}[C_n] \sim \frac{a}{\mathrm{H}(\mathbf{t})}\, n \ln n$, where $\mathrm{H}(\mathbf{t})$ is given by equation* (4.1) *on page 328.*

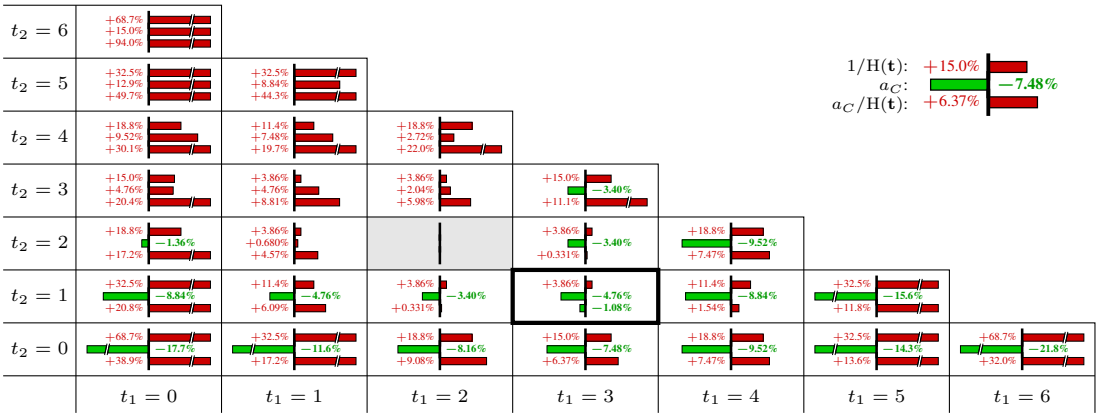


Figure 2: Inverse of discrete entropy (top), number of comparisons per partitioning step (middle) and overall comparisons (bottom) for all $\mathbf{t}$ with $k = 8$, relative to the tertiles case $\mathbf{t} = (2, 2, 2)$.

$t_1 \backslash t_2$	0	1	2	3
0	1.9956	1.8681	2.0055	2.4864
1	1.7582	**1.7043**	1.9231	
2	1.7308	1.7582		
3	1.8975			

(a) $a_C/\mathrm{H}(\mathbf{t})$

$t_1 \backslash t_2$	0	1	2	3
0	0.4907	0.4396	0.4121	**0.3926**
1	0.6319	0.5514	0.5220	
2	0.7967	0.7143		
3	1.0796			

(b) $a_S/\mathrm{H}(\mathbf{t})$

$t_1 \backslash t_2$	0	1	2	3
0	20.840	**18.791**	19.478	23.293
1	20.440	19.298	21.264	
2	22.830	22.967		
3	29.378			

(c) $a_{BC}/\mathrm{H}(\mathbf{t})$

Table 1: $\frac{a_C}{\mathrm{H}(\mathbf{t})}$, $\frac{a_S}{\mathrm{H}(\mathbf{t})}$ and $\frac{a_{BC}}{\mathrm{H}(\mathbf{t})}$ for all $\mathbf{t}$ with $k = 5$. Rows resp. columns give t_1 and t_2; t_3 is then $k - 2 - t_1 - t_2$. The symmetric choice $\mathbf{t} = (1, 1, 1)$ is shaded, the minimum is printed in bold.

Theorem 7.1 has first been proven by Hennequin (1991, Proposition III.9) using arguments on the Cauchy-Euler differential equations that the recurrence implies for the generating function of $\mathbb{E}[C_n]$. The tool box of handy and ready-to-apply theorems has grown considerably since then. In Appendix E of the extended version, we give a concise and elementary proof using the *Continuous Master Theorem* (Roura, 2001): we show that the distribution of the *relative* subproblem sizes converges to a *Beta distribution* and that then a continuous version of the recursion tree argument allows to solve our recurrence. An alternative tool closer to Hennequin's original arguments is offered by Chern et al. (2002).

Theorem 4.1 now directly follows by using Lemma 6.1 on the partitioning costs from Lemma 5.1, 5.2 and 5.3 and plugging the result into Theorem 7.1.

8 Discussion — Asymmetries Everywhere

With Theorem 4.1, we can find the optimal sampling parameter $\mathbf{t}$ for any given sample size k. As an example, Figure 2 shows how $\mathrm{H}(\mathbf{t})$, a_C and the overall number of comparisons behave for all possible $\mathbf{t}$ with sample size $k = 8$: the discrete entropy decreases symmetrically as we move away from the center $\mathbf{t} = (2, 2, 2)$; this corresponds to the effect of less evenly distributed subproblem sizes. The individual partitioning steps, however, are cheap for *small* values of t_2 and optimal in the extreme point $\mathbf{t} = (6, 0, 0)$. For minimizing the *overall* number of comparisons — the ratio of latter two numbers — we have to find a

suitable trade-off between the center and the extreme point $(6, 0, 0)$; in this case the minimal total number of comparisons is achieved with $\mathbf{t} = (3, 1, 2)$.

Apart from this trade-off between the evenness of subproblem sizes and the number of comparisons per partitioning, Table 1 shows that the optimal choices for $\mathbf{t}$ w. r. t. comparisons, swaps and Bytecodes heavily differ. The partitioning costs are, in fact, in *extreme conflict* with each other: for all $k \geq 2$, the minimal values of a_C, a_S and a_{BC} among all choices of $\mathbf{t}$ for sample size k are attained for $\mathbf{t} = (k-2, 0, 0)$, $\mathbf{t} = (0, k-2, 0)$ and $\mathbf{t} = (0, 0, k-2)$, respectively. Intuitively this is so, as the strategy minimizing partitioning costs in isolation is to make the cheapest path through the partitioning loop execute as often as possible, which naturally leads to extreme choices for $\mathbf{t}$. It then depends on the actual numbers, where the total costs are minimized. It is thus not possible to minimize all cost measures at once, and the rivaling effects described above make it hard to reason about optimal parameters merely on a qualitative level. The number of executed Bytecode instructions is certainly more closely related to actual running time than the pure number of comparisons and swaps, while it remains platform independent and deterministic.[ii] We hope that the sensitivity of the optimal sampling parameter to the chosen cost measure renews the interest in instruction-level analysis in the style of Knuth. Focusing only on abstract cost measures leads to *suboptimal* choices in Yaroslavskiy's Quicksort!

It is interesting to note in this context that the implementation in Oracle's Java 7 runtime library — which uses $\mathbf{t} = (1, 1, 1)$ — executes asymptotically *more* Bytecodes (on random permutations) than $Y^w_{\mathbf{t}}$ with $\mathbf{t} = (0, 1, 2)$, despite using the same sample size $k = 5$. Whether this also results in a performance gain in practice, however, depends on details of the runtime environment (Wild et al., 2013c).

Continuous ranks. It is natural to ask for the optimal *relative ranks* of P and Q if we are not constrained by the discrete nature of pivot sampling. In fact, one might want to choose the sample size depending on those optimal relative ranks to find a discrete order statistic that falls close to the continuous optimum.

We can compute the optimal relative ranks by considering the limiting behavior of $Y^w_{\mathbf{t}}$ as $k \to \infty$. Formally, we consider the following family of algorithms: let $(t_l^{(j)})_{j\in\mathbb{N}}$ for $l = 1, 2, 3$ be three sequences of non-negative integers and set $k^{(j)} := t_1^{(j)} + t_2^{(j)} + t_3^{(j)} + 2$ for every $j \in \mathbb{N}$. Assume that we have $k^{(j)} \to \infty$ and $t_l^{(j)}/k^{(j)} \to \tau_l$ with $\tau_l \in [0, 1]$ for $l = 1, 2, 3$ as $j \to \infty$. Note that we have $\tau_1+\tau_2+\tau_3 = 1$ by definition. For each $j \in \mathbb{N}$, we can apply Theorem 4.1 for $Y^w_{\mathbf{t}^{(j)}}$ and then consider the limiting behavior of the total costs for $j \to \infty$.[iii] For $\mathrm{H}(\mathbf{t})$, equation (4.2) shows convergence to the entropy function $\mathrm{H}^*(\boldsymbol{\tau}) = -\sum_{l=1}^{3} \tau_l \ln(\tau_l)$ and for the numerators a_C, a_S and a_{BC}, it is easily seen that

$$a_C^{(j)} \;\to\; a_C^* \;:=\; 1 + \tau_2 + (2\tau_1 + \tau_2)\tau_3\,, \tag{8.1}$$

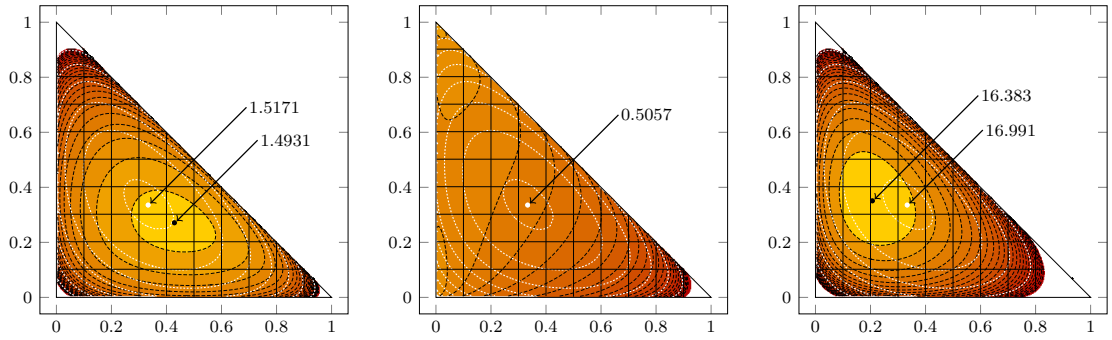
$$a_S^{(j)} \;\to\; a_S^* \;:=\; \tau_1 + (\tau_1 + \tau_2)\tau_3\,, \tag{8.2}$$

$$a_{BC}^{(j)} \;\to\; a_{BC}^* \;:=\; 10 + 13\tau_1 + 5\tau_2 + (\tau_1 + \tau_2)(\tau_1 + 11\tau_3)\,. \tag{8.3}$$

Together, the overall number of comparisons, swaps and Bytecodes converge to $a_C^*/\mathrm{H}^*(\boldsymbol{\tau})$, $a_S^*/\mathrm{H}^*(\boldsymbol{\tau})$ resp. $a_{BC}^*/\mathrm{H}^*(\boldsymbol{\tau})$; see Figure 3 for plots. We could not find a way to compute the minima of these functions analytically. However, all three functions have isolated minima that can be approximated well by numerical methods.

[ii] Counting the number of executed Bytecode instructions still ignores many important effects on actual running time, *e. g.*, costs of branch mispredictions in pipelined execution, cache misses and the influence of just-in-time compilation.

[iii] Letting the sample size go to infinity implies non-constant overhead per partitioning step for our implementation, which is not negligible any more. For the analysis here, you can assume an oracle that provides us with the desired order statistic in $O(1)$.



(a) $a_C^*/\mathrm{H}^*(\boldsymbol{\tau})$ (b) $a_S^*/\mathrm{H}^*(\boldsymbol{\tau})$ (c) $a_{BC}^*/\mathrm{H}^*(\boldsymbol{\tau})$

Figure 3: Contour plots for the limits of the leading term coefficient of the overall number of comparisons, swaps and executed Bytecode instructions, as functions of $\boldsymbol{\tau}$. τ_1 and τ_2 are given on x- and y-axis, respectively, which determine τ_3 as $1 - \tau_1 - \tau_2$. Black dots mark global minima, white dots show the center point $\tau_1 = \tau_2 = \tau_3 = \frac{1}{3}$. (For swaps no minimum is attained in the open simplex, see main text). Black dashed lines are level lines connecting "equi-cost-ant" points, *i. e.* points of equal costs. White dotted lines mark points of equal entropy $\mathrm{H}^*(\boldsymbol{\tau})$.

The number of comparisons is minimized for $\boldsymbol{\tau}_C^* \approx (0.428846, 0.268774, 0.302380)$. For this choice, the expected number of comparisons is asymptotically $1.4931\, n \ln n$. For swaps, the minimum is not attained inside the open simplex, but for the extreme points $\boldsymbol{\tau}_S^* = (0, 0, 1)$ and $\boldsymbol{\tau}_S^{*\prime} = (0, 1, 0)$. The minimal value of the coefficient is 0, so the expected number of swaps drops to $o(n \ln n)$ for these extreme points. Of course, this is a very bad choice w. r. t. other cost measures, *e. g.*, the number of comparisons becomes quadratic, which again shows the limitations of tuning an algorithm to one of its basic operations in isolation. The minimal asymptotic number of executed Bytecodes of roughly $16.3833\, n \ln n$ is obtained for $\boldsymbol{\tau}_{BC}^* \approx (0.206772, 0.348562, 0.444666)$.

We note again that the optimal choices heavily differ depending on the employed cost measure and that the minima differ significantly from the symmetric choice $\boldsymbol{\tau} = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$.

9 Conclusion

In this paper, we gave the precise leading term asymptotic of the average costs of Quicksort with Yaroslavskiy's dual-pivot partitioning method and selection of pivots as arbitrary order statistics of a constant size sample. Our results confirm earlier empirical findings (Yaroslavskiy, 2010; Wild et al., 2013c) that the inherent asymmetries of the partitioning algorithm call for a systematic skew in selecting the pivots — the tuning of which requires a quantitative understanding of the delicate trade-off between partitioning costs and the distribution of subproblem sizes for recursive calls. Moreover, we have demonstrated that this tuning process is very sensitive to the choice of suitable cost measures, which firmly suggests a detailed analyses in the style of Knuth, instead of focusing on the number of comparisons and swaps only.

Future work. A natural extension of this work would be the computation of the linear term of costs, which is not negligible for moderate n. This will require a much more detailed analysis as sorting the samples and dealing with short subarrays contribute to the linear term of costs, but then allows to compute the optimal choice for w, as well. While in this paper only expected values were considered, the distribu-

tional analysis of Section 5 can be used as a starting point for analyzing the distribution of overall costs. Yaroslavskiy's partitioning can also be used in Quickselect (Wild et al., 2013a); the effects of generalized pivot sampling there are yet to be studied. Finally, other cost measures, like the number of symbol comparisons (Vallée et al., 2009; Fill and Janson, 2012), would be interesting to analyze.

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Analytic combinatorics of chord and hyperchord diagrams with k crossings

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Abstract. Using methods from Analytic Combinatorics, we study the families of perfect matchings, partitions, chord diagrams, and hyperchord diagrams on a disk with a prescribed number of crossings. For each family, we express the generating function of the configurations with exactly k crossings as a rational function of the generating function of crossing-free configurations. Using these expressions, we study the singular behavior of these generating functions and derive asymptotic results on the counting sequences of the configurations with precisely k crossings. Limiting distributions and random generators are also studied.

Keywords: Quasi-Planar Configurations — Chord Diagrams — Analytic Combinatorics — Generating Functions

1 Introduction

Quasi-planar chord diagrams. Let V be a set of n points on the unit circle. A *chord diagram* on V is a set of chords between points of V. We say that two chords *cross* when their relative interior intersect. The *crossing graph* of a chord diagram is the graph with a vertex for each chord and an edge between any two crossing chords. The enumeration properties of crossing-free (or planar) chord diagrams have been widely studied in the literature, see in particular the results of P. Flajolet and M. Noy in [FN99]. From the work of J. Touchard [Tou52] and J. Riordan [Rio75], we know a remarkable explicit formula for the distribution of crossings among all perfect matchings, which was exploited in [FN00] to derive, among other parameters, the limit distribution of the number of crossings for matchings with many chords.

