THE POWER OF BIDIAGONAL MATRICES*

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Abstract. Bidiagonal matrices are widespread in numerical linear algebra, not least because of their use in the standard algorithm for computing the singular value decomposition and their appearance as LU factors of tridiagonal matrices. We show that bidiagonal matrices have a number of interesting properties that make them powerful tools in a variety of problems, especially when they are multiplied together. We show that the inverse of a product of bidiagonal matrices is insensitive to small componentwise relative perturbations in the factors if the factors or their inverses are nonnegative. We derive componentwise rounding error bounds for the solution of a linear system $Ax = b$, where A or A^{-1} is a product $B_1 B_2 \dots B_k$ of bidiagonal matrices, showing that strong results are obtained when the B_i are nonnegative or have a checkerboard sign pattern. We show that given the factorization of an $n \times n$ totally nonnegative matrix A into the product of bidiagonal matrices, $\|A^{-1}\|_\infty$ can be computed in $O(n^2)$ flops and that in floating-point arithmetic the computed result has small relative error, no matter how large $\|A^{-1}\|_\infty$ is. We also show how factorizations involving bidiagonal matrices of some special matrices, such as the Frank matrix and the Kac–Murdock–Szegö matrix, yield simple proofs of the total nonnegativity and other properties of these matrices.

Key words. Bidiagonal matrix, totally nonnegative matrix, condition number, matrix function, Vandermonde system, Toeplitz matrix, the Frank matrix, the Pascal matrix, the Kac–Murdock–Szegö Matrix.

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1. Introduction.

Bidiagonal matrices

$$B = \begin{bmatrix} b_{11} & b_{12} & & \\ & b_{22} & \ddots & \\ & & \ddots & b_{n-1,n} \\ & & & b_{nn} \end{bmatrix} \in \mathbb{C}^{n\times n}$$

have $2n - 1$ parameters, appearing on two diagonals. Despite their simplicity, bidiagonal matrices are powerful tools in a variety of problems, especially when they are multiplied together. Their properties and uses have been explained by various authors, but the full range of them may be underappreciated. Indeed, in the 1139-page book *Matrix Mathematics* [4] the word "bidiagonal" appears on only one page and bidiagonal matrices appear little in the *Handbook of Linear Algebra* [31] apart from in the chapter by Fallat [17].

The purpose of this work is to show the utility of bidiagonal matrices, and in particular to show how factorizations of matrices into bidiagonal factors can be exploited. Our main contributions are as follows, where $A = B_1 B_2 \dots B_k$ with each B_i either upper bidiagonal or lower bidiagonal.

- We show that small componentwise perturbations in the B_i produce small componentwise perturbations in A^{-1} if the B_i or the B_i^{-1} are nonnegative (Theorem 2.3).
- We show that the condition number $\kappa_\infty(A) = \|A\|_\infty \|A^{-1}\|_\infty$ can be computed in $O(kn)$ flops when the B_i are nonnegative or have a checkerboard sign pattern, without explicitly forming A (section 3).
- We give a unified derivation of backward error bounds and forward error bounds for the computed solution of $Ax = b$ when A or A^{-1} is a product of bidiagonal matrices and the system is solved using the factors (section 4).

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- We show that for a totally nonnegative $n \times n$ matrix A, $\kappa_\infty(A)$ can be computed in $O(n^2)$ flops, given a factorization of A into a product of bidiagonal matrices and that the computed solution is highly accurate (Algorithm 5.5).
- We explore functions of bidiagonal matrices and show that the exponential of a totally nonnegative bidiagonal matrix is totally nonnegative.
- We give new observations on how factorizations involving bidiagonal matrices can help us to understand properties of some well-known matrices (section 8).

Bidiagonal matrices arise in some classical contexts in numerical linear algebra, which we briefly summarize as they will not be the focus of our attention.

Computing the singular value decomposition (SVD). The first step of the Golub–Reinsch algorithm for computing the SVD is a two-sided reduction by Householder transformations to upper bidiagonal form B, as proposed by Golub and Kahan [22]. The SVD of B is then computed by the QR algorithm implicitly applied to B^*B, and this can be done in a way that guarantees high relative accuracy in all the computed singular values of B [10].

LU factorization of tridiagonal matrices. If $A \in \mathbb{C}^{n\times n}$ is tridiagonal and has an LU factorization $A = LU$ then L is unit lower bidiagonal and U is upper bidiagonal.

Lanczos bidiagonalization. For large, sparse matrices the solution to a linear system or the least squares solution to an overdetermined system can be computed using a method based on unitary reduction to bidiagonal form by the Lanczos process [5, sec. 7.6], [22], [41].

