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## Bidiagonal decompositions of Vandermonde-type matrices of arbitrary rank <sup>☆,☆☆</sup>



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### ABSTRACT

We present a method to derive new explicit expressions for bidiagonal decompositions of Vandermonde and related matrices such as the  $(q-, h-)$  Bernstein-Vandermonde ones, among others. These results generalize the existing expressions for nonsingular matrices to matrices of arbitrary rank. For totally nonnegative matrices of the above classes, the new decompositions can be computed efficiently and to high relative accuracy componentwise in floating point arithmetic. In turn, matrix computations (e.g., eigenvalue computation) can also be performed efficiently and to high relative accuracy.

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## 1. Introduction

A matrix is totally nonnegative (TN) if all of its minors are nonnegative [1–3]. The bidiagonal decompositions of the TN matrices have become an important tool in the study of these matrices [4,5] and for performing matrix computations with them accurately and efficiently [6–8]. The bidiagonal decompositions of many classical TN matrices such as Vandermonde and many related matrices are well known, but contain singularities when some of the nodes coincide. For example, a

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$3 \times 3$  Vandermonde matrix with nodes  $x, y, z$  is decomposed as [6]:

$$\begin{bmatrix} 1 & x & x^2 \\ 1 & y & y^2 \\ 1 & z & z^2 \end{bmatrix} = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ 1 & 1 & \\ & \frac{z-y}{y-x} & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & y-x & \\ & & (z-x)(z-y) \end{bmatrix} \\ \times \begin{bmatrix} 1 & x & \\ & 1 & y \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & x \\ & & 1 \end{bmatrix}. \tag{1}$$

This decomposition is undefined when  $x = y$ , which is unfortunate, since the Vandermonde matrix is very well defined for any values of the nodes.

By relaxing the requirement that the bidiagonal factors have ones on the main diagonal, we show how to rearrange the factors in (1), so that the new decomposition contains no singularities and is valid for any values of the nodes and is thus valid for a Vandermonde matrix of arbitrary rank. For example, the  $3 \times 3$  Vandermonde from (1) can be decomposed as

$$\begin{bmatrix} 1 & x & x^2 \\ 1 & y & y^2 \\ 1 & z & z^2 \end{bmatrix} = \begin{bmatrix} 1 & & \\ & 1 & z-y \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ 1 & y-x & \\ & 1 & z-x \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} \\ \times \begin{bmatrix} 1 & x & \\ & 1 & y \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & x \\ & & 1 \end{bmatrix}, \tag{2}$$

which is valid for any values of the nodes  $x, y, z$ .

Many classes of other TN matrices share the exact same singularities in their bidiagonal decompositions, e.g., the Bernstein–Vandermonde, their  $q$ -,  $h$ -, and rational generalizations, Lupaş, Said-Ball matrices, etc. [6,9–16]. We call these matrices Vandermonde-type below (see Section 3).

The method that allowed us to obtain the decomposition (2) from (1) applies to all Vandermonde-type matrices (Section 5) and is the main contribution of this paper. The starting point for our method is the existing bidiagonal decompositions of the Vandermonde-type matrices, which are valid only when these matrices are both TN and nonsingular. Our method takes these decompositions as a starting point and produces new bidiagonal decompositions valid for matrices of arbitrary rank, regardless of whether they are TN or not – see Corollary 4.1.

While the computational complexity of the transformed bidiagonal decomposition of an  $n \times n$  matrix remains  $O(n^2)$ , the new expressions are simpler.

In terms of accuracy, just like their non-singular counterparts, the new decompositions remain insusceptible to subtractive cancellation, and thus all of the entries of these decompositions can be computed to high relative accuracy when the matrix is TN. By “high relative accuracy” we mean that for each entry its sign and most of its leading significant digits are computed correctly (see Section 8).

The Vandermonde-type matrices have many applications that are well referenced in the papers we cite above that deal with the nonsingular case. For example, the Lupaş matrices (Appendix A.1) have direct applications in CAGD [11,17]. For TN Vandermonde-type matrices, the new results in this paper allow for matrix computations with them to be performed to high relative accuracy very efficiently (in  $O(n^3)$  time) using the methods of [8] now also when these matrices are singular – see Section 9 for a numerical example.

The efficiency and high relative accuracy is particularly relevant, for example, in eigenvalue computations since the corresponding matrices are unsymmetric. The error bounds for the eigenvalues computed by the conventional algorithms (such as the ones in LAPACK [18]) [19] imply that none of the eigenvalues are guaranteed to be accurate, although the largest ones typically are – see the example in Section 9. In contrast, the results of this paper now allow for all eigenvalues to be efficiently computed to high relative accuracy and, in particular, the zero eigenvalues are computed exactly.

The paper is organized as follows. In Section 2 we review the bidiagonal decompositions of nonsingular TN matrices. In Section 3 we present the formal definition of Vandermonde-type matrix and, in Section 4, we show how to remove the singularities in its bidiagonal decomposition. We demonstrate how our method applies to the particular class of  $q$ -Bernstein–Vandermonde matrices in Section 5. Our method is also directly applicable to derivative matrices, such as generalized Vandermonde matrices, Laguerre matrices, etc., which are submatrices or products of Vandermonde matrices and other nonsingular TN matrices (Section 6). In Section 7, we present a method to make the bottom right-hand corner entry of all bidiagonal factors in the corresponding bidiagonal decompositions equal to 1 – this is a requirement for the methods of [8] to work. We discuss accuracy issues in Section 8 and present numerical experiments in Section 9. The explicit formulas for the decompositions of several Vandermonde-type matrices are in Appendix.

## 2. Bidiagonal decompositions of TN matrices

Our focus in this paper is on the class of TN matrices, but the formulas and methods we present are valid without the requirement of total nonnegativity (Corollary 4.1 below). The bidiagonal decompositions of the TN matrices serve as a major tool in their study and computations with them. We review those here [2,4].



