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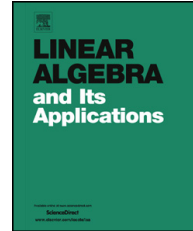
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Error analysis, perturbation theory and applications of the bidiagonal decomposition of rectangular totally positive h-Bernstein-Vandermonde matrices[☆]

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ABSTRACT

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A fast and accurate algorithm to compute the bidiagonal decomposition of rectangular totally positive h-Bernstein-Vandermonde matrices is presented. The error analysis of the algorithm and the perturbation theory for the bidiagonal decomposition of totally positive h-Bernstein-Vandermonde matrices are addressed. The computation of this bidiagonal decomposition is used as the first step for the accurate and efficient computation of the singular values of rectangular totally positive h-Bernstein-Vandermonde matrices and for solving least squares problems whose coefficient matrices are such matrices.

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Bidiagonal decomposition
High relative accuracy

1. Introduction

The h -Bernstein bases are a generalization of the Bernstein basis which for $h > 0$ share many properties with the standard Bernstein basis (the case $h = 0$). They were introduced in approximation theory by Stancu [27,28], and rediscovered in the field of Computer Aided Geometric Design by Goldman [15], and Barry and Goldman [1,2]. More recently the h -Bernstein bases have been studied also in this field in [26].

An h -Bernstein-Vandermonde matrix is a generalization of the Vandermonde matrix obtained when replacing the monomial basis by an h -Bernstein basis [24].

The design of accurate algorithms to work with structured totally positive matrices is a current topic of research in numerical linear algebra since, although numerical linear algebra problems can be solved for these matrices by means of standard algorithms, the usual ill-conditioning of structured totally positive matrices may cause inaccurate results when standard algorithms are used (see, for example, [19,9,20,21,4,22,5,23,6,7]).

Let us recall that a matrix is *totally positive* (resp. *strictly totally positive*) if all its minors are nonnegative (resp. positive), and they are also known in the literature as totally nonnegative (resp. totally positive) [10,25].

Our aim in this work is to continue the study of totally positive h -Bernstein-Vandermonde matrices initiated in [24]. In particular, we will start with the extension to the rectangular case of the algorithm for computing with high relative accuracy the bidiagonal decomposition of square totally positive h -Bernstein-Vandermonde matrices presented in [24]. Then, we will focus on two research topics that have not been considered in the square case: the error analysis of the algorithm and the perturbation theory for the bidiagonal factorization of totally positive h -Bernstein-Vandermonde matrices. In addition, we will examine the solution of two important numerical linear algebra problems for these matrices, namely singular value computation and least squares problems.

Let us remind that an algorithm computes to high relative accuracy if it only multiplies, divides, adds (resp. subtracts) real numbers with like (resp. differing) signs, and otherwise only adds or subtracts input data [8].

The rest of the paper is organized as follows. Some basic results on Neville elimination, the main theoretical tool on which our algorithm for computing the bidiagonal decomposition is based, and on total positivity are summarized in Section 2. Section 3 is devoted to the bidiagonal decomposition of a rectangular h -Bernstein-Vandermonde matrix, along with the algorithm for computing it. In Section 4 the algorithms to compute the singular values and to solve the least squares problems are presented. The error analysis of our algorithm for computing the bidiagonal factorization is carried out in Section 5, while the perturbation theory is addressed in Section 6. Finally, numerical experiments showing the good performance of our algorithms are included in Section 7.

2. Basic results on Neville elimination and total positivity

Some basic results on Neville elimination and total positivity, which will be essential for obtaining the results presented in the next section, are briefly recalled here. Our notation follows the notation used in [11] and [13]. Given $k, n \in \mathbb{N}$ ($1 \leq k \leq n$), $Q_{k,n}$ will denote the set of all increasing sequences of k positive integers less than or equal to n .

Let A be an $l \times n$ real matrix. For $k \leq l, m \leq n$, and for any $\alpha \in Q_{k,l}$ and $\beta \in Q_{m,n}$, we will denote by $A[\alpha|\beta]$ the $k \times m$ submatrix of A containing the rows numbered by α and the columns numbered by β .

The fundamental theoretical tool for obtaining the results presented in this paper is the *Neville elimination* [11,13,14], a procedure that makes zeros in a matrix by adding to a given row an appropriate multiple of the previous one.

Let $A = (a_{i,j})_{1 \leq i \leq l; 1 \leq j \leq n}$ be a matrix where $l \geq n$. The Neville elimination of A consists of $n - 1$ steps resulting in a sequence of matrices $A_1 := A \rightarrow A_2 \rightarrow \dots \rightarrow A_n$, where $A_t = (a_{i,j}^{(t)})_{1 \leq i \leq l; 1 \leq j \leq n}$ has zeros below its main diagonal in the $t - 1$ first columns. The matrix A_{t+1} is obtained from A_t ($t = 1, \dots, n - 1$) by using the following formula:

$$a_{i,j}^{(t+1)} := \begin{cases} a_{i,j}^{(t)}, & \text{if } i \leq t \\ a_{i,j}^{(t)} - (a_{i,t}^{(t)} / a_{i-1,t}^{(t)}) a_{i-1,j}^{(t)}, & \text{if } i \geq t + 1 \text{ and } j \geq t + 1 \\ 0, & \text{otherwise.} \end{cases}$$