In perturbation and rounding error analyses products of terms of the form $1 + \delta_i$ arise. Their distance from 1 will be bounded using the following result [28, Lem. 3.1].

Lemma 1.1. *If $|\delta_i| \le \delta$ and $\rho_i = \pm 1$ for $i = 1\colon n$, and $n\delta < 1$, then*

$$\prod_{i=1}^{n}(1+\delta_i)^{\rho_i} = 1 + \theta_n, \quad |\theta_n| \le \frac{n\delta}{1-n\delta}. \tag{1.1}$$

We also need a componentwise bound for perturbations in a matrix product [28, Lem. 3.8]. Here and throughout, $|A| = (|a_{ij}|)$ and inequalities between matrices hold componentwise.

Lemma 1.2. *If $X_j + \Delta X_j \in \mathbb{C}^{n\times n}$ satisfies $|\Delta X_j| \le \delta_j |X_j|$ for $j = 1\colon m$ then*

$$\left|\prod_{j=1}^{m}(X_j + \Delta X_j) - \prod_{j=1}^{m} X_j\right| \le \left(\prod_{j=1}^{m}(1+\delta_j) - 1\right)\prod_{j=1}^{m}|X_j|.$$

We use the standard model of floating-point arithmetic [28, sec. 2.2] and denote by u the unit roundoff. We need the constant, for $nu < 1$,

$$\gamma_n = \frac{nu}{1-nu}.$$

We will make use of the one-parameter bidiagonal matrix

$$T_n(\theta) = \begin{bmatrix} 1 & \theta & & & \\ & 1 & \theta & & \\ & & 1 & \ddots & \\ & & & \ddots & \theta \\ & & & & 1 \end{bmatrix} \in \mathbb{C}^{n\times n}. \tag{1.2}$$

2. Basic Properties of Bidiagonal Matrices. First we consider the inverse of a nonsingular bidiagonal matrix. It is instructive to look at the 4×4 case:

$$\begin{bmatrix} a & x & 0 & 0 \\ & b & y & 0 \\ & & c & z \\ & & & d \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{a} & -\frac{x}{ab} & \frac{xy}{abc} & -\frac{xyz}{abcd} \\ & \frac{1}{b} & -\frac{y}{bc} & \frac{yz}{bcd} \\ & & \frac{1}{c} & -\frac{z}{cd} \\ & & & \frac{1}{d} \end{bmatrix}.$$

Notice that every element in the upper triangle is a product of off-diagonal elements of B and inverses of diagonal elements, that the superdiagonals have alternating signs attached, and that there are no additions. These properties hold for general n, as the explicit form of the inverse in the following result shows.

Lemma 2.1. *If $B \in \mathbb{C}^{n\times n}$ is nonsingular and upper bidiagonal then*

$$(B^{-1})_{ij} = \frac{1}{b_{jj}} \prod_{k=i}^{j-1} \left(\frac{-b_{k,k+1}}{b_{kk}} \right), \quad j \ge i. \tag{2.1}$$

We will make use of the fact that when B has nonnegative elements, B^{-1} has a checkerboard (alternating) sign pattern.

We introduce the comparison matrix $M(A)$ of $A \in \mathbb{C}^{n\times n}$:

$$\big(M(A)\big)_{ij} = \begin{cases} |a_{ii}|, & i = j, \\ -|a_{ij}|, & i \ne j. \end{cases}$$

It is easy to see that

$$|B^{-1}| = M(B)^{-1}, \tag{2.2}$$

an observation that we will need later.

Using the representation (2.1) of the inverse we can bound the effect of a componentwise perturbation of B. Let

$$\tau = \frac{(2n-1)\delta}{1-(2n-1)\delta}. \tag{2.3}$$

Theorem 2.2. *If $B \in \mathbb{C}^{n\times n}$ is a nonsingular bidiagonal matrix and ΔB is a perturbation satisfying $|\Delta B| \le \delta |B|$ then*

$$\left|(B + \Delta B)^{-1} - B^{-1}\right| \le \tau |B^{-1}|,$$

where τ is defined in (2.3).