As with  $\mathcal{BD}(A)$ , the matrix  $B$  stores the nontrivial offdiagonal entries of  $L_i$  and  $U_i$  as well as the diagonal entries of  $D$ , exactly as in (4):

$$\begin{aligned} b_{ij} &= (L_{n-i+j})_{i,i-1}, \quad i > j, \\ b_{ij} &= (U_{n-j+i})_{j-1,j}, \quad i < j, \\ b_{ii} &= D_{ii}. \end{aligned}$$

The matrix  $C$  stores the diagonal entries of  $L_i$  and  $U_i$  as

$$c_{ij} = \begin{cases} (L_{n-i+j})_{i-1,i-1}, & i > j, \\ (U_{n-j+i})_{j-1,j-1}, & i < j. \end{cases}$$

In this arrangement,  $c_{ij}$ ,  $i > j$ , is the diagonal entry in  $L_{n-i+j}$  immediately above  $b_{ij}$  and similarly for  $i < j$  and  $U_{n-j+i}$ . The entries  $c_{ii}$ ,  $i = 1, 2, \dots, n + 1$  as well as the entries  $c_{1,n+1}$  and  $c_{n+1,1}$  are unused. This is the same construction as the one given in formula (9) in [8], except that we now allow for the  $(n, n)$  entry in  $L_i$  and  $U_i$  to be any nonnegative number and not necessarily equal 1. This is the reason we need an  $(n + 1) \times (n + 1)$  matrix to host the entries  $c_{ij}$ : the nontrivial diagonal entries of  $L_1, L_2, \dots, L_{n-1}$  are of lengths 2, 3,  $\dots$ ,  $n$ , and similarly for the  $U_i$ 's.

As we explain in Section 7, we can always make the  $(n, n)$  entry in the  $L_i$ 's and  $U_i$ 's equal to 1, so that the algorithms of [8] be used, but the formulas are more elegant without that restriction, which can be imposed after in software.

Thus, in this paper we start with the known ordinary bidiagonal decomposition  $M = \mathcal{BD}(A)$  of a nonsingular matrix  $A$ , (3), and produce the singularity-free bidiagonal decomposition  $[B, C] = \mathcal{SBD}(A)$ , (6), which is defined for a matrix  $A$  of arbitrary rank.

The new singularity-free bidiagonal decomposition (6) is not unique, but this is inconsequential – for the purposes of accurate computations, any accurate decomposition of a TN matrix as a product of nonnegative bidiagonals is an equally good input [6].

### 3. Vandermonde-type matrices

The ordinary Vandermonde matrices are the starting point of our investigation as the approach extends analogously to all other classes of matrices in this paper.

An  $n \times n$  Vandermonde matrix  $A$  with nodes  $x_1, x_2, \dots, x_n$  is defined as

$$A = \left[ x_i^{j-1} \right]_{i,j=1}^n. \tag{7}$$

When the nodes are distinct, it has an ordinary bidiagonal decomposition (3),  $V = \mathcal{BD}(A)$ , such that [6]

$$\begin{aligned} v_{ii} &= \prod_{k=1}^{i-1} (x_i - x_k), & 1 \leq i \leq n, \\ v_{ij} &= \prod_{k=i-j}^{i-2} \frac{x_i - x_{k+1}}{x_{i-1} - x_k}, & 1 \leq j < i \leq n, \\ v_{ij} &= x_i, & 1 \leq i < j \leq n. \end{aligned} \tag{8}$$

In the following definition, we take a more general stance, where the lower bidiagonal factors and the diagonal have additional factors, which contain no singularities.

**Definition 1.** An  $n \times n$  matrix  $A = [a_{ij}]_{i,j=1}^n$  is said to be of *Vandermonde-type* with nodes  $x_1, x_2, \dots, x_n$  on an (open or closed) interval  $D$ , if it satisfies all of the conditions below:

1.  $a_{ij} = f_j(x_i)$ , where  $f_j(x)$  is a rational function of  $x$  for  $j = 1, 2, \dots, n$ ;
2.  $A$  is TN when  $x_1 < x_2 < \dots < x_n$  and all  $x_i \in D$ ,  $i = 1, 2, \dots, n$ ;
3.  $A$  has an ordinary bidiagonal decomposition,  $M = \mathcal{BD}(A)$ , such that

$$m_{ij} = s_{ij}v_{ij}, \tag{9}$$

for  $1 \leq j \leq i \leq n$ , where  $v_{ij}$  are defined as in (8), and the entries  $s_{ij}$  for  $1 \leq j \leq i \leq n$  and the entries  $m_{ji}$  for  $1 \leq j < i \leq n$  are rational functions of  $x_1, x_2, \dots, x_n$ , with no singularities when  $x_i \in D$ ,  $i = 1, 2, \dots, n$ .

A Vandermonde-type matrix is thus fully specified by the entries  $s_{ij}$  for  $1 \leq j \leq i \leq n$  and the entries  $m_{ji}$  for  $1 \leq j < i \leq n$ .

From the above definition, the ordinary Vandermonde matrix (7) is a Vandermonde-type matrix on  $(0, \infty)$  with  $s_{ij} = 1$  for  $1 \leq j \leq i \leq n$  and  $m_{ji} = v_{ji} = x_j$  for  $1 \leq j < i \leq n$ .

In the literature, the Vandermonde-type matrices sometimes have  $n + 1$  nodes, with the indexing starting at 0, e.g.,  $x_0, x_1, \dots, x_n$ . For consistency, in this paper, all Vandermonde-type matrices are  $n \times n$  and their nodes are  $x_1, x_2, \dots, x_n$ .

4. Singularity-free bidiagonal decompositions of Vandermonde-type matrices

In this section, we show how to remove the singularities in the ordinary bidiagonal decomposition (3) for Vandermonde-type matrices and obtain a singularity-free bidiagonal decomposition (6).

If  $M = \mathcal{BD}(A)$  is the ordinary bidiagonal decomposition (3) of a Vandermonde-type matrix, from (9) we have  $m_{ii} = s_{ii}v_{ii}$ ,  $i = 1, 2, \dots, n$ , and thus the diagonal factor  $D$  can be factored as  $D = D_n \cdot D'$ , so that

$$A = L^{(1)}L^{(2)} \dots L^{(n-1)} \cdot D_n \cdot D' \cdot U^{(n-1)} \dots U^{(1)},$$

where

$$D_n = \text{diag}(v_{11}, \dots, v_{nn}) \tag{10}$$

and  $D' = \text{diag}(s_{11}, \dots, s_{nn})$ .