A more recent trend studies chord diagrams with some but restricted crossings. The several ways to restrict their crossings lead to various notions of *quasi-planar chord diagrams*. Among others, it is interesting to study chord diagrams

(i) with at most k crossings, or
(ii) with no $(k+2)$-crossing (meaning $k+2$ pairwise crossing edges), or
(iii) where each chord crosses at most k other chords, or
(iv) which become crossing-free when removing at most k well-chosen chords.

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These conditions are natural restrictions on the crossing graphs of the chord diagrams. Namely, the crossing graphs have respectively (i) at most k edges, (ii) no $(k+2)$-clique, (iii) vertex degree at most k, and (iv) a vertex cover of size k. For $k=0$, all these conditions coincide and lead to crossing-free chord diagrams.

Families of $(k+2)$-crossing-free chord diagrams have been studied in recent literature. On the one hand, $(k+2)$-crossing-free matchings (as well as their $(k+2)$-nesting-free counterparts) were enumerated in [CDD$^+$07]. On the other hand, maximal $(k+2)$-crossing-free chord diagrams, also called $(k+1)$-triangulations, were enumerated in [Jon05], see also [PS09]. As far as we know, Conditions (i), (iii) and (iv), as well as other natural notions of quasi-planar chord diagrams, still remain to be studied in details. We focus in this paper on the Analytic Combinatorics of chord diagrams under Condition (i).

Rationality of generating functions. In this paper, we study enumeration and asymptotic properties for different families of configurations: perfect matchings, partitions, chord diagrams, and hyperchord diagrams (our results also extend to partitions and hyperchord diagrams with prescribed block sizes, see [PR13]). Examples of these configurations are represented in Figure 1.

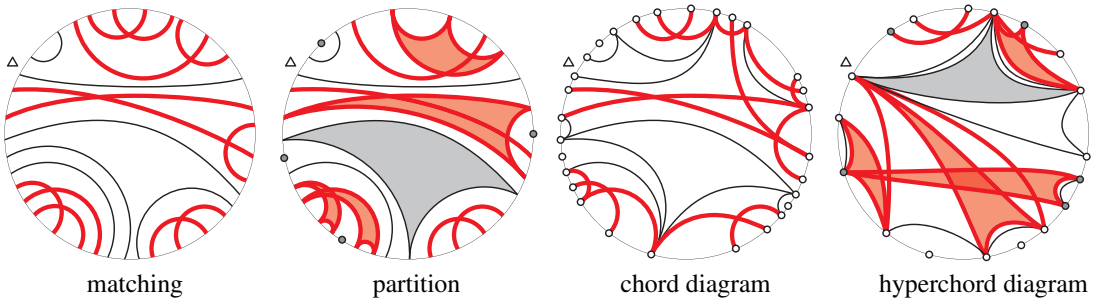

Fig. 1: The four families of (hyper)chord configurations studied in this paper. Their cores are highlighted in bold red.

Let $\mathcal{C}$ denote one of these families of configurations. To avoid handling symmetries, we insert a root in each configuration between two consecutive vertices, and we consider two rooted configurations C and C' of $\mathcal{C}$ as equivalent if there is a continuous bijective automorphism of the circle which sends the root, the vertices, and the (hyper)chords of C to that of C'. We focus on three parameters of the configurations of $\mathcal{C}$: their number n of vertices, their number m of (hyper)chords, and their number k of crossings. Note that for hyperchord diagrams and partitions, we count all crossings involving two chords contained in two distinct hyperchords. We denote by $\mathcal{C}(n,m,k)$ the set of configurations in $\mathcal{C}$ with n vertices, m (hyper)chords and k crossings, and we let $\mathbf{C}_k(x,y) := \sum_{n,m\in\mathbb{N}} |\mathcal{C}(n,m,k)|\, x^n y^m$ denote the generating function of the configurations in $\mathcal{C}$ with precisely k crossings. Our first result concerns the rationality of this function.

Theorem 1 *The generating function $\mathbf{C}_k(x,y)$ of configurations in $\mathcal{C}$ with exactly k crossings is a rational function of the generating function $\mathbf{C}_0(x,y)$ of planar configurations in $\mathcal{C}$ and of the variables x and y.*

The idea behind this result is to confine crossings of the configurations of $\mathcal{C}$ to finite subconfigurations. Namely, we define the *core configuration* $C^\star$ of a configuration $C \in \mathcal{C}$ to be the subconfiguration formed by all (hyper)chords of C involved in at least one crossing. The key observation is that

(i) there are only finitely many core configurations with k crossings, and
(ii) any configuration C of $\mathcal{C}$ with k crossings can be constructed from its core configuration $C^\star$ by inserting crossing-free subconfigurations in the connected components of the complement of $C^\star$ in the disk.

This translates in the language of generating functions to a rational expression of $\mathbf{C}_k(x,y)$ in terms of $\mathbf{C}_0(x,y)$ and its successive derivatives with respect to x, which in turn are rational in $\mathbf{C}_0(x,y)$ and the variables x and y. Similar decomposition ideas were used for example by E. Wright in his study of graphs with fixed excess [Wri77, Wri78], or more recently by G. Chapuy, M. Marcus, G. Schaeffer in their enumeration of unicellular maps on surfaces [CMS09].

Note that Theorem 1 extends a specific result of M. Bóna [Bón99] who proved that the generating function of the partitions with k crossings is a rational function of the generating function of the Catalan numbers. We note that his method was slightly different. The advantage of our decomposition scheme is to be sufficiently elementary and general to apply to the various families of configurations mentioned above.

Asymptotic analysis and random generation. From the expression of the generating function $\mathbf{C}_k(x,y)$ in terms of $\mathbf{C}_0(x,y)$, we can extract the asymptotic behavior of configurations in $\mathcal{C}$ with k crossings.

Theorem 2 *For $k \geq 1$, the number of configurations in $\mathcal{C}$ with k crossings and n vertices is*

$$[x^n]\,\mathbf{C}_k(x,1) \underset{n\to\infty}{=} \Lambda\, n^\alpha\, \rho^{-n}\,(1+o(1)),$$

for certain constants $\Lambda, \alpha, \rho \in \mathbb{R}$ depending on the family $\mathcal{C}$ and on the parameter k as follows.

family	*constant* Λ	*exponent* α	*singularity* ρ^{-1}	*Prop.*
matchings[(i)]	$\dfrac{\sqrt{2}\,(2k-3)!!}{4^{k-1}\,k!\,\Gamma\left(k-\frac{1}{2}\right)}$	$k-\dfrac{3}{2}$	2	*11*
partitions	$\dfrac{(2k-3)!!}{2^{3k-1}\,k!\,\Gamma\left(k-\frac{1}{2}\right)}$	$k-\dfrac{3}{2}$	4	*13*
chord diagrams	$\dfrac{\left(-2+3\sqrt{2}\right)^{3k}\sqrt{-140+99\sqrt{2}}\,(2k-3)!!}{2^{3k+1}\,(3-4\sqrt{2})^{k-1}\,k!\,\Gamma(k-\frac{1}{2})}$	$k-\dfrac{3}{2}$	$6+4\sqrt{2}$	*17*
hyperchord diagrams[(ii)]	$\simeq \dfrac{1.034^{3k}\;0.003655\,(2k-3)!!}{0.03078^{k-1}\,k!\,\Gamma(k-\frac{1}{2})}$	$k-\dfrac{3}{2}$	$\simeq 64.97$	*21*

From the rational expression of the generating function $\mathbf{C}_k(x,y)$, we also derive random generation schemes for the configurations in $\mathcal{C}$ with precisely k crossings, using the methods developed in [DFLS04].

Overview. Due to space limitation, we have decided to present the detailed analysis only for perfect matchings with k crossings, since we believe that it already gives the flavor of our results and illustrates our method, while remaining technically elementary. For the remaining families, we only report our results and skip the detailed analysis. We refer the interested reader to the long version of this paper [PR13].

(i) The asymptotic estimate for the number of matchings with n vertices is obviously only valid when n is even.
(ii) The expression of ρ^{-1} and Λ for hyperchord diagrams is obtained from approximations of roots of polynomials, and approximate evaluations of analytic functions. Details can be found in Propositions 19 and 21.

2 Perfect matchings

2.1 Perfect matchings and their cores

In this section, we consider the family $\mathcal{M}$ of perfect matchings with endpoints on the unit circle. Each perfect matching M of $\mathcal{M}$ is *rooted*: we mark (with the symbol $\triangle$) an arc of the circle between two endpoints of M. See Figure 1 (left). Let $\mathcal{M}(n,k)$ denote the set of matchings in $\mathcal{M}$ with n vertices and k crossings. We denote by $\mathbf{M}_k(x) := \sum_{n\in\mathbb{N}} |\mathcal{M}(n,k)|\, x^n$ the generating function of perfect matchings with exactly k crossings, where x encodes the number of vertices.

Let M be a perfect matching with some crossings. Our goal is to isolate the contribution of the chords of M involved in crossings from that of the chords of M with no crossings.

Definition 3 *A core matching is a perfect matching where each chord is involved in a crossing. It is a k-core matching if it has exactly k crossings. The core $M^\star$ of a perfect matching M is the submatching of M formed by all its chords involved in at least one crossing. See Figure 1 (left).*

Let K be a core matching. We let $n(K)$ denote its number of vertices and $k(K)$ denote its number of crossings. We call *regions* of K the connected components of the complement of K in the unit disk. A region has i *boundary arcs* if its intersection with the unit circle has i connected arcs. We let $n_i(K)$ denote the number of regions of K with i boundary arcs, and we set $\mathbf{n}(K) := (n_i(K))_{i\in[k(K)]}$ (all regions of K have at most $k(K)$ boundary arcs). Since a crossing only involves 2 chords, a k-core matching can have at most $2k$ chords. This immediately implies that there are only finitely many k-core matchings.

Definition 4 *We encode the finite list of all possible k-core matchings K and their parameters $n(K)$ and $\mathbf{n}(K) := (n_i(K))_{i\in[k]}$ in the k-core matching polynomial*

$$\mathbf{KM}_k(\mathbf{x}) := \mathbf{KM}_k(x_1,\dots,x_k) := \sum_{\substack{K \text{ } k\text{-core} \\ \text{matching}}} \frac{\mathbf{x}^{\mathbf{n}(K)}}{n(K)} := \sum_{\substack{K \text{ } k\text{-core} \\ \text{matching}}} \frac{1}{n(K)} \prod_{i\in[k]} {x_i}^{n_i(K)}.$$

Example 5 *The 7-core of the matching of Figure 1 (left) contributes to $\mathbf{KM}_7(\mathbf{x})$ as $\frac{1}{24}\,{x_1}^{17}{x_2}^2x_3$.*

Remark 6 *There is an efficient enumeration algorithm to generate all connected matchings (i.e. whose crossing graph is connected), from which we can easily compute the k-core matching polynomial $\mathbf{KM}_k(\mathbf{x})$. We refer to [PR13, Sections 2.2 and 2.3] for details on this algorithm.*

2.2 Generating function of matchings with k crossings

We study perfect matchings with k crossings focussing on their k-cores. For this, we consider the following weaker notion of rooting of perfect matchings. We say that a perfect matching with k crossings is *weakly rooted* if we have marked an arc between two consecutive vertices of its k-core. Note that a rooted perfect matching is automatically weakly rooted (the weak root marks the arc of the k-core containing the root of the matching), while a weakly rooted perfect matching corresponds to several rooted perfect matchings. To overcome this technical problem, we use the following rerooting argument.

Lemma 7 *Let K be a k-core with $n(K)$ vertices. The number $M_K(n)$ of rooted matchings on n vertices with core K and the number $\bar{M}_K(n)$ of weakly rooted matchings on n vertices with core K are related by*

$$n(K)M_K(n) = n\bar{M}_K(n).$$

Observe now that we can construct any perfect matching with k crossings by inserting crossing-free submatchings in the regions left by its k-core. From the k-core matching polynomial $\mathbf{KM}_k(\mathbf{x})$, we can therefore derive the following expression of the generating function $\mathbf{M}_k(x)$.

Proposition 8 *For any $k \geq 1$, the generating function $\mathbf{M}_k(x)$ of the rooted perfect matchings with k crossings is given by*

$$\mathbf{M}_k(x) = x\frac{d}{dx}\mathbf{KM}_k\left(x_i \leftarrow \frac{x^i}{(i-1)!}\frac{d^{i-1}}{dx^{i-1}}\left(x^{i-1}\mathbf{M}_0(x)\right)\right).$$

In particular, $\mathbf{M}_k(x)$ is a rational function of $\mathbf{M}_0(x)$ and x.

Proof: Consider a rooted crossing-free perfect matching M. We say that M is *i-marked* if we have placed $i-1$ additional marks between consecutive vertices of M. Note that we can place more than one mark between two consecutive vertices but that the root is always distinguishable from the other marks. Since we have $\binom{n+i-1}{i-1}$ possible ways to place these $(i-1)$ additional marks, the generating function of the i-marked crossing-free perfect matchings is given by

$$\frac{1}{(i-1)!}\frac{d^{i-1}}{dx^{i-1}}\left(x^{i-1}\mathbf{M}_0(x)\right).$$

Consider now a weakly rooted perfect matching M with $k \geq 1$ crossings. We decompose this matching into several submatchings as follows. On the one hand, the core $M^\star$ contains all crossings of M. This core is rooted by the root of M. On the other hand, each region R of $M^\star$ contains a (possibly empty) crossing-free submatching M_R. We root this submatching M_R as follows:

(i) if the root of M is not the region R, then M_R is just rooted by the root of M;

(ii) otherwise, M_R is rooted on the boundary arc of $M^\star$ just before the root of M in clockwise direction.

Moreover, we place additional marks on the remaining boundary arcs of the complement of R in the unit disk. We thus obtain a rooted i-marked crossing-free submatching M_R in each region R of $M^\star$ with i boundary arcs. Conversly, we can reconstruct the weakly rooted perfect matching M from its rooted core $M^\star$ and its rooted i-marked crossing-free submatchings M_R.

By this bijection, we thus obtain the generating function of weakly rooted perfect matchings with k crossings. From this generating function, and by application of Lemma 7, we derive the generating function $\mathbf{M}_k(x)$ of rooted perfect matchings with k crossings:

$$\begin{aligned}\mathbf{M}_k(x) &= \sum_{\substack{K \ k\text{-core} \\ \text{matching}}} \frac{x}{n(K)}\frac{d}{dx}x^{n(K)}\prod_{i\geq 1}\left(\frac{1}{(i-1)!}\frac{d^{i-1}}{dx^{i-1}}\left(x^{i-1}\mathbf{M}_0(x)\right)\right)^{n_i(K)} \qquad (1)\\ &= x\frac{d}{dx}\mathbf{KM}_k\left(x_i \leftarrow \frac{x^i}{(i-1)!}\frac{d^{i-1}}{dx^{i-1}}\left(x^{i-1}\mathbf{M}_0(x)\right)\right).\end{aligned}$$

Since $\mathbf{M}_0(x) = \frac{1-\sqrt{1-4x^2}}{2x^2}$ satisfies the functional equation $\mathbf{M}_0(x) = 1 + x^2\,\mathbf{M}_0(x)^2$, all its successive derivatives, and thus $\mathbf{M}_k(x)$, are rational in $\mathbf{M}_0(x)$ and x. □

Example 9 *Since $\mathbf{KM}_1(\mathbf{x}) = \frac{1}{4}\,x_1{}^4$, we obtain the coefficients of $\mathbf{M}_1(x)$ (see Seq. A002694 in OIES):*

$$\mathbf{M}_1(x) = \frac{x^4\,\mathbf{M}_0(x)^4}{1-2x^2\,\mathbf{M}_0(x)} = \frac{\left(1-\sqrt{1-4x^2}\right)^4}{16x^4\sqrt{1-4x^2}} = x^4 + 6\,x^6 + 28\,x^8 + 120\,x^{10} + 495\,x^{12} + 2002\,x^{14}\ldots$$

2.3 Asymptotic analysis

We now describe the asymptotic behavior of the number of perfect matchings with $k \geq 1$ crossings. The method consists in studying the asymptotic behavior of $\mathbf{M}_0(x)$ and of all its derivatives around their dominant singularities, and to exploit the rational expression of $\mathbf{M}_k(x)$ in terms of $\mathbf{M}_0(x)$ and x given in Proposition 8. Along the way, we naturally study which k-cores have the main asymptotic contributions. For that, we need the following lemma, whose detailed proof can be found in [PR13, Lemma 2.13].