Proof. Assume, without loss of generality, that B is upper bidiagonal. Write $\Delta b_{ij} = \delta_{ij} b_{ij}$, where $|\delta_{ij}| \le \delta$. From (2.1) we obtain

$$\begin{aligned} (B+\Delta B)^{-1}_{ij} - (B^{-1})_{ij} &= \frac{1}{b_{jj}(1+\delta_{jj})} \prod_{k=i}^{j-1} \left(\frac{-b_{k,k+1}(1+\delta_{k,k+1})}{b_{kk}(1+\delta_{kk})} \right) - \frac{1}{b_{jj}} \prod_{k=i}^{j-1} \left(\frac{-b_{k,k+1}}{b_{kk}} \right) \\ &= (B^{-1})_{ij} \left(\frac{1}{1+\delta_{jj}} \prod_{k=i}^{j-1} \left(\frac{1+\delta_{k,k+1}}{1+\delta_{kk}} \right) - 1 \right) \\ &= (B^{-1})_{ij} \theta_{2(j-i)+1}, \end{aligned}$$

where $|\theta_k| \le \gamma_k = k\delta/(1-k\delta)$ by Lemma 1.1. ∎

This result, which is essentially the same as [28, Prob. 22.8], shows that a componentwise relative perturbation in B produces a componentwise relative perturbation in B^{-1} at most about $2n$ times larger: a strong result that does not hold for triangular matrices in general.

We now extend this result to a product of bidiagonal matrices. In all the products of bidiagonal matrices in this paper each matrix can be upper bidiagonal or lower bidiagonal.

THEOREM 2.3. *Let $B = B_1 B_2 \dots B_k \in \mathbb{C}^{n\times n}$, where the B_i are nonsingular bidiagonal matrices, and let $B + \varDelta B = (B_1 + \varDelta B_1)(B_2 + \varDelta B_2)\dots(B_k + \varDelta B_k)$, where $|\varDelta B_i| \le \delta |B_i|$ for all i. Then*

$$\left|(B+\varDelta B)^{-1} - B^{-1}\right| \le \left((1+\tau)^k - 1\right)|B_k^{-1}||B_{k-1}^{-1}|\dots|B_1^{-1}|, \tag{2.4}$$

where τ is defined in (2.3), and if the B_i or the B_i^{-1} are all nonnegative then

$$\left|(B+\varDelta B)^{-1} - B^{-1}\right| \le \left((1+\tau)^k - 1\right)|B^{-1}|. \tag{2.5}$$

Proof. We have

$$\begin{aligned}(B+\varDelta B)^{-1} &= (B_k + \varDelta B_k)^{-1}(B_{k-1}+\varDelta B_{k-1})^{-1}\dots(B_1+\varDelta B_1)^{-1}\\ &= (B_k^{-1}+E_k)(B_{k-1}^{-1}+E_{k-1})\dots(B_1^{-1}+E_1),\end{aligned}$$

where by Theorem 2.2, $|E_i| \le \tau|B_i^{-1}|$, $i = 1\colon k$. Hence by Lemma 1.2,

$$|(B+\varDelta B^{-1}) - B^{-1}| \le \left((1+\tau)^k - 1\right)|B_k^{-1}||B_{k-1}^{-1}|\dots|B_1^{-1}|.$$

The bound (2.5) is immediate if the B_i^{-1} are all nonnegative. If the B_i are all nonnegative. then (2.5) follows from considering the checkerboard sign pattern of the inverses; see Theorem 3.2 below. ◻

The bound (2.5) shows that if the B_i or the B_i^{-1} are all nonnegative then componentwise relative perturbations in the B_i produce componentwise relative perturbation in the inverse of the product at most about a factor $2nk$ times larger.

Like the inverse, the singular values of a bidiagonal matrix are very well behaved under componentwise perturbations. Let $\sigma_i(B)$ denote the ith largest singular value of B.

THEOREM 2.4. *Let $B \in \mathbb{C}^{n\times n}$ and $B + \varDelta B$ be upper bidiagonal and suppose that $(B + \varDelta B)_{ii} = \alpha_{2i-1} b_{ii}$ and $(B+\varDelta B)_{i,i+1} = \alpha_{2i} b_{i,i+1}$, where the α_i are nonzero. Then*

$$\frac{\sigma_i(B)}{\mu} \le \sigma_i(B+\varDelta B) \le \mu\sigma_i(B), \quad i = 1\colon n,$$

where

$$\mu = \prod_{i=1}^{2n-1} \max(|\alpha_i|, |\alpha_i^{-1}|).$$

Proof. We can write $B + \varDelta B = D_1 B D_2$, where

$$D_1 = \operatorname{diag}\left(\alpha_1, \frac{\alpha_1\alpha_3}{\alpha_2}, \frac{\alpha_1\alpha_3\alpha_5}{\alpha_2\alpha_4}, \dots\right), \qquad D_2 = \operatorname{diag}\left(1, \frac{\alpha_2}{\alpha_1}, \frac{\alpha_2\alpha_4}{\alpha_1\alpha_3}, \frac{\alpha_2\alpha_4\alpha_6}{\alpha_1\alpha_3\alpha_5}, \dots\right).$$