Since there are no singularities in the product  $D' \cdot U^{(n-1)} \dots U^{(1)}$ , it suffices to remove the singularities in the remaining factors, i.e., in the product

$$L^{(1)}L^{(2)} \dots L^{(n-1)}D_n. \tag{11}$$

**Theorem 4.1.** Let  $L^{(i)}$ ,  $i = 1, 2, \dots, n - 1$  be the lower bidiagonal factors in the ordinary bidiagonal decomposition (3) of a Vandermonde-type matrix, whose nontrivial entries are defined as in (9) and  $D_n$  be defined as in (10). Then

$$L_1L_2 \dots L_{n-1} = L^{(1)}L^{(2)} \dots L^{(n-1)}D_n,$$

where

$$L_i = \begin{bmatrix} 1 & & & & & & & & \\ & \ddots & & & & & & & \\ & & 1 & & & & & & \\ & & s_{n-i+1,1} & x_{n-i+1} - x_{n-i} & & & & & \\ & & & s_{n-i+2,2} & x_{n-i+2} - x_{n-i} & & & & \\ & & & & \ddots & \ddots & & & \\ & & & & & s_{ni} & x_n - x_{n-i} & & \end{bmatrix}. \tag{12}$$

**Proof.** It suffices to observe just the initial step, i.e., that

$$D_{n-1} \cdot L_{n-1} = L^{(n-1)} \cdot D_n, \tag{13}$$

where  $D_{n-1}$  is a diagonal matrix, such that  $(D_{n-1})_{ii} = 1$  for  $i = 1, 2$ , and

$$(D_{n-1})_{ii} = \prod_{k=2}^{i-1} (x_i - x_k), \quad i = 3, 4, \dots, n.$$

In other words, the  $(n - 1) \times (n - 1)$  bottom right principal submatrix of  $D_{n-1}$  is the diagonal factor in the ordinary bidiagonal decomposition of an  $(n - 1) \times (n - 1)$  ordinary Vandermonde matrix with nodes  $x_2, x_3, \dots, x_n$ .

Since both  $D_n$  and  $D_{n-1}$  are diagonal and both  $L^{(n-1)}$  and  $L_{n-1}$  are lower bidiagonal, we have bidiagonals on each side of (13). To establish that those are equal, it suffices to show that the corresponding diagonal and offdiagonal entries are the same. Since  $L^{(n-1)}$  is unit lower bidiagonal, the diagonal entry in the product on the right,  $L^{(n-1)}D_n$  is  $(D_n)_{ii}$ . Thus, for  $i > 1$ ,

$$(D_n)_{ii} = \prod_{k=1}^{i-1} (x_i - x_k) = \left( \prod_{k=2}^{i-1} (x_i - x_k) \right) \cdot (x_i - x_1) = (D_{n-1})_{ii}(L_{n-1})_{ii},$$

since  $(L_{n-1})_{ii} = x_i - x_1$  by (12). Also,  $(D_n)_{11} = 1$ , so the diagonal entries on both sides of (13) are equal.

Since  $(L_{n-1})_{i+1,i} = s_{i+1,i}$ , the offdiagonal entry in position  $(i + 1, i)$  on the left side of (13) is  $s_{i+1,i}(D_{n-1})_{i+1,i+1}$ . Also, from (4),

$$L_{i+1,i}^{(n-1)} = m_{i+1,i} = s_{i+1,i}v_{i+1,i} = s_{i+1,i} \prod_{j=1}^{i-1} \frac{x_{i+1} - x_{j+1}}{x_i - x_j}$$

and thus

$$\begin{aligned}
 s_{i+1,i}(D_{n-1})_{i+1,i+1} &= s_{i+1,i} \prod_{j=2}^i (x_{i+1} - x_j) \\
 &= s_{i+1,i} \prod_{j=1}^{i-1} (x_{i+1} - x_{j+1}) \\
 &= s_{i+1,i} \prod_{j=1}^{i-1} \frac{x_{i+1} - x_{j+1}}{x_i - x_j} \prod_{j=1}^{i-1} (x_i - x_j) \\
 &= s_{i+1,i} v_{i+1,i}(D_n)_{ii} \\
 &= (L^{(n-1)})_{i+1,i} (D_n)_{ii},
 \end{aligned}$$

which is the  $(i + 1, i)$  entry on the right hand side of (13).

Therefore the offdiagonal entries on each side of (13) are also equal and (13) is fully established.

Completely analogously, we establish that  $D_{k-1}L_{k-1} = L^{(k-1)}D_k$  for  $k = n - 1, n - 2, \dots, 2$ , and for the product (11) we have

$$\begin{aligned}
 L^{(1)}L^{(2)} \dots L^{(n-1)}D_n &= L^{(1)}L^{(2)} \dots \underline{L^{(n-2)}}D_{n-1}L_{n-1} \\
 &= L^{(1)}L^{(2)} \dots \underline{L^{(n-3)}}D_{n-2}L_{n-2}L_{n-1} \\
 &= \dots \\
 &= \underline{L^{(1)}}D_2L_2 \dots L_{n-1} \\
 &= \underline{D_1}L_1L_2 \dots L_{n-1}, \quad \text{and since } D_1 = I, \\
 &= L_1L_2 \dots L_{n-1}.
 \end{aligned}$$

The factors that change on each step are underlined.

In other words, we “walk” the matrix  $D_n$  through the product (11) right-to-left, canceling the denominators in each  $L^{(k)}$  and factoring a slightly different diagonal matrix,  $D_{k-1}$ , out the left until we end up with just  $D_1 = I$ , which we drop. □

The ordinary bidiagonal decompositions exist for nonsingular TN matrices, however very simple singular TN matrices such as  $\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$  (let alone non-TN ones) do not have ordinary bidiagonal decompositions. Thus the fact that all Vandermonde-type matrices have singularity-free bidiagonal decompositions regardless of their rank or total nonnegativity is remarkable, which we prove below.

**Corollary 4.1.** *The singularity-free bidiagonal decomposition (6) of a Vandermonde-type matrix  $A$  is valid for any complex values of the nodes  $x_1, x_2, \dots, x_n$  for which the matrices on both sides of (6) are defined.*

**Proof.** Since it is derived from the ordinary bidiagonal decomposition (3), the singularity-free bidiagonal decomposition (6) is valid when  $A$  is nonsingular and TN. This remains the case when all the nodes of  $A$  are strictly increasing inside an open interval  $(a, b)$  contained in the interval  $D$  of total nonnegativity of  $A$ .

