

# Further results on the inducibility of $d$ -ary trees\*

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## Abstract

A subset of leaves of a rooted tree induces a new tree in a natural way. The density of a tree  $D$  inside a larger tree  $T$  is the proportion of such leaf-induced subtrees in  $T$  that are isomorphic to  $D$  among all those with the same number of leaves as  $D$ . The inducibility of  $D$  measures how large this density can be as the size of  $T$  tends to infinity. In this paper, we explicitly determine the inducibility in some previously unknown cases and find general upper and lower bounds, in particular in the case where  $D$  is balanced, i.e., when its branches have at least almost the same size. Moreover, we prove a result on the speed of convergence of the maximum density of  $D$  in strictly  $d$ -ary trees  $T$  (trees where every internal vertex has precisely  $d$  children) of a given size  $n$  to the inducibility as  $n \rightarrow \infty$ , which supports an open conjecture.

## 1 Introduction and statement of results

The inducibility of rooted trees is a recently introduced invariant that captures how often a fixed rooted tree can occur “inside” a large rooted tree. By a  $d$ -ary tree, we mean a rooted tree whose internal (non-leaf) vertices all have at least two and at most  $d$  children. In the special cases  $d = 2$  and  $d = 3$ , we speak of *binary* and *ternary* trees, respectively. A rooted tree is called *strictly  $d$ -ary* if every internal vertex has exactly  $d$  children. For our purposes, it is natural to measure the size of a rooted tree  $T$  by the number of leaves, which we denote by  $\|T\|$ . A subset  $S$  of leaves of a  $d$ -ary tree induces another  $d$ -ary tree in a natural way: we first take the smallest subtree of  $T$  that contains all the leaves in  $S$ , and then repeatedly suppress all vertices with only one child by contracting the two adjacent edges to a single edge, until no vertex with a single child remains. The procedure is illustrated in Figure 1. The resulting

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tree is called a *leaf-induced subtree*. Its root is precisely the most recent common ancestor of the leaves in  $S$ .

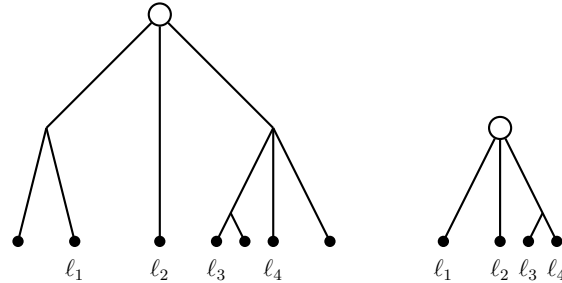


Figure 1: A ternary tree (left) and the subtree induced by four leaves  $\{\ell_1, \ell_2, \ell_3, \ell_4\}$  (right).

A *copy* of a fixed  $d$ -ary tree  $D$  is any leaf-induced subtree that is isomorphic to  $D$ ; we denote the number of distinct copies of  $D$  in  $T$  by  $c(D, T)$ . In other words,  $c(D, T)$  is the number of subsets of the leaf set of  $T$  that induce a tree isomorphic to  $D$ . A normalised version of this quantity is the *density*  $\gamma(D, T)$ , which is defined as

$$\gamma(D, T) = \frac{c(D, T)}{\binom{\|T\|}{\|D\|}}.$$

This can be seen as the probability that a leaf subset of  $T$ , chosen uniformly at random among all sets of  $\|D\|$  leaves, induces a subtree isomorphic to  $D$ . Thus it always lies between 0 and 1. Now we finally define the  $d$ -ary *inducibility* of a fixed  $d$ -ary tree  $D$  as the limit superior of the density as the size of  $T$  tends to infinity:

$$I_d(D) = \limsup_{\substack{\|T\| \rightarrow \infty \\ T \text{ } d\text{-ary tree}}} \gamma(D, T) = \limsup_{n \rightarrow \infty} \max_{\substack{\|T\|=n \\ T \text{ } d\text{-ary tree}}} \gamma(D, T). \tag{1}$$

It is a nontrivial fact, proven in [4], that one can replace  $\limsup$  by an ordinary limit in the second expression. Moreover, it is possible to restrict  $T$  to strictly  $d$ -ary trees without changing the value of the limit (also proven in [4]):

$$I_d(D) = \lim_{n \rightarrow \infty} \max_{\substack{\|T\|=n \\ T \text{ } d\text{-ary tree}}} \gamma(D, T) = \lim_{n \rightarrow \infty} \max_{\substack{\|T\|=(d-1)n+1 \\ T \text{ strictly } d\text{-ary tree}}} \gamma(D, T). \tag{2}$$

Note here that  $\|T\| \equiv 1 \pmod{d-1}$  for every strictly  $d$ -ary tree  $T$  (which is well-known and easy to show), hence the restriction to values of the form  $(d-1)n+1$ .

The definition described above parallels the notion of inducibility of graphs, which is defined in an analogous way (“copies” being isomorphic embeddings). Its investigation began with a paper by Pippenger and Golumbic [12], and there is a substantial amount of literature on this parameter (see [1, 8, 10, 11] for some recent examples).

Bubeck and Linial defined a similar concept [2, Problem 4]: for two (unrooted) trees  $S$  and  $T$ , let  $C(S, T)$  be the number of copies (isomorphic embeddings) of  $S$  in

$T$ . Moreover, let  $Z_k(T)$  be the number of  $k$ -vertex subtrees of  $T$ . The inducibility of  $S$  in the sense of Bubeck and Linial is the limit superior of the quotient  $\frac{C(S,T)}{Z_{|S|}(T)}$  (i.e., the proportion of subtrees of  $T$  that are isomorphic to  $S$  among all subtrees of the same size as  $S$ ) as the size of  $T$  tends to infinity, similar to (1). There are two important differences: the trees in the setting of [2] are not rooted, and subtrees are induced by arbitrary vertices rather than leaves. A consequence of the latter is that the denominator  $Z_{|S|}(T)$  depends on the full structure of  $T$  rather than its size only, which can complicate matters. Bubeck and Linial asked in particular whether there are trees other than paths and stars whose inducibility can get arbitrarily close to 1, and whether there is a constant  $\epsilon > 0$  such that there are infinitely many trees of inducibility  $\geq \epsilon$ . Both questions were settled recently by Chan, Král, Mohar, and Wood [3]: the answer to the former is negative (there is a constant  $\epsilon_1 > 0$  such that every tree that is neither a path nor a star has inducibility at most  $1 - \epsilon_1$ ), while the answer to the latter is affirmative.

The definition of inducibility in (1) in terms of leaf-induced subtrees first appears in an article by Czabarka, Székely and the second author of this paper [5], originally only in the binary case. The maximum value of  $I_d(D)$  is equal to 1, and it is attained precisely when  $D$  is a *binary caterpillar*, i.e., a binary tree whose internal vertices form a path rooted at one of its ends (see [4]). Note that this is trivial if  $\|D\| = 1$  or  $\|D\| = 2$ , since there are no other trees of the same size in these cases. On the other hand, the following lower bound was shown in [4] to hold for all  $d$ -ary trees with  $k > 1$  leaves:

$$I_d(D) \geq \frac{(k - 1)!}{k^{k-1} - 1},$$

with equality for the star when  $k = d$ . In particular, we have  $I_d(D) > 0$  for all  $d$ -ary trees  $D$ . The minimum  $\min_{\|D\|=k} I_d(D)$  is not known in general, though. In this context, it is worth mentioning that the quantity

$$\liminf_{\substack{\|T\| \rightarrow \infty \\ T \text{ } d\text{-ary tree}}} \gamma(D, T) = \liminf_{n \rightarrow \infty} \min_{\substack{\|T\|=n \\ T \text{ } d\text{-ary tree}}} \gamma(D, T),$$

which is the minimum analogue of the inducibility, is much better understood. Specifically, it was shown in [6] that this quantity is always equal to 0 unless  $D$  is a binary caterpillar, in which case an explicit formula can be given.

While the limit in (2) is difficult to evaluate, it can be used to approximate  $I_d(D)$ ; this method was applied in [7] to two concrete examples. For this purpose, information on the speed of convergence is crucial. Define  $I_d(D; n)$  and  $i_d(D; n)$  as

$$I_d(D; n) = \max_{\substack{\|T\|=n \\ T \text{ } d\text{-ary tree}}} \gamma(D, T) \quad \text{and} \quad i_d(D; n) = \max_{\substack{\|T\|=(d-1)n+1 \\ T \text{ strictly } d\text{-ary tree}}} \gamma(D, T), \quad (3)$$

so that  $I_d(D) = \lim_{n \rightarrow \infty} I_d(D; n) = \lim_{n \rightarrow \infty} i_d(D; n)$ . It was shown in [4] that

$$I_d(D) \leq I_d(D; n) \leq I_d(D) + \frac{\|D\|(\|D\| - 1)}{n}, \quad (4)$$

so the sequence of maximum densities converges to the limit with an error term of order at most  $\mathcal{O}(n^{-1})$ . There are concrete examples (see [5]) showing that the order of magnitude of this error term cannot be improved in general. In the case where only strictly  $d$ -ary trees are considered, it was shown in [4] that

$$i_d(D; n) = I_d(D) + \mathcal{O}(n^{-1/2}). \tag{5}$$

Here and in the following,  $\mathcal{O}$ -constants may depend on  $d$  and  $D$ , but nothing else. It is an open question whether the order of the error term in (5) can be improved.