An extension for singular values of a result of Ostroswki for eigenvalues [15, Thm. 3.1] gives

$$\frac{\sigma_i(B)}{\|D_1^{-1}\|_2\|D_2^{-1}\|_2} \le \sigma_i(B+\varDelta B) \le \sigma_i(B)\|D_1\|_2\|D_2\|_2.$$

Using $\|D_1\|_2\|D_2\|_2 = \max_i |(D_1)_{ii}| \max_i |(D_2)_{ii}| \le \mu$ (taking account of cancellation in the product) and $\|D_1^{-1}\|_2\|D_2^{-1}\|_2 \le \mu$ gives the result. ◻

Theorem 2.4 is from Demmel and Kahan [10, Cor. 2] and the proof is from Eisenstat and Ipsen [15, Cor. 4.2]. The theorem shows that relative perturbations of magnitude at most $\tau = \max_i |1 - \alpha_i| \ll 1$ to the elements on the diagonal and superdiagonal of an upper bidiagonal matrix produce relative changes of at most $(1-\tau)^{2n-1} - 1 \approx (2n-1)\tau$ in each singular value. This is a much stronger result than for general perturbations of a general $n \times n$ matrix, where it is only the absolute changes in the singular values that are bounded: $|\sigma_k(A + \varDelta A) - \sigma_k(A)| \le \sigma_1(\varDelta A) = \|\varDelta A\|_2$, $k = 1\colon n$ [32, Cor. 7.3.5].

Theorem 2.4 does not extend to a product of bidiagonal matrices, as the following example shows. Let

$$A = I = \begin{bmatrix} 1 & x \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -x \\ 0 & 1 \end{bmatrix} =: B_1 B_2,$$
$$A + \varDelta A = \begin{bmatrix} 1 & 2x\delta \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & x(1+\delta) \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -x(1-\delta) \\ 0 & 1 \end{bmatrix} =: (B_1 + \varDelta B_1)(B_2 + \varDelta B_2),$$

where $\delta > 0$, $x > 0$, and $x\delta \gg 1$. Here, B_1 and B_2 have undergone a componentwise relative change δ. The singular values of A are $\sigma_1 = 1$ and $\sigma_2 = 1$, and those of $A + \varDelta A$ are approximately $\widehat{s}_1 = 2x\delta$ and $\widehat{s}_2 = (2x\delta)^{-1}$ (since $x\delta \gg 1$). Hence the relative change in σ_1 is $|\sigma_1 - \widehat{s}_1|/\sigma_1 \approx 2x\delta \gg 1$ and that in σ_2 is $|\sigma_2 - \widehat{s}_2|/\sigma_2 \approx 1 - 1/(2x\delta) \approx 1$. We conclude that relative changes in bidiagonal matrices $B_1, B_2, \dots, B_k$ can induce a much larger relative change in the singular values of their product. The situation is different for a product of *nonnegative* bidiagonal matrices $B_1, B_2, \dots B_k$: small componentwise relative changes in the B_i produce only small relative changes in the singular values of the product $B_1, B_2, \dots B_k$, as shown by Koev [34, Cor. 7.3].

The next result reveals some further interesting properties of the singular values of a bidiagonal matrix.

Theorem 2.5. *Let $B \in \mathbb{C}^{n \times n}$ be bidiagonal.*

(a) *$|B| = DBF$, where D and F are unitary diagonal matrices. Hence B and $|B|$ have the same singular values.*

(b) *If b_{ii} and $b_{i,i+1}$ are nonzero for all i then the singular values of B are distinct.*

Proof. (a): Let $D = \operatorname{diag}(d_i)$ and $F = \operatorname{diag}(f_i)$ with $f_1 = 1$. We take $d_1 = \operatorname{sign}(b_{11})^*$, $f_2 = \operatorname{sign}(d_1 b_{12})^*$, $d_2 = \operatorname{sign}(b_{22} f_2)^*$, $f_3 = \operatorname{sign}(d_2 b_{23})^*$, and so on, where $\operatorname{sign}(z) = z/|z|$ if $z \ne 0$ or 1 otherwise. Then $|B| = DBF$, where D and F have diagonal elements of modulus 1 and so are unitary. Therefore if $B = U\Sigma V^*$ is an SVD of B then $|B| = (DU)\Sigma(V^*F)$ is an SVD of $|B|$.