In this process the element

$$p_{i,j} := a_{i,j}^{(j)} \quad 1 \leq j \leq n, \quad j \leq i \leq l$$

is called (i, j) *pivot* of the Neville elimination of A . The process would break down if any of the pivots $p_{i,j}$ ($1 \leq j \leq n, j \leq i \leq l$) were zero. In that case we can move the corresponding rows to the bottom and proceed with the new matrix, as described in [11]. The Neville elimination can be done without row exchanges if all the pivots are nonzero, as it will happen in our situation. The pivots $p_{i,i}$ are called *diagonal pivots*. If all the pivots $p_{i,j}$ are nonzero, then $p_{i,1} = a_{i,1} \forall i$ and, by Lemma 2.6 of [11]

$$p_{i,j} = \frac{\det A[i - j + 1, \dots, i | 1, \dots, j]}{\det A[i - j + 1, \dots, i - 1 | 1, \dots, j - 1]} \quad 1 < j \leq n, \quad j \leq i \leq l. \tag{1}$$

The element

$$m_{i,j} = \frac{p_{i,j}}{p_{i-1,j}} \quad 1 \leq j \leq n, \quad j < i \leq l, \tag{2}$$

is called *multiplier* of the Neville elimination of A . The matrix $U := A_n$ is upper triangular and has the diagonal pivots on its main diagonal.

The *complete Neville elimination* of a matrix A consists of performing the Neville elimination of A for obtaining U and then continue with the Neville elimination of U^T . The (i, j) pivot (resp., multiplier) of the complete Neville elimination of A is the (j, i) pivot (resp. multiplier) of the Neville elimination of U^T , if $j \geq i$. When no row exchanges are needed in the Neville elimination of A and U^T , we say that the complete Neville elimination of A can be done without row and column exchanges, and in this case the multipliers of the complete Neville elimination of A are the multipliers of the Neville elimination of A if $i \geq j$ and the multipliers of the Neville elimination of A^T if $j \geq i$.

Let us point out here that our approach uses results related to Neville elimination as a theoretical tool but it does not apply the Neville elimination algorithm for obtaining the bidiagonal factorization of h-Bernstein-Vandermonde matrices.

Neville elimination characterizes the strictly totally positive matrices as follows [11]:

Theorem 1. *A matrix is strictly totally positive if and only if its complete Neville elimination can be performed without row and column exchanges, the multipliers of the Neville elimination of A and A^T are positive, and the diagonal pivots of the Neville elimination of A are positive.*

As it is shown in [24], the h-Bernstein-Vandermonde matrices are strictly totally positive when $h \geq 0$ and the nodes $\{x_i\}_{1 \leq i \leq n}$ satisfy $0 < x_1 < x_2 < \dots < x_n < 1$.

3. Bidiagonal decomposition

The *h-Bernstein basis* of the space $\Pi_n(x)$ of polynomials of degree less than or equal to n on the interval $[0, 1]$ is

$$\mathcal{B}_{h,n} = \left\{ B_i^n(x; h) = \binom{n}{i} \frac{\prod_{k=0}^{i-1} (x + kh) \prod_{k=0}^{n-i-1} (1 - x + kh)}{\prod_{k=0}^{n-1} (1 + kh)} : i = 0, \dots, n \right\},$$

where $h \in \mathbb{R}$ [26].

The matrix

$$A = \begin{pmatrix} \binom{n}{0} \frac{\prod_{k=0}^{n-1} (1 - x_1 + kh)}{\prod_{k=0}^{n-1} (1 + kh)} & \binom{n}{1} \frac{x_1 \prod_{k=0}^{n-2} (1 - x_1 + kh)}{\prod_{k=0}^{n-1} (1 + kh)} & \dots & \binom{n}{n} \frac{\prod_{k=0}^{n-1} (x_1 + kh)}{\prod_{k=0}^{n-1} (1 + kh)} \\ \binom{n}{0} \frac{\prod_{k=0}^{n-1} (1 - x_2 + kh)}{\prod_{k=0}^{n-1} (1 + kh)} & \binom{n}{1} \frac{x_2 \prod_{k=0}^{n-2} (1 - x_2 + kh)}{\prod_{k=0}^{n-1} (1 + kh)} & \dots & \binom{n}{n} \frac{\prod_{k=0}^{n-1} (x_2 + kh)}{\prod_{k=0}^{n-1} (1 + kh)} \\ \vdots & \vdots & \ddots & \vdots \\ \binom{n}{0} \frac{\prod_{k=0}^{n-1} (1 - x_{l+1} + kh)}{\prod_{k=0}^{n-1} (1 + kh)} & \binom{n}{1} \frac{x_{l+1} \prod_{k=0}^{n-2} (1 - x_{l+1} + kh)}{\prod_{k=0}^{n-1} (1 + kh)} & \dots & \binom{n}{n} \frac{\prod_{k=0}^{n-1} (x_{l+1} + kh)}{\prod_{k=0}^{n-1} (1 + kh)} \end{pmatrix}$$

is the h-Bernstein-Vandermonde matrix (hBV matrix in the sequel) for the h-Bernstein basis $\mathcal{B}_{h,n}$ and the nodes $\{x_i\}_{1 \leq i \leq l+1}$. From now on, we will consider $h \geq 0$, since it is the case in which h-Bernstein bases share many properties with the standard Bernstein basis (the case $h = 0$) [26], and we will assume $0 < x_1 < x_2 < \dots < x_{l+1} < 1$. In this