This paper contributes to all the aforementioned questions. In particular, we determine the precise value of  $I_d(D)$  in some new cases. Among the trees to which our method applies are what we call *even  $d$ -ary trees* (based on the property that the leaves in these trees are “evenly distributed”). This extends previous results in the binary case [5]. The even  $d$ -ary tree with  $k$  leaves, denoted  $E_k^d$ , is defined recursively as follows:

- For  $k \leq d$ ,  $E_k^d$  is a star, consisting only of the root and  $k$  leaves.
- If  $k > d$ , we express it as  $k = ds + b$ , with  $b \in \{0, 1, \dots, d - 1\}$ . Take  $d - b$  copies of  $E_s^d$  and  $b$  copies of  $E_{s+1}^d$ , and connect a new common root to each of their roots by an edge to obtain  $E_k^d$ .

Figure 2 shows the even ternary trees with up to nine leaves.

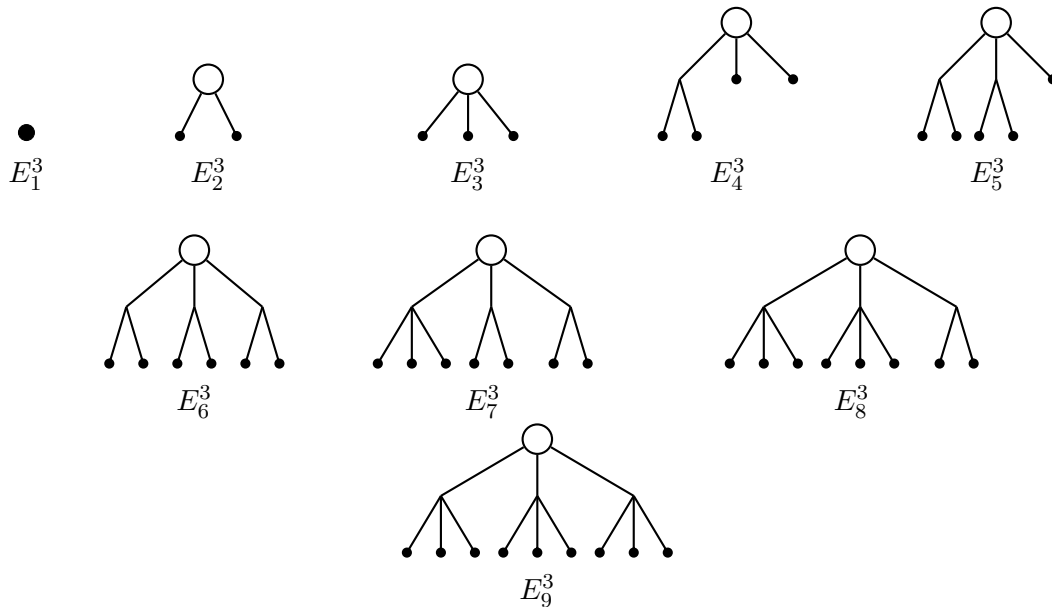


Figure 2: All even ternary trees with at most nine leaves.

While in general, the trees  $T$  that attain the maximum in (3) seem to be difficult to determine, we find evidence (looking at small instances) that there is an explicit answer for even trees, namely that the even  $d$ -ary tree  $E_n^d$  always has the greatest number of copies of the tree  $E_k^d$  over all  $n$ -leaf  $d$ -ary trees:

**Conjecture 1.1** *Let  $d \geq 2$  and  $k \geq 1$  be two fixed integers. Then we have*

$$I_d(E_k^d; n) = \gamma(E_k^d, E_n^d)$$

for every  $n \geq 1$ .

We verify that this holds in the limit as  $n \rightarrow \infty$ . The following theorem gives an explicit formula for  $I_d(E_k^d)$ .

**Theorem 1.2** *Let the constants  $c_k$  be defined recursively by  $c_0 = c_1 = 1$ , and by*

$$c_{ds+b} = \binom{d}{b} \frac{c_s^{d-b} \cdot c_{s+1}^b}{d^{ds+b} - d}$$

for every  $s \geq 0$  and every  $b \in \{0, 1, \dots, d - 1\}$ . Then we have

$$I_d(E_k^d) = k! \cdot c_k$$

for every  $k$ .

As an example, Table 1 indicates the value of  $I_3$  for the first few even ternary trees.

Table 1: Some values of  $I_3(E_k^3)$ .

$k$	1	2	3	4	5	6	7	8	9	10	11	12
$I_3(E_k^3)$	1	1	$\frac{1}{4}$	$\frac{6}{13}$	$\frac{3}{8}$	$\frac{15}{121}$	$\frac{15}{208}$	$\frac{35}{2186}$	$\frac{7}{5248}$	$\frac{1575}{255886}$	$\frac{4725}{453596}$	$\frac{1247400}{194594881}$

In addition, we show that the asymptotic formula

$$i_d(E_k^d; n) = I_d(E_k^d) + \mathcal{O}(n^{-1})$$

as  $n \rightarrow \infty$  holds for all even trees  $E_k^d$ , lending support to the conjecture that the error term in (5) can generally be improved to  $\mathcal{O}(n^{-1})$ .

Theorem 1.2 will be proven as part of a general approach in which a strictly  $d$ -ary version of even trees plays a major role. For the inducibility of arbitrary  $d$ -ary trees, our approach yields both a general lower bound (Theorem 2.3) and an upper bound (Proposition 3.1). In both cases, the bounds are determined recursively by decomposing a rooted tree into its *branches*, i.e., the smaller trees that result as components when the root is removed. As it turns out, the inducibility of a tree can often be bounded in terms of the product of the inducibilities of its branches, both from above and below.

As a particularly simple example, we have

$$I_d(D) \leq \prod_{i=1}^d I_d(D_i)$$

for every  $d$ -ary tree  $D$  with branches  $D_1, D_2, \dots, D_d$  with the property that no two nonisomorphic branches  $D_i, D_j$  have the same size (Corollary 3.3). We provide a more general version of this inequality as well as further upper and lower bounds of a similar nature. We also demonstrate in some examples how they are applied to compute or approximate the inducibility in different cases.

## 2 A special limit

The proof of Theorem 1.2 (as well as other results) relies on a general recursion for the number of copies  $c(D, T)$  of a tree  $D$  inside a larger tree  $T$ , based on the decomposition of a rooted tree into its branches. It will be useful for notational purposes to allow empty trees (in particular, as branches of a tree) with no leaf. If  $D$  is empty, then we set  $c(D, T) = 1$ ; accordingly, we will also set  $I_d(D) = 1$  if  $D$  is empty. If  $T$  is empty, but  $D$  is not, then  $c(D, T) = 0$ .

For a  $d$ -ary tree  $D$  with branches  $D_1, D_2, \dots, D_d$  (some of which are allowed to be empty), we define the equivalence relation  $\sim_D$  on the set of all permutations of  $[d] = \{1, 2, \dots, d\}$  as follows: for two permutations  $\pi$  and  $\pi'$  of  $[d]$ ,

$$(\pi(1), \pi(2), \dots, \pi(d)) \sim_D (\pi'(1), \pi'(2), \dots, \pi'(d))$$

if for every  $j \in [d]$ , the tree  $D_{\pi(j)}$  is isomorphic to  $D_{\pi'(j)}$  as a rooted tree (i.e., there is a root-preserving isomorphism between the two; two empty trees are of course considered isomorphic). Moreover, let  $M(D)$  be a complete set of representatives of all equivalence classes of  $\sim_D$ . One verifies easily that all these equivalence classes have the same cardinality.

With all this notation in mind, we can state and prove the following lemma, which will be used repeatedly in various places of this paper.

**Lemma 2.1** *Let  $T$  be a  $d$ -ary tree with branches  $T_1, T_2, \dots, T_d$  (some of which might be empty). Then for every  $d$ -ary tree  $D$  with branches  $D_1, D_2, \dots, D_d$  (some of which might also be empty), we have*

$$c(D, T) = \sum_{i=1}^d c(D, T_i) + \sum_{\pi \in M(D)} \prod_{j=1}^d c(D_{\pi(j)}, T_j).$$

*Proof.* Recall that  $c(D, T)$  denotes the number of subsets of leaves of  $T$  that induce a copy of  $D$ . A subset of leaves of  $T$  belongs to either a single branch of  $T$  or different branches of  $T$ .

The number of subsets of leaves that belong to a single branch of  $T$  and induce a copy of  $D$  is given by  $\sum_{i=1}^d c(D, T_i)$ . On the other hand, the number of copies of  $D$  in which its branches  $D_{\pi(1)}, D_{\pi(2)}, \dots, D_{\pi(d)}$  are induced by subsets of leaves of  $T_1, T_2, \dots, T_d$ , respectively, is given by  $\prod_{j=1}^d c(D_{\pi(j)}, T_j)$ . This term needs to be summed over all distinct (non-isomorphic, to be precise) permutations of the branches  $D_1, D_2, \dots, D_d$ , for which  $M(D)$  provides a set of representatives. Hence, the formula follows.  $\square$

For our next step, we introduce the natural analogue of even  $d$ -ary trees in the class of strictly  $d$ -ary trees:

- The tree  $H_0^d$  consists only of a single leaf.