(b): The singular values of B are the square roots of the eigenvalues of $T = |B|^*|B|$, by (a). The matrix T is symmetric tridiagonal with positive superdiagonal and subdiagonal elements, so the eigenvalues of T are distinct [42, Lem. 7.7.1], and hence so are the singular values of B. ∎

It is interesting to note that the SVD codes in both LINPACK [12] and LAPACK [3] reduce $A \in \mathbb{C}^{m \times n}$ to a real bidiagonal matrix, so that the QR iteration can be carried out in real arithmetic, but they do so in different ways. LINPACK reduces A to bidiagonal form by Householder transformations and then explicitly carries out the diagonal scaling given in part (a) of Theorem 2.5. LAPACK reduces A to bidiagonal form using elementary unitary matrices of the form $P = I - \rho vv^*$ with generally nonreal ρ that are chosen so that the reduced bidiagonal matrix is real [36].

3. The Condition Number of a Matrix Product. Suppose a matrix $X \in \mathbb{C}^{n \times n}$ is given in factored form $X = A_1 A_2 \dots A_k$, where $A_i \in \mathbb{C}^{n \times n}$ for all i, and that we wish to compute or estimate the condition number $\kappa_\infty(X) = \|X\|_\infty \|X^{-1}\|_\infty$ without explicitly forming X. Initially we will make no assumptions about the A_i, but later we will specialize to bidiagonal A_i. For dense matrices the cost of forming X is $2(k-1)n^3$ flops, whereas we would like to compute or estimate $\kappa_\infty(X)$ at the cost of a few matrix–vector products with X, that is, in a small multiple of $2(k-1)n^2$ flops.

The condition number estimation problem is well studied [28, Chap. 15]. Here we focus on the problem of *exactly* computing the condition number. Recall that the ∞-norm satisfies

$$\|X\|_\infty = \|\,|X|\,\|_\infty = \|\,|X|e\,\|_\infty,$$

where $e = [1, 1, \dots, 1]^T$.

In general we cannot compute $\|A_1 A_2 \dots A_k\|_\infty$ without forming the matrix product. However, if the equality

$$|A_1 A_2 \dots A_k| = |A_1||A_2| \dots |A_k| \tag{3.1}$$

holds then

$$\|A_1 A_2 \dots A_k\|_\infty = \|\,|A_1||A_2| \dots |A_k|\,\|_\infty = \|\,|A_1||A_2| \dots |A_k|e\,\|_\infty \tag{3.2}$$

and we can evaluate the right-hand side in $O(kn^2)$ flops as opposed to the $O(kn^3)$ flops that are required if we explicitly form the product. If the A_i are bidiagonal then the costs are $3kn$ flops compared with up to $O(kn^2)$ flops if the product is explicitly formed, since in general the product fills in.

The equality (3.1) obviously holds when the B_i are all nonnegative. It can also hold because all additions in the product $A_1 A_2 \dots A_k$ are of like-signed numbers, so that there is no cancellation. Important such cases are when the A_i are nonnegative and when each A_i has a checkerboard (alternating) sign pattern, which can be expressed as

$$A_i = \pm\Sigma|A_i|\Sigma, \quad i = 1\colon k, \tag{3.3}$$

where

$$\Sigma = \mathrm{diag}\big(1, -1, 1, \dots, (-1)^{n-1}\big). \tag{3.4}$$

Theorem 3.1. *If the matrices A_i, $i = 1\colon k$, satisfy (3.3) then*

$$A_1 A_2 \dots A_k = \pm\Sigma|A_1||A_2| \dots |A_k|\Sigma \tag{3.5}$$

and hence

$$|A_1 A_2 \dots A_k| = |A_1||A_2| \dots |A_k|. \tag{3.6}$$

Proof. If the A_i satisfy (3.3) then

$$A_1 A_2 \dots A_k = \pm\Sigma|A_1|\Sigma \cdot \Sigma|A_2|\Sigma \dots \Sigma|A_k|\Sigma = \pm\Sigma|A_1||A_2| \dots |A_k|\Sigma,$$

which is (3.5), and (3.6) follows immediately, □

We conclude that if the A_i are nonnegative or have a checkerboard sign pattern then we can compute $\|A_1 A_2 \dots A_k\|_\infty$ in $O(kn^2)$ flops.

If $B_1, B_2, \dots, B_k$ are bidiagonal and nonnegative then from Lemma 2.1 it is clear that B_i^{-1} has a checkerboard sign pattern, that is, it satisfies (3.3). Therefore by (3.6),

$$|B_k^{-1} B_{k-1}^{-1} \dots B_1^{-1}| = |B_k^{-1}||B_{k-1}^{-1}| \dots |B_1^{-1}|. \tag{3.7}$$

The same is true if the B_i have a checkerboard sign pattern.