Lemma 10 *The following assertions are equivalent for an (unrooted) k-core matching K:*
(i) K belongs to the family of the k-core matchings whose first five elements are shown in Figure 2.
(ii) $n_1(K) = 3k$, $n_k(K) = 1$ and $n_i(K) = 0$ for all other values of i (here, $k \geq 2$).
(iii) K maximizes $n_1(K)$ among all possible k-core matchings (here, $k \geq 3$).
(iv) K maximizes the potential $\phi(K) := \sum_{i>1}(2i-3)\, n_i(K)$ among all possible k-core matchings.
We call a k-core matching maximal *if it satisfies these conditions.*

Fig. 2: Maximal core matchings (unrooted) for $k = 1, \dots, 5$.

Proposition 11 *For any $k \geq 1$, the number of perfect matchings with k crossings and $n = 2m$ vertices is*

$$[x^{2m}]\, \mathbf{M}_k(x) \underset{m\to\infty}{=} \frac{(2k-3)!!}{2^{k-1}\, k!\, \Gamma\big(k-\frac{1}{2}\big)}\, m^{k-\frac{3}{2}}\, 4^m\, (1+o(1)),$$

where $(2k-3)!! := (2k-3)\cdot(2k-5)\cdots 3\cdot 1$ and $(-1)!! = 1$.

Proof: We assume here that $k \geq 2$ (the case $k = 1$ can be derived from a direct analysis of the expression of $\mathbf{M}_1(x)$ given in Example 9). We first study the asymptotic behavior of $\mathbf{M}_0(x)$ and of all its derivatives around their dominant singularities. The generating function $\mathbf{M}_0(x)$ defines an analytic function around the origin. Its dominant singularities are located at $x = \pm\frac{1}{2}$. Denoting by $X_+ := \sqrt{1-2x}$, the singular expansions of $\mathbf{M}_0(x)$ and its derivative around $x = \frac{1}{2}$ are

$$\mathbf{M}_0(x) \underset{x\sim\frac{1}{2}}{=} 2 - 2\sqrt{2}\, X_+ + O\left({X_+}^2\right), \qquad \frac{d}{dx}\mathbf{M}_0(x) \underset{x\sim\frac{1}{2}}{=} 2\sqrt{2}\, {X_+}^{-1} + O(1),$$

$$\text{and} \qquad \frac{d^i}{dx^i}\mathbf{M}_0(x) \underset{x\sim\frac{1}{2}}{=} 2\sqrt{2}\,(2i-3)!!\, {X_+}^{1-2i} + O\left({X_+}^{2-2i}\right) \qquad \text{for all } i \geq 2,$$

where $(2i-3)!! := (2i-3)\cdot(2i-5)\cdots 3\cdot 1$. These expansions are valid in a dented domain at $x = \frac{1}{2}$, [FS09].

We now exploit the expression of the generating function $\mathbf{M}_k(x)$ given by Equation (1) in the proof of Proposition 8. The dominant singularities of $\mathbf{M}_k(x)$ are located at $x = \pm\frac{1}{2}$. We provide the full analysis

around $x = \frac{1}{2}$, the computation for $x = -\frac{1}{2}$ being similar. For conciseness in the following expressions, we set by convention $(-1)!! = 1$. We therefore obtain:

$$\begin{aligned}
\mathbf{M}_k(x) &= x\frac{d}{dx} \sum_{\substack{K \ k\text{-core} \\ \text{matching}}} \frac{1}{n(K)} \prod_{i\geq 1} \left(\frac{x^i}{(i-1)!} \frac{d^{i-1}}{dx^{i-1}} \big(x^{i-1}\mathbf{M}_0(x)\big) \right)^{n_i(K)} \\
&\underset{x\sim\frac{1}{2}}{=} \frac{1}{2}\frac{d}{dx} \sum_{\substack{K \ k\text{-core} \\ \text{matching}}} \frac{1}{n(K)} \prod_{i>1} \left(\frac{\sqrt{2}\,(2i-5)!!}{4^{i-1}\,(i-1)!}\, {X_+}^{3-2i} + O\left({X_+}^{4-2i}\right) \right)^{n_i(K)} \\
&\underset{x\sim\frac{1}{2}}{=} \frac{1}{2} \sum_{\substack{K \ k\text{-core} \\ \text{matching}}} \frac{\phi(K)}{n(K)} \prod_{i>1} \left(\frac{\sqrt{2}\,(2i-5)!!}{4^{i-1}\,(i-1)!} \right)^{n_i(K)} {X_+}^{-\phi(K)-2} + O\left({X_+}^{-\phi(K)-1}\right),
\end{aligned}$$

where $\phi(K) := \sum_{i>1}(2i-3)\,n_i(K)$ is the potential function introduced in Lemma 10. Observe that in order to obtain the second equality, we used the fact that $k > 1$, and thus, that there exists k-cores K such that $n_i(K) \neq 0$ when $i > 1$. Combining Lemma 10 and the Transfer Theorem of singularity analysis [FO90], we conclude that the main contribution in the asymptotic of the previous sum arises from maximal k-cores, as they maximize the value $2 + \phi(K)$. By Lemma 10, there are exactly 4 rooted maximal k-cores with $n_1(K) = 3k$, $n_k(K) = 1$, $n(K) = 4k$, and $\phi(K) = 2k - 3$. Hence,

$$\begin{aligned}
[x^n]\,\mathbf{M}_k(x) &\underset{x\sim\frac{1}{2}}{=} [x^n]\,\frac{1}{2} \sum_{\substack{K \ k\text{-core} \\ \text{matching}}} \frac{\phi(K)}{n(K)} \prod_{i>1} \left(\frac{\sqrt{2}\,(2i-5)!!}{4^{i-1}\,(i-1)!} \right)^{n_i(K)} {X_+}^{-\phi(K)-2} + O\left({X_+}^{-\phi(K)-1}\right) \\
&\underset{x\sim\frac{1}{2}}{=} \frac{2\sqrt{2}\,(2k-3)!!}{4^k\,k!}\,[x^n]\ \sqrt{1-2x}^{\,1-2k} + O\left((1-2x)^{1-k}\right) \\
&\underset{n\to\infty}{=} \frac{2\sqrt{2}\,(2k-3)!!}{4^k\,k!\,\Gamma\left(k-\frac{1}{2}\right)}\, n^{k-\frac{3}{2}}\, 2^n\,(1+o(1)),
\end{aligned}$$

where the last equality is obtained by application of the Transfer Theorem of singularity analysis [FO90].

Finally, we obtain the stated result by adding the expressions obtained when studying $\mathbf{M}_k(x)$ around $x = \frac{1}{2}$ and $x = -\frac{1}{2}$. In fact, one can check that the asymptotic estimate of $[x^n]\,\mathbf{M}_k(x)$ around $x = -\frac{1}{2}$ is the same but with an additional multiplicative constant $(-1)^n$. Consequently, the contribution is equal to 0 when n is odd and to the estimate in the statement when n is even. □

2.4 Random generation

The composition scheme presented in Proposition 8 can also be exploited in order to provide Boltzmann samplers for random generation of perfect matchings with k crossings. Throughout this section we consider a positive real number $\theta < \frac{1}{2}$, which acts as a "control-parameter" for the random sampler (see [DFLS04] for further details). The Boltzmann sampler works in three steps:

(i) We first decide which is the core of our random object.
(ii) Once this core is chosen, we complete the matching by means of non-crossing matchings.
(iii) Finally, we place the root of the resulting perfect matching with k crossings.

We start with the choice of the k-core. For each k-core K, let $\mathbf{M}_K(x)$ denote the generating function of matchings with k crossings and whose k-core is K, where x marks as usual the number of vertices. Note that this generating function is computed as in Proposition 8, using only the contribution of the k-core K. Therefore, we have

$$\mathbf{M}_k(x) = \sum_{\substack{K \ k\text{-core} \\ \text{matching}}} \mathbf{M}_K(x)\,.$$

This sum defines a probability distribution as follows: once fixed the parameter θ, let $p_K = \frac{\mathbf{M}_K(\theta)}{\mathbf{M}_k(\theta)}$. This set of values defines a discrete probability distribution $\{p_K\}_{\substack{K \ k\text{-core} \\ \text{matching}}}$, which can be easily simulated.

Once we have fixed the core of the random matching, we continue in the second step filling in its regions with crossing-free perfect matchings. For this purpose it is necessary to have a procedure to generate crossing-free perfect matchings, namely $\Gamma\mathbf{M}_0(\theta)$. As $\mathbf{M}_0(\theta)$ satisfies the recurrence relation $\mathbf{M}_0(\theta) = 1 + \theta^2\mathbf{M}_0(\theta)^2$, a Boltzmann sampler $\Gamma\mathbf{M}_0(\theta)$ can be defined in the following way. Let $p = \frac{1}{\Gamma\mathbf{M}_0(\theta)}$. Then, using the language of [DFLS04],

$$\Gamma\mathbf{M}_0(\theta) \coloneqq \mathrm{Bern}(p) \longrightarrow \varnothing \mid (\Gamma\mathbf{M}_0(\theta)\ ,\ \bullet - \bullet\,,\ \Gamma\mathbf{M}_0(\theta)),$$

where $\bullet - \bullet$ means that the Boltzmann sampler is generating a single chord (or equivalently, two vertices in the border of the circle). This Boltzmann sampler is defined when $\theta < \frac{1}{2}$, in which case the defined branching process is subcritical. In such situation the algorithm stops in finite expected time, see [DFLS04].

Once this random sampler is performed, we can deal with a term of the form $\frac{d^{i-1}}{dx^{i-1}}x^{i-1}\mathbf{M}_0(\theta)$. Indeed, once a random crossing-free perfect matching $\Gamma\mathbf{M}_0(\theta)$ of size $n(\Gamma\mathbf{M}_0(\theta))$ is generated, there exist

$$\binom{n(\Gamma\mathbf{M}_0(\theta)) + i - 1}{i-1}$$

i-marked crossing-free perfect matchings arising from $\Gamma\mathbf{M}_0(\theta)$. Hence, with uniform probability we can choose one of these i-marked crossing-free perfect matchings. As this argument follows for each choice of i, and $\mathbf{KM}_K(\mathbf{x})$ is a polynomial, we can combine the generator of i-marked crossing-free diagrams with the Boltzmann sampler for the cartesian product of combinatorial classes (recall that we need to provide the substitution $x_i \leftarrow \frac{x^i}{(i-1)!}\frac{d^{i-1}}{dx^{i-1}}\left(x^{i-1}\mathbf{M}_0(x)\right)$).

Finally, we need to apply the root operator, which can be done by means of similar arguments as in the case of i-marked crossing-free diagrams.

Concerning the statistics of the random variable N corresponding to the size of the element generated by means of the previous random sampler, as it is shown in [DFLS04], the expected value $\mathbb{E}[N]$ and the variance $\mathbb{V}\mathrm{ar}[N]$ of the random variable N satisfy

$$\mathbb{E}[N] = \theta\,\frac{\mathbf{M}_k'(\theta)}{\mathbf{M}_k(\theta)} \qquad \text{and} \qquad \mathbb{V}\mathrm{ar}[N] = \frac{\theta^2(\mathbf{M}_k''(\theta)\,\mathbf{M}_k(\theta) - \theta\,\mathbf{M}_k'(\theta)^2) + \theta\,\mathbf{M}_k'(\theta)}{\mathbf{M}_k(\theta)^2}.$$

Hence, when θ tends to $\frac{1}{2}$, the expected value of the generated element tends to infinity, and the variance for the expected size also diverges.

3 Extension to other families of chord diagrams

3.1 Partitions

We first extend our results to the family $\mathcal{P}$ of partitions of point sets on the unit circle. See Figure 1. As before, the partitions are rooted by a mark on an arc between two vertices. A *crossing* between two blocks U, V of a partition P is a pair of crossing chords u_1u_2 and v_1v_2 where $u_1, u_2 \in U$ and $v_1, v_2 \in V$. We count crossings with multiplicity: two blocks U, V cross as many times as the number of such pairs of crossing chords among U and V. Note that perfect matchings are particular partitions where all blocks have size 2. Applying the same method as in Section 2.2, we obtain an expression of the generating function $\mathbf{P}_k(x, y)$ of partitions with k crossings in terms of the k-core partition polynomial $\mathbf{KP}_k(\mathbf{x}, y)$.

Proposition 12 *For any $k \geq 1$, the generating function $\mathbf{P}_k(x, y)$ of partitions with k crossings is given by*

$$\mathbf{P}_k(x, y) = x\frac{d}{dx}\mathbf{KP}_k\left(x_i \leftarrow \frac{x^i}{(i-1)!}\frac{d^{i-1}}{dx^{i-1}}\big(x^{i-1}\mathbf{P}_0(x, y)\big), y\right).$$

In particular, $\mathbf{P}_k(x, y)$ is a rational function of $\mathbf{P}_0(x, y)$ and x.

From this expression, we can extract as in Section 2.3 asymptotic estimates for the number of partitions with k crossings, and we can as well construct efficient random generators as in Section 2.4.

Proposition 13 *For any $k \geq 1$, the number of partitions with k crossings and n vertices is*

$$[x^n]\,\mathbf{P}_k(x, 1) \underset{n\to\infty}{=} \frac{(2k-3)!!}{2^{3k-1}\,k!\,\Gamma\big(k-\frac{1}{2}\big)}\,n^{k-\frac{3}{2}}\,4^n\,(1+o(1)).$$

Remark 14 *Our results on matchings and partitions can even be extended to analyze the generating function $\mathbf{P}_k^S(\mathbf{x}, y)$ of partitions with k crossings and whose block sizes all belong to S. In contrast to Proposition 12 which can be directly adapted to this context, the asymptotic analysis of $\mathbf{P}_k^S(\mathbf{x}, y)$ involves more technical tools, including the theory of A. Meir and J. Moon on the singular behavior of generating functions defined by a smooth implicit function schema [MM89]. See [PR13, Section 2.10].*

3.2 Chord diagrams

We now consider the family $\mathcal{D}$ of all chord diagrams on the unit circle. Remember that a chord diagram is given by a set of vertices on the unit circle, and a set of chords between them. In particular, we allow isolated vertices, as well as several chords incident to the same vertex, but not multiple chords with the same two endpoints. We are interested in the generating function $\mathbf{D}_k(x, y)$ of chord diagrams with k crossings. The generating function $\mathbf{D}_0(x, y)$ of crossing-free chord diagrams was studied in [FN99].