- If  $n > 0$ , we write  $n - 1 = ds + b$ , with  $b \in \{0, 1, \dots, d - 1\}$ . Take  $d - b$  copies of  $H_s^d$  and  $b$  copies of  $H_{s+1}^d$ , and connect a new common root to each of their roots by an edge to obtain  $H_n^d$ . For future purposes, let us write  $s_1(n) = s_2(n) = \dots = s_{d-b}(n) = s$  and  $s_{d-b+1}(n) = s_{d-b+2}(n) = \dots = s_d(n) = s + 1$  to encode the branches.

See Figure 3 for an example. One easily shows that  $H_n^d$  is a strictly  $d$ -ary tree with  $(d - 1)n + 1$  leaves for every  $n$ . As in the sequence of even  $d$ -ary trees, the leaves are as evenly distributed among the branches as possible. We first prove that  $\gamma(D, H_n^d)$  converges to a positive limit for every fixed  $d$ -ary tree  $D$ , which immediately provides a lower bound on the inducibility.

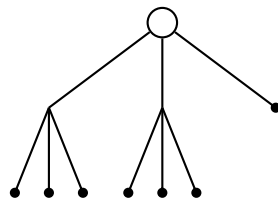


Figure 3: The tree  $H_3^3$ .

**Definition 2.2** For every  $d$ -ary tree  $D$ , let  $\eta_d(D)$  be determined recursively as follows: it is equal to 1 when  $D$  is empty or only consists of a single vertex. Otherwise, let  $D_1, D_2, \dots, D_d$  be the branches of  $D$  (some possibly empty), and define  $M(D)$  as in Lemma 2.1. Now set

$$\eta_d(D) = \binom{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \frac{|M(D)|}{d^{\|D\|} - d} \prod_{i=1}^d \eta_d(D_i).$$

**Theorem 2.3** For every  $d$ -ary tree  $D$ , we have

$$\gamma(D, H_n^d) = \eta_d(D) + \mathcal{O}(n^{-1}),$$

where the constant implied by the  $\mathcal{O}$ -term only depends on  $d$  and  $D$ .

*Proof.* Define  $\phi(D) = \frac{(d-1)^{\|D\|} \eta_d(D)}{\|D\|!}$ , which satisfies the recursion

$$\phi(D) = \frac{|M(D)|}{d^{\|D\|} - d} \prod_{i=1}^d \phi(D_i). \tag{6}$$

Let us set  $k = \|D\|$  and  $\ell_i = \|D_i\|$  for simplicity and use induction on  $k$  to prove that there exists a nonnegative constant  $\kappa(D)$  such that

$$|c(D, H_n^d) - \phi(D)n^k| \leq \kappa(D)n^{k-1} \tag{7}$$

holds for all  $n \geq 1$ . This is straightforward for  $k = 0$ , where  $D$  is the empty tree,  $c(D, H_n^d) = 1$  and  $\phi(D) = 1$ , so that we can take  $\kappa(D) = 0$ . Likewise, the cases

$k = 1$  (where  $c(D, H_n^d) = \|H_n^d\| = (d - 1)n + 1$  and  $\phi(D) = d - 1$ ) and  $k = 2$  (where  $c(D, H_n^d) = \binom{\|H_n^d\|}{2} = \binom{(d-1)n+1}{2}$  and  $\phi(D) = \frac{(d-1)^2}{2}$ ) are easy.

For the induction step, we apply the recursion of Lemma 2.1: for the tree  $T = H_n^d$ , the branches  $T_j$  are of the form  $H_{s_j(n)}^d$ , where  $s_j(n) = \lfloor \frac{n-1}{d} \rfloor$  or  $s_j(n) = \lfloor \frac{n-1}{d} \rfloor + 1$ . So for every  $j$ , we have

$$c(D_{\pi(j)}, T_j) = \phi(D_{\pi(j)}) \|T_j\|^{\ell_{\pi(j)}} + \mathcal{O}(\|T_j\|^{\ell_{\pi(j)}-1}) = \phi(D_{\pi(j)}) \left(\frac{n}{d}\right)^{\ell_{\pi(j)}} + \mathcal{O}(n^{\ell_{\pi(j)}-1})$$

by the induction hypothesis, applied to  $D_{\pi(j)}$ . From this, it follows that the final sum in Lemma 2.1 (with  $T = H_n^d$ ) is equal to

$$\sum_{\pi \in M(D)} \prod_{j=1}^d \left( \phi(D_{\pi(j)}) \left(\frac{n}{d}\right)^{\ell_{\pi(j)}} \left(1 + \mathcal{O}(n^{-1})\right) \right) = |M(D)| \prod_{i=1}^d \phi(D_i) \left(\frac{n}{d}\right)^k \left(1 + \mathcal{O}(n^{-1})\right).$$

Thus, we can conclude that

$$c(D, H_n^d) = \sum_{i=1}^d c(D, H_{s_i(n)}^d) + |M(D)| \prod_{i=1}^d \phi(D_i) \left(\frac{n}{d}\right)^k + \mathcal{O}(n^{k-1}).$$

In particular, there exists a positive constant  $C(D)$  such that

$$\left| c(D, H_n^d) - \sum_{i=1}^d c(D, H_{s_i(n)}^d) - |M(D)| \prod_{i=1}^d \phi(D_i) \left(\frac{n}{d}\right)^k \right| \leq C(D) n^{k-1} \tag{8}$$

for all  $n \geq 1$ . We choose  $\kappa(D)$  in such a way that (7) holds for  $1 \leq n \leq d$ , and

$$\kappa(D) \geq \sup_{n \geq 1} \frac{\phi(D) \sum_{i=1}^d |s_i(n)^k - \left(\frac{n}{d}\right)^k| + C(D) n^{k-1}}{n^{k-1} - \sum_{i=1}^d s_i(n)^{k-1}}.$$

This choice will be justified later. To see why the supremum is positive and finite, note first that the denominator is always positive, as  $\sum_{i=1}^d s_i(n)^{k-1} \leq (\sum_{i=1}^d s_i(n))^{k-1} = (n - 1)^{k-1}$ . The numerator is clearly positive, so the fraction is positive for every  $n$ . Moreover, since  $s_i(n) = \frac{n}{d} + \mathcal{O}(1)$  for each  $i$ , the numerator is  $\mathcal{O}(n^{k-1})$ , and the denominator is  $n^{k-1}(1 - d^{2-k}) + \mathcal{O}(n^{k-2})$ . The factor  $1 - d^{2-k}$  is positive as we are assuming  $k \geq 3$ . Therefore, the quotient remains bounded as  $n \rightarrow \infty$ .

Now we prove by induction on  $n$  that (7) holds for all  $n \geq 1$  with this choice of  $\kappa(D)$ . For  $1 \leq n \leq d$ , it holds by our choice of  $\kappa(D)$ . For  $n > d$ , we can apply the induction hypothesis to  $c(D, H_{s_i(n)}^d)$  for all  $i$  in (8), which is possible since  $s_i(n) \geq 1$  for all  $i$ . This yields

$$\left| c(D, H_n^d) - \sum_{i=1}^d \phi(D) s_i(n)^k - |M(D)| \prod_{i=1}^d \phi(D_i) \left(\frac{n}{d}\right)^k \right| \leq \kappa(D) \sum_{i=1}^d s_i(n)^{k-1} + C(D) n^{k-1}$$



by the triangle inequality. Applying the triangle inequality one more time gives us

$$\begin{aligned} & \left| c(D, H_n^d) - d \cdot \phi(D) \left(\frac{n}{d}\right)^k - |M(D)| \prod_{i=1}^d \phi(D_i) \left(\frac{n}{d}\right)^k \right| \\ & \leq \kappa(D) \sum_{i=1}^d s_i(n)^{k-1} + \phi(D) \sum_{i=1}^d \left| s_i(n)^k - \left(\frac{n}{d}\right)^k \right| + C(D)n^{k-1}. \end{aligned}$$

By the recursion for  $\phi(D)$ , we have  $|M(D)| \prod_{i=1}^d \phi(D_i) = (d^k - d)\phi(D)$ , and by our choice of  $\kappa(D)$ , we have

$$\phi(D) \sum_{i=1}^d \left| s_i(n)^k - \left(\frac{n}{d}\right)^k \right| + C(D)n^{k-1} \leq \kappa(D) \left( n^{k-1} - \sum_{i=1}^d s_i(n)^{k-1} \right).$$

Thus

$$\begin{aligned} & \left| c(D, H_n^d) - d \cdot \phi(D) \left(\frac{n}{d}\right)^k - (d^k - d)\phi(D) \left(\frac{n}{d}\right)^k \right| \\ & \leq \kappa(D) \sum_{i=1}^d s_i(n)^{k-1} + \kappa(D) \left( n^{k-1} - \sum_{i=1}^d s_i(n)^{k-1} \right), \end{aligned}$$

which finally reduces to

$$\left| c(D, H_n^d) - \phi(D)n^k \right| \leq \kappa(D)n^{k-1},$$

completing the induction with respect to  $n$  and thus also the induction with respect to  $k$ . □

Note that

$$\eta_d(D) = \lim_{n \rightarrow \infty} \gamma(D, H_n^d) \leq I_d(D)$$

holds by definition, so Theorem 2.3 provides a lower bound on the inducibility. We now show that this lower bound is in fact sharp for (among others) even trees, thereby proving Theorem 1.2. This is achieved by proving a matching upper bound, which is derived in the following.