$$m_{i,j} = \frac{(1 - x_{i-j} + (n - j + 1)h) \prod_{k=1}^{j-1} (x_i - x_{i-k}) \prod_{k=0}^{n-j} (1 - x_i + kh)}{\prod_{k=1}^{j-1} (x_{i-1} - x_{i-1-k}) \prod_{k=0}^{n-j+1} (1 - x_{i-1} + kh)}, \quad (4)$$

where $j = 2, \dots, n + 1$, $i = j + 1, \dots, l + 1$. The quantities $\tilde{m}_{i,j}$ are the multipliers of the Neville elimination of A^T , and their expression is

$$\tilde{m}_{i,j} = \frac{n - i + 2}{i - 1} \cdot \frac{(x_j + (i - j - 1)h) \prod_{k=1}^{j-1} (1 - x_k + (n - i + 2)h)}{\prod_{k=1}^j (1 - x_k + (n - i + 1)h)}, \quad (5)$$

where $j = 1, \dots, n$, $i = j + 1, \dots, n + 1$. Finally, the i th diagonal entry of D is the diagonal pivot of the Neville elimination of A and its expression is

$$p_{i,i} = \binom{n}{i - 1} \frac{\prod_{k < i} (x_i - x_k) \prod_{k=0}^{n-i} (1 - x_i + kh)}{\prod_{k=1}^{n-i} (1 + kh) \prod_{k=1}^{i-1} (1 - x_k + (n - i + 1)h)} \quad (6)$$

where $i = 1, \dots, n + 1$.

Proof. It is analogous to the one carried out in theorems 3.3 and 3.4 of [24] for the case in which A is a square hBV matrix. To obtain equations (3)-(6) explicit expressions of the determinants involved in (1) and (2) are calculated. \square

Based on the previous theorem, we present a fast and accurate algorithm for computing the bidiagonal decomposition of a rectangular strictly totally positive hBV matrix A . From now on we will follow the notation in [19], where $\mathcal{BD}(A)$ is used for denoting the matrix containing the multipliers and pivots in the bidiagonal decomposition of the matrix A , as it is described below.

Given the degree n of the h-Bernstein basis we are considering, the value $h \geq 0$ and the nodes $\{x_i\}_{1 \leq i \leq l+1}$ (where $0 < x_1 < x_2 < \dots < x_{l+1} < 1$ and $l > n$) corresponding to A , the algorithm we have called TNBDhBVR (see Algorithm 1) returns a matrix $M = \mathcal{BD}(A)$ such that

$$\begin{aligned} M_{i,i} &= p_{i,i} & i &= 1, \dots, n + 1, \\ M_{i,j} &= m_{i,j} & j &= 1, \dots, n + 1; i = j + 1, \dots, l + 1, \\ M_{i,j} &= \tilde{m}_{j,i} & i &= 1, \dots, n; j = i + 1, \dots, n + 1, \end{aligned}$$

where $m_{i,j}$ are the multipliers of the Neville elimination of A , $\tilde{m}_{i,j}$ are the multipliers of the Neville elimination of A^T and $p_{i,i}$ are the diagonal pivots of the Neville elimination of A .

The algorithm, which does not construct the hBV matrix A , is an extension to the rectangular case of the algorithm presented in [24] for computing the bidiagonal decomposition of a square strictly totally positive hBV matrix. In order to facilitate the understanding of the error analysis carried out in Section 5, the pseudocode of the algorithm TNBDhBVR is included here.

Algorithm 1

Input: The vector c containing the nodes $\{x_i\}_{1 \leq i \leq l+1}$, the value $h \geq 0$, and the degree n of the h -Bernstein basis.

Output: $M = \mathcal{BD}(A)$

1: function $z = \text{TNBDhBVR}(c, n, h)$

- $m_{i,j}$ computation:

2: for $i=2:l+1$

3: $aux = \frac{1-x_i}{1-x_{i-1}}$;

4: for $k=1:n-1$

5: $aux = aux \cdot \frac{(1-x_i)+kh}{(1-x_{i-1})+kh}$;

6: end

7: $M_{i,1} = aux$;

8: end

9: for $i=3:l+1$

10: $M_{i,2} = \frac{(x_i-x_{i-1})((1-x_{i-2})+(n-1)h)}{(x_{i-1}-x_{i-2})((1-x_i)+(n-1)h)} M_{i,1}$;

11: end

12: for $j=2:n$

13: for $i=j+2:l+1$

14: $M_{i,j+1} = \frac{(x_i-x_{i-j})((1-x_{i-j-1})+(n-j)h)((1-x_{i-1})+(n-j+1)h)}{(x_{i-1}-x_{i-j-1})((1-x_i)+(n-j)h)((1-x_{i-j})+(n-j+1)h)} M_{i,j}$;

15: end

16: end

- $\tilde{m}_{i,j}$ computation:

17: for $j=2:n+1$

18: $M_{1,j} = \frac{(n-j+2)(x_1+(j-2)h)}{(j-1)((1-x_1)+(n-j+1)h)}$;

19: end

20: for $j=3:n+1$

21: for $i=1:j-2$

22: $M_{i+1,j} = \frac{(x_{i+1}+(j-i-2)h)((1-x_i)+(n-j+2)h)}{((x_i+(j-i-1)h)((1-x_{i+1})+(n-j+1)h)} M_{i,j}$;

23: end

24: end

- $p_{i,i}$ computation:

25: $aux=1$

26: for $k=1:n$

27: $aux = aux \cdot \frac{x_{n+1}-x_k}{1-x_k}$;

28: end

29: $M_{n+1,n+1} = aux$;

30: $B = \text{zeros}(1,n+1)$;

31: $B_1 = 1$;

32: for $i=1:n$

33: $B_{i+1} = \frac{n-i+1}{i} B_i$;

34: end

35: for $i=1:n$

36: $aux = B_i(1-x_i)$;

37: for $k=1:i-1$

38: $aux = aux \cdot \frac{x_i-x_k}{(1-x_k)+(n-i+1)h}$;

39: end

40: for $k=1:n-i$

41: $aux = aux \cdot \frac{(1-x_i)+kh}{1+kh}$;

42: end

43: $M_{i,i} = aux$;

44: end

Looking at Algorithm 1 it is observed that TNBDhBVR preserves high relative accuracy, and it has a computational cost of $O(ln)$ arithmetic operations. For a more detailed explanation see [24].

4. Accurate computations with rectangular hBV matrices

Given a totally positive hBV matrix A , algorithms for solving two fundamental problems in numerical linear algebra, namely singular value computation and the least squares problem, are given in this section. In the particular case of A being square, accurate and efficient algorithms for solving linear systems, computing eigenvalues and calculating the inverse for these types of matrices can be found in [24].

The algorithms developed in this section are both accurate and efficient, and are based on the accurate algorithm for computing $\mathcal{BD}(A)$ presented in Section 3.

We must note that, due to the ill-conditioning of hBV matrices [24], standard algorithms to solve the two previously cited problems will generally provide less accurate results. The reason is that, as these algorithms do not take into account the particular structure of the matrix, they can suffer from inaccurate **cancellation**. In our approach, on the contrary, the exploitation of the specific structure of hBV matrices will provide accurate results. This becomes clear in the numerical experiments of Section 7.

4.1. Singular values and condition number

Let $A \in \mathbb{R}^{(l+1) \times (n+1)}$ be a rectangular hBV matrix for the nodes $\{x_i\}_{1 \leq i \leq l+1}$, where $0 < x_1 < x_2 < \dots < x_{l+1} < 1$, $l > n$ and $h \geq 0$. For matrix A , Algorithm 2 computes the singular values of A with high relative accuracy.

Algorithm 2

Input: The vector c containing the nodes $\{x_i\}_{1 \leq i \leq l+1}$, the value $h \geq 0$, and the degree n of the h-Bernstein basis.

Output: A vector $z \in \mathbb{R}^{n+1}$ containing the singular values of A .

1: function $z = \text{TNSingularValueshBVR}(c, n, h)$

2: $B = \text{TNBDhBVR}(c, n, h);$

3: $z = \text{TNSingularValues}(B);$

The command `TNSingularValues` provides the singular values of a totally positive matrix with bidiagonal decomposition stored in matrix B . Its implementation in MATLAB can be obtained from [18]. It preserves high relative accuracy and has a computational cost of $O(ln^2)$ arithmetic operations [19]. This cost dominates the computational cost of `TNBDhBVR`, which is $O(ln)$ (see Section 3). Thus, the number of arithmetic operations required by Algorithm 2 is $O(ln^2)$.

Let us notice that the accurate computation of the singular values of A allows us to compute the 2 -norm condition number of A accurately, just dividing the greatest by the smallest singular value of A . A numerical experiment showing this fact is included in Section 7.

4.2. The least squares problem

Let $b \in \mathbb{R}^{l+1}$ be a data vector, and let us consider the overdetermined linear system $Ax = b$, whose coefficient matrix A is the rectangular hBV matrix for the nodes

$\{x_i\}_{1 \leq i \leq l+1}$ (where $0 < x_1 < x_2 < \dots < x_{l+1} < 1$, $l > n$) and $h \geq 0$. The least squares problem to be solved consists of computing a vector $x \in \mathbb{R}^{n+1}$ which minimizes $\|b - Ax\|_2$. Since A is a strictly totally positive matrix, it has full rank $n + 1$. Hence, the solution of the least squares problem is unique, and the method of G. H. Golub [16] based on the QR decomposition is adequate for solving this least squares problem [3].

For completeness we include the following result (see Section 1.3.1 in [3]), which will be essential in the construction of our algorithm.

Theorem 3. *Let $Ax = b$ be a linear system where $A \in \mathbb{R}^{(l+1) \times (n+1)}$, $l \geq n$, $x \in \mathbb{R}^{n+1}$ and $b \in \mathbb{R}^{l+1}$. Assume that $\text{rank}(A) = n + 1$, and let the QR decomposition of A be given by*

$$A = Q \begin{bmatrix} R \\ 0 \end{bmatrix},$$

where $Q \in \mathbb{R}^{(l+1) \times (l+1)}$ is an orthogonal matrix and $R \in \mathbb{R}^{(n+1) \times (n+1)}$ is an upper triangular matrix with positive diagonal entries. Then the solution of the least squares problem $\min_x \|b - Ax\|_2$ is obtained from

$$\begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = Q^T b, \quad Rx = d_1, \quad r = Q \begin{bmatrix} 0 \\ d_2 \end{bmatrix},$$

where $d_1 \in \mathbb{R}^{n+1}$, $d_2 \in \mathbb{R}^{l-n}$ and $r = b - Ax$. In particular $\|r\|_2 = \|d_2\|_2$.