Proposition 15 ([FN99, Equation (22)]) *The generating function $\mathbf{D}_0(x, y)$ of crossing-free chord diagrams satisfies the functional equation*

$$y\,\mathbf{D}_0(x, y)^2 + \big(x^2(1+y) - x(1+2y) - 2y\big)\,\mathbf{D}_0(x, y) + x(1+2y) + y = 0.$$

Therefore, all derivatives $\frac{d^i}{dx^i}\mathbf{D}_0(x, y)$ are rational functions in $\mathbf{D}_0(x, y)$ and x. Moreover, we have

$$\mathbf{D}_0(x, 1) \underset{x\sim\rho}{=} \alpha - \beta\sqrt{1-\rho^{-1}x} + O(1-\rho^{-1}x),$$

where $\rho^{-1} = 6 + 4\sqrt{2}$, $\alpha = -1 + 3\frac{\sqrt{2}}{2}$, *and* $\beta = \frac{1}{2}\sqrt{-140+99\sqrt{2}}$.

As for matchings, we can construct any chord diagram with k crossings by inserting crossing-free subdiagrams in the regions left by its k-core. We can therefore derive the following expression for the generating function $\mathbf{D}_k(x,y)$ of diagrams with k crossings, in terms of the generating function $\mathbf{D}_0(x,y)$ of crossing-free diagrams, of the k-core diagram polynomial $\mathbf{KD}_k(x,y)$, and of the polynomials

$$\mathbf{D}_0^n(y) := [x^n]\,\mathbf{D}_0(x,y) \qquad \text{and} \qquad \mathbf{D}_0^{\leq p}(x,y) := \sum_{n\leq p} \mathbf{D}_0^n(y)\,x^n = \sum_{\substack{n\leq p\\ m\geq 0}} |\mathcal{D}(n,m,0)|\,x^n y^m.$$

Proposition 16 *For any $k \geq 1$, the generating function $\mathbf{D}_k(x,y)$ of chord diagrams with k crossings is given by*

$$\mathbf{D}_k(x,y) = x\frac{d}{dx}\mathbf{KD}_k\left(x_{0,j} \leftarrow \frac{\mathbf{D}_0^j(y)}{x^j},\ x_{i,j} \leftarrow \frac{x^i}{(i-1)!}\frac{d^{i-1}}{dx^{i-1}}\frac{\mathbf{D}_0(x,y)-\mathbf{D}_0^{\leq i+j}(x,y)}{x^{i+j+1}},\ y\right).$$

In particular, $\mathbf{D}_k(x,y)$ is a rational function of $\mathbf{D}_0(x,y)$ and x.

Similarly to our asymptotic analysis in Section 2.3, we can obtain asymptotic results for the number of chord diagrams with k crossings, in terms of the constants ρ, α, and β defined in Proposition 15. Random generators can as well be constructed, see [PR13, Section 3.6].

Proposition 17 *For any $k \geq 1$, the number of chord diagrams with k crossings and n vertices is*

$$[x^n]\,\mathbf{D}_k(x,1) \underset{n\to\infty}{=} \frac{\alpha^{3k}\,\beta\,(2k-3)!!}{(2\rho)^{k-1}\,k!\,\Gamma(k-\frac{1}{2})}\,n^{k-\frac{3}{2}}\,\rho^{-n}\,(1+o(1)).$$

3.3 Hyperchord diagrams

As from matchings to partitions, we can finally extend our results from chord diagrams to hyperchord diagrams. A *hyperchord* is the convex hull of finitely many points of the unit circle. Given a point set V on the circle, a *hyperchord diagram* on V is a set of hyperchords with vertices in V. Note that we allow isolated vertices in hyperchord diagrams. As for partitions, a *crossing* between two hyperchords U, V is a pair of crossing chords u_1u_2 and v_1v_2, with $u_1, u_2 \in U$ and $v_1, v_2 \in V$. We consider the family $\mathcal{H}$ of hyperchord diagrams, and we want to analyze the generating function $\mathbf{H}_k(x,y)$ of hyperchord diagrams with k crossings, counted with multiplicities. As for chord diagrams, our first step is to study the generating function $\mathbf{H}_0(x,y)$ of crossing-free hyperchord diagrams, extending the results of P. Flajolet and M. Noy for chord diagrams [FN99] that we presented in Proposition 15.

Proposition 18 *The generating function $\mathbf{H}_0(x,y)$ of crossing-free hyperchord diagrams satisfies the functional equation*

$$p_3(x,y)\,\mathbf{H}_0(x,y)^3 + p_2(x,y)\,\mathbf{H}_0(x,y)^2 + p_1(x,y)\,\mathbf{H}_0(x,y) + p_0(x,y) = 0,$$

where

$$\begin{aligned}
p_0(x,y) :=& -2x^2 - x + 2xy^3 + y^2 + x^2y^4 - 7x^2y - 7x^2y^2 - x^2y^3 - 3xy,\\
p_1(x,y) :=& -2x^3 - 2x^3y^4 - 8x^3y + 2x - 3y^2 - 12x^3y^2 - 8x^3y^3\\
&+ 6xy - x^2y^4 + x^2 + 4x^2y + 4x^2y^2 - 4xy^3,\\
p_2(x,y) :=& x^2y^3 + x^2 + 3x^2y^2 - x - 3xy + 2xy^3 + 3x^2y + 3y^2,\\
p_3(x,y) :=& -y^2.
\end{aligned}$$

We use this functional equation to derive the asymptotic behavior of $\mathbf{H}_0(x, y)$.

Proposition 19 *The smallest singularity of the generating function $\mathbf{H}_0(x, 1)$ of crossing-free hyperchord diagrams is located at the smallest real root $\rho \simeq 0.015391$ of the polynomial*

$$R(x) := 256\,x^4 - 768\,x^3 + 736\,x^2 - 336\,x + 5.$$

Moreover, when y varies uniformly in a small neighborhood of 1, the singular expansion of $\mathbf{H}_0(x, y)$ is

$$\mathbf{H}_0(x, y) \underset{y\sim 1}{=} h_0(y) - h_1(y)\sqrt{1 - \frac{x}{\rho(y)}} + O\left(1 + \frac{x}{\rho(y)}\right),$$

valid in a domain dented at $\rho(y)$ (for each choice of y), where $h_0(y)$, $h_1(y)$ and $\rho(y)$ are analytic functions around $y = 1$, with $\rho(1) = \rho \simeq 0.015391$, $h_0(1) \simeq 1.034518$ and $h_1(1) \simeq 0.00365515$.

Using a similar method as in Section 2.2, we obtain the following expression of the generating function $\mathbf{H}_k(x, y)$ of hyperchord diagrams with k crossings, in terms of the k-core hyperchord diagram polynomial $\mathbf{KH}_k(\mathbf{x}, y)$, and of the polynomials

$$\mathbf{H}_0^n(y) := [x^n]\,\mathbf{H}_0(x, y) \qquad \text{and} \qquad \mathbf{H}_0^{\leq p}(x, y) := \sum_{n\leq p} \mathbf{H}_0^n(y)\,x^n = \sum_{\substack{n\leq p\\ m\geq 0}} |\mathcal{H}(n, m, 0)|\,x^n y^m.$$

Proposition 20 *For any $k \geq 1$, the generating function $\mathbf{H}_k(x, y)$ of the hyperchord diagrams with k crossings is given by*

$$\mathbf{H}_k(x, y) = x\frac{d}{dx}\mathbf{KH}_k\left(x_{0,j} \leftarrow \frac{\mathbf{H}_0^j(y)}{x^j},\ x_{i,j} \leftarrow \frac{x^i}{(i-1)!}\frac{d^{i-1}}{dx^{i-1}}\frac{\mathbf{H}_0(x, y) - \mathbf{H}_0^{\leq i+j}(x, y)}{x^{i+j+1}},\ y\right).$$

In particular, $\mathbf{H}_k(x, y)$ is a rational function of the function $\mathbf{H}_0(x, y)$ and of the variables x and y.

Finally, using the expression of the generating function $\mathbf{H}_k(x, y)$ given by Proposition 20, we can derive the asymptotic behavior of the number of hyperchord diagrams with k crossings. The analysis is identical to that of the proof of Proposition 17.

Proposition 21 *For any $k \geq 1$, the number of hyperchord diagrams with k crossings and n vertices is*

$$[x^n]\,\mathbf{D}_k(x, 1) \underset{n\to\infty}{=} \frac{h_0(1)^{3k}\,h_1(1)\,(2k-3)!!}{(2\rho)^{k-1}\,k!\,\Gamma(k-\frac{1}{2})}\,n^{k-\frac{3}{2}}\,\rho^{-n}\,(1 + o(1)),$$

where $\rho \simeq 0.015391$ is the smallest real root of $R(x) := 256\,x^4 - 768\,x^3 + 736\,x^2 - 336\,x + 5$, and where $h_0(1) \simeq 1.034518$ and $h_1(1) \simeq 0.00365515$.

Remark 22 *Our results on chord and hyperchord diagrams can as well be extended to analyze the generating function $\mathbf{H}_k^S(\mathbf{x}, y)$ of hyperchord diagrams with k crossings and whose hyperchord sizes all belong to S, although the results are more difficult to express. We refer the reader to [PR13, Section 3.8].*

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The Ising model on graphs: grammar and applications to bipartite enumeration

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Abstract. We adapt the grammar introduced by Chapuy, Fusy, Kang and Shoilekova to study the Ising model on graphs which are defined by their 3-connected components. This approach permits to encode simultaneously counting formulas for the graph family under study as well as the generating function for the corresponding bipartite family of graphs. In particular, using our approach it is possible to avoid the often encountered difficult integration step which appears when relating the generating function of networks and the generating function of 2-connected graphs.

As a first application of our method, we asymptotically enumerate labelled bipartite series-parallel graphs with n vertices, and we study the probability that a bipartite series-parallel graph of size n chosen uniformly at random from all object of size n is connected.

Keywords: graph enumeration, analytic combinatorics, singularity analysis

1 Introduction

There has been a growing interest in the enumeration of families of labelled graphs in the last twenty years. An important breakthrough was achieved in this area in [GN09], where the authors were able to asymptotically count the number of labelled planar graphs on n vertices. The methods developed in their work have been applied very successfully to other families of graphs ([BGKN07, CFG$^+$11, GN09, GNR13]). In more applied terms, these results yield efficient uniform random generators for labelled planar graphs [Fus09], based on Boltzmann samplers [DFLS04, FFP07].

The results on planar graphs are based on generating function methods and analytic tools, joint with previously obtained results on the map enumeration setting. A *map* is a connected planar graph which is embedded in the plane, and a graph is *c-(vertex)-connected* if we are required to remove at least c vertices before the graph is disconnected. In general, when enumerating c-connected graphs or maps with c being a small constant it is natural to proceed from 3-connected to 2-connected, and later from 2-connected to connected structures where graphical decomposition theorems are represented by functional compositions of the corresponding generating functions. Using techniques from map enumeration as well

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as Whitney's Theorem (which tells us that any 3-connected planar graph has a unique embedding on the sphere [Die05, Theorem 4.3.2]) 2-connected labelled planar graphs were counted asymptotically for the first time in [BGW00]. This was a crucial step in the enumeration of planar graphs as well as other graph classes.

In contrast to all the previous research, less is known about enumerative results of the corresponding families of bipartite graphs. The bipartite condition introduces technical difficulties, including the integration step between networks and 2-connected graphs. Solving the integration step was one of the most crucial contributions of [GN09]. As a first step to circumvent this difficulty for the enumeration of bipartite graphs, we present here an extension of a grammar first presented in [CFKS08] (see also [GLLW09] for a similar treatment using the language of the theory of species).

The main idea behind the grammar is to avoid the integration step (or, in combinatorial terms, the unrooting step) by a clever application of the Dissymmetry Theorem for trees. The Dissymmetry Theorem itself provides a way to unroot special, tree-like structures and we refer to [BLL98] for more details. As a first application we use our grammar to asymptotically enumerate the number of labelled bipartite series-parallel graphs with n vertices as well as their structure (number of components). In particular, we obtain precise expressions for the order of magnitude of the number of bipartite series-parallel graphs on n vertices. This is the first time that a non-trivial bipartite planar family of graphs is enumerated and a first step towards the study of bipartite planar graphs from a combinatorial, analytic and probabilistic point of view.

More generally, our results should extend to bipartite families of so-called *subcritical* graph families (see [DFK$^+$11] for a technical definition) and thus providing a precise asymptotic picture of the structural properties of graphs sampled randomly from such bipartite families. Amongst others these parameter would include the expected number of edges and the number of cut-vertices.

Outline: In the following (Section 2) we introduce some notations and definitions before deducing the grammar for 2-coloured closed classes of graphs in Section 3. Subsequently in Section 4 we apply this grammar to the class of bipartite series-parallel graphs and obtain explicit expressions for the corresponding generating functions. Finally, in Section 5 we analyse these generating functions in order to asymptotically count bipartite series-parallel graphs and to analyse their asymptotic structure (number of components). In Section 6 we describe future work and further research directions.

2 Preliminaries

We consider simple graphs on the vertex set $\{1, \dots, n\}$. A set of graphs is a *class*, if it is closed under isomorphisms. Following [GNR13], a class $\mathcal{G}$ of graphs is *closed* if $G \in \mathcal{G}$ if and only if every 3-connected component of G is in $\mathcal{G}$. A closed class is also sometimes referred to as *stable under Tutte's decomposition*, see [CFKS08]. A graph is *bipartite* if and only if it is properly 2-colourable, which means that there exists a 2-colouring of the vertices such that two vertices of the same colour are not adjacent. Equivalently a graph is bipartite if and only if all cycles have even length.

We are going to define our main model by colouring vertices using two colours. We use vertex colouring as an intermediate tool in order to distinguish between two types of edges. More precisely, a 2-coloured vertex graph defines two types of edges: *monochromatic* and *non-monochromatic*, depending on whether the end-vertices have the same colour or not (non-monochromatic edges are also usually called *frustrated*). Notice that for any 2-coloured vertex graph a permutation of the two colours does not change the edge

type. This last observation is crutial in order to forget about the colours of the vertices, and consider only the type of edges that are defined.

Let $\mathcal{G}$ be a class of labelled graphs where edges are either *monochromatic* or *frustrated*. We observe that bipartite graphs in $\mathcal{G}$ correspond to the graphs in $\mathcal{G}$ where all edges are frustrated. We will usually call this edge colouring model the *Ising model* over the graph family $\mathcal{G}$ due to its connections with the usual Ising model in statistical physics (see for instance [BFG07, BMS, BBM11]).

Let g_{n,k_1,k_2} be the number of graphs in the coloured class $\mathcal{G}$ on n labelled vertices with k_1 frustrated edges and k_2 monochromatic edges. The generating function of all graphs in the labelled class $\mathcal{G}$ where x marks the number of vertices, y_1 marks the number of non-monochromatic edges and y_2 marks the number of monochromatic edges is defined as

$$G(x, y_1, y_2) = \sum_{n,k_1,k_2} g_{n,k_1,k_2} y_1^{k_1} y_2^{k_2} \frac{x^n}{n!}.$$

Denote by $\bar{\mathcal{G}} \subset \mathcal{G}$ the subclass of bipartite graphs in $\mathcal{G}$. Similarly, let $\mathcal{C}$, $\mathcal{B}$ be the class of connected and 2-connected graphs in $\mathcal{G}$ (with generating functions and $C(x, y_1, y_2)$ and $B(x, y_1, y_2)$, respectively) and let $\bar{\mathcal{C}}$, $\bar{\mathcal{B}}$ denote the corresponding class of connected and 2-connected bipartite graphs in $\mathcal{G}$ (with generating functions and $\bar{C}(x, y)$ and $\bar{B}(x, y)$, respectively). The generating functions are related as follows

$$\bar{G}(x, y) = G(x, y, 0),\ \bar{C}(x, y) = C(x, y, 0),\ \bar{B}(x, y) = B(x, y, 0).$$

Observe that for $y_1 = 0$, $y_2 = y$ the function $G(x, 0, y)$ corresponds to the generating function of the class of graphs without a 2-colouring (an uncoloured graph can be interpreted as a graph where all edges are monochromatic).