### 3 Upper bounds involving branches

We first need some notation. For a fixed  $d \geq 2$  and a given  $d$ -ary tree  $D$  with branches  $D_1, D_2, \dots, D_d$  (some of them possibly empty), we define the  $d$ -dimensional real function

$$Z_D(x_1, x_2, \dots, x_d) = \frac{1}{1 - \sum_{i=1}^d x_i^{\|D\|}} \sum_{\pi \in M(D)} \prod_{j=1}^d x_j^{\|D_{\pi(j)}\|}.$$

It follows from the definition that this function is always symmetric in its variables. This is because  $\pi \sim_D \pi'$  implies that  $D_{\pi(j)}$  and  $D_{\pi'(j)}$  are isomorphic for all  $j$ , thus  $\|D_{\pi(j)}\| = \|D_{\pi'(j)}\|$  for all  $j$ . It follows that the final product is the same for all members of an equivalence class of  $\sim_D$ , and we can write  $Z_D$  as

$$Z_D(x_1, x_2, \dots, x_d) = \frac{1}{1 - \sum_{i=1}^d x_i^{\|D\|}} \cdot \frac{|M(D)|}{d!} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\|D_{\pi(j)}\|}, \tag{9}$$

the sum now being over the set  $S_d$  of all permutations. For example, when  $D$  is the even ternary tree  $E_7^3$  with seven leaves, as shown in Figure 2, the function is given by

$$Z_{E_7^3}(x_1, x_2, x_3) = \frac{x_1^3 x_2^2 x_3^2 + x_1^2 x_2^3 x_3^2 + x_1^2 x_2^2 x_3^3}{1 - x_1^7 - x_2^7 - x_3^7}.$$

The following proposition bounds the inducibility of a tree  $D$  in terms of the inducibilities of its branches and the function  $Z_D$ .

**Proposition 3.1** *Let  $D$  be a  $d$ -ary tree with branches  $D_1, D_2, \dots, D_d$  (some of them possibly empty). Then the following inequality holds:*

$$I_d(D) \leq \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right) \left( \prod_{i=1}^d I_d(D_i) \right) \sup_{\substack{0 \leq x_1, x_2, \dots, x_d < 1 \\ x_1 + x_2 + \dots + x_d = 1}} Z_D(x_1, x_2, \dots, x_d). \tag{10}$$

The benefit of this proposition is that the combinatorial problem is translated to a purely analytic question. The supremum on the right side of the inequality can be determined explicitly in many cases. In order to prove the proposition, we first need a technical lemma on the supremum occurring in (10) that will also be useful at a later point.

**Lemma 3.2** *Let  $D$  be a  $d$ -ary tree, and let  $D_1, D_2, \dots, D_d$  be its branches (some of which might be empty). Moreover, let  $m_j$  be the number of branches with  $j$  leaves for every  $j \geq 0$ . We have*

$$\sup_{\substack{0 \leq x_1, x_2, \dots, x_d < 1 \\ x_1 + x_2 + \dots + x_d = 1}} Z_D(x_1, x_2, \dots, x_d) \leq \frac{|M(D)| \prod_{j \geq 0} m_j!}{d!} \cdot \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right)^{-1}.$$

*In particular, if  $D$  has the property that no two nonisomorphic branches have the same size, then*

$$\sup_{\substack{0 \leq x_1, x_2, \dots, x_d < 1 \\ x_1 + x_2 + \dots + x_d = 1}} Z_D(x_1, x_2, \dots, x_d) \leq \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right)^{-1}.$$

*Finally, if  $D$  has only two nonempty branches  $D_1, D_2$  with  $\|D_1\| = 1$  and  $\|D_2\| > 1$ , then*

$$\sup_{\substack{0 \leq x_1, x_2, \dots, x_d < 1 \\ x_1 + x_2 + \dots + x_d = 1}} Z_D(x_1, x_2, \dots, x_d) = \frac{1}{\|D\|}.$$

*Proof.* Let us use the abbreviations  $k = \|D\|$  and  $\ell_i = \|D_i\|$ . Recall that we can write the function  $Z_D$  as

$$Z_D(x_1, x_2, \dots, x_d) = \frac{1}{1 - \sum_{i=1}^d x_i^k} \cdot \frac{|M(D)|}{d!} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\ell_{\pi(j)}}.$$

We apply the multinomial theorem to  $(x_1 + x_2 + \dots + x_d)^k$  and split the resulting terms according to the exponents of  $x_1, x_2, \dots, x_d$  into permutations of  $(k, 0, \dots, 0)$ , permutations of  $(\ell_1, \ell_2, \dots, \ell_d)$ , and the rest. The terms corresponding to permutations of  $(k, 0, \dots, 0)$  are clearly  $\sum_{i=1}^d x_i^k$ . Monomials where the exponents form a permutation of  $(\ell_1, \ell_2, \dots, \ell_d)$  have a coefficient of  $\binom{k}{\ell_1, \ell_2, \dots, \ell_d}$ , and the sum of all such monomials can be expressed as

$$\frac{1}{\prod_{j \geq 0} m_j!} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\ell_{\pi(j)}},$$

since each of them occurs precisely  $\prod_{j \geq 0} m_j!$  times in the sum over all permutations in  $S_d$ . So the contribution to the expansion of  $(x_1 + x_2 + \dots + x_d)^k$  according to the multinomial theorem can be expressed as

$$\frac{1}{\prod_{j \geq 0} m_j!} \binom{k}{\ell_1, \ell_2, \dots, \ell_d} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\ell_{\pi(j)}}.$$

The remaining terms corresponding to exponents that are not permutations of  $(k, 0, \dots, 0)$  or  $(\ell_1, \ell_2, \dots, \ell_d)$  are clearly nonnegative whenever the variables  $x_1, x_2, \dots, x_d$  are, so we obtain

$$(x_1 + x_2 + \dots + x_d)^k \geq \sum_{i=1}^d x_i^k + \frac{1}{\prod_{j \geq 0} m_j!} \binom{k}{\ell_1, \ell_2, \dots, \ell_d} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\ell_{\pi(j)}}.$$

If additionally  $x_1 + x_2 + \dots + x_d = 1$ , then we can easily manipulate this to get

$$\begin{aligned} Z_D(x_1, x_2, \dots, x_d) &= \frac{1}{1 - \sum_{i=1}^d x_i^k} \cdot \frac{|M(D)|}{d!} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\ell_{\pi(j)}} \\ &\leq \frac{|M(D)| \prod_{j \geq 0} m_j!}{d!} \binom{k}{\ell_1, \ell_2, \dots, \ell_d}^{-1}, \end{aligned}$$

which proves the first part.

If we assume that two branches  $D_i, D_j$  of  $D$  are isomorphic if and only if  $\|D_i\| = \|D_j\|$ , then the equivalence relation  $\sim_D$  is given by

$$\pi \sim_D \pi' \iff \ell_{\pi(j)} = \ell_{\pi'(j)} \text{ for all } j.$$

Accordingly, the elements of  $M(D)$  correspond to all distinct permutations of  $(\ell_1, \ell_2, \dots, \ell_d)$ , and we have

$$|M(D)| = \frac{d!}{\prod_{j \geq 0} m_j!},$$

giving us the second part of the lemma.

For the proof of the final part of the lemma, we merely need to show that the upper bound can be reached in the limit for a suitable sequence of vectors  $(x_1, x_2, \dots, x_d)$ . Note that under the given conditions, the function  $Z_D$  is given by

$$\begin{aligned} Z_D(x_1, x_2, \dots, x_d) &= \frac{\sum_{\{i,j\} \subseteq [d]} (x_i x_j^{k-1} + x_i^{k-1} x_j)}{1 - \sum_{i=1}^d x_i^k} \\ &= \frac{(\sum_{i=1}^d x_i) (\sum_{i=1}^d x_i^{k-1}) - (\sum_{i=1}^d x_i^k)}{1 - \sum_{i=1}^d x_i^k}. \end{aligned}$$

If we set  $x_1 = x_2 = \dots = x_{d-1} = \epsilon$  and  $x_d = 1 - (d - 1)\epsilon$ , the numerator is readily seen to be  $(d - 1)\epsilon + \mathcal{O}(\epsilon^2)$ , while the denominator is  $(d - 1)k\epsilon + \mathcal{O}(\epsilon^2)$ . Hence we have

$$\lim_{\epsilon \rightarrow 0^+} Z_D(\epsilon, \epsilon, \dots, \epsilon, 1 - (d - 1)\epsilon) = \frac{1}{k},$$

which completes the proof of the lemma. □

*Proof of Proposition 3.1.* Let us first consider the case that  $D$  has only two leaves. We can then assume that both  $D_1$  and  $D_2$  are single vertices, and all other branches empty. Thus  $I_d(D) = I_d(D_1) = I_d(D_2) = \dots = I_d(D_d) = 1$ . Moreover,

$$Z_D(x_1, x_2, \dots, x_d) = \frac{\sum_{\{i,j\} \subseteq [d]} x_i x_j}{1 - \sum_{i=1}^d x_i^2} = \frac{(\sum_{i=1}^d x_i)^2 - \sum_{i=1}^d x_i^2}{2(1 - \sum_{i=1}^d x_i^2)}.$$

If  $x_1 + x_2 + \dots + x_d = 1$ , this actually simplifies to  $\frac{1}{2}$ , so the supremum in the inequality is  $\frac{1}{2}$ , and the statement of the proposition holds.