Algorithm 3 is based on Theorem 3 and provides the solution of the least squares problem we are considering.

Algorithm 3

Input: The vector c containing the nodes $\{x_i\}_{1 \leq i \leq l+1}$, the value $h \geq 0$, the degree n of the h -Bernstein basis, and the vector $b \in \mathbb{R}^{l+1}$.

Output: The solution vector $x \in \mathbb{R}^{n+1}$ and the minimum residual $r = b - Ax$.

1: function $[x, r] = \text{TNLeastSquareshBV}(c, n, h, b)$

2: $B = \text{TNBDhBVR}(c, n, h)$;

3: $[Q, R] = \text{TNQR}(B)$;

4: $d = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = Q^T b$;

5: $x = \text{TNSolve}(R, d_1)$;

6: $r = Q \begin{bmatrix} 0 \\ d_2 \end{bmatrix}$;

The algorithm TNQR has been developed by P. Koev and, given the bidiagonal factorization of A , it computes the matrix Q and the bidiagonal factorization of the matrix R with high relative accuracy. Let us point out here that if A is strictly totally positive, then R is totally positive, a fact carefully analyzed in [12]. TNQR is based on Givens rotations and has a computational cost of $O(l^2 n)$ arithmetic operations if the matrix Q is required [20]. Its implementation in MATLAB can be obtained from [18].

Lines 4 and 6 are performed by using the standard matrix multiplication command of MATLAB.

The command `TNSolve` solves the linear system $Ax = b$, where A is a strictly totally positive matrix, starting from the bidiagonal decomposition of A and using backward substitution. Its implementation in MATLAB is available in the package `TNTool` of P. Koev [18] and it guarantees high relative accuracy provided that the data vector has alternating sign pattern. The computational cost of applying it is of $O(n^2)$ arithmetic operations.

Taking into account that the cost of `TNBDhBVR` is $O(ln)$ (see Section 3), the computational cost of the whole algorithm is $O(l^2n)$.

Although for the least squares problem our approach does not guarantee high relative accuracy, numerical experiments illustrating its good behaviour are presented in Section 7.

5. Error analysis

In this section the error analysis of the algorithm `TNBDhBVR` for computing the bidiagonal factorization of a rectangular totally positive hBV matrix included in Section 3 is accomplished.

For our error analysis we use the standard model of floating point arithmetic (see section 2.2 of [17]):

Let x, y be floating point numbers and let ϵ be the *machine precision*. Then we have

$$fl(x \odot y) = (x \odot y)(1 + \delta)^{\pm 1}, \quad \text{where } |\delta| \leq \epsilon, \quad \odot \in \{+, -, \times, /\}.$$

Our error analysis of algorithm `TNBDhBVR` (Algorithm 1) is summarized in the following theorem:

Theorem 4. *Let A be an hBV matrix for the h -Bernstein basis $\mathcal{B}_{h,n}$ ($h \geq 0$) and the nodes $\{x_i\}_{1 \leq i \leq l+1}$, where $0 < x_1 < x_2 < \dots < x_{l+1} < 1$ and $l \geq n$. Let $\mathcal{BD}(A) = (b_{i,j})_{1 \leq i \leq l+1; 1 \leq j \leq n+1}$ be the matrix representing the exact bidiagonal decomposition of A and $(\widehat{b}_{i,j})_{1 \leq i \leq l+1; 1 \leq j \leq n+1}$ be the matrix representing the computed bidiagonal decomposition of A by means of the algorithm `TNBDhBVR` in floating point arithmetic with machine precision ϵ . Then*

$$|\widehat{b}_{i,j} - b_{i,j}| \leq \frac{(22n - 9)\epsilon}{1 - (22n - 9)\epsilon} b_{i,j}, \quad i = 1, \dots, l + 1; \quad j = 1, \dots, n + 1.$$

Proof. Accumulating the relative errors in the style of Higham (see Chapter 3 of [17], [9], [19] and [21]) in the computation of the multipliers $m_{i,j}$ by means of the algorithm `TNBDhBVR` included in Section 3 we obtain

$$|\widehat{m}_{i,j} - m_{i,j}| \leq \frac{(22n - 9)\epsilon}{1 - (22n - 9)\epsilon} m_{i,j}, \quad j = 1, \dots, n + 1; \quad i = j + 1, \dots, l + 1, \quad (7)$$

where $\widehat{m}_{i,j}$ are the multipliers $m_{i,j}$ computed in floating point arithmetic. Proceeding in the same way for the computation of the $\widetilde{m}_{i,j}$ we derive

$$|\widehat{m}_{i,j} - \widetilde{m}_{i,j}| \leq \frac{(12n-5)\epsilon}{1-(12n-5)\epsilon} \widetilde{m}_{i,j}, \quad j = 1, \dots, n; \quad i = j+1, \dots, n+1, \quad (8)$$

where $\widehat{m}_{i,j}$ are the multipliers $\widetilde{m}_{i,j}$ computed in floating point arithmetic. Analogously

$$|\widehat{p}_{i,i} - p_{i,i}| \leq \frac{(7n-5)\epsilon}{1-(7n-5)\epsilon} p_{i,i}, \quad i = 1, \dots, n+1, \quad (9)$$

where $\widehat{p}_{i,i}$ are the diagonal pivots $p_{i,i}$ computed in floating point arithmetic.