The  $(i, j)$ th entries on each side of (6) are rational functions of  $x_i$  for all  $i, j = 1, 2, \dots, n$ . Indeed, on the left hand side,  $a_{ij} = f_j(x_i)$ , is a rational function of  $x_i$  by Definition 1. On the right hand side, the  $(i, j)$ th entry is a polynomial in the entries of the factors of (6). These entries are obtained via the construction in Section 4 from the entries of the ordinary bidiagonal decomposition (3), which are rational functions of the nodes  $x_1, x_2, \dots, x_n$  as either quotients of minors of  $A$  or products of quotients of minors of  $A$  [6, Prop. (3.1)].

Since all rational functions are meromorphic on  $\mathbb{C}$ , and the equality between the  $(i, j)$ th entries on each side of (6) holds on an open interval in  $\mathbb{R}$  containing  $x_i$ :  $x_{i-1} < x_i < x_{i+1}$ , for  $1 < i < n$  and  $a < x_1 < x_2, x_{n-1} < x_n < b$  for  $i = 1, i = n$ , respectively, the Identity Theorem [20, Thm. 3.2.6], implies that this equality holds for any complex values of the nodes where these entries are defined. □

As a direct application to the ordinary Vandermonde matrices for example, as is evident from the formulas in Section 5.1, the above Corollary immediately implies that their singularity-free bidiagonal decomposition is valid for any complex nodes .

### 5. Our method and explicit formulas for Vandermonde-type matrices

Our method for producing a singularity-free bidiagonal decomposition for an  $n \times n$  Vandermonde-type matrix  $A$  of arbitrary rank works as follows:



5.2. *q*-Bernstein–Vandermonde matrices

The *q*-Bernstein–Vandermonde matrices are expressed in terms of *q*-integers and *q*-binomial coefficients: given  $q > 0$  and any nonnegative integer  $r$ , a *q*-integer  $[r]$  is defined as

$$[r] = \begin{cases} (1 - q^r)/(1 - q), & q \neq 1, \\ r, & q = 1. \end{cases} \tag{18}$$

For a nonnegative integer  $r$ , a *q*-factorial is defined as

$$[r]! = \begin{cases} [r][r - 1] \cdots [1], & r \neq 1, \\ 1, & r = 0. \end{cases}$$

The *q*-binomial coefficient is defined as

$$\begin{bmatrix} n \\ r \end{bmatrix} = \frac{[n][n - 1] \cdots [n - r + 1]}{[r]!}$$

for integers  $n \geq r \geq 0$  and as zero otherwise.

The *q*-Bernstein–Vandermonde matrices generalize the Bernstein–Vandermonde matrices [12,14], which are the  $q = 1$  case. The nonsingular case was developed in [10].

The *q*-Bernstein polynomials of degree  $n$  for  $0 < q \leq 1$  are defined in [22] as

$$b_{i,q}^n(x) = \begin{bmatrix} n \\ i \end{bmatrix} x^i \prod_{s=0}^{n-i-1} (1 - q^s x), \quad x \in [0, 1], \quad i = 0, 1, \dots, n. \tag{19}$$

An  $n \times n$  *q*-Bernstein–Vandermonde matrix  $A$  with nodes  $x_1, x_2, \dots, x_n$  is defined as

$$A = [b_{j-1,q}^{n-1}(x_i)]_{i,j=1}^n \tag{20}$$

and is TN when

$$0 \leq x_1 \leq x_2 \leq \dots \leq x_n < 1. \tag{21}$$

When the nodes  $x_i, i = 1, 2, \dots, n$ , are also distinct, it has an ordinary bidiagonal decomposition  $M = \mathcal{BD}(A)$  with parameters [10]

$$m_{ij} = \frac{1 - q^{n-j}x_{i-j}}{1 - q^{n-j}x_{i-1}} \prod_{s=0}^{n-1-j} \frac{1 - q^s x_i}{1 - q^s x_{i-1}} \underbrace{\prod_{k=i-j}^{i-2} \frac{x_i - x_{k+1}}{x_{i-1} - x_k}}_{v_{ij}},$$

$$m_{ji} = \frac{[n - i + 1]}{[i - 1]} \cdot \frac{x_j}{1 - q^{n-i}x_j} \prod_{k=1}^{j-1} \frac{1 - q^{n-i+1}x_k}{1 - q^{n-i}x_k}, \tag{22}$$

for  $1 \leq j < i \leq n$  and

$$m_{ii} = \begin{bmatrix} n - 1 \\ i - 1 \end{bmatrix} \frac{\prod_{s=0}^{n-1-i} (1 - q^s x_i)}{\prod_{k=1}^{i-1} (1 - q^{n-i} x_k)} \underbrace{\prod_{k=1}^{i-1} (x_i - x_k)}_{v_{ii}}$$

for  $1 \leq i \leq n$ .

With the entries of the ordinary bidiagonal decomposition of the ordinary Vandermonde matrix  $v_{ij}$  defined as in (8), we have that  $m_{ij} = s_{ij}v_{ij}$  for  $1 \leq j \leq i \leq n$ , where

$$s_{ij} = \frac{1 - q^{n-j}x_{i-j}}{1 - q^{n-j}x_{i-1}} \prod_{s=0}^{n-1-j} \frac{1 - q^s x_i}{1 - q^s x_{i-1}}, \tag{23}$$

$$s_{ii} = \begin{bmatrix} n - 1 \\ i - 1 \end{bmatrix} \frac{\prod_{s=0}^{n-1-i} (1 - q^s x_i)}{\prod_{k=1}^{i-1} (1 - q^{n-i} x_k)}. \tag{24}$$

The *q*-Bernstein–Vandermonde matrix is therefore a Vandermonde-type matrix on  $[0, 1)$ .

As described at the beginning of this section, we obtain the singularity-free bidiagonal decomposition of  $A$  by removing the factors  $v_{ij}$  from  $m_{ij}$  for  $i \geq j$  and setting  $c_{ij} = x_{i-1} - x_{i-j}$  for  $2 \leq j < i \leq n + 1$ .

The decomposition  $[B, C] = \mathcal{SBD}(A)$  is thus fully defined as in (14)–(17) with the  $s_{ij}, i \leq j$ , defined in (23) and (24) and  $m_{ji}, i > j$ , defined in (22).

The singularity-free bidiagonal decomposition of a *q*-Bernstein–Vandermonde matrix can be computed to high relative accuracy in  $O(n^2)$  time using the routine STNBDqBernsteinVandermonde in our package STNTool [21].