For the rest of the proof, we can assume that  $D$  has more than two leaves. As before, let us use the abbreviations  $k = \|D\|$  and  $\ell_i = \|D_i\|$ . We know from the proof of Theorem 3 in [4] that

$$0 \leq I_d(D; n) - I_d(D) \leq \frac{k(k - 1)}{n} \tag{11}$$

for all  $n \geq k$ . Consider a sequence  $T_1, T_2, \dots$  of  $d$ -ary trees such that  $\|T_n\| \rightarrow \infty$  as  $n \rightarrow \infty$  and  $c(D, T_n)$  is the maximum of  $c(D, T)$  over all trees  $T$  with the same number of leaves as  $T_n$ . Denote the branches of  $T_n$  by  $T_{n,1}, T_{n,2}, \dots, T_{n,d}$  (some of these branches are allowed to be empty). One can assume that  $T_{n,1}$  is the branch of  $T_n$  with the greatest number of leaves for every  $n$ . Set  $\alpha_{n,i} = \|T_{n,i}\|/\|T_n\|$  for every  $i \in [d]$  and every  $n$  (the proportion of leaves belonging to  $T_{n,i}$ ), and set  $\beta_n = 1 - \alpha_{n,1}$ .

We distinguish two cases based on whether  $\beta_n$  is “large” (bounded below by a positive constant) or “small” (going to 0 along a subsequence) as  $n \rightarrow \infty$ .

**Case 1:** Suppose that  $\beta_n$  is bounded below by a positive constant  $\delta$  as  $n \rightarrow \infty$ . We can assume that  $\delta \leq \frac{1}{d}$ . Note that  $\beta_n$  is automatically bounded above by  $\frac{d-1}{d}$  by definition. It follows that

$$1 - \sum_{i=1}^d \alpha_{n,i}^k \geq 1 - \alpha_{n,1}^k - \left( \sum_{i=2}^d \alpha_{n,i} \right)^k = 1 - (1 - \beta_n)^k - \beta_n^k \geq 1 - (1 - \delta)^k - \delta^k \quad (12)$$

for all  $n$ , since the function  $x \mapsto 1 - (1 - x)^k - x^k$  is increasing for  $x \in [0, \frac{1}{2}]$  and decreasing for  $x \in [\frac{1}{2}, 1]$ . Now we apply Lemma 2.1:

$$c(D, T_n) = \sum_{i=1}^d c(D, T_{n,i}) + \sum_{\pi \in M(D)} \prod_{j=1}^d c(D_{\pi(j)}, T_{n,j}).$$

In view of (11), it gives us

$$\begin{aligned} I_d(D) \binom{\|T_n\|}{k} &\leq c(D, T_n) \leq \sum_{i=1}^d \left( I_d(D) + \frac{k(k-1)}{\|T_{n,i}\|} \right) \binom{\|T_{n,i}\|}{k} \\ &\quad + \sum_{\pi \in M(D)} \prod_{j=1}^d \left( I_d(D_{\pi(j)}) + \frac{\ell_{\pi(j)}(\ell_{\pi(j)} - 1)}{\|T_{n,j}\|} \right) \binom{\|T_{n,j}\|}{\ell_{\pi(j)}}, \end{aligned}$$

which implies that

$$\begin{aligned} I_d(D) \binom{\|T_n\|}{k} &\leq \sum_{i=1}^d \left( I_d(D) \frac{\|T_{n,i}\|^k}{k!} + \frac{\|T_{n,i}\|^{k-1}}{(k-2)!} \right) \\ &\quad + \sum_{\pi \in M(D)} \prod_{j=1}^d \left( I_d(D_{\pi(j)}) \frac{\|T_{n,j}\|^{\ell_{\pi(j)}}}{\ell_{\pi(j)}!} + N(T_{n,j}, D_{\pi(j)}) \right), \end{aligned}$$

where  $N(T_{n,j}, D_{\pi(j)})$  is equal to  $\|T_{n,j}\|^{\ell_{\pi(j)}-1}/(\ell_{\pi(j)} - 2)!$  if  $\ell_{\pi(j)} \geq 2$ , and 0 otherwise. Consequently,

$$\left( \|T_n\|^k - \sum_{i=1}^d \|T_{n,i}\|^k \right) I_d(D) \leq k! \sum_{\pi \in M(D)} \prod_{j=1}^d I_d(D_{\pi(j)}) \frac{\|T_{n,j}\|^{\ell_{\pi(j)}}}{\ell_{\pi(j)}!} + \mathcal{O}(\|T_n\|^{k-1}),$$

as  $\|T_{n,j}\| < \|T_n\|$  for all  $j \in [d]$  and all  $n$ . Dividing through by  $\|T_n\|^k$ , we get

$$\left( 1 - \sum_{i=1}^d \alpha_{n,i}^k \right) I_d(D) \leq \frac{k!}{\ell_1! \ell_2! \cdots \ell_d!} \sum_{\pi \in M(D)} \prod_{j=1}^d I_d(D_{\pi(j)}) \alpha_{n,j}^{\ell_{\pi(j)}} + \mathcal{O}(\|T_n\|^{-1}).$$

Now using the fact that  $1 - \sum_{i=1}^d \alpha_{n,i}^k$  is bounded below by a positive constant as  $n \rightarrow \infty$  by (12), we deduce that

$$\begin{aligned} I_d(D) &\leq \left( \prod_{i=1}^d I_d(D_i) \right) \binom{k}{\ell_1, \ell_2, \dots, \ell_d} Z_D(\alpha_{n,1}, \alpha_{n,2}, \dots, \alpha_{n,d}) + \mathcal{O}(\|T_n\|^{-1}) \\ &\leq \left( \prod_{i=1}^d I_d(D_i) \right) \binom{k}{\ell_1, \ell_2, \dots, \ell_d} \sup_{\substack{0 \leq x_1, x_2, \dots, x_d < 1 \\ x_1 + x_2 + \dots + x_d = 1}} Z_D(x_1, x_2, \dots, x_d) + \mathcal{O}(\|T_n\|^{-1}). \end{aligned}$$

Finally, we take the limit as  $n \rightarrow \infty$ , giving us the desired result in the first case.

**Case 2:** If  $\beta_n$  is not bounded below by a positive constant, then  $\liminf_{n \rightarrow \infty} \beta_n = 0$  and we can assume (without loss of generality, by considering a subsequence if necessary) that the limit of  $\beta_n$  is actually 0 as  $n \rightarrow \infty$ . Denote by  $T_n \setminus T_{n,1}$  the tree that is obtained by removing the branch  $T_{n,1}$  from  $T_n$  (and possibly the root of  $T_n$  if there is only one other nonempty branch). We first prove two auxiliary claims.

*Claim 1:* We claim that the number of copies of  $D$  in  $T_n$  that involve more than one leaf of  $T_n \setminus T_{n,1}$  is at most of order  $\mathcal{O}(\beta_n^2 \|T_n\|^k)$ .

For the proof of this claim, note that by definition, the number of copies of  $D$  in  $T_n$  that involve more than one leaf of  $T_n \setminus T_{n,1}$  is at most

$$\begin{aligned} \sum_{j=2}^k \binom{\|T_n\| - \|T_{n,1}\|}{j} \binom{\|T_{n,1}\|}{k-j} &\leq \sum_{j=2}^k \frac{(\|T_n\| - \|T_{n,1}\|)^j \|T_{n,1}\|^{k-j}}{j!(k-j)!} \\ &= \|T_n\|^k (1 - \alpha_{n,1})^2 \sum_{j=2}^k \frac{(1 - \alpha_{n,1})^{j-2} \alpha_{n,1}^{k-j}}{j!(k-j)!} \\ &\leq \|T_n\|^k \beta_n^2 \sum_{j=2}^k \frac{1}{j!(k-j)!}. \end{aligned}$$

This completes the proof of Claim 1. It follows that the proportion of copies of  $D$  in  $T_n$  that involve more than one leaf of  $T_n \setminus T_{n,1}$  is at most of order  $\mathcal{O}(\beta_n^2)$  among all subsets of  $k$  leaves of  $T_n$ .

*Claim 2:* We further claim that  $D$  must have only two nonempty branches, one of which is a single leaf.