Therefore, looking at the inequalities given by (7), (8) and (9) and taking into account that $\widehat{m}_{i,j}$, $\widetilde{m}_{i,j}$ and $\widehat{p}_{i,i}$ are the entries of $(\widehat{b}_{i,j})_{1 \leq i \leq l+1; 1 \leq j \leq n+1}$, we conclude that

$$|\widehat{b}_{i,j} - b_{i,j}| \leq \frac{(22n-9)\epsilon}{1-(22n-9)\epsilon} b_{i,j}, \quad i = 1, \dots, l+1; \quad j = 1, \dots, n+1. \quad \square$$

This result shows that TNBDhBVR computes the bidiagonal decomposition of an hBV matrix accurately in floating point arithmetic.

6. Perturbation theory

In his work [19], P. Koev showed that if a totally positive matrix A is represented as a product of nonnegative bidiagonal matrices, then small relative perturbations in the entries of the bidiagonal factors produce only small relative perturbations in the eigenvalues and singular values of A . More precisely, $\mathcal{BD}(A)$ determines the eigenvalues and the singular values of A accurately, and the appropriate structured condition number of each eigenvalue and/or singular value with respect to perturbations in $\mathcal{BD}(A)$ is at most $2n^2$ (see Corollary 7.3 in [19]).

These results reveal the importance of the study of the perturbation theory for the bidiagonal decomposition $\mathcal{BD}(A)$ of a totally positive matrix A . This study in the case in which A is a totally positive hBV matrix is carried out in this section, and so the sensitivity of its $\mathcal{BD}(A)$ with respect to perturbations in the nodes x_i of A is analyzed. Specifically, we prove that small relative perturbations in the nodes of an hBV matrix A produce only small relative perturbations in its bidiagonal factorization $\mathcal{BD}(A)$.

We start by defining the quantities we need to find an appropriate condition number, in a similar way to the work developed in [19,21–23].

Definition 1. Let A be a strictly totally positive hBV matrix for the h-Bernstein basis $\mathcal{B}_{h,n}$ and the nodes $\{x_i\}_{1 \leq i \leq l+1}$ and let $x'_i = x_i(1 + \delta_i)$ be the perturbed nodes for $1 \leq i \leq l+1$, where $|\delta_i| \ll 1$. We define:

$$rel_gap_x \equiv \min_{i \neq j} \frac{|x_i - x_j|}{|x_i| + |x_j|},$$

$$rel_gap_1 \equiv \min_i \frac{|1 - x_i|}{|x_i|},$$

$$\theta \equiv \max_i \frac{|x_i - x'_i|}{|x_i|} = \max_i |\delta_i|,$$

$$\alpha \equiv \min\{rel_gap_x, rel_gap_1\},$$

$$\kappa_h \equiv \frac{1}{\alpha},$$

where $\theta \ll rel_gap_x, rel_gap_1$.

The following theorem is the main result of this section.

Theorem 5. *Let A and A' be strictly totally positive hBV matrices for the h -Bernstein basis $\mathcal{B}_{h,n}$ and the nodes $\{x_i\}_{1 \leq i \leq l+1}$ and $x'_i = x_i(1 + \delta_i)$ for $1 \leq i \leq l + 1$, where $|\delta_i| \leq \theta \ll 1$. Let $\mathcal{BD}(A)$ and $\mathcal{BD}(A')$ be the matrices representing the bidiagonal decomposition of A and the bidiagonal decomposition of A' , respectively. Then*

$$|(\mathcal{BD}(A'))_{i,j} - (\mathcal{BD}(A))_{i,j}| \leq \frac{(2n + 2)\kappa_h\theta}{1 - (2n + 2)\kappa_h\theta} (\mathcal{BD}(A))_{i,j}.$$

Proof. Taking into account that $|\delta_i| \leq \theta$, it can easily be shown that

$$x'_i - x'_j = (x_i - x_j)(1 + \delta_{i,j}), \quad |\delta_{i,j}| \leq \frac{\theta}{rel_gap_x}, \tag{10}$$

$$x'_j + kh = (x_j + kh)(1 + \delta'_j), \quad |\delta'_j| \leq \theta, \tag{11}$$

and

$$1 - x'_j + kh = (1 - x_j - kh)(1 + \delta''_j), \quad |\delta''_j| \leq \frac{\theta}{rel_gap_1}. \tag{12}$$

Accumulating the perturbations in the style of Higham (see Chapter 3 of [17], [19] and [21]) using the formulae (3) and (4) for the $m_{i,j}$, and (10) and (12) we obtain

$$m'_{i,j} = m_{i,j}(1 + \bar{\delta}), \quad |\bar{\delta}| \leq \frac{(2n + 2)\kappa_h\theta}{1 - (2n + 2)\kappa_h\theta},$$

where $m'_{i,j}$ are the entries of $\mathcal{BD}(A')$ below the main diagonal. Proceeding in the same way by using Equation (5), and (11) and (12) we get

$$\tilde{m}'_{i,j} = \tilde{m}_{i,j}(1 + \bar{\delta}), \quad |\bar{\delta}| \leq \frac{(2n)\frac{\theta}{rel_gap_1}}{1 - (2n)\frac{\theta}{rel_gap_1}},$$

where $\tilde{m}'_{i,j}$ are the entries of $\mathcal{BD}(A')$ above the main diagonal. Analogously, and using in this case Equation (6), and (10) and (12) we get

$$p'_{i,i} = p_{i,i}(1 + \bar{\delta}), \quad |\bar{\delta}| \leq \frac{(2n+1)\kappa_h\theta}{1 - (2n+1)\kappa_h\theta},$$

where $p'_{i,i}$ are the diagonal elements of $\mathcal{BD}(A')$. Finally, considering the last three inequalities we conclude that

$$|(\mathcal{BD}(A'))_{i,j} - (\mathcal{BD}(A))_{i,j}| \leq \frac{(2n+2)\kappa_h\theta}{1 - (2n+2)\kappa_h\theta} (\mathcal{BD}(A))_{i,j}. \quad \square$$