### 6. Derivative Vandermonde matrices

Our results apply to other classes of matrices which are not directly Vandermonde-type. These include

- submatrices of Vandermonde-type matrices,
- products of Vandermonde-type matrices and other matrices, whose ordinary bidiagonal decompositions are known and contain no singularities.

The former include the generalized Vandermonde matrices. The latter include the Laguerre matrices, the Bessel matrices, and Wronskian matrices of a basis of exponential polynomials. We address these separately.

The *generalized Vandermonde* matrices

$$G_\lambda(x_1, \dots, x_n) = \left[ x_i^{j-1+\lambda_{n-j+1}} \right]_{i,j=1}^n$$

are defined for integer *partitions*  $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_n)$ , where  $\lambda_i$  are integers such that  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0$ . They are submatrices of ordinary Vandermonde matrices (obtained by removing appropriate columns). Their singularity-free bidiagonal decompositions can thus be obtained by starting with the singularity-free bidiagonal decomposition of the ordinary Vandermonde matrix, derived in Section 5.1, and removing the appropriate columns employing the methods of [8].

The singularity-free bidiagonal decomposition of a generalized Vandermonde matrix can be computed to high relative accuracy in  $O(\lambda_1 n^2)$  time using the STNBDGeneralizedVandermonde routine in our package STNTool [21].

Several classes of TN matrices are products of a TN ordinary Vandermonde matrix (call it  $V$ ) and a second TN matrix (call it  $A$ ) whose ordinary bidiagonal decomposition is known and contains no singularities. These include:

- Laguerre [23],
- Bessel matrices [24], and
- Wronskian matrices of a basis of exponential polynomials [25].

The singularity-free bidiagonal decomposition of the product  $VA$  (or  $AV$ ) can be obtained using the method for computing the singularity-free bidiagonal decomposition of a product of TN matrices from [8, sec. 6] (implemented in the routine STNProduct in our package STNTool [21]) with the singularity-free bidiagonal decomposition of  $V$  from Section 3 and the ordinary bidiagonal decomposition of  $A$ .

### 7. The $(n, n)$ entry of the bidiagonal factors must equal 1 for computations

The algorithms of [8] require that the  $(n, n)$  entry of every bidiagonal factor in the singularity-free bidiagonal decomposition of a TN matrix be equal to 1. These algorithms rely heavily on this fact and it turns out that the assumption that this is always the case can be made without any loss of generality.

To that end, in this section, we present a method to “fix” any singularity-free bidiagonal decomposition (6) so that the bottom right-hand corner entries of all bidiagonal factors,  $L_1, L_2, \dots, L_{n-1}$  and  $U_1, U_2, \dots, U_{n-1}$  equal to 1.

We do so by “moving” the non-unit  $(n, n)$  entries of each lower bidiagonal factor into  $D$  and adjusting the  $(n, n - 1)$  entries accordingly:

For any bidiagonal matrix  $L_i$  and diagonal matrix  $D_i = \text{diag}(1, 1, \dots, 1, x_i), i = 1, 2, \dots, n - 1$ , we can make the bottom right hand corner entry of the product  $D_i L_i$  equal to one by factoring a new diagonal factor  $\bar{D}_{i+1}$  out of the right. Namely,

$$D_i L_i = \bar{L}_i \bar{D}_{i+1}, \tag{25}$$

where  $\bar{L}_i$  equals  $L_i$ , except for  $(\bar{L}_i)_{nn} = 1, (\bar{L}_i)_{n,n-1} = L_{n,n-1} x_i$ . Then  $\bar{D}_{i+1} = \text{diag}(1, 1, \dots, x_i, L_{nn})$ .

This allows us, by starting with  $D_1 = I$ , to move the bottom right hand corner entries of the lower bidiagonal factors of  $SBD(A)$  into the diagonal factor,  $D$ :

$$\begin{aligned} A &= L_1 L_2 \cdots L_{n-1} \cdot D \cdot U_{n-1} U_{n-2} \cdots U_1 & (26) \\ &= \underline{D_1} L_1 L_2 \cdots L_{n-1} \cdot D \cdot U_{n-1} U_{n-2} \cdots U_1, \quad \text{since } D_1 = I, \\ &= \bar{L}_1 \underline{D_2} L_2 \cdots L_{n-1} \cdot D \cdot U_{n-1} U_{n-2} \cdots U_1, \quad \text{using } D_1 L_1 = \bar{L}_1 D_2 \text{ as in (25)}, \\ &= \dots \\ &= \bar{L}_1 \bar{L}_2 \cdots \underline{D_{n-1}} L_{n-1} \cdot D \cdot U_{n-1} U_{n-2} \cdots U_1 \\ &= \bar{L}_1 \bar{L}_2 \cdots \bar{L}_{n-1} \cdot (D_n D) \cdot U_{n-1} U_{n-2} \cdots U_1 \end{aligned}$$

(the factors being transformed on each step using (25) are underlined).

The procedure is analogous for the upper bidiagonal factors.

Thus, if (26) is a singularity-free bidiagonal decomposition of the TN matrix  $A$ , then

$$A = \bar{L}_1 \bar{L}_2 \cdots \bar{L}_{n-1} \cdot \bar{D} \cdot \bar{U}_{n-1} \bar{U}_{n-2} \cdots \bar{U}_1$$

is a singularity-free idagonal decomposition of  $A$  with all  $(n, n)$  entries of  $\bar{L}_i$  and  $\bar{U}_i, i = 1, 2, \dots, n$ , equal to 1.

The matrices  $\bar{L}_i, \bar{U}_i, i = 1, 2, \dots, n - 1$ , and  $\bar{D}$  differ from the matrices  $L_i, U_i$  and  $D$ , respectively, only in

$$(\bar{L}_i)_{n,n} = (\bar{U}_i)_{n,n} = 1$$

and

$$\begin{aligned} (\bar{L}_i)_{n,n-1} &= (L_i)_{n,n-1} \prod_{k=1}^{i-1} (L_k)_{n,n}, \\ (\bar{U}_i)_{n,n-1} &= (U_i)_{n,n-1} \prod_{k=1}^{i-1} (U_k)_{n,n}, \\ \bar{D}_{nn} &= D_{nn} \prod_{k=1}^{n-1} (L_k)_{n,n} \prod_{k=1}^{n-1} (U_k)_{n,n}. \end{aligned}$$

The routine `STNFixBottomRightOfBD` in our package `STNTool` [21] implements the technique from this section.