Indeed, suppose that  $D$  does not have this shape. Then the subsets of leaves of  $T_n$  that induce a copy of  $D$  come in two types: either the  $k$  leaves are all leaves of  $T_{n,1}$ , or more than one of the  $k$  leaves is a leaf of  $T_n \setminus T_{n,1}$ . So this gives us

$$c(D, T_n) = c(D, T_{n,1}) + \mathcal{O}(\beta_n^2 \|T_n\|^k) \tag{13}$$

by Claim 1. It was established in the proof of (11) (see [4, Theorem 3]) that

$$0 \leq I_d(D; j) - I_d(D; j + 1) \leq \frac{k(k-1)}{j(j+1)}.$$

Summing all these inequalities for  $j = m, m + 1, \dots, n - 1$ , we find that

$$0 \leq I_d(D; m) - I_d(D; n) \leq k(k - 1) \left( \frac{1}{m} - \frac{1}{n} \right).$$

Thus we have

$$I_d(D; m) - I_d(D; n) = \mathcal{O} \left( \frac{n - m}{mn} \right)$$

as  $m \leq n$  and  $m \rightarrow \infty$ . In particular, since  $T_n$  was assumed to contain the maximum number of copies of  $D$  among all trees of the same size,

$$\gamma(D, T_{n,1}) - \gamma(D, T_n) \leq I_d(D; \|T_{n,1}\|) - \gamma(D, T_n) = \mathcal{O} \left( \frac{\|T_n\| - \|T_{n,1}\|}{\|T_n\| \cdot \|T_{n,1}\|} \right). \tag{14}$$

Using (14), formula (13) implies that

$$c(D, T_n) \leq \frac{\binom{\|T_{n,1}\|}{k}}{\binom{\|T_n\|}{k}} c(D, T_n) + \mathcal{O} \left( \|T_{n,1}\|^k \cdot \frac{\|T_n\| - \|T_{n,1}\|}{\|T_n\| \cdot \|T_{n,1}\|} + \beta_n^2 \|T_n\|^k \right).$$

Thus

$$\left( 1 - \frac{\binom{\|T_{n,1}\|}{k}}{\binom{\|T_n\|}{k}} \right) c(D, T_n) \leq \mathcal{O}(\beta_n \|T_{n,1}\|^{k-1} + \beta_n^2 \|T_n\|^k),$$

and using the asymptotic formula

$$\binom{\|T_n\|}{k} - \binom{\|T_{n,1}\|}{k} \sim (\|T_n\| - \|T_{n,1}\|) \frac{\|T_n\|^{k-1}}{(k-1)!} = \frac{\|T_n\|^k \beta_n}{(k-1)!}, \tag{15}$$

which holds since  $\|T_n\| \sim \|T_{n,1}\|$ , we derive

$$\gamma(D, T_n) \leq \mathcal{O}(\|T_n\|^{-1} + \beta_n).$$

Therefore

$$I_d(D) = \lim_{n \rightarrow \infty} \gamma(D, T_n) \leq 0$$

as  $\lim_{n \rightarrow \infty} \beta_n = 0$ . This contradicts the fact that  $I_d(D)$  is strictly positive (which was mentioned in the introduction and also follows from Theorem 2.3). Thus the proof of Claim 2 is complete.

Back to the main argument, we can now assume (by Claim 2) that  $D$  has only two nonempty branches, one of which ( $D_1$ , say) is the tree that has only one vertex. Since we are assuming that  $k > 2$ , the second nonempty branch  $D_2$  of  $D$  has at least two leaves. Using Claim 1, we get

$$c(D, T_n) = c(D, T_{n,1}) + (\|T_n\| - \|T_{n,1}\|)c(D_2, T_{n,1}) + \mathcal{O}(\beta_n^2 \|T_n\|^k).$$

Following the same course of reasoning used to prove Claim 2, it is not difficult to see that

$$\begin{aligned} & \left(1 - \frac{\binom{\|T_{n,1}\|}{k}}{\binom{\|T_n\|}{k}}\right) c(D, T_n) \\ & \leq (\|T_n\| - \|T_{n,1}\|) \binom{\|T_{n,1}\|}{k-1} \gamma(D_2, T_{n,1}) + \mathcal{O}(\beta_n \|T_n\|^{k-1} + \beta_n^2 \|T_n\|^k). \end{aligned}$$

It follows from the asymptotic formula (15) now that

$$\gamma(D, T_n) - \gamma(D_2, T_{n,1}) \leq \mathcal{O}(\|T_n\|^{-1} + \beta_n).$$

Applying  $\liminf$  to both sides of this inequality, we get

$$I_d(D) - \limsup_{n \rightarrow \infty} \gamma(D_2, T_{n,1}) = \liminf_{n \rightarrow \infty} (\gamma(D, T_n) - \gamma(D_2, T_{n,1})) \leq 0,$$

which implies that

$$I_d(D) \leq \limsup_{n \rightarrow \infty} \gamma(D_2, T_{n,1}) \leq I_d(D_2).$$

This completes the proof of Case 2 and thus the entire proposition once we invoke the final part of Lemma 3.2.  $\square$

The following corollary is a direct consequence of Proposition 3.1 combined with the first and second part of Lemma 3.2.

**Corollary 3.3** *Let  $D$  be a  $d$ -ary tree, and let  $D_1, D_2, \dots, D_d$  be its branches (some of which might be empty). Moreover, let  $m_j$  be the number of branches with  $j$  leaves for every  $j \geq 0$ . Then we have*

$$I_d(D) \leq \frac{|M(D)| \prod_{j \geq 0} m_j!}{d!} \prod_{i=1}^d I_d(D_i).$$

If  $D$  has the property that no two nonisomorphic branches have the same size, then this reduces to

$$I_d(D) \leq \prod_{i=1}^d I_d(D_i).$$

Further improvements rely on our ability to determine (or estimate) the supremum over the function  $Z_D$  occurring in Proposition 3.1. This will be achieved for a special class of trees in the following section.

## 4 Balanced trees

Recall from Theorem 2.3 that  $\eta_d(D)$ , as described in Definition 2.2, provides a lower bound on the inducibility:  $\eta_d(D) \leq I_d(D)$ . Simple instances where equality holds are the empty tree or trees with only one or two leaves. It turns out that there are many more such cases, which is a consequence of the following theorem:



**Theorem 4.1** *Let  $D$  be a  $d$ -ary tree with branches  $D_1, D_2, \dots, D_d$  (some of which may be empty). If  $I_d(D_i) = \eta_d(D_i)$  for all branches and the supremum of  $Z_D(x_1, x_2, \dots, x_d)$  under the conditions  $0 \leq x_i < 1$  and  $x_1 + x_2 + \dots + x_d = 1$  is attained when  $x_1 = x_2 = \dots = x_d = \frac{1}{d}$ , i.e.,*

$$\sup_{\substack{0 \leq x_1, x_2, \dots, x_d < 1 \\ x_1 + x_2 + \dots + x_d = 1}} Z_D(x_1, x_2, \dots, x_d) = Z_D\left(\frac{1}{d}, \frac{1}{d}, \dots, \frac{1}{d}\right) = \frac{|M(D)|}{d^{\|D\|} - d},$$

then we also have  $I_d(D) = \eta_d(D)$ .

*Proof.* Let us compare the recursion for  $\eta_d$ ,

$$\eta_d(D) = \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right) \frac{|M(D)|}{d^{\|D\|} - d} \prod_{i=1}^d \eta_d(D_i), \tag{16}$$

to the upper bound in Proposition 3.1:

$$I_d(D) \leq \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right) \left( \prod_{i=1}^d I_d(D_i) \right) \sup_{\substack{0 \leq x_1, x_2, \dots, x_d < 1 \\ x_1 + x_2 + \dots + x_d = 1}} Z_D(x_1, x_2, \dots, x_d). \tag{17}$$

The similarities are obvious. Plugging  $x_1 = x_2 = \dots = x_d = \frac{1}{d}$  into the representation (9), we obtain

$$Z_D\left(\frac{1}{d}, \frac{1}{d}, \dots, \frac{1}{d}\right) = \frac{1}{1 - \sum_{i=1}^d d^{-\|D_i\|}} \cdot \frac{|M(D)|}{d!} \sum_{\pi \in S_d} d^{-\|D\|} = \frac{|M(D)|}{d^{\|D\|} - d}.$$

Thus we can combine (16) and (17), giving us

$$\begin{aligned} \eta_d(D) \leq I_d(D) &\leq \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right) \frac{|M(D)|}{d^{\|D\|} - d} \prod_{i=1}^d I_d(D_i) \\ &= \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right) \frac{|M(D)|}{d^{\|D\|} - d} \prod_{i=1}^d \eta_d(D_i) = \eta_d(D), \end{aligned}$$

which implies that  $I_d(D) = \eta_d(D)$ . □

Let us now define a class of trees for which the supremum condition of Theorem 4.1 is satisfied. A *balanced  $d$ -ary tree* is a  $d$ -ary tree whose branches  $D_1, D_2, \dots, D_d$  (some of which may be empty) satisfy  $|\|D_i\| - \|D_j\|| \leq 1$  for all  $i, j$ , i.e., the number of leaves in two different branches differs at most by 1. In particular, this means that a balanced  $d$ -ary tree is either a star or has root degree  $d$ . Figure 4 shows an example of a balanced 4-ary tree.