Therefore, we see that the quantity $(2n+2)\kappa_h$ is an appropriate *structured condition number* of A with respect to the perturbations in the data x_i . This result is analogous to the results of [9,19] in the sense that the relevant quantities for the determination of a structured condition number are the *relative* separations between the nodes. As it happens in [21,22], in this case important quantities for the determination of a structured condition number are also the relative distances between the nodes and 1.

Combining this theorem with Corollary 7.3 in [19], which states that small componentwise relative perturbations of $\mathcal{BD}(A)$ cause only small relative perturbation in the eigenvalues λ_i and singular values σ_i of A , we obtain that

$$|\lambda'_i - \lambda_i| \leq O(n^3\kappa_h\theta)\lambda_i \quad \text{and} \quad |\sigma'_i - \sigma_i| \leq O(n^3\kappa_h\theta)\sigma_i,$$

where λ'_i and σ'_i are the eigenvalues and the singular values of A' . That is, small relative perturbations in the nodes of an hBV matrix A produce only small relative perturbations in its eigenvalues and in its singular values.

7. Numerical examples

Two numerical tests illustrating the good behaviour of the algorithms developed in the previous sections are shown. In the first of them, the singular values of several rectangular hBV matrices are computed. Classical algorithms for calculating singular values of ill-conditioned totally positive matrices only compute the largest singular values with guaranteed relative accuracy, whereas the tiny singular values may be computed with no relative accuracy at all [19]. This fact has consequences in some applications, such as the computation of the condition number of a matrix as the ratio between its largest and its smallest singular value. The second example is devoted to the solution of three least squares problems.

Example 1. Let us consider the three h-Bernstein bases $\mathcal{B}_{h,n}$ for $n = 20$, and $h = 0.2$, $h = 0.5$ and $h = 1$. We also take the 31 nodes

Table 1
Relative errors of the singular values of $A_{0.2}$, $A_{0.5}$ and A_1 .

h=0.2			h=0.5			h=1		
σ_i	Alg 2	svd	σ_i	Alg 2	svd	σ_i	Alg 2	svd
2.3e+00	3.9e-16	3.9e-16	2.6e+00	1.7e-16	1.7e-16	2.9e+00	3.1e-16	1.5e-16
1.6e+00	1.4e-16	1.4e-16	1.9e+00	9.3e-16	1.2e-16	2.2e+00	4.1e-16	0
8.2e-01	4.1e-16	4.1e-16	6.7e-01	8.3e-16	0	5.1e-01	4.3e-16	2.2e-16
5.4e-01	4.1e-16	2.1e-16	3.2e-01	5.2e-16	3.5e-16	1.7e-01	6.4e-16	1.6e-16
2.8e-01	7.9e-16	5.9e-16	1.1e-01	1.3e-16	3.9e-16	3.5e-02	6.0e-16	6.0e-16
1.3e-01	2.1e-16	2.1e-16	2.9e-02	1.2e-16	5.9e-16	5.6e-03	7.8e-16	1.4e-15
4.7e-02	5.9e-16	1.5e-16	6.0e-03	0	7.3e-16	6.6e-04	3.3e-16	6.6e-16
1.4e-02	7.3e-16	3.7e-16	9.8e-04	2.2e-16	2.0e-15	6.1e-05	1.2e-15	2.6e-14
3.8e-03	1.1e-16	9.2e-16	1.4e-04	6.0e-16	8.2e-14	4.7e-06	1.6e-15	1.0e-12
9.6e-04	1.2e-15	1.6e-14	1.7e-05	5.8e-16	7.3e-13	3.3e-07	8.0e-16	1.6e-11
1.9e-04	2.9e-16	1.4e-14	1.7e-06	8.5e-16	1.6e-12	1.8e-08	5.5e-16	1.1e-10
3.5e-05	3.9e-16	6.6e-13	1.6e-07	1.0e-15	3.5e-11	8.9e-10	5.8e-16	5.5e-09
5.5e-06	6.2e-16	3.0e-12	1.2e-08	1.4e-16	4.8e-10	3.7e-11	5.3e-16	8.4e-08
7.4e-07	7.2e-16	9.2e-12	7.9e-10	7.8e-16	9.7e-09	1.3e-12	0	4.1e-06
9.3e-08	2.9e-16	4.7e-11	4.8e-11	2.7e-16	1.9e-07	4.2e-14	1.1e-15	1.9e-05
9.5e-09	1.7e-16	1.0e-09	2.3e-12	1.2e-15	1.6e-06	1.1e-15	1.1e-15	1.9e-03
8.7e-10	7.1e-16	6.6e-09	1.0e-13	2.5e-16	5.0e-05	2.5e-17	0	1.6e-02
6.2e-11	8.3e-16	2.1e-08	3.4e-15	1.6e-15	1.8e-03	4.5e-19	4.3e-16	1.4e+01
3.7e-12	8.7e-16	6.0e-07	9.4e-17	1.3e-15	7.2e-02	6.7e-21	1.7e-15	9.3e+02
1.4e-13	1.7e-15	5.4e-05	1.7e-18	1.5e-15	1.1e+01	6.5e-23	4.0e-15	7.6e+04
5.3e-15	1.8e-15	1.6e-04	2.9e-20	6.1e-16	3.5e+02	5.9e-25	1.9e-15	4.5e+06