THEOREM 3.2. *Let $B_1, B_2, \dots, B_k \in \mathbb{R}^{n\times n}$ be nonsingular bidiagonal matrices. If B_i is nonnegative for all i or has a checkerboard sign pattern for all i then*

$$|B_k^{-1}B_{k-1}^{-1}\dots B_1^{-1}| = |B_k^{-1}||B_{k-1}^{-1}|\dots|B_1^{-1}| = M(B_k)^{-1}M(B_{k-1})^{-1}\dots M(B_1)^{-1}. \tag{3.8}$$

Proof. For nonnegative B_i the result follows from (3.7) on recalling (2.2). From (2.1) it is clear that B_i having a checkerboard sign pattern is equivalent to either B_i^{-1} or $-B_i^{-1}$ being nonnegative and equal to $M(B_i)^{-1}$, which gives the second part of the result. ∎

From (3.8) we have

$$\|B_k^{-1}B_{k-1}^{-1}\dots B_1^{-1}\|_\infty = \|M(B_k)^{-1}M(B_{k-1})^{-1}\dots M(B_1)^{-1}e\|_\infty, \tag{3.9}$$

and the right-hand side can be computed in $3kn$ flops, whereas explicitly forming the product on the left (using substitutions) costs $3kn^2/2$ flops. We conclude that when the B_i are nonnegative for all i or all have a checkerboard sign pattern, $\kappa_\infty(B_1B_2\dots B_k)$ can be computed exactly in $6kn$ flops. Since $\|A\|_1 = \|A^T\|_\infty$, the 1-norm condition number can be computed at the same cost by working with the transpose of the product.

In the case $k = 1$, (3.9) reduces to the result that $\|B^{-1}\|_\infty = \|M(B)^{-1}\|_\infty = \|M(B)^{-1}e\|_\infty$ [25, sec. 2].

We can also compute the condition number of Skeel [44],

$$\mathrm{cond}(A, x) = \frac{\|\,|A^{-1}||A||x|\,\|_\infty}{\|x\|_\infty},$$

exactly in $6kn$ flops for $A = B_1B_2\dots B_k$ with nonnegative B_i:

$$\mathrm{cond}(B_1B_2\dots B_k, x) = \frac{\|\,M(B_k)^{-1}\dots M(B_1)^{-1}B_1\dots B_k|x|\,\|_\infty}{\|x\|_\infty}.$$

If the B_i have checkerboard sign patterns then the same formula holds with $B_1B_2\dots B_k$ replaced by $|B_1||B_2|\dots|B_k|$.

We will make use of (3.9) for totally nonnegative matrices in Section 5.

4. Linear Systems. We consider a linear system $Ax = b$ in which A is either a product of bidiagonal matrices or a product of inverses of bidiagonal matrices. Our interest is in what can be said about the backward error and forward error when such a system is solved in floating-point arithmetic.

4.1. Product of Bidiagonal Matrices. Suppose $A = B_1B_2\dots B_k$ is a product of k bidiagonal matrices. We can solve the system by solving k bidiagonal systems by substitution. Standard rounding error analysis [28, Lem. 8.2] shows that the computed $\widehat{x}$ satisfies

$$(B_1 + \Delta B_1)(B_2 + \Delta B_2)\dots(B_k + \Delta B_k)\widehat{x} = b, \quad |\Delta B_i| \le \gamma_2|B_i|, \quad i = 1\colon k. \tag{4.1}$$

Hence the residual is

$$\begin{aligned}|b - B_1B_2\dots B_k\widehat{x}| &= \big|\big((B_1 + \Delta B_1)(B_2 + \Delta B_2)\dots(B_k + \Delta B_k) - B_1B_2\dots B_k\big)\widehat{x}\big|\\ &\le \big((1+\gamma_2)^k - 1\big)|B_1||B_2|\dots|B_k||\widehat{x}|,\end{aligned}$$

by Lemma 1.2. If the B_i are all nonnegative or, by Theorem 3.1, if they have a checkerboard sign pattern, then the bound becomes

$$|b - A\widehat{x}| \le \big((1+\gamma_2)^k - 1\big)|A||\widehat{x}| = \big(2ku + O(u^2)\big)|A||\widehat{x}|, \tag{4.2}$$

which shows that the componentwise relative backward error is small—an ideal backward error result. We note that this result has used the triangularity of the B_i but not their bidiagonal structure (except through the constant in (4.1)).