For example, by implementing the technique from this section to the singularity-free bidiagonal decomposition of our  $3 \times 3$  example (2) we obtain a new singularity-free bidiagonal decomposition with all  $(n, n)$  entries of all bidiagonal factors now equal to 1:

$$\begin{aligned} \begin{bmatrix} 1 & x & x^2 \\ 1 & y & y^2 \\ 1 & z & z^2 \end{bmatrix} &= \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & y-x & \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & \\ & & (z-y)(z-x) \end{bmatrix} \\ &\times \begin{bmatrix} 1 & x & \\ & 1 & y \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & x \\ & & 1 \end{bmatrix}. \end{aligned}$$

### 8. Numerical accuracy

In the standard “ $1 + \delta$ ” model of floating point arithmetic [26], to which the IEEE 754 double precision arithmetic [27] conforms, the result of any floating point calculation is assumed to satisfy

$$\text{fl}(a \odot b) = (a \odot b)(1 + \delta), \tag{27}$$

where  $\odot \in \{+, -, \times, /\}$ ,  $|\delta| \leq \varepsilon$ , and  $\varepsilon$  is tiny and is called *machine precision*.

For a computed quantity,  $\hat{x}$  to have *high relative accuracy*, it means that it satisfies an error bound with its true counterpart,  $x$

$$|\hat{x} - x| \leq \theta|x|,$$

where  $\theta$  is a modest multiple of  $\varepsilon$ . In other words, the sign and most significant digits of  $x$  must be correct. In particular, if  $x = 0$ , it must be computed exactly.

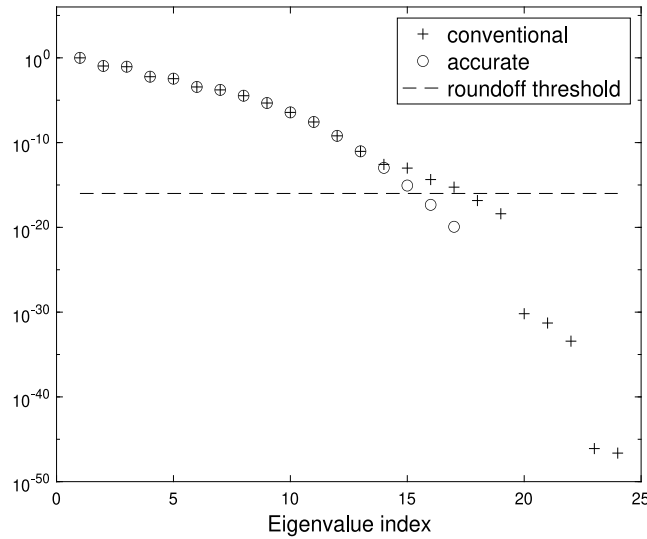
The above model directly implies that the accuracy in numerical calculations is lost due to one phenomenon only, known as subtractive cancellation [28]. It occurs when a subtraction of previously rounded off quantities results in the loss of significant digits. Multiplication, division, and addition of same-sign quantities preserve the relative accuracy. Subtraction of initial data such as the nodes  $x_i$  is also fine, since initial data is assumed to be exact: (27) tells us the result of that subtraction is computed to high relative accuracy. The only subtractions in any singularity-free bidiagonal decomposition presented in this paper are between exact initial data: either in the form  $x_i - x_j$  between the nodes  $x_i$  of the Vandermonde-type matrix as in (16) or  $1 - x_i$  between the exact double precision floating point number 1 and a node  $x_i$  as in (29), (31), and (32).

Detailed error analyses for the ordinary bidiagonal decompositions of all nonsingular TN Vandermonde-type matrices presented in this paper have already been performed in the corresponding papers (e.g., [14] for the Bernstein-Vandermonde matrices, etc.). All those decompositions are computable to high relative accuracy componentwise.

The new singularity-free bidiagonal decompositions inherit the same componentwise error bounds and are thus also computable to high relative accuracy: the offdiagonal entries in the bidiagonal factors  $L_i$  and  $U_i$  as well as the diagonal entries of the diagonal factor  $D$  in the singularity-free bidiagonal decomposition (6) are the same as the corresponding entries in the ordinary bidiagonal decomposition (3) except for the factors  $v_{ij}$  from (8). The diagonal entries in the bidiagonal factors  $L_i$  and  $U_i$  in (6) are either equal to 1 or are of the form  $x_i - x_j$ , the latter computable with relative error bounded by the machine precision,  $\varepsilon$ , per (27).

### 9. Numerical experiments

We performed extensive numerical tests to verify the correctness of the formulas we derived in this paper as well as their inherent accuracy in numerical computations. We present one illustrative example in Fig. 1. Using the formulas in



**Fig. 1.** The eigenvalues of a  $24 \times 24$   $q$ -Bernstein-Vandermonde matrix as computed by the conventional eigenvalue algorithms of LAPACK as implemented by MATLAB's `eig` and also by forming the accurate singularity-free bidiagonal decomposition as in Section 5 and then using the accurate eigenvalue algorithm of [8].

Section 5.2, we computed the eigenvalues of the  $24 \times 24$   $q$ -Bernstein-Vandermonde matrix  $A$  with parameter  $q = 0.1$  and nodes

0.1, 0.2, 0.2, 0.2, 0.3, 0.31, 0.32, 0.33, 0.34, 0.35, 0.36, 0.37, 0.38, 0.39,

0.5, 0.6, 0.7, 0.7, 0.7, 0.7, 0.7, 0.7, 0.8, 0.9.

A  $q$ -Bernstein-Vandermonde matrix with distinct nodes is nonsingular [10], thus the 17 rows corresponding to distinct nodes are linearly independent. The repeated nodes (0.2, three times, and 0.7, six times) correspond to repeated rows in the matrix and thus the rank of the matrix is 17.

We started with the singularity-free bidiagonal decomposition of  $A$ , computed using the formulas in Section 5.2, and implemented in our software package STNTool [21] as the routine STNBDqBernsteinVandermonde. We computed the eigenvalues using the algorithm STNEigenValues [8]. The matrix  $A$  is never explicitly formed or needed in this part of the computation, which is not only accurate (as we see below), but also very efficient: The singularity-free bidiagonal decomposition takes  $O(n^2)$  time and the eigenvalues take an additional  $O(n^3)$  time [8].