It turns out that balanced  $d$ -ary trees always satisfy the supremum condition of Theorem 4.1. Among other things, this will imply Theorem 1.2.

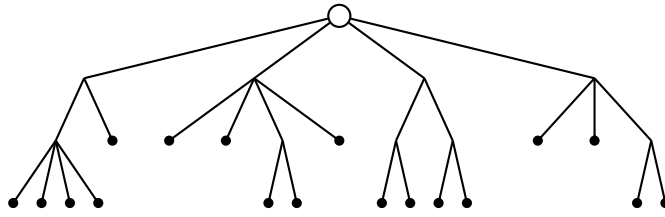


Figure 4: A balanced 4-ary tree.

**Lemma 4.2** *For every balanced  $d$ -ary tree  $D$  with branches  $D_1, D_2, \dots, D_d$  (some of which may be empty), we have*

$$\sup_{\substack{0 \leq x_1, x_2, \dots, x_d < 1 \\ x_1 + x_2 + \dots + x_d = 1}} Z_D(x_1, x_2, \dots, x_d) = \frac{|M(D)|}{d^{\|D\|} - d}.$$

In the proof of this lemma, we rely on *Muirhead’s inequality* (see [9, p. 44-45]). Let  $A = (a_1, a_2, \dots, a_d)$  and  $B = (b_1, b_2, \dots, b_d)$  be vectors of real numbers with  $a_1 \geq a_2 \geq \dots \geq a_d$  and  $b_1 \geq b_2 \geq \dots \geq b_d$ . We say that the vector  $A$  *majorizes* the vector  $B$  if  $\sum_{i=1}^d a_i = \sum_{i=1}^d b_i$  and for every  $j \in \{1, 2, \dots, d - 1\}$ ,

$$\sum_{i=1}^j a_i \geq \sum_{i=1}^j b_i.$$

Muirhead’s inequality states that for nonnegative real numbers  $x_1, x_2, \dots, x_d$ , we have

$$\sum_{\pi \in S_d} \prod_{i=1}^d x_i^{a_{\pi(i)}} \geq \sum_{\pi \in S_d} \prod_{i=1}^d x_i^{b_{\pi(i)}}$$

if  $A$  majorizes  $B$ , the sum being over all permutations of  $[d] = \{1, 2, \dots, d\}$ . For our purposes, the following special case is particularly relevant: let  $k$  be a positive integer, and write it as  $k = ds + b$ , with  $b \in \{0, 1, \dots, d - 1\}$ . It is not difficult to see that the vector  $(s + 1, \dots, s + 1, s, \dots, s)$  ( $b$  copies of  $s + 1$ , followed by  $d - b$  copies of  $s$ ) is majorized by all other vectors of  $d$  nonnegative integers with sum  $k$ .

Let us now get to the proof of Lemma 4.2.

*Proof of Lemma 4.2.* Let us write  $k = \|D\|$  as in previous proofs. Since  $D$  is balanced, there exists a positive integer  $s$  such that each branch of  $D$  contains either  $s$  or  $s + 1$  leaves. Writing  $k = ds + b$ , where  $b \in \{0, 1, \dots, d - 1\}$ , we have  $b$  branches with  $s + 1$  leaves, and  $d - b$  branches with  $s$  leaves.

We write the function  $Z_D$  according to (9) as

$$Z_D(x_1, x_2, \dots, x_d) = \frac{1}{1 - \sum_{i=1}^d x_i^k} \cdot \frac{|M(D)|}{d!} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\|D_{\pi(j)}\|}.$$

As mentioned before, the vector of branch sizes  $(\|D_1\|, \|D_2\|, \dots, \|D_d\|) = (s + 1, \dots, s + 1, s, \dots, s)$  (without loss of generality in decreasing order) is majorized

by all other ordered nonnegative integer vectors of the same length and sum. We expand

$$\left(\sum_{i=1}^d x_i\right)^k - \sum_{i=1}^d x_i^k$$

by means of the multinomial theorem and group the terms according to the vector of exponents. Each of the resulting groups has the form

$$C \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{a_{\pi(j)}}$$

for a suitable constant  $C$  and a vector  $(a_1, a_2, \dots, a_d)$  whose sum of entries is  $k$ . Since each vector  $(a_1, a_2, \dots, a_d)$  majorizes  $(\|D_1\|, \|D_2\|, \dots, \|D_d\|)$ , we can apply Muirhead’s theorem repeatedly to obtain

$$\left(\sum_{i=1}^d x_i\right)^k - \sum_{i=1}^d x_i^k \geq \frac{d^k - d}{d!} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\|D_{\pi(j)}\|}.$$

If the sum of the  $x_i$ s is equal to 1, then this immediately yields

$$Z_D(x_1, x_2, \dots, x_d) = \frac{1}{1 - \sum_{i=1}^d x_i^k} \cdot \frac{|M(D)|}{d!} \sum_{\pi \in S_d} \prod_{j=1}^d x_j^{\|D_{\pi(j)}\|} \leq \frac{|M(D)|}{d^k - d}.$$

Equality holds in Muirhead’s inequality if and only if all  $x_i$  are equal, so this is also the case for our inequality: when  $x_1 = x_2 = \dots = x_d = \frac{1}{d}$ , the upper bound is attained (as we have already seen in the proof of Theorem 4.1). This proves the lemma. □

The following theorem is now straightforward.

**Theorem 4.3** *For a balanced  $d$ -ary tree  $D$  with branches  $D_1, D_2, \dots, D_d$  (some of which may be empty), the inequality*

$$I_d(D) \leq \frac{|M(D)|}{d^{\|D\|} - d} \left( \|D_1\|, \|D_2\|, \dots, \|D_d\| \right) \prod_{i=1}^d I_d(D_i)$$

holds for every  $d$ . Furthermore, if  $I_d(D_i) = \eta_d(D_i)$  for all  $i$ , then we also have  $I_d(D) = \eta_d(D)$ .

*Proof.* The first part is a consequence of Proposition 3.1 and Lemma 4.2. The second part follows from Theorem 4.1 together with Lemma 4.2. □

The upper bound in Theorem 4.3 can be extended to trees which have fewer than  $d$  nonempty branches, but are otherwise balanced (i.e., the number of leaves in any

two nonempty branches differs at most by 1). In this case, the same approach yields the inequality

$$I_d(D) \leq \frac{|M(D)|}{\Sigma(D)} \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right) \prod_{i=1}^d I_d(D_i),$$

where  $\Sigma(D)$  is defined as follows: let  $r$  be the number of nonempty branches of  $D$ , and let  $V(D)$  be the set of all vectors  $(k_1, k_2, \dots, k_d)$  with  $0 \leq k_i < \|D\|$  for all  $i$ ,  $k_1 + k_2 + \dots + k_d = \|D\|$ , and at least  $d - r$  of the entries  $k_i$  equal to 0. Then

$$\Sigma(D) = \sum_{(k_1, k_2, \dots, k_d) \in V(D)} \binom{\|D\|}{k_1, k_2, \dots, k_d}.$$

Let us now look at an application of Theorem 4.3.

*Proof of Theorem 1.2.* Let us define  $E_0^d$  to be the empty tree, which is consistent with the recursive definition. We have  $I_d(E_0^d) = \eta_d(E_0^d) = I_d(E_1^d) = \eta_d(E_1^d) = 1$ . Since even trees are balanced and their branches are again even trees, it follows by induction on  $k$  from the second part of Theorem 4.3 that  $I_d(E_k^d) = \eta_d(E_k^d)$  for all  $k$ . Setting  $c_k = I_d(E_k^d)/k! = \eta_d(E_k^d)/k!$ , we have  $c_0 = c_1 = 1$ . The recursive definition of  $\eta_d$  yields

$$c_{ds+b} = \frac{\eta_d(E_{ds+b}^d)}{(ds+b)!} = \frac{|M(E_{ds+b}^d)|}{d^{ds+b} - d} \left( \frac{\eta_d(E_s^d)}{s!} \right)^{d-b} \left( \frac{\eta_d(E_{s+1}^d)}{(s+1)!} \right)^b.$$

The even tree  $E_{ds+b}^d$  has two types of branches ( $E_s^d$  and  $E_{s+1}^d$ ), occurring  $d - b$  and  $b$  times respectively. Thus the elements of  $M(E_{ds+b}^d)$  correspond precisely to the  $b$ -element subsets of  $[d]$ . So  $|M(E_{ds+b}^d)| = \binom{d}{b}$ , and it follows that

$$c_{ds+b} = \frac{\binom{d}{b}}{d^{ds+b} - d} c_s^{d-b} c_{s+1}^b,$$

which is precisely the recursion stated in Theorem 1.2. □

A complete  $d$ -ary tree is a strictly  $d$ -ary tree in which all leaves are at the same distance from the root; the complete  $d$ -ary tree with  $d^h$  leaves (whose distance from the root is  $h$ ) is denoted by  $C_h^d$ . It is not difficult to see that complete  $d$ -ary trees are precisely the even trees of the form  $E_{d^h}^d$ , see for instance  $E_9^3$  in Figure 2. As a corollary of Theorem 1.2, we obtain an explicit formula for the inducibility of a complete  $d$ -ary tree.