To obtain a forward error bound we rewrite (4.1) as

$$\widehat{x} = (B_k + \Delta B_k)^{-1}(B_{k-1} + \Delta B_{k-1})^{-1} \dots (B_1 + \Delta B_1)^{-1} b.$$

Then

$$\begin{aligned} |\widehat{x} - x| &\le \Big|(B_k + \Delta B_k)^{-1}(B_{k-1} + \Delta B_{k-1})^{-1} \dots (B_1 + \Delta B_1)^{-1} - B_k^{-1} B_{k-1}^{-1} \dots B_1^{-1}\Big||b| \\ &\le \big((1+\tau)^k - 1\big)|B_k^{-1}||B_{k-1}^{-1}| \dots |B_1^{-1}||b| \end{aligned} \tag{4.3}$$

by Theorem 2.3, where

$$\tau = \frac{(2n-1)\gamma_2}{1-(2n-1)\gamma_2}. \tag{4.4}$$

If the B_i are all nonnegative or have a checkerboard sign pattern then by Theorem 3.2 this inequality becomes

$$|\widehat{x} - x| \le \big(2k(2n-1)u + O(u^2)\big)|A^{-1}||b|. \tag{4.5}$$

The bound (4.5) is a strong forward error bound because it is the same as a bound for the change in x induced by a small componentwise relative perturbation of of b: $b \to b + \Delta b$ with $|\Delta b| \le 4knu|b|$ [28, Thm. 7.4].

4.2. Product of Inverses of Bidiagonal Matrices. Now suppose that it is A^{-1} rather than A that is a product of bidiagonal matrices: $A^{-1} = B_1 B_2 \dots B_k$. Now we solve $Ax = b$ by forming $x = A^{-1} b = B_1 B_2 \dots B_k b$ and the computed $\widehat{x}$ satisfies

$$\widehat{x} = (B_1 + \Delta B_1)(B_2 + \Delta B_2) \dots (B_k + \Delta B_k) b, \quad |\Delta B_i| \le \gamma_2 |B_i|, \quad i = 1\colon k. \tag{4.6}$$

Then the forward error is

$$\begin{aligned} |\widehat{x} - x| &= \Big|\big((B_1 + \Delta B_1)(B_2 + \Delta B_2) \dots (B_k + \Delta B_k) - B_1 B_2 \dots B_k\big) b\Big|, \\ &\le \big((1+\gamma_2)^k - 1\big)|B_1||B_2| \dots |B_k||b|, \end{aligned} \tag{4.7}$$

by Lemma 1.2. If the B_i are all nonnegative or have a checkerboard sign pattern then by Theorem 3.1, $|B_1||B_2| \dots |B_k| = |B_1 B_2 \dots B_k|$, so

$$|\widehat{x} - x| \le \big((1+\gamma_2)^k - 1\big)|A^{-1}||b|. \tag{4.8}$$

Now we turn to the residual. Note first that by (4.6),

$$b = (B_k + \Delta B_k)^{-1}(B_{k-1} + \Delta B_{k-1})^{-1} \dots (B_1 + \Delta B_1)^{-1} \widehat{x}.$$

Hence

$$|b - A\widehat{x}| = \Big|\big[(B_k + \Delta B_k)^{-1}(B_{k-1} + \Delta B_{k-1})^{-1} \dots (B_1 + \Delta B_1)^{-1} - B_k^{-1} B_{k-1}^{-1} \dots B_1^{-1}\big]\widehat{x}\Big|$$

and by Lemma 1.2 and Theorem 2.3 we obtain, with τ given by (4.4),

$$\begin{aligned} |b - A\widehat{x}| &\le \big((1+\tau)^k - 1\big)|B_k^{-1}||B_{k-1}^{-1}| \dots |B_1^{-1}||\widehat{x}| \\ &= \big(2k(2n-1)u + O(u^2)\big)|B_k^{-1}||B_{k-1}^{-1}| \dots |B_1^{-1}||\widehat{x}|. \end{aligned}$$

If the B_i are all nonnegative or have a checkerboard sign pattern then by Theorem 3.2 this bound can be written

$$|b - A\widehat{x}| \le \big(2k(2n-1)u + O(u^2)\big)|A||\widehat{x}|, \tag{4.9}$$

which again shows a small componentwise relative backward error.

Our conclusion is that whether it is A or A^{-1} that is a product of bidiagonal matrices we have the same satisfactory form of forward error bounds (4.5) and (4.8) and residual bounds (4.2) and (4.9) when the B_i are all nonnegative or have a checkerboard sign pattern.