For comparison, in double precision floating point arithmetic [27], we formed  $A$  explicitly and computed its eigenvalues using the conventional eigenvalue algorithm of LAPACK [18] (as implemented by `eig` in MATLAB [29]). As expected, only the largest eigenvalues of  $A$  are computed accurately by `eig`. Further, since  $A$  is unsymmetric and its largest eigenvalue is about 1, the complete loss of relative accuracy occurs in all eigenvalues smaller than about  $10^{-12}$ , a value much larger machine precision (about  $10^{-16}$ ). The zero eigenvalues are lost to roundoff. This behavior is fully expected and justified for the general, structure-ignoring algorithms of LAPACK. It also underscores the utility of developing special algorithms for structured matrices, which deliver results to high relative accuracy with the same  $O(n^3)$  efficiency.

For verification, we formed  $A$ , then computed its eigenvalues, in 60 decimal digit arithmetic using the software package Mathematica. All nonzero eigenvalues computed by STNEigenValues agreed with those computed by Mathematica to at least 14 significant decimal digits. No amount of extra precision will allow us to reliably compute the zero eigenvalues using the conventional eigenvalue algorithms of LAPACK, thus the only reason we know the algorithm from [8] computed the correct number of zero eigenvalues (7) is because we know that the rank of the matrix is 17.<sup>1</sup>

MATLAB implementations of the algorithms described in this paper are available online [21].

**Data availability**

No data was used for the research described in the article.

<sup>1</sup> Since the graph is log-scale, the zero eigenvalues are not depicted and the negative and complex eigenvalues returned by the conventional algorithm are displayed by their absolute values.

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### Appendix

Here we present the explicit formulas for the singularity-free bidiagonal decompositions of the following Vandermonde-type matrices:

- $h$ -Bernstein–Vandermonde
- Lupaş
- rational Bernstein–Vandermonde, and
- Cauchy–Vandermonde matrices with one multiple pole.

This is not a complete list of Vandermonde-type matrices as this is an active area of research, but since we derived these formulas before realizing that all matrices of the Vandermonde-type follow the same pattern, we share them here and have implemented them in software [\[21\]](#).

#### A.1. Lupaş matrices

The Lupaş  $q$ -analogues of the Bernstein functions of degree  $n$  for  $0 < q \leq 1$  are defined as [\[30\]](#)

$$l_{i,q}^n(x) = \frac{a_{i,q}^n(x)}{w_q^n(x)}, \quad x \in [0, 1], \quad i = 0, 1, \dots, n,$$

where

$$a_{i,q}^n(x) = \begin{bmatrix} n \\ i \end{bmatrix} q^{\frac{i(i-1)}{2}} x^i (1-x)^{n-i},$$

$$w_q^n(x) = \sum_{i=0}^n a_{i,q}^n(x) = \prod_{i=2}^n (1-x + q^{i-1}x).$$

For case  $q = 1$  the Lupaş  $q$ -analogues of the Bernstein functions coincide with the Bernstein polynomials.

An  $n \times n$  Lupaş matrix  $A$  with nodes  $x_1, x_2, \dots, x_n$  is defined in [\[11\]](#) as

$$A = [l_{j-1,q}^{n-1}(x_i)]_{i,j=1}^n.$$

For  $0 \leq x_1 \leq x_2 \leq \dots \leq x_n < 1$ , the matrix  $A$  is TN [\[11, Thm. 2.1\]](#). It is also a Vandermonde-type matrix on  $[0, 1)$  with a singularity-free bidiagonal decomposition  $[B, C] = \mathcal{SBD}(A)$  defined as in [\(14\)–\(17\)](#) with parameters

$$s_{ij} = \frac{(1-x_i)^{n-j}(1-x_{i-j-1})}{(1-x_{i-1})^{n+1-j}} \prod_{k=1}^{n-2} \frac{1-x_{i-1} + q^k x_{i-1}}{1-x_i + q^k x_i},$$

$$m_{ji} = \frac{[n-i+1]q^{i-2}x_j}{[i-1](1-x_j)},$$

for  $1 \leq j < i \leq n$  and

$$s_{ii} = \begin{bmatrix} n-1 \\ i-1 \end{bmatrix} \frac{q^{\frac{(i-1)(i-2)}{2}} (1-x_i)^{n-i}}{\prod_{k=2}^{n-1} (1-x_i + q^{k-1}x_i) \prod_{k=0}^{i-1} (1-x_k)}$$

for  $1 \leq i \leq n$ .

The singularity-free bidiagonal decomposition of a Lupaş matrix can be computed to high relative accuracy in  $O(n^2)$  time using the routine STNBDLupas in our package STNTool [\[21\]](#).

#### A.2. $h$ -Bernstein–Vandermonde matrices

These matrices are generalization of the Bernstein–Vandermonde matrices [\[12,14\]](#), which are the  $h = 0$  case. The nonsingular case was developed in [\[15\]](#).

The  $h$ -Bernstein polynomials of degree  $n$  for a real parameter  $h \geq 0$  are defined in [15] as

$$b_{i,h}^n(x) = \binom{n}{i} \frac{\prod_{k=0}^{i-1}(x+kh) \prod_{k=0}^{n-i-1}(1-x+kh)}{\prod_{k=0}^{n-1}(1+kh)}, \quad x \in [0, 1], \quad 0 \leq i \leq n. \tag{28}$$

An  $n \times n$   $h$ -Bernstein-Vandermonde matrix with nodes  $x_1, x_2, \dots, x_n$  is defined as

$$A = [b_{j-1,h}^{n-1}(x_i)]_{i,j=1}^n.$$

For  $0 \leq x_1 \leq x_2 \leq \dots \leq x_n < 1$ ,  $A$  is a TN Vandermonde-type matrix [15] on  $[0, 1]$  and has a singularity-free bidiagonal decomposition  $[B, C] = \mathcal{SBD}(A)$  defined as in (14)–(17) with parameters

$$s_{ij} = \frac{1-x_{i-j}+(n-j)h}{1-x_{i-1}+(n-j)h} \prod_{k=0}^{n-j-1} \frac{1-x_i+kh}{1-x_{i-1}+kh}, \tag{29}$$

$$m_{ji} = \frac{n-i+1}{i-1} \cdot \frac{(x_j+(i-j-1)h) \prod_{k=1}^{j-1}(1-x_k+(n-i+1)h)}{\prod_{k=1}^j(1-x_k+(n-i)h)},$$

for  $1 \leq j < i \leq n$  and

$$s_{ii} = \binom{n-1}{i-1} \frac{\prod_{k=0}^{n-i-1}(1-x_i+kh)}{\prod_{k=1}^{n-i-1}(1+kh) \prod_{k=1}^{i-1}(1-x_k+(n-i)h)}$$

for  $1 \leq i \leq n$ .