$$\frac{1}{100} < \frac{1}{60} < \frac{1}{45} < \frac{1}{40} < \frac{1}{30} < \frac{1}{21} < \frac{1}{19} < \frac{1}{12} < \frac{1}{11} < \frac{1}{10} < \frac{1}{7} < \frac{1}{5} < \frac{1}{4} < \frac{2}{7} < \frac{1}{3} < \frac{2}{5} < \frac{3}{7} < \frac{1}{2} < \frac{6}{11} < \frac{3}{5} < \frac{31}{50} < \frac{2}{3} < \frac{18}{25} < \frac{3}{4} < \frac{4}{5} < \frac{6}{7} < \frac{9}{10} < \frac{13}{14} < \frac{19}{20} < \frac{39}{40} < \frac{99}{100}.$$

We denote by $A_{0.2}$, $A_{0.5}$ and A_1 the hBV matrices associated to the nodes above and the h-Bernstein bases $\mathcal{B}_{0.2,20}$, $\mathcal{B}_{0.5,20}$ and $\mathcal{B}_{1,20}$, respectively.

We compute the singular values σ_i ($i = 1, \dots, 21$) of $A_{0.2}$, $A_{0.5}$ and A_1 by using Algorithm 2 and the command `svd` of MATLAB. In order to compare the relative errors obtained when computing the singular values by these two methods we use the singular values σ_i computed with *Maple* by means of the command `SingularValues` of the package *LinearAlgebra* as follows: the singular values are stored by *Maple* as the roots of polynomials by means of the function `RootOf` (which is a placeholder for representing the roots), and then they are evaluated to 50 digits by means of the command `evalf`. The results are given in Table 1.

In Table 2, the relative errors obtained when computing the 2-norm condition number of the matrices $A_{0.2}$, $A_{0.5}$ and A_1 by using our approach and the command `cond` of MATLAB are presented. The condition number considered as exact $\kappa_2(A)$ is the one obtained in *Maple* by dividing the largest singular value of A by the smallest one computed as explained above. They are also showed in Table 2.

Looking at the results in Table 1 we observe that our algorithm computes all the singular values of the hBV matrices $A_{0.2}$, $A_{0.5}$ and A_1 accurately, while the standard command `svd` of MATLAB only computes accurately their largest singular values, and

Table 2Relative errors of the 2-norm condition number of $A_{0.2}$, $A_{0.5}$ and A_1 .

h	κ_2	Alg 2	cond
0.2	$4.3e + 14$	$1.2e - 15$	$1.6e - 04$
0.5	$8.9e + 19$	$9.2e - 16$	1.0
1	$4.9e + 24$	$1.3e - 15$	1.0

Table 3Relative errors of the least squares problem for $A_{0.2}$, $A_{0.5}$ and A_1 .

h	(Alg 3) $_x$	(Alg 3) $_r$	(A\b) $_x$	(A\b) $_r$
0.2	$1.3e - 15$	$1.2e - 15$	$1.0e + 00$	$3.9e - 01$
0.5	$4.8e - 16$	$2.0e - 15$	$1.0e + 00$	$8.8e - 01$
1	$1.4e - 15$	$1.4e - 15$	$1.0e + 00$	$1.0e + 00$

the smallest ones without any accuracy. The same situation appears when computing the condition number of $A_{0.2}$, $A_{0.5}$ and A_1 (see Table 2). While our approach computes the three condition numbers accurately, the ones computed by `cond` of MATLAB are not accurate at all.

Furthermore, we notice that our algorithm computes accurate singular values regardless of the 2-norm condition number of the hBV matrices, but this fact does not occur when using `svd` of MATLAB (see Table 1 and Table 2).

Example 2. Let us consider the same hBV matrices $A_{0.2}$, $A_{0.5}$ and A_1 as in Example 1, and the data vector

$$b = (-1, 0, 2, 2, 1, 3, -2, 6, 5, -3, 0, 4, 1, -2, -3, -1, 0, 6, -2, -4, 7, 0, 1, 5, 11, 2, 3, 1, 0, 5, -4)^T.$$

In Table 3 we present the relative errors obtained when solving the least squares problem $\min_x \|b - A_h x\|_2$ (for $h = 0.2, 0.5, 1$) by means of Algorithm 3 and the command `A\b` from MATLAB. They are denoted by (Alg 3) $_x$ and (A\b) $_x$, respectively. The relative errors corresponding to the computation of the minimum residual by using Algorithm 3 and `A\b` of MATLAB by (Alg 3) $_r$ and (A\b) $_r$, respectively. In the computation of the relative errors the exact solution vector and the exact minimum residual obtained in *Maple* are used.

Looking at Table 3 we notice that our approach computes accurately the solutions and the residuals of the considered least squares problems. In contrast, the command `A\b` of MATLAB returns results no accurate at all.

Declaration of competing interest

42Q3 None declared.

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