In order to define a recursive construction of $\mathcal{G}$ we are going to use the symbolic constructions for labelled combinatorial classes as defined in Chapter II of [FS09], and specially the disjoint union, the labelled product, the set construction and the sequence construction. See Table 1.

Construction		Generating function
Union	$\mathcal{A} + \mathcal{B}$	$A(x, y_1, y_2) + B(x, y_1, y_2)$
Product	$\mathcal{A} \times \mathcal{B}$	$A(x, y_1, y_2) \cdot B(x, y_1, y_2)$
Sequence	$\mathrm{Seq}(\mathcal{A})$	$(1 - A(x, y_1, y_2))^{-1}$
Set	$\mathrm{Set}(\mathcal{A})$	$\exp(A(x, y_1, y_2))$

Tab. 1: The Symbolic Method. In the table, GFs associated to classes $\mathcal{A}$ and $\mathcal{B}$ are $A(x, y_1, y_2)$ and $B(x, y_1, y_2)$, respectively.

We use letters v, e_1, e_2 to denote a single vertex, a frustrated and a monochromatic edge, respectively (encoded by x, $\frac{1}{2}x^2y_1$ and $\frac{1}{2}x^2y_2$ respectively). As usually, graphs in $\mathcal{G}$ can be *vertex-* or *edge-rooted* meaning that there is one distinguished vertex or edge, respectively, in every graph. For a class of graphs $\mathcal{G}$ denote by $\mathcal{G}'$ the class of *vertex-pointed* graphs, that is the class where in every graph there is one distinguished vertex, and the distinguished vertex is *unlabelled*. Similarly, for a class of graphs $\mathcal{G}$ denote by $\overrightarrow{\mathcal{G}}$ the class of *edge-rooted* graphs, that is the class where in each graph there is one distinguished edge (called the root) that is oriented, and all the vertices are labelled except the extremities of the root (which are deleted from the graph).

Furthermore, we need two non-standard types of substitution.

Vertex substitution: for class of graphs (possibly 2-coloured) $\mathcal{A}$ (unrooted, vertex-pointed or rooted) and a class of vertex-pointed, 2-coloured graph $\mathcal{B}^{'}$ (with generating function $B(x, y_1, y_2)$) the class $\mathcal{C} = \mathcal{A} \circ_v \mathcal{B}^{'}$ is the class of graphs obtained by taking a graph in $G \in \mathcal{A}$ and substituting a vertex-pointed graph $G_v \in \mathcal{B}^{'}$ at each vertex in G. As the distinguished vertex of G_v is unlabelled, this translates into

$$C(x, y_1, y_2) = A(xB(x, y_1, y_2), y_1, y_2).$$

We observe that for the vertex substitution the 2-colouring does not matter: as we consider a colouring of a graph up to permuting the two colours, we can guarantee that the distinguished vertex in G_v and the vertex in G which we are going to replace by G_v are of the same colour.

Edge substitution: as we are looking at classes of 2-coloured graphs, we have two different types of edges namely, frustrated and monochromatic ones. Given a 2-coloured graph class $\mathcal{A}$ and a class of properly 2-coloured edge-rooted graphs $\overrightarrow{\mathcal{B}}$ (with counting formula $B(x, y_1, y_2)$), where the root-edge is oriented, the class $\mathcal{C} = \mathcal{A} \circ_{e_1} \overrightarrow{\mathcal{B}}$ is obtained by taking a graph $G \in \mathcal{A}$ called the *core*, replacing each frustrated edge $e = \{u, v\}$ in G by a graph $\overrightarrow{G} \in \overrightarrow{\mathcal{B}}$ (replace u by the start of the root-edge of $G^{'}$ and v by the end-vertex of the root edge), and deleting the root-edge of $\overrightarrow{G}$. For the corresponding generating functions this translates to

$$C(x, y_1, y_2) = A(x, B(x, y_1, y_2), y_2). \tag{1}$$

Similarly, given a 2-coloured graph class $\mathcal{A}$ and a class of monochromatic edge-rooted graphs $\overrightarrow{\mathcal{B}}$ (with counting formula $B(x, y_1, y_2)$), where the root-edge is oriented, the class $\mathcal{C} = \mathcal{A} \circ_{e_2} \overrightarrow{\mathcal{B}}$ is obtained by taking a core $G \in \mathcal{A}$, replacing each monochromatic labelled edge $e = \{u, v\}$ in G by a graph $\overrightarrow{G} \in \overrightarrow{\mathcal{B}}$, and deleting the root-edge of $\overrightarrow{G}$. For the generating function we obtain the analogue of Equation (1)

$$C(x, y_1, y_2) = A(x, y_1, B(x, y_1, y_2)).$$

We will use expressions of the form $\mathcal{A} \circ_{e_1} \overrightarrow{\mathcal{B}}_1 \circ_{e_2} \overrightarrow{\mathcal{B}}_2$ to express a double edge substitution: for a core in $\mathcal{A}$ we substitute frustrated edges by elements of $\overrightarrow{\mathcal{B}}_1$ and monochromatic edges by elements of $\overrightarrow{\mathcal{B}}_2$, respectively.

Our strategy explains as follows: we obtain a complete grammar for the class $\mathcal{G}$ which only depends on the 3-connected components in $\mathcal{G}$. This grammar then translates into a system of functional equations describing the generating function $G(x, y_1, y_2)$ associated to the Ising model over the graph family. Once we have found this grammar and the generating function $G(x, y_1, y_2)$ we also have found a complete description of the generating function of bipartite graphs $\overline{G}(x, y) = G(x, y, 0)$. Hence in the following we restrict our attention to decomposing $\mathcal{G}$.

3 The grammar for coloured classes

Let $\mathcal{G}$ be a closed class of labelled graphs with monochromatic and frustrated edges. By definition, closed classes are fully characterized by their 3-connected components and the expansion of the generating function corresponding to the classes $\mathcal{G}$ and $\mathcal{C}$ will only depend on the generating function of the subclass of the 2-connected graphs $\mathcal{B} \subset \mathcal{G}$.

Recall that $\mathcal{C}$ denotes the family of connected graphs in $\mathcal{G}$. Decomposing graphs from a closed class into connected components is easy, as the class $\mathcal{G}$ is decomposable in the sense of [Kol99]: a graph is in $\mathcal{G}$ if and only if each component is in $\mathcal{G}$. This implies

$$\mathcal{G} = \mathrm{Set}\,(\mathcal{C})\,,$$

and $G(x, y_1, y_2) = \exp(C(x, y_1, y_2))$.

Let us encode now the generating function $C(x, y_1, y_2)$ in terms of 2-connected graphs. Recall that a maximal 2-connected induced subgraph is called a *block*. For uncoloured closed classes, vertex-pointed connected graphs $\mathcal{C}'$ can be constructed recursively using the 2-connected graphs $\mathcal{B}$ in the class, by taking a collection of vertex-pointed blocks, gluing them together at their distinguished vertices and replacing every non-distinguished vertex in a block by a connected graph. We observe that the exact same construction holds for graphs in our model. Hence

$$\mathcal{C}' = \mathrm{Set}(\mathcal{B}' \circ_v \mathcal{C}')$$

which is a result of [BLL98]. This equation easily translates to the enumerative setting: by applying the symbolic language we get that

$$x\frac{\partial}{\partial x}C(x, y_1, y_2) = x \exp\left(\frac{\partial B}{\partial x}\left(x\frac{\partial}{\partial x}C(x, y_1, y_2), y_1, y_2\right)\right).$$

Hence it remains to decompose 2-connected graphs into 3-connected components. Let us start by decomposing networks. A *network* is a connected graph with two distinguished (virtual) vertices, called poles, such that the graph obtained by adding an edge between the two poles (if missing) is 2-connected. In the counting formulas the two poles are not labelled. As shown in [Tra58] a network can be of four different types: a single edge, a series network, a parallel network or an h-network. A network is *series* if it is obtained by a cycle C with a distinguished edge e, whose endpoints become the poles and every edge apart from e is replaced by a network. A network is *parallel* if it is obtained by gluing two or more networks along the poles. A network is an *h-network* if it is obtained from a 3-connected graph G, which is rooted at an edge, by replacing every edge of G apart from the root edge, by an arbitrary network. To obtain a full grammar of graphs with our model, we have to distinguish between networks where the root edge is either monochromatic or frustrated.

Let $\mathcal{D}$ denote the class of networks. Let $\mathcal{D}_{\circ-\bullet}$, $\mathcal{D}_{\bullet-\bullet}$ be the set of networks where the root edge defines a frustrated or a monochromatic edge, respectively. Similarly, let $\mathcal{S}_{\bullet-\bullet}$, $\mathcal{P}_{\bullet-\bullet}$, $\mathcal{H}_{\bullet-\bullet}$ denote the set of series, parallel and 3-connected networks where the root edge is monochromatic, and $\mathcal{S}_{\circ-\bullet}$, $\mathcal{P}_{\circ-\bullet}$,$\mathcal{H}_{\circ-\bullet}$ denote the set of series, parallel and 3-connected networks where the root edge is frustrated. Let $\mathcal{T}$ be the family of 3-connected graphs in $\mathcal{G}$, and let $\mathcal{T}_{\circ-\bullet}$, $\mathcal{T}_{\bullet-\bullet}$ be the class of 2-coloured 3-connected graphs in $\mathcal{G}$ where the root edge is frustrated and monochromatic, respectively.

The construction of networks in [Tra58] taking into account the colouring of the vertices then translates

into the following symbolic equations

$$\begin{aligned}
\mathcal{D}_{\circ-\bullet} &= e_1 + \mathcal{S}_{\circ-\bullet} + \mathcal{P}_{\circ-\bullet} + \mathcal{H}_{\circ-\bullet}\\
\mathcal{D}_{\bullet-\bullet} &= e_2 + \mathcal{S}_{\bullet-\bullet} + \mathcal{P}_{\bullet-\bullet} + \mathcal{H}_{\bullet-\bullet}\\
\mathcal{S}_{\bullet-\bullet} &= (\mathcal{D}_{\bullet-\bullet} - \mathcal{S}_{\bullet-\bullet}) \times v \times \mathcal{S}_{\bullet-\bullet} + (D_{\circ-\bullet} - \mathcal{S}_{\circ-\bullet}) \times v \times \mathcal{S}_{\circ-\bullet}\\
\mathcal{S}_{\circ-\bullet} &= (\mathcal{D}_{\bullet-\bullet} - \mathcal{S}_{\bullet-\bullet}) \times v \times \mathcal{S}_{\circ-\bullet} + (D_{\circ-\bullet} - \mathcal{S}_{\circ-\bullet}) \times v \times \mathcal{S}_{\bullet-\bullet}\\
\mathcal{P}_{\circ-\bullet} &= e_1 \times \mathrm{Set}_{\geq 1}(\mathcal{D}_{\circ-\bullet} - \mathcal{P}_{\circ-\bullet} - e_1) + \mathrm{Set}_{\geq 2}(\mathcal{D}_{\circ-\bullet} - \mathcal{P}_{\circ-\bullet} - e_1)\\
\mathcal{P}_{\bullet-\bullet} &= e_2 \times \mathrm{Set}_{\geq 1}(\mathcal{D}_{\bullet-\bullet} - \mathcal{P}_{\bullet-\bullet} - e_2) + \mathrm{Set}_{\geq 2}(\mathcal{D}_{\bullet-\bullet} - \mathcal{P}_{\bullet-\bullet} - e_2)\\
\mathcal{H}_{\circ-\bullet} &= \mathcal{T}_{\circ-\bullet} \circ_{e_1} \mathcal{D}_{\circ-\bullet} \circ_{e_2} \mathcal{D}_{\bullet-\bullet}\\
\mathcal{H}_{\bullet-\bullet} &= \mathcal{T}_{\bullet-\bullet} \circ_{e_1} \mathcal{D}_{\circ-\bullet} \circ_{e_2} \mathcal{D}_{\bullet-\bullet}.
\end{aligned} \tag{2}$$

However, relating the class of (coloured) networks $\mathcal{D}$ to the class of 2-connected (coloured) graphs $\mathcal{B}$ is highly non-trivial, due to the integration step needed to obtain the counting formula for 2-connected graphs in terms of networks. In order to avoid this integration step we are going to adapt an idea of [CFKS08].

Let us briefly recall Tutte's decomposition and the definition of a RMT-trees. Following Tutte's decomposition Theorem (see [Tut66]) every 2-connected graph can be decomposed into 3-connected components using *split operations*. For a 2-connected graph G a *split candidate* is a set $\{E_1, E_2, u, v\}$ where $E(G) = E_1 \cup E_2$ is a partition of the edges of G and deleting the vertices $u, v \in V(G)$ yields a disconnected graph with components $G[E_1]$ and $G[E_2]$. Furthermore, $G[E_2]$ has to be 2-connected and $G[E_1]$ is a graph such that E_1 cannot be partitioned into two nonempty sets E_{11}, E_{22} which only intersect in the set $\{u, v\}$.

For a given graph G and a split candidate $\{E_1, E_2, u, v\}$ the corresponding split operation is defined as follows: add an edge e between u and v. This is called the *virtual edge*. Cut along the edge e, i.e. separate the two graphs $G[E_1]$, $G[E_2]$ and add the (virtual) edge e to both graphs. Continue to perform split operations until there is no split candidate left. The resulting final structure after all possible split operations have been performed is a collection of graphs called the *bricks*. The resulting bricks are independent of the order in which the split operations are performed, see [Tut66].

Furthermore, Tutte showed that a brick graph has to be of one of the following types: multi-edge graph (M-brick), ring-graph (R-brick), or 3-connected graph with at least 4 vertices (T-brick). Similarly to the block graph, one can translate Tutte's decomposition into a graph structure. For a graph G let the *RMT-tree* be the graph with vertex set equal to the set of bricks of G and edge-set corresponding to the virtual edges of the Tutte decomposition of G. As shown in [Tut66] the resulting graph is really a tree and by the maximality of the decomposition two R-bricks as well as two M-bricks are never adjacent.

We are now going to use this decomposition. Recall that e_1, e_2 are the frustrated and monochromatic edge graphs with counting series $\frac{1}{2}x^2y_1$, $\frac{1}{2}x^2y_2$, respectively, and let $\mathcal{A}$ denote the class of graphs in $\mathcal{B}$ with at least three edges. Then

$$\mathcal{B} = e_1 + e_2 + \mathcal{A}.$$

Following [CFKS08] let $\mathcal{B}^\bullet$ ($\mathcal{B}^{\bullet-\bullet}$, $\mathcal{B}^{\bullet\to\bullet}$) be the class of graphs in $\mathcal{B}$ such that the RMT-tree has a distinguished vertex (edge, directed edge respectively). Next we are going to apply the generalized Dissymmetry Theorem. In its original form the Dissymmetry Theorem allows to characterize unrooted trees in terms of edge-rooted and vertex-rooted trees, see [BLL98]. In its generalized version, it allows a similar result for graph classes which are tree-like, i.e. which can be associated with special families of trees.