The singularity-free bidiagonal decomposition of an  $h$ -Bernstein-Vandermonde matrix can be computed to high relative accuracy in  $O(n^2)$  time using the routine `STNBdBernsteinVandermonde` in our package `STNTool` [21].

### A.3. Rational Bernstein-Vandermonde matrices

A rational Bernstein-Vandermonde matrix with nodes  $x_1, x_2, \dots, x_n$  and positive weights  $w_1, w_2, \dots, w_n$  is defined as [9]:

$$R = [r_{j-1}^{n-1}(x_i)]_{i,j=1}^n,$$

where

$$r_{j-1}^{n-1}(x) = \frac{w_j b_{j-1}^{n-1}(x)}{W(x)}, \quad x \in [0, 1], \quad j \in \{1, 2, \dots, n\}, \tag{30}$$

and  $W(x) = \sum_{j=1}^n w_j b_{j-1}^{n-1}(x)$ . The functions  $b_i^n(x)$  are the Bernstein polynomials of degree  $n$ . They equal the  $q$ -Bernstein polynomials (19) for  $q = 1$  and the  $h$ -Bernstein polynomials (28) for  $h = 0$ , i.e.,

$$b_i^n(x) = \binom{n}{i} x^i (1-x)^{n-i}, \quad i \in \{0, 1, \dots, n\}, \quad x \in [0, 1].$$

For  $0 < x_1 \leq x_2 \leq \dots \leq x_n < 1$ , the matrix  $R$  is TN [9, Thm. 3.1], which is of Vandermonde-type on  $(0, 1)$  and has a singularity-free bidiagonal decomposition  $[B, C] = \mathcal{SBD}(R)$  defined as in (14)–(17) with parameters

$$s_{ij} = \frac{W(x_{i-1})(1-x_i)^{n-j}(1-x_{i-j})}{W(x_i)(1-x_{i-1})^{n-j+1}}, \tag{31}$$

$$m_{ji} = \frac{w_i}{w_{i-1}} \cdot \frac{n-i+1}{i-1} \cdot \frac{x_j}{1-x_j}, \tag{32}$$

for  $1 \leq j < i \leq n$  and

$$s_{ii} = \binom{n-1}{i-1} \frac{w_i(1-x_i)^{n-i}}{W(x_i) \prod_{k=1}^{i-1}(1-x_k)}$$

for  $1 \leq i \leq n$ .

While we like the above expressions for their symmetry, an alternative singularity-free bidiagonal decomposition of  $R$  can be obtained by recognizing, from (20) and (30), that  $R = W_1^{-1} A W_2$ , where  $A$  is the  $q$ -Bernstein-Vandermonde matrix for  $q = 1$ , and

$$W_1 = \text{diag}(W(x_1), W(x_2), \dots, W(x_n))$$

$$W_2 = \text{diag}(w_1, w_2, \dots, w_n)$$

are positive diagonal matrices. Thus if  $\mathcal{SBD}(A)$  is given by (6), then  $R$  has a singularity-free bidiagonal decomposition

$$R = (W_1^{-1} L_1) L_2 \cdots L_{n-1} D U_{n-1} U_{n-2} \cdots (U_1 W_2), \tag{33}$$

where the first and last factors in the parentheses,  $W_1^{-1}L_1$  and  $U_1W_2$ , are nonnegative bidiagonal matrices with the same nonzero pattern as  $L_1$  and  $U_1$ , respectively. Thus (33) is another bidiagonal decomposition of  $R$  and an example of how the nonuniqueness of the singularity-free bidiagonal decomposition (6) can play out.

The singularity-free bidiagonal decomposition of a rational Bernstein–Vandermonde matrix can be computed to high relative accuracy in  $O(n^2)$  time using the routine `STNBDRationalBernsteinVandermonde` in our package `STNTool` [21].

#### A.4. Cauchy–Vandermonde matrices with one multiple pole

A Cauchy–Vandermonde matrix with nodes  $x_1, \dots, x_n$  and one pole  $d$  of multiplicity  $s \geq 1$  is defined as [31]

$$A = \begin{bmatrix} \frac{1}{(x_1+d)^s} & \cdots & \frac{1}{x_1+d} & 1 & x_1 & \cdots & x_1^{n-s-1} \\ \frac{1}{(x_2+d)^s} & \cdots & \frac{1}{x_2+d} & 1 & x_2 & \cdots & x_2^{n-s-1} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ \frac{1}{(x_n+d)^s} & \cdots & \frac{1}{x_n+d} & 1 & x_n & \cdots & x_n^{n-s-1} \end{bmatrix}$$

and is totally nonnegative when  $0 \leq x_1 \leq x_2 \leq \dots \leq x_n$  and  $d > 0$ . It is a Vandermonde-type matrix on  $[0, \infty)$  for  $d > 0$  and has a decomposition  $[B, C] = \mathcal{SBD}(A)$  with parameters

$$s_{ij} = \left( \frac{x_{i-1} + d}{x_i + d} \right)^s,$$

$$m_{ji} = \begin{cases} x_j + d, & 0 < i - j \leq s \\ x_j, & i - j > s \end{cases},$$

for  $1 \leq j < i \leq n$  and

$$s_{ii} = \frac{1}{(x_i + d)^s}$$

for  $1 \leq i \leq n$ .

The singularity-free bidiagonal decomposition of a Cauchy–Vandermonde matrix with one multiple pole can be computed to high relative accuracy in  $O(n^2)$  time using the routine `STNBDCauchyVandermonde1pole` in our package `STNTool` [21].

#### A.5. Other Vandermonde-type matrices

The method presented in this section can be used analogously to derive singularity-free bidiagonal decompositions of other Vandermonde-type matrices, for example:

- Said-Ball Vandermonde [13,16],
- Rational Said-Ball Vandermonde [9],
- Collocation and Wronskian matrices of Jacobi polynomials [32].

This is likely an incomplete list as this currently appears to be an area of active research.

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