**Corollary 4.4** *For the complete  $d$ -ary tree of height  $h$ , we have*

$$I_d(C_h^d) = (d^h)! \prod_{i=0}^{h-1} \left( d^{d^{h-i}} - d \right)^{-d^i}.$$

*Proof.* Note that  $I_d(C_h^d) = (d^h)! c_{d^h}$ , and the recursion

$$c_{d^h} = \frac{1}{d^{d^h} - d} c_{d^{h-1}}^d$$

holds. The stated formula follows easily by induction. □

Balanced trees are by far not the only trees that satisfy the supremum condition of Theorem 4.1. For example, one can show that all binary trees where one branch has  $\ell \geq 2$  leaves and the other  $\ell + 2$  leaves satisfy it. This implies, among other instances, that the binary tree  $T_1$  in Figure 5 has inducibility  $I_2(T_1) = \eta_2(T_1) = \frac{45}{217}$ . The tree  $T_2$  in the same figure can also be shown to satisfy the conditions of Theorem 4.1 (even though it is not balanced), and one obtains  $I_3(T_2) = \eta_3(T_2) = \frac{15}{121}$ .

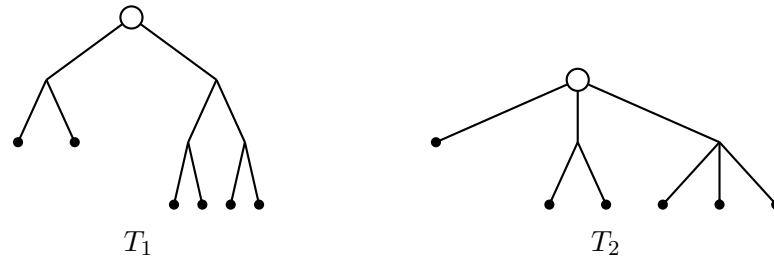


Figure 5: Further examples satisfying the conditions of Theorem 4.1.

Unfortunately, it does not seem easy to characterise the cases when the supremum condition of Theorem 4.1 is satisfied. An answer to this open question would be extremely useful.

We conclude this section with a result on the speed of convergence of the maximum density over strictly  $d$ -ary trees to the inducibility.

**Theorem 4.5** *If  $I_d(D) = \eta_d(D)$ , then we have*

$$i_d(D; n) = I_d(D) + \mathcal{O}(n^{-1}). \tag{18}$$

*Proof.* The lower bound is a consequence of Theorem 2.3, since

$$i_d(D; n) \geq \gamma(D, H_n^d) = \eta_d(D) + \mathcal{O}(n^{-1}).$$

The upper bound follows directly from (4):

$$i_d(D; n) \leq I_d(D; (d - 1)n + 1) \leq I_d(D) + \frac{\|D\|(\|D\| - 1)}{(d - 1)n + 1}.$$

□

As mentioned in the introduction, this result gives support to the conjecture that (18) holds for arbitrary trees  $D$  (in general, it has only been proven with an error term  $\mathcal{O}(n^{-1/2})$ ). As we have seen in this section, there are many examples for which the condition  $I_d(D) = \eta_d(D)$  holds, such as all even trees.

## 5 Further bounds

Even when Theorem 4.3 does not yield the precise value of the inducibility, it often gives us very good bounds. In the case where  $D$  has  $d$  identical branches, the following theorem shows that it is at least “almost sharp”.

**Theorem 5.1** *Let  $d \geq 2$  be a fixed integer and  $D$  a  $d$ -ary tree. Assume that  $D$  has  $d$  branches all of which are isomorphic to the same  $d$ -ary tree, say  $D'$ . Then we have*

$$\frac{\|D\|!}{d^{\|D\|}} \left( \frac{I_d(D')}{\|D'\|!} \right)^d \leq I_d(D) \leq \frac{\|D\|!}{d^{\|D\|} - d} \left( \frac{I_d(D')}{\|D'\|!} \right)^d.$$

*Proof.* The lower bound is a special case of [4, Theorem 9], while the upper bound is a direct consequence of Theorem 4.3.  $\square$

We conclude with a lower bound on the inducibility of a tree in terms of the inducibilities of its branches, of which the lower bound in the previous theorem is also a special case.

**Theorem 5.2** *Let  $D$  be a  $d$ -ary tree with branches  $D_1, D_2, \dots, D_d$  (some of which may be empty). The following inequality holds:*

$$I_d(D) \geq \left( \frac{\|D\|}{\|D_1\|, \|D_2\|, \dots, \|D_d\|} \right) \|D\|^{-\|D\|} \prod_{i=1}^d \|D_i\|^{\|D_i\|} \prod_{i=1}^d I_d(D_i).$$

Here, we set  $0^0 = 1$  if  $\|D_i\| = 0$  for some  $i$ .

*Proof.* Let us write  $k = \|D\|$  and  $\ell_i = \|D_i\|$  as in previous proofs. For each  $D_i$ , we can find a sequence of rooted trees  $T_n^{(i)}$  such that  $\|T_n^{(i)}\| = n$  and  $\lim_{n \rightarrow \infty} \gamma(D_i, T_n^{(i)}) = I_d(D_i)$ . Now define a new sequence of trees  $T_n$  as follows:

- For each  $i \in [d]$ , take a copy of the tree  $T_{\ell_i n}^{(i)}$ , which has  $\ell_i n$  leaves (if  $\ell_i = 0$ , this is the empty tree).
- Add a new root, which is connected to the roots of all these trees by an edge.

Note that the tree  $T_n$  has  $\sum_{i=1}^d (\ell_i n) = kn$  leaves. If we take a leaf set in the  $i$ -th branch that induces a copy of  $D_i$  for each  $i$ , then the union of all these leaf sets induces a copy of  $D$ . Therefore, we have

$$c(D, T_n) \geq \prod_{i=1}^d c(D_i, T_{\ell_i n}^{(i)}).$$

This also follows easily from Lemma 2.1. Now note that  $c(D_i, T_{\ell_i n}^{(i)}) = \binom{\ell_i n}{\ell_i} \gamma(D_i, T_{\ell_i n}^{(i)})$  and  $c(D, T_n) = \binom{kn}{k} \gamma(D, T_n)$ . It follows that

$$\gamma(D, T_n) \geq \frac{\prod_{i=1}^d \binom{\ell_i n}{\ell_i}}{\binom{kn}{k}} \prod_{i=1}^d \gamma(D_i, T_{\ell_i n}^{(i)}).$$

As  $n \rightarrow \infty$ , the right side of this inequality tends to

$$\frac{\prod_{i=1}^d \frac{\ell_i^{\ell_i}}{\ell_i!}}{\frac{k^k}{k!}} \prod_{i=1}^d I_d(D_i) = \binom{k}{\ell_1, \ell_2, \dots, \ell_d} k^{-k} \prod_{i=1}^d \ell_i^{\ell_i} \prod_{i=1}^d I_d(D_i),$$

so it follows that

$$I_d(D) \geq \limsup_{n \rightarrow \infty} \gamma(D, T_n) \geq \binom{k}{\ell_1, \ell_2, \dots, \ell_d} k^{-k} \prod_{i=1}^d \ell_i^{\ell_i} \prod_{i=1}^d I_d(D_i),$$

which completes the proof. □

Let us illustrate the results of this section with two final examples, which are shown in Figure 6.

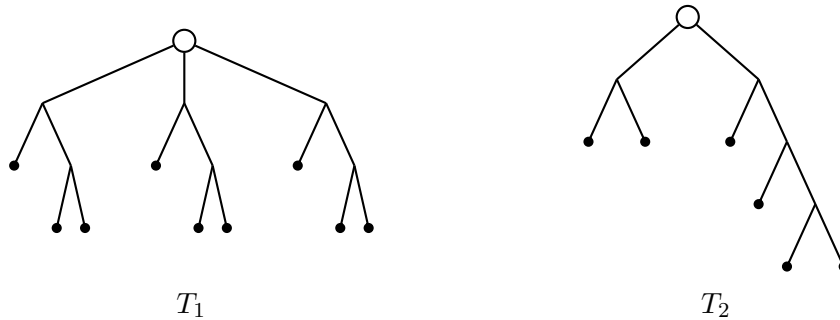


Figure 6: Two final examples.

For the ternary tree  $T_1$  on the left, Theorem 5.1 yields  $0.08535 \approx \frac{560}{6561} \leq I_3(T_1) \leq \frac{7}{82} \approx 0.08537$ , giving us an excellent approximation. The lower bound provided by Theorem 2.3 is much weaker in this case, as  $\eta_3(T_1) = \frac{189}{5248} \approx 0.03601$ . For the binary tree  $T_2$  on the right, Theorem 5.2 yields  $I_2(T_2) \geq \frac{80}{243} \approx 0.32922$ , which is stronger than the lower bound  $\eta_2(T_2) = \frac{60}{217} \approx 0.27650$ . An upper bound can be obtained from Proposition 3.1, which gives us  $I_2(T_2) \leq \frac{15}{31} \approx 0.48387$ . We do not know the precise value in either of the two cases, though.

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