Applying the (extended) Dissymmetry Theorem [CFKS08, Theorem 3.1] then yields

$$\mathcal{A} = \mathcal{B}^{\bullet} + \mathcal{B}^{\bullet-\bullet} - \mathcal{B}^{\bullet\to\bullet} \tag{3}$$

Furthermore, the three classes $\mathcal{B}^{\bullet}$, $\mathcal{B}^{\bullet-\bullet}$, $\mathcal{B}^{\bullet\to\bullet}$ can be partitioned into subclasses according to the type of the distinguished node in the RMT-tree. Let $\mathcal{B}_R$, $\mathcal{B}_M$, $\mathcal{B}_T$ stand for rooted graphs from $\mathcal{B}$ where the distinguished node in the RMT-tree is an R-, M-, T-node, respectively. Similarly let $\mathcal{B}_{M-R}$ be the graphs where the rooted edge in the RMT-tree is between vertices of type R and M, etc. Taking into account simplifications such as $\mathcal{B}_{R\to M} \backsimeq \mathcal{B}_{M\to R} \backsimeq B_{R-M}$ Equation (3) becomes

$$\mathcal{B} = \mathcal{B}_R + \mathcal{B}_M + \mathcal{B}_T - \mathcal{B}_{R-M} - \mathcal{B}_{R-T} - \mathcal{B}_{M-T} - \mathcal{B}_{T\to T} + \mathcal{B}_{T-T} \tag{4}$$

which is Equation (13) in [CFKS08]. It remains to decompose the families in (4).

Let $\mathcal{R}$ be the class of ring-graphs that are unoriented cycles with at least three edges which are either monochromatic or frustrated and let $\mathcal{M}$ be the class of multi-edge graphs, with at least three edges. Furthermore, let $\mathcal{T}$ be the family of 3-connected graphs in $\mathcal{G}$ with at least four vertices and with both monochromatic and frustrated edges. For every graph in $\mathcal{B}_R$ each edge e of the distinguished R-brick is either real or virtual. If e is a real edge, the graph attached to it on the side not incident to the R-brick is naturally rooted at e and hence is a network. Given that two R-bricks are never adjacent the network has to be non-series. Taking into account the different colourings of the edges of the ring-graph and the type of edge on the (virtual) roots of the networks we obtain the following specification

$$\mathcal{B}_R = \mathcal{R} \circ_{e_1} (\mathcal{D}_{\circ-\bullet} - \mathcal{S}_{\circ-\bullet}) \circ_{e_2} (\mathcal{D}_{\bullet-\bullet} - \mathcal{S}_{\bullet-\bullet}). \tag{5}$$

Similarly, every graph in $\mathcal{B}_M$ can be constructed by taking a multi-edge graph in $\mathcal{M}$ and substituting edges for non-parallel network. The networks have to be non-parallel as two M-bricks are never adjacent. Taking into account the different types of the edges although in a multi-edge all edges have to necessarily be of the same type we obtain

$$\mathcal{B}_M = \mathcal{M} \circ_{e_1} (\mathcal{D}_{\circ-\bullet} - \mathcal{P}_{\circ-\bullet}) \circ_{e_2} (\mathcal{D}_{\bullet-\bullet} - \mathcal{P}_{\bullet-\bullet}). \tag{6}$$

Furthermore, we have

$$\mathcal{B}_T = \mathcal{T} \circ_{e_1} \mathcal{D}_{\circ-\bullet} \circ_{e_2} \mathcal{D}_{\bullet-\bullet}.$$

In the next step, we decompose 2-connected graphs with a distinguished edge in the RMT-tree. We obtain

$$\mathcal{B}_{R-M} = v^2 \times (\mathcal{S}_{\circ-\bullet} \times \mathcal{P}_{\circ-\bullet} + \mathcal{S}_{\bullet-\bullet} \times \mathcal{P}_{\bullet-\bullet})/\sim, \tag{7}$$

where $\sim$ identifies graphs in $\mathcal{B}_{R-M}$ if they are the same up to exchanging the direction of the virtual edge between the two poles. Similarly,

$$\begin{aligned}
\mathcal{B}_{M-T} &= v^2 \times (\mathcal{P}_{\circ-\bullet} \times \mathcal{H}_{\circ-\bullet} + \mathcal{P}_{\bullet-\bullet} \times \mathcal{H}_{\bullet-\bullet})/\sim \\
\mathcal{B}_{R-T} &= v^2 \times (\mathcal{S}_{\circ-\bullet} \times \mathcal{H}_{\circ-\bullet} + \mathcal{S}_{\bullet-\bullet} \times \mathcal{H}_{\bullet-\bullet})/\sim \\
\mathcal{B}_{T\to T} &= v^2 \times (\mathcal{H}_{\circ-\bullet} \times \mathcal{H}_{\circ-\bullet} + \mathcal{H}_{\bullet-\bullet} \times \mathcal{H}_{\bullet-\bullet})/\sim \\
\mathcal{B}_{T-T} &= v^2 \times (\mathcal{H}_{\circ-\bullet} \times \mathcal{H}_{\circ-\bullet} + \mathcal{H}_{\bullet-\bullet} \times \mathcal{H}_{\bullet-\bullet})/(\sim, H\leftrightarrow)
\end{aligned}$$

where $/(\sim, H\leftrightarrow)$ means up to exchanging the two pole vertices and up to orienting the distinguished virtual edge.

4 Translating the grammar into generating functions

The previous grammar provides an explicit description of a closed class of graphs in terms of its 3-connected components. We are now going to apply it to series-parallel graphs. Recall that in this particular situation, the class $\mathcal{T}$ of 3-connected graphs with at least four vertices is empty. We are interested in the generating function of bipartite series-parallel graphs. Hence we put $y_1 = y$ and $y_2 = 0$. Using these observations the set of symbolic equations (2) from Section 3 translates and simplifies to the following set of equations

$$\begin{aligned} D_{\bullet-\bullet}(x,y,0) := D_1 &= -1 + \exp\left(\frac{x\left({D_1}^3 x - D_1 {D_2}^2 x + {D_1}^2 + {D_2}^2\right)}{{D_1}^2 x^2 - {D_2}^2 x^2 + 2xD_1 + 1}\right) \\ D_{\circ-\bullet}(x,y,0) := D_2 &= y + y\left(\exp\left(\frac{xD_2\left(x{D_1}^2 - x{D_2}^2 + 2D_1\right)}{{D_1}^2 x^2 - {D_2}^2 x^2 + 2xD_1 + 1}\right) - 1\right) \\ &\quad + \exp\left(\frac{xD_2\left(x{D_1}^2 - x{D_2}^2 + 2D_1\right)}{{D_1}^2 x^2 - {D_2}^2 x^2 + 2xD_1 + 1}\right) - 1. \end{aligned} \tag{8}$$

The expressions for the generating functions of series networks easily follow

$$\begin{aligned} S_{\bullet-\bullet}(x,y,0) := S_1 &= \frac{x\left({D_1}^3 x - D_1 {D_2}^2 x + {D_1}^2 + {D_2}^2\right)}{{D_1}^2 x^2 - {D_2}^2 x^2 + 2xD_1 + 1} \\ S_{\circ-\bullet}(x,y,0) := S_2 &= \frac{xD_2\left(x{D_1}^2 - x{D_2}^2 + 2D_1\right)}{{D_1}^2 x^2 - {D_2}^2 x^2 + 2xD_1 + 1}. \end{aligned}$$

Recall that for series-parallel graphs the class $\mathcal{H}$ of networks build from 3-connected graphs is empty. Hence equation (4) translates into

$$B(x,y,0) = \frac{1}{2}x^2y^2 + B_R(x,y,0) + B_M(x,y,0) - B_{R-M}(x,y,0)$$

where by equations (5),(6),(7) we have

$$\begin{aligned} B_R(x,y,0) &= R(x, D_1 - S_1, D_2 - S_2) \\ B_M(x,y,0) &= \frac{x^2}{2}\exp_{\geq 3}(S_1) + \frac{x^2}{2}(y\exp_{\geq 2}(S_2) + \exp_{\geq 3}(S_2)) \\ B_{R-M}(x,y,0) &= \frac{x^2}{2}(S_1\,(D_1 - S_1) + S_2\,(D_2 - S_2)). \end{aligned}$$

Here $R(x, y_1, y_2)$ stands for the generating function of vertex ring-graphs with monochromatic and frustrated edges, which is equal to

$$R(x,y_1,y_2) = -\frac{1}{4}\log\left((-xy_1 - y_2x + 1)\,(-xy_1 + y_2x + 1)\right) - \frac{1}{4}x^2{y_2}^2 - \frac{1}{2}xy_1 - \frac{1}{4}x^2{y_1}^2.$$

We observe that by using the same grammar but putting $y_1 = 0$, $y_2 = y$ (no colours) we recover the system of equations for series-parallel graphs studied in [BGKN07].

5 Asymptotic enumeration of bipartite series-parallel graphs

We are now presenting our main result which is a precise asymptotic estimate of the number of connected and general bipartite series-parallel graphs with n vertices:

Theorem 5.1 (Asymptotic behaviour of bipartite series-parallel graphs) *The number of connected and general bipartite (labelled) series-parallel graphs with n vertices is asymptotically equal to*

$$c_n \sim c \cdot n^{-5/2} \cdot \gamma^n \cdot n!$$
$$g_n \sim g \cdot n^{-5/2} \cdot \gamma^n \cdot n!$$

where $\gamma = 4.22044$, $c = 0.021446$ and $g = 0.026499$ are computable constants.

The proof of Theorem 5.1 is based on singularity analysis of the corresponding generating functions. We refer to [FS09, Chapter VI] for an introduction to these analytic techniques. Let us briefly sketch the ideas behind the proof of this theorem. We start studying the system of equations (8). One can check that the singular nature of $D_{\circ-\bullet}(x,1,0)$ and $D_{\bullet-\bullet}(x,1,0)$ are both of square-root type, by means of the so-called Drmota-Lalley-Woods Theorem (see [Drm97]).

Once the singular behaviour of both $D_{\circ-\bullet}(x,1,0)$ and $D_{\bullet-\bullet}(x,1,0)$ is known, we conclude that the dominant singularity of $B(x,1,0)$ is determined by the dominant nature of the pair $D_{\circ-\bullet}(x,1,0)$, $D_{\bullet-\bullet}(x,1,0)$ (which have, in fact, the same singularities). Let us mention that the singular nature of $B(x,1,0)$ (namely, the counting formula for 2-connected bipartite series-parallel graphs) is of type $3/2$ instead of $1/2$. This fact can be interpreted by combinatorial means as the unrooting step which is required when relating the network level to the 2-connected level. In the singular expansion of $B(x,1,0)$ this 'unrooting' results in a cancelation of the square-root type terms and the hence the singular nature is of of type $3/2$.

Going from the 2-connected to the connected level the singularity is moved due to the existence of a branch point of the equation relating $B(x,1,0)$ and $C(x,1,0)$. Recall that $C(x,1,0)$ stands for the exponential generating function associated with connected bipartite series-parallel graphs. This tells us that the class of bipartite series-parallel graphs fits into the subcritical graph scheme, studied in full detail in [DFK$^+$11]. Finally, by applying the classic transfer theorems of singularity analysis [FS09, Thm VI.2] we deduce the asymptotic behaviour of the coefficients.

Furthermore, we are interested in the asymptotic behaviour of R_n which denotes the random graph chosen uniformly at random over all bipartite series-parallel graphs on n vertices. By [BBCR00, Theorem 1.1] the previous result gives the distribution of the number of connected components of R_n:

Theorem 5.2 (Distribution for the number of connected components) *Let $\kappa(R_n)$ denote the number of connected components of a random bipartite series-parallel graph. Then, as $n \to \infty$*

$$\kappa(R_n) \to 1 + \mathrm{Po}(C(\gamma^{-1}))$$

where $\mathrm{Po}(C(\gamma^{-1}))$ *stands for the Poisson distribution of parameter $C(\gamma^{-1}) = 0.21158$.*

In particular, the probability that a random bipartite series-parallel graph is connected is asymptotically equal to $p = 0.80930$. In the following table we compare the parameters obtained in this paper with the parameters known in the case of general series-parallel graphs which can be found in [BGKN07]

Parameter	Series-Parallel	Bipartite Series-Parallel
γ	9.07359	4.22043
p	0.88904	0.80930

Tab. 2: Constants for series-parallel graphs and for bipartite series-parallel graphs. γ is the growth constant of the class and p stands for the probability of connectedness of a graph with n vertices chosen sampled uniformly at random.

6 Further research

As mentioned in the previous section, the family of bipartite series-parallel graphs fits into the subcritical scheme. Consequently, many important parameters can be studied using the general framework developed in [DFK$^+$11]. In particular, the number of edges in the random bipartite series-parallel graph R_n will follow a normal limiting distribution with linear expectation and linear variance. The precise constants on the expectation and the variance can be obtained explicitly by applying the so-called *Quasi-Powers Theorem* on perturbation of singularities, see [Hwa98]). A wide variety of parameters of the random graph R_n can be analyzed, including the number of cut-vertices, the number of blocks and the number of copies of a fixed subgraph. All these parameters all follow Gaussian limit laws. We believe that similar results would also hold when considering families of bipartite graphs defined by a *finite* list of 3-connected components.

Finally, the system of equations presented in this extended abstract provides a first step towards the analysis of the more involved problem of studying the asymptotic number of bipartite (labelled) planar graphs with n vertices. In order to apply our grammar we need the counting formulas for 3-connected planar graphs carrying an Ising model. Again, by Whitney's Theorem, this family is essentially equivalent to the family of 3-connected planar maps carrying this statistical model. As it is explicitly pointed out in [BBM11] (see also [BM08]) the expressions for the generating functions obtained in the context of these special types of map are algebraic but very involved. Hence a major problem in this direction is to deduce from [BBM11] counting formulas for coloured 3-connected planar maps, then translate them to the graph setting and finally apply our methodology.

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A Linear-Time Algorithm for Sampling Graphs with Given Degrees

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Abstract. We introduce a new algorithm for the asymptotically uniform sampling of graphs with given degrees, combining elements of combinatorial and Markov Chain Monte Carlo methods into a hybrid strategy. Under a typical sparseness condition, the runtime is linear in the number of edges, improving upon the previous best runtime by a factor equal to the maximum degree. We go on to show that this idea is applicable to a variety of other combinatorial families.

Keywords: Uniform Sampling, Graphs with Given Degrees, Perfect Matching, Markov Chain Coupling

1 Introduction

Consider the following statistic: the mean Erdős number (among people who have one) is 4.65 (Grossman, 2004). It is natural to ask whether this is a sociological statistic describing mathematicians' propensity to collaborate, or a graph-theoretical constant that arises from the construction of the collaboration graph.

Answering this question statistically requires sampling labelled graphs with given degree sequence, which maintains mathematicians' identities and propensities to collaborate while randomising the choice of coauthors. More generally, sampling graphs with given degrees is useful for a statistical study of any graph for which only one instance exists, such as Darwin's finches (Chen et al., 2005) or network motifs (Alon, 2007).

In this paper, we introduce a new algorithm for sampling graphs with given degrees asymptotically uniformly, in the sense that the total variation distance to uniformity vanishes as the number of edges increases. The improvements over previous algorithms are:

1. The runtime is linear in the number of edges, which is faster than the previous best algorithm (Bayati, Kim and Saberi, 2010) by a factor equal to the maximum degree. It is also best possible in the sense that a sublinear runtime is impossible, since each edge needs to be generated.

2. Asymptotic uniformity also holds for the important counterexample of Bezáková et al. (2012), for which other algorithms produce exponentially skewed outputs.

3. The strategy can be generalised to many combinatorial structures other than graphs.

Algorithm A. Sampling labelled graphs with given degrees $(d_1, \ldots, d_n)$.

1. Run Algorithm B (see below) to obtain a random multigraph. Call the edges that are loops or part of multiple edges "bad", and the remaining edges "good".
2. Pick 2 good edges uniformly at random, and pick any bad edge. Perform a 3-swap (see below) if the new edges it would produce are all good, otherwise do nothing.
3. Repeat Step 2 until no bad edges remain.

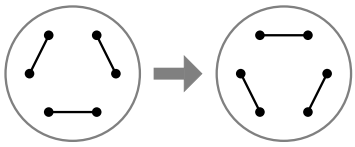

Fig. 1: A 3-swap takes 3 edges (α, β), (γ, δ) and (ζ, η), and replaces them with 3 new edges (β, γ), (δ, ζ) and (η, α). When selecting edges randomly, the order of endpoints is also randomised.

Let $(d_1, \ldots, d_n)$ be the prescribed degree sequence, with n vertices, $m = \frac{1}{2}\sum_i d_i$ edges, and maximum degree $d = \max_i d_i$. A classical sampling algorithm (Bender and Canfield, 1978; Bollobás, 1980) produces a multigraph with the given degrees.

Algorithm B. Classical sampling algorithm for multigraphs with given degrees.

1. Divide the first vertex into d_1 "edge-endpoints", the second vertex into d_2 edge-endpoints, and so on, until one obtains $\sum_i d_i = 2m$ edge-endpoints in n groups.
2. Choose a random matching of these $2m$ edge-endpoints, by picking edges between pairs of unmatched edge-endpoints at random until all are matched.
3. Collapse the groups of edge-endpoints back into vertices to obtain a labelled multigraph with the given degree sequence.

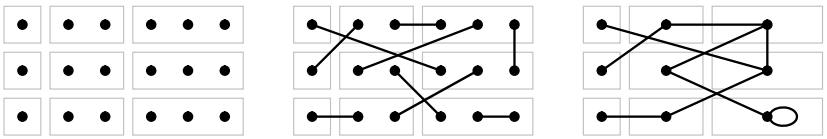

Fig. 2: Example for Algorithm B with degrees $(1, 1, 1, 2, 2, 2, 3, 3, 3)$. From left to right: (1) dividing vertices into groups of edge-endpoints; (2) randomly matching pairs of edge-endpoints; and (3) collapsing groups of edge-endpoints back into vertices. This realisation contains a loop, so the output is not simple.

An easy computation (see Lemma 4) shows that the output of Algorithm B restricted to simple graphs is uniformly distributed. Thus, one can obtain a simple graph by rejecting samples until one appears, but the probability that this happens is only $O(e^{-(d-1)^2/4})$ (Wormald, 1984). Many subsequent improvements (McKay and Wormald, 1990; Steger and Wormald, 1999; Bayati, Kim and Saberi, 2010) are based on the perfect matching idea, typically requiring a sparseness condition like $d = O(m^{1/4})$, which we will also assume.

The best matching-based algorithms require $O(d)$ steps to add each edge, in order to check that the edge does not already exist. Our runtime improvement comes from allowing multiple edges initially, so that edges can be added in $O(1)$ steps. Each 3-swap still requires $O(d)$ steps to check whether edges exist, but it will turn out that only $O(d^2)$ such moves are necessary, thereby reducing the runtime from $O(md)$ to $O(m + d^3) = O(m)$.

The use of a Markov chain in our algorithm is reminiscent of Markov Chain Monte Carlo (MCMC), which was applied to this problem by Jerrum and Sinclair (1990) and Bezáková, Bhatnagar and Vigoda (2006). The best MCMC algorithm produces an asymptotically uniform output without requiring a sparseness assumption, but unfortunately the runtime of $O(n^4m^3d\log^5 n)$ is prohibitive in practice.

Another strategy is Sequential Importance Sampling (SIS) (Chen et al., 2005; Blanchet, 2009; Blitzstein and Diaconis, 2010), which produces samples of known non-uniformity, which can then be appropriately weighted to give an unbiased estimate of the desired statistic.

While SIS works for all inputs, Bezáková et al. (2012) showed that the sample can be exponentially far from uniform, and thus almost always produces an underestimate with occasional extreme overestimates. This counterexample also causes exponentially bad behaviour in all non-MCMC sampling algorithms, while Algorithm A works well with a slight modification. This will be discussed in more detail in Section 2.2.

Algorithm	Runtime	Sparseness
Algorithm B with rejection	$O(me^{(d^2-1)/4})$	All
McKay-Wormald	$O(m^2d^2)$	$d = O(m^{1/4})$
Bayati-Kim-Saberi	$O(md)$	$d = O(m^{1/4-\epsilon})$
Chen-Diaconis-Holmes-Liu	$O(n^3)$	SIS
Blitzstein-Diaconis	$O(n^2m)$	SIS
Bezáková-Bhatnagar-Vigoda	$O(n^4m^3d\log^5 n)$	All
Algorithm A	$O(m)$	$d = o(m^{1/4})$

Fig. 3: Comparison of algorithms for sampling graphs with given degrees, showing runtime and required sparseness constraint for asymptotic uniformity.

The idea behind why Algorithm A should output an asymptotically uniform graph is one we will call *Expand and Contract*. Complicated combinatorial families are usually embedded inside simpler ones, and a basic sampling strategy is to take samples from the larger family and reject until a member of the smaller family is obtained. Expanding the state space is a common theme in many separate literatures, such as generating functions (Flajolet and Sedgewick, 2009), the Boltzmann sampler (Duchon et al., 2004) and auxilliary variables (Andersen and Diaconis, 2007).

Given a uniform sample from a superset $\mathcal{S}$, one often needs to wait an exponentially long time before an element of the desired subset $\mathcal{S}_0 \subset \mathcal{S}$ is obtained. Instead, we will use a contraction phase, where the

superset is partitioned into slices $\mathcal{S} = \mathcal{S}_0 \sqcup \cdots \sqcup \mathcal{S}_k$ corresponding to some notion of distance from the desired subset, and the sample evolves via a Markov chain that is forced to reduce this distance.

Asymptotic uniformity comes from a reverse coupling argument. Since the initial sample is uniform on each slice $\mathcal{S}_i$, we can couple the initial state of our chain with another chain that stays exactly uniform on each slice $\mathcal{S}_i$, reducing the problem to showing that the probability of decoupling before reaching $\mathcal{S}_0$ is small.

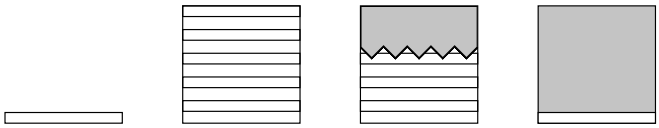

Fig. 4: Expand and Contract. From left to right: (1) the set $\mathcal{S}_0$; (2) expansion to $\mathcal{S} = \mathcal{S}_0 \sqcup \cdots \sqcup \mathcal{S}_k$; (3) and (4) contraction back to $\mathcal{S}_0$. Uniformity is gained through expansion; the goal is the ensure it is not lost during contraction.

In Section 3, we will demonstrate this idea for a variety of other combinatorial families.

2 Graphs with Given Degrees

2.1 Main Results

Let $(d_1, \ldots, d_n)$ denote a degree sequence, with n vertices, $m = \frac{1}{2}\sum_i d_i$ edges and maximum degree $d = \max_i d_i$. We will also let X_t denote the Markov chain described in Algorithm A. In this section, we will show that if $d = o(m^{1/4})$, then Algorithm A runs in $O(m)$ time, and the output is asymptotically uniform in total variation as $m \to \infty$.

We will mostly be concerned with studying the behaviour of the *bad edges* (loops and multiple edges), and begin by bounding the initial number of bad edges, which is a minor refinement of the bound of McKay and Wormald (1990).

Lemma 1 *If a family of degree sequences satisfies the maximum degree bound $d = o(\sqrt{m})$ as $m \to \infty$, then the number of bad edges in the output of Algorithm B is $b = O(d^2)$ with high probability, in the sense that there is $C < \infty$ such that $\mathbb{P}[b > Cd^2] \to 0$.*

We omit the proof here as the techniques are well-known; please see the full version of this paper for details. The key idea is that since the number of perfect matchings between $2m$ edge-endpoints is $(2m)!/2^m m!$, the number of matchings containing any specified set of $k = o(\sqrt{m})$ pairs is

$$\frac{(2m-2k)!}{2^{m-k}(m-k)!} \Big/ \frac{(2m)!}{2^m m!} = \frac{2^k m(m-1)\cdots(m-k+1)}{2m(2m-1)\cdots(2m-2k+1)} \simeq (2m)^{-k}. \tag{1}$$

By using Equation 1 to estimate the probability of various combinations of edges occuring in the output of Algorithm B, we can obtain a bound on the number of bad edges.

Theorem 2 *If a family of degree sequences satisfies the maximum degree bound $d = o(\sqrt{m})$ as $m \to \infty$, Algorithm A terminates in at most $O(m)$ steps with high probability. More precisely, the runtime of Algorithm A is equal to the runtime of Algorithm B plus at most an additional $O(d^2)$ steps.*

Proof: Let (α, β) be a bad edge, and let (γ, δ) and (ζ, η) be randomly chosen good edges. By Lemma 1, there are $\Theta(m^2)$ choices for these good edges with high probability. We will count the number of these choices that result in any bad edges upon a 3-swap.

The new edge (β, γ) is bad if either $\beta = \gamma$ or (β, γ) already exists as an edge. In both cases, (γ, δ) must lie within the ball of radius 2 centred at β in the graph distance metric. Hence, there are $O(md^2)$ choices of the two good edges that result in a bad edge at (β, γ).

Similarly, there are also $O(md^2)$ choices that result in a bad edge at (η, α). For the new edge (δ, ζ), by the same argument, for each choice of (γ, δ), there are at most $O(d^2)$ choices of (ζ, η) that create a bad edge, again resulting in $O(md^2)$ choices that result in a bad edge.

For each choice of bad edge (α, β), there are $2(m - b)(m - b - 1)$ choices for the two good edges in a 3-swap (including the 4 choices for vertex order), $O(md^2) = o(m^2)$ of which create new bad edges. Hence no new bad edges are created with high probability, so the number of steps taken is bounded by the number of bad edges.

By Lemma 1, there are $O(d^2) = o(m)$ bad edges, so the runtime is dominated by the $O(m)$ steps required for Algorithm B. □

It remains to bound the distance to uniformity of the output. For this, we will need to keep track of the bad edges in the following way.

Definition 3 *Let a bad edge set $B = \{(\alpha_1, \beta_1, k_1), \ldots, (\alpha_\ell, \beta_\ell, k_\ell)\}$ be defined as a set of vertex pairs $(\alpha_1, \beta_1), \ldots, (\alpha_\ell, \beta_\ell)$ with prescribed multiplicities $k_1, \ldots, k_\ell$. Let $\mathcal{S}_B$ denote the set of multigraphs with bad edge set B, in the sense that its multiplicities agree with B where they are defined, and there are no bad edges outside of B. For simplicity, we will use the term bad edge set to refer to both B and $\mathcal{S}_B$.*

Note that a bad edge set can prescribe a simple edge, in the same way that a simple edge left over after the removal of a double edge is still considered bad. For example, the bad edge set $\{(1, 1, 2), (1, 2, 1)\}$ consists of all multigraphs with a double loop at vertex 1 and a single edge between vertices 1 and 2.

Lemma 4 *For any bad edge set $B = \{(\alpha_1, \beta_1, k_1), \ldots, (\alpha_\ell, \beta_\ell, k_\ell)\}$, the distribution of the initial state X_0 restricted to B is uniform.*

Proof: This probability of a multigraph is proportional to the number of matchings that give rise to it, which is $\prod_i d_i!$ for a simple graph since each permutation of the edge-endpoints at each vertex results in a distinct matching, and decreases by a factor of $2^k k!$ for each k-tuple loop and $k!$ for each k-tuple non-loop edge. Since each multigraph in B has the same number of k-tuple loops and k-tuple non-loops, they have the same initial probability. □

Thus, our Markov chain is initially uniform restricted to each bad edge set, and we wish to prove that its final state is close to uniform restricted to each bad edge set (keeping in mind that only the empty bad edge set is possible). The idea for the proof is in essence a reverse coupling argument: find a chain Y_t that always stays uniform restricted to each bad edge set, couple X_0 and Y_0, and show that the chance of decoupling is small.

Theorem 5 *If $d = o(m^{1/4})$, then the total variation distance to uniform of the output of Algorithm A converges to 0 as $m \to \infty$.*

Proof: Let $B_0, B_1, \ldots$ be a fixed sequence of bad edge sets, let $\mathcal{B}_t = \{X_0 \in S_{B_0}, \ldots, X_t \in S_{B_t}\}$ be the event that the sample path follows this sequence up to time t, and let $\mathcal{L}(X_t \,|\, \mathcal{B}_t)$ denote the conditional distribution of X_t restricted to this event. Write this distribution as a linear combination

$$\mathcal{L}(X_t \,|\, \mathcal{B}_t) = u_t U_{B_t} + (1 - u_t) E_t,$$

where U_{B_t} is the uniform measure on $\mathcal{S}_{B_t}$ and $0 \le u_t \le 1$ is the largest number so that the above equation holds with E_t a signed measure with total absolute mass at most 1. Note $1 - u_t$ bounds the total variation distance to uniformity of X_t given $\mathcal{B}_t$, since

$$\big|\big|\mathcal{L}(X_t \,|\, \mathcal{B}_t) - U_{B_t}\big|\big|_{TV} = (1 - u_t)\,\big|\big|E_t - U_{B_t}\big|\big|_{TV} \le 1 - u_t.$$

At each step, at most one bad edge is removed and no new bad edges can be created, so we can restrict our attention to sequences of bad edge sets where either $B_{t+1} = B_t$, or B_{t+1} reduces a prescribed multiplicity by 1, removing it altogether if it drops to 0.

Case 1: $B_{t+1} = B_t$. Since the transition probabilities within S_{B_t} are symmetric, uniformity is preserved, hence $u_{t+1} \ge u_t$.

Case 2: B_{t+1} reduces the multiplicity of a k-tuple loop (α, α, k) from B_t.

For any multigraph in $\mathcal{S}_{B_t}$, there are $2(m - b)(m - b - 1)$ possible 3-swaps that remove a loop at α, accounting for the $\binom{m-b}{2}$ choices of two good edges and 4 choices of vertex order. By the argument in Theorem 2, all but $O(md^2) = o(m^{3/2})$ of these are admissible, hence each multigraph in S_{B_t} has $(1 + o(m^{-1/2}))2(m - b)(m - b - 1)$ connections to $S_{B_{t+1}}$.

For any multigraph in $\mathcal{S}_{B_{t+1}}$, let c_α be the number of good edges incident at vertex α, which depends only on B_{t+1} and not on the multigraph itself. There are $\binom{c_\alpha}{2}$ choices for two edges incident at α, and for each choice, there are $m - b - c_\alpha - O(d^2)$ choices of another good edge and 2 choices of vertex order such that a 3-swap creates no new bad edges except for an additional loop at α. Thus, each multigraph in $\mathcal{S}_{B_{t+1}}$ can be reached from $(1 + o(m^{-1/2}))c_\alpha(c_\alpha - 1)(m - b - c_\alpha)$ multigraphs in $\mathcal{S}_{B_t}$ via a 3-swap.

Let Q be the transition matrix of the Markov chain given the sample path of bad edge sets, so that

$$\mathbb{P}(X_{t+1} = y \,|\, \mathcal{B}_{t+1}) = \sum_x \mathbb{P}(X_t = x \,|\, \mathcal{B}_t) Q(x, y).$$

Then, for any $y \in B_{t+1}$, the mass at y under $Q(U_{B_t})$ is given by

$$\sum_x U_{B_t}(x) Q(x, y) = \frac{1}{|S_{B_t}|} \frac{(1 + o(m^{-1/2}))c_\alpha(c_\alpha - 1)(m - b - c_\alpha)}{(1 + o(m^{-1/2}))2(m - b)(m - b - 1)}.$$

This probability is within a factor of $1 + o(m^{-1/2})$ of a constant, so the uniformity in this transition decreases by at most this factor, hence $u_{t+1} \ge (1 - o(m^{-1/2}))u_t$.

Case 3: B_{t+1} reduces the multiplicity of a k-tuple non-loop (α, β, k) from B_t. A similar counting argument shows that again, we have $u_{t+1} = (1 - O(m^{-1/2}))u_t$.

There is a remaining issue: if the bad edge set contains a double edge $(\alpha, \beta, 2)$, then removing a bad edge (α, β) still leaves a prescribed single edge $(\alpha, \beta, 1)$, but any given edge typically does not exist

for a uniformly random multigraph satisfying our sparseness condition. The solution is to expand the definition of "bad edge" to include single edges left over from double edges. Once such a single bad edge is removed, the remaining prescribed multiplicity is $(\alpha, \beta, 0)$, and removing this prescription altogether by replacing B_{t+1} by $B'_{t+1} = B_{t+1} \setminus \{(\alpha, \beta, 0)\}$ decreases the uniformity by a factor of $|\mathcal{S}_{B'_{t+1}}|/|\mathcal{S}_{B_{t+1}}|$.

Using (1), the edge (α, β) occurs with probability at most $d_\alpha d_\beta / 2m = o(m^{-1/2})$, so again, we have $u_{t+1} = (1 - o(m^{-1/2}))u_t$. Since the number of changes in the bad edge set is bounded by the initial badness, and each change reduces uniformity by a factor of $1 - o(m^{-1/2})$, the uniformity of the output is $u_\infty = (1 - o(m^{-1/2}))^{o(\sqrt{m})} = 1 - o(1)$. □

Remark 6 *The need for 3-swaps instead simpler 2-swaps is limited to Case 2 of the proof. With 2-swaps, in order to count the number of ways to reconstruct a loop at α, we need to evaluate the number of triangles incident at α, which varies by a factor greater than $1 + o(m^{-1/2})$.*

2.2 Multi-star graphs

Definition 7 *A multi-star degree sequence is one of the form $(1, \ldots, 1, d_1, \ldots, d_k)$, where the number of 1s is equal to $d_1 + \cdots + d_k$. This corresponds to the degree sequence of a disjoint union of k star graphs. We consider k to be fixed, while the degrees grow with m. Call a vertex of degree 1 a leaf, and a vertex of degree d_i a hub.*

For $k = 1$, this is a star graph, and for $k = 2$, this is counterexample of Bezáková et al. (2012), who showed that for such degree sequences, the algorithm of Chen et al. (2005) produces a bipartite graph that is exponentially far from uniform. In fact, every existing non-MCMC sampling algorithm suffers the same exponentially bad behaviour under this single counterexample, while MCMC still carries the prohibitive runtime from the general case.

In non-MCMC algorithms, edges are added sequentially with probability proportional to degree, so the edge between the two hubs has $\Theta(1)$ probability of being added at each of $m = 2d$ steps. Thus, the probability of obtaining a graph with no edge between hubs is $e^{-\Theta(d)}$, while the probability under the uniform measure is $2/d^2$. This is exponentially far from uniform under the following metric.

Definition 8 *The probability ratio metric between two probability measures μ and ν on a common finite set S is*

$$d(\mu, \nu) = \max_{x \in S} \big| \log \mu(x) - \log \nu(x) \big|.$$

We say these two measures are exponentially far apart when $d(\mu, \nu)$ grows super-linearly with $\log n$, which corresponds to the existence of a state $x \in S$ such that the ratio $\mu(x)/\nu(x)$ gets exponentially large or exponentially small.

Note that this metric requires the probability of every state to be close to uniform, and is stronger than total variation. This is necessary since under total variation, a sampling algorithm that never produces a graph where the hubs are not connected can still be considered uniform, since the probability of such a graph is $2/d^2$.

We will show that a slightly modified version of the Expand and Contract algorithm performs remarkably well. Note that the degree sequence is in no way sparse, in fact, $d = \Theta(m)$. The fact that we nonetheless obtain good results suggests that the strategy is far more robust than we are currently able to prove.

Algorithm A′. Expand and Contract for multi-star graphs. Requires an additional input T, the number of extra steps to run the chain.

1. Run Algorithm B to obtain a random multigraph.
2. Pick a random bad edge (α, β) and a random good edge (γ, δ), and replace them with (β, γ) and (δ, α) if both these new edges are good, otherwise do nothing. Repeat until no bad edges remain.
3. Pick two random good edges and perform the same swap, repeating T times.

Theorem 9 *For any multi-star degree sequence, there exists $T = O(\log m)$ such that Algorithm A′ terminates in time $O(m)$ with high probability, and the resulting graph is within $O(1/m)$ of uniform in the probability ratio metric.*

The proof is fairly long and is omitted here; it can be found in the full version of this paper. The idea is to exploit the symmetry under relabelling of vertices; since k is bounded, the number of equivalence classes under relabelling is small, and the projection of the Markov chain onto the equivalence classes can be readily understood.

2.3 Erdős numbers

As mentioned in the introduction, the statistical study of Erdős numbers is a natural application for sampling graphs with given degrees. The underlying data structure is the collaboration graph, which is formed by taking the vertex set to be the set of all mathematicians, and adding an edge between every pair of mathematicians who have coauthored a publication. Many statistical questions can be answered by comparing the observed collaboration graph to typical graphs with the same degree sequences, where the rationale for fixing the degree sequence is that Erdős numbers would not be as interesting if Erdős did not have by far the highest number of collaborators of any mathematician.

Using the Expand and Contract algorithm, and the degree sequence of the collaboration graph generously provided by the Erdős Number Project (Grossman, 2004), we generated random graphs with this degree sequence to study the mean Erdős number (the mean graph distance to Erdős among mathematicians within the same connected component). In 10,000 trials, the mean Erdős number of a random graph with the same degree sequence was 4.119 on average, with a sample standard deviation of 0.025, indicating very tight concentration around the mean.

In contrast, the actual mean Erdős number in the real world is 4.686[(i)], which is 22 standard deviations higher than the expected number. This indicates that there are strong sociological factors that govern the distribution of Erdős numbers, although it is not clear what these factors might one. One possible explanation is that mathematicians are more likely to find new collaborators who are already close to themselves in the collaboration graph, and thus the reduction in mean Erdős number from each new collaboration is lower than if collaborations were chosen at random.

[(i)] This mean Erdős number of 4.686 differs from the 4.65 cited in the introduction because it was computed using older data (2000), since the full collaboration graph for the newer data (2004) was not available.

3 Other Combinatorial Families

Graphs are only one of a rich world of combinatorial families. In this section, we will explore a variety of other examples for which the Expand and Contract strategy provides a workable sampling algorithm. We begin with some simple motivating examples.

3.1 Subsets of a given size

Let $\mathcal{S}_0$ be the subsets of $[n] = \{1, 2, \ldots, n\}$ with cardinality k, where $\epsilon n \leq k \leq (1-\epsilon)n$ as $n \to \infty$ for some $\epsilon > 0$. We will expand to the superset $\mathcal{S}$ of all subsets of $[n]$, partitioned so that $\mathcal{S}_i$ consists of the subsets of cardinality $k \pm i$. The Expand and Contract algorithm is as follows:

1. Pick a random subset of $[n]$ by including elements independently with probability k/n.
2. Pick an element of $[n]$ and include or exclude it with probability $\frac{1}{2}$ each, rejecting moves which cause the cardinality to move further away from k.
3. Repeat until the cardinality is k.

Suppose the initial cardinality is c, and without loss of generality assume $c > k$. At each step with cardinality i, the cardinality decreases by 1 with probability $i/2n$. Hence, the number of steps required is bounded by a sum of independent geometric random variables with probability of success $i/2n$, which has mean

$$\frac{2n}{c} + \frac{2n}{c-1} + \cdots + \frac{2n}{k+1} = 2n\big(\log c - \log k + O(\tfrac{1}{k})\big).$$

Since $c = k + O(\sqrt{n})$ and $k = \Theta(n)$, $c/k = 1 + O(n^{-1/2})$, so the expected number of steps is $O(\sqrt{n})$. Using Markov's inequality to bound the number of steps by its mean, the runtime is dominated by the $O(n)$ steps to pick the initial subset.

Since both the initial state and the Markov chain are invariant under relabelling of points, the output is uniform by symmetry. The best existing algorithms (Knuth, 1969; Pak, 1998) also run in $O(n)$ time.

3.2 Permutations

Let $\mathcal{S}_0 = S_n$ be the permutations of n. Expand to the superset $\mathcal{S}$ of functions $[n] \to [n]$, partitioned so that $\mathcal{S}_i$ is the set of functions whose range has cardinality $n - i$. The Expand and Contract algorithm is as follows:

1. Pick a uniformly random function $[n] \to [n]$, keeping track of "bad" points in the domain which map to a point that has already been picked in the range.
2. Pick a bad point and map it to a uniformly random point in $[n]$, rejecting the move if a point already in the range is picked.
3. Repeat until the function is surjective.

A coupon-collector bound shows that the runtime is $O(n \log n)$. This is somewhat slower than the best existing algorithms (Knuth, 1969; Pak, 1998), which run in time $O(n)$. Since both the initial state and the transition probabilities are invariant under relabelling of the codomain, the output is a uniformly random permutation.

3.3 General linear group

Let $\mathcal{S}_0 = GL_n(\mathbb{F}_q)$ be the invertible $n \times n$ matrices over a finite field $\mathbb{F}_q$. Expand to the superset $\mathcal{S}$ of all $n \times n$ matrices, partitioned so that $\mathcal{S}_i$ is the set of matrices with rank $n - i$. The Expand and Contract algorithm is as follows:

1. Pick n random vectors in $\mathbb{F}_q^n$ as the columns of a $n \times n$ matrix. Find a maximal set of linearly independent columns by Gaussian elimination.
2. Pick a linearly dependent column and replace it with a random vector in $\mathbb{F}_q^n$, rejecting moves that do not increase the rank of the matrix.
3. Repeat until the matrix is full rank.

Since the initial rank is $n - O(1)$, each step takes $O(n^3)$ time to perform Gaussian elimination, and succeeds with probability $1 - o(1)$, the overall runtime is $O(n^3)$, which agrees with the best existing algorithms (Diaconis and Shahshahani, 1986; Pak, 1998).

The initial state and the transition probabilities depend only on the set of linear dependences between columns, which are invariant under Gaussian elimination. Since $\mathcal{S}_0$ forms a single orbit under Gaussian elimination, the output is exactly uniform.

3.4 Directed and bipartite graphs with given degrees

The same techniques used in Section 2 for simple graphs carry over to directed graphs. Algorithm B splits vertices into in-edges and out-edges to be matched randomly, while a 3-swap randomises only the order of edges while the order of endpoints is determined by direction. Similarly, bipartite graphs can be considered as directed graphs where every vertex has either in-degree 0 or out-degree 0. Please see the full version of the paper for details.

3.5 Lattice points on a sphere

Let $\mathcal{S}_0$ be the set of tuples $(a_1, \ldots, a_n)$ of non-negative integers with $a_1^2 + \cdots + a_n^2 = E = Cn$. This has the quantum mechanical interpretation of configurations of n non-interacting bosons in an infinite one-dimensional well, with total energy E and average energy C (Chatterjee and Diaconis, 2013). Expand to the superset $\mathcal{S}$ of all tuples of non-negative integers, partitioned so that $\mathcal{S}_i$ consists of the tuples whose sum of squares is $E \pm i$. The Expand and Contract algorithm is as follows:

1. Pick each component of an n-tuple independently from a geometric distribution G with probability of success p chosen so that $\mathbb{E}[G^2] = C$. This results in an overall energy close to E, with the choice of geometric distribution corresponding to the physical fact that particle energies should follow the Boltzmann distribution.
2. Pick a component at random and either add or subtract 1 with equal probability, rejecting moves where the energy gets further away from E, or moves that introduce a negative component.
3. Repeat until the energy is E.

At each step, the energy can get closer to E by changing a 1 to 0 or a 0 to 1 depending on whether it is initially above or below E. Thus, there is $\Theta(1)$ probability of getting closer, so only $O(\sqrt{n})$ moves are required, hence the runtime is dominated by the $O(n)$ moves required to generate the initial tuple.

Unfortunately, it is difficult to prove anything about uniformity in this example. This represents the typical situation with Expand and Contract: describing an algorithm is easy, proving a runtime bound is also fairly easy, while proving uniformity is difficult.

3.6 Magic squares

Let $\mathcal{S}_0$ be the set ot $n \times n$ magic squares, that is, the set of $n \times n$ matrices whose entries are a permutation of $\{1, \ldots, n^2\}$ and whose row, column and diagonal sums are all equal to $\frac{1}{2}n(n^2+1)$. Despite being a classical combinatorial family studied since antiquity, the existing literature contains little discussion of uniform sampling. Ardell (1994) showed how to generate a magic square using a genetic algorithm, while Kitajima and Kikuchi (2013) used a technique similar to ours to estimate the number of magic squares up to size $n \leq 30$, but neither result bounds the running time or the distance to uniformity.

We will expand to the superset $\mathcal{S}$ of matrices whose entries are a permutation of $\{1, \ldots, n^2\}$, partitioned so that $\mathcal{S}_i$ consists of those matrices whose row, column and diagonal sums differ from $\frac{1}{2}n(n^2+1)$ by i in the L^1 norm. The Expand and Contract algorithm is as follows

1. Pick a random $n \times n$ matrix whose entries are a permutation of $\{1, \ldots, n^2\}$.
2. Swap two random entries of the matrix. If this moves the state from $\mathcal{S}_i$ to $\mathcal{S}_j$, reject the move with probability $\alpha^{j^2-i^2}$, where the choice of a quadratic energy function and $\alpha = 0.937$ were determined to be experimentally optimal.
3. Repeat until a magic square is obtained.

We are unable to prove any results about either the running time or the uniformity of the algorithm. However, it does seem to work reasonably well in practice, demonstrating the robustness of the Expand and Contract strategy in being able to describe a plausible algorithm for almost any combinatorial family. For the 7040 magic squares of size 4×4, the empirical distribution was distance 0.130 from uniform in total variance, and the empirical probability of any magic square was within a factor of 2.196 from uniform. For larger squares, the extremely large state space prevented a similar simulation, but the algorithm nonetheless succeeded in producing magic squares up to size 50×50, after which the runtime became prohibitive on an AMD *Phenom II* CPU.

4 Conclusion

For graphs with given degrees, we described a $O(m)$ algorithm for asymptotically uniform sampling, which improves upon the previous best runtime of $O(md)$ by a factor equal to the maximum degree. There is a sparseness condition we require, $d = o(m^{1/4})$, which appears independently in several other algorithms, namely McKay and Wormald (1990) and Bayati, Kim and Saberi (2010), and seems to be the critial value at which bad edges become "common" instead of "rare" in the classical perfect matching algorithm.

An immediate goal is to extend the class of possible inputs. The fact that Expand and Contract works well for the non-sparse multi-star example suggests that it might be possible to weaken the sparseness condition. One possible improvement is in selection of the bad edge: the current algorithm chooses bad edges deterministically for simplicity, but a suitable randomisation should result in a more uniform output.

There are countless other combinatorial families for which sampling algorithms would be useful. We demonstrated the versatility of the Expand and Contract strategy via a few motivating examples in Section 3, and hope that many other useful algorithms will arise from this idea in future.

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