4.3. Application to Vandermonde Systems. An application of these results is to the Björck–Pereyra algorithm for solving a Vandermonde system $Vy = b$ in $O(n^2)$ flops [6], where $V = (x_j^{i-1}) \in \mathbb{C}^{n\times n}$ for given points $x_i \in \mathbb{C}$. This algorithm uses a factorization of V^{-1} into a product of $2n-2$ bidiagonal matrices $B_{2n-2}, \dots, B_1$ given in terms of the points x_i. When $0 \le x_1 < x_2 < \cdots < x_n$ the bidiagonal factors have positive diagonal and nonpositive off-diagonal elements. Therefore the B_i have a checkerboard sign pattern and so $|B_{2n-2}| \dots |B_1| = |B_{2n-2} \dots B_1| = |A^{-1}|$ by (3.7). From (4.8) and (4.9) we have

$$\begin{aligned}
|\widehat{y} - y| &\le \big(2(2n-2)u + O(u^2)\big)|V^{-1}||b|,\\
|b - V\widehat{y}| &\le \big(2(2n-2)(2n-1)u + O(u^2)\big)|V||\widehat{y}|,
\end{aligned}$$

which reproduce [26, Thm. 2.3] and the monomial case of [27, Cor. 4.1], respectively. Since V^{-1} has a checkerboard sign pattern, if $(-1)^i b_i \ge 0$ then $|V^{-1}||b| = |V^{-1}b| = |y|$, and $\widehat{y}$ therefore has a small componentwise relative error. The analysis in [27] makes use of the bidiagonal factorization, but that in [26] does not.

4.4. Application to Pascal Systems. We give a numerical illustration of the use of the bidiagonal factorization for solving the linear system $P_n x = b$, where P_n is the symmetric positive definite $n \times n$ Pascal matrix with

$$p_{ij} = \binom{i+j-2}{j-1} = \frac{(i+j-2)!}{(i-1)!(j-1)!} \tag{4.10}$$

and $b = e_n/n$, where e_n is the nth unit vector. The Pascal matrix has a known factorization as a product of $2n-1$ bidiagonal matrices, as we explain in section 8.3. We solve the system using the bidiagonal factorization, solving the bidiagonal systems by substitution. We also solve the system for the explicitly formed P using the MATLAB backslash operator (which exploits the symmetric positive definiteness of P_n but not its bidiagonal factorization). The working precision is double precision, with $u \approx 1.1 \times 10^{-16}$. Table 4.1 shows the relative errors $\|x - \widehat{x}\|_\infty / \|x\|_\infty$, for which we take as the exact solution x the solution computed at a precision of 500 decimal digits using the Multiprecision Computing Toolbox [39] and then rounded to double precision. We restrict to $n \le 25$ to ensure that P is exactly representable at the working precision. We see that substitution with the bidiagonal factorization yields errors of $O(u)$ that satisfy the bound (4.5), whereas the MATLAB backslash function produces much larger errors, which usually exceed (4.5).

5. Totally Nonnegative Matrices. A matrix $A \in \mathbb{R}^{n\times n}$ is totally nonnegative if every minor (determinant of a square submatrix) is nonnegative and totally positive if every minor is positive. We will need the following key result, which is a direct consequence of the Binet–Cauchy theorem on determinants [32, sec. 0.8.7].

Theorem 5.1. *If $A, B \in \mathbb{R}^{n\times n}$ are totally nonnegative then so is AB.*

Table 4.1: Relative errors for the computed solution to a linear system $P_n x = b$ with P_n the $n \times n$ Pascal matrix.

n	Relative errors: Bidiagonal factorization	Relative errors: `P\b`	Error bound (4.5)
5	9.25e-17	9.25e-16	7.99e-15
10	1.50e-16	4.94e-9	3.80e-14
15	6.36e-17	1.05e-3	9.02e-14
20	1.34e-16	3.12e-12	1.65e-13
25	1.68e-16	2.76e-11	2.61e-13

Bidiagonal matrices play a key role in the theory of totally nonnegative matrices. Indeed a nonnegative bidiagonal matrix is totally nonnegative. In the proof of this result we will need the elementary lower bidiagonal matrix

$$L_k(\ell_{k+1,k}) = I + \ell_{k+1,k} e_{k+1} e_k^T, \tag{5.1}$$

which differs from the identity matrix only in the $(k+1,k)$ position, which contains $\ell_{k+1,k}$.

Theorem 5.2. *A bidiagonal matrix $B \in \mathbb{R}^{n\times n}$ with nonnegative elements is totally nonnegative.*

Proof. Without loss of generality we take B to be lower bidiagonal. We first assume that B is nonsingular. Since $0 \neq \det(B) = b_{11}b_{22}\dots b_{nn}$, the b_{ii} are all positive, so with $D = \mathrm{diag}(b_{ii})$ and $\ell_{i+1,i} = b_{i+1,i}/b_{i+1,i+1} \geq 0$, $i = 1\colon n-1$, we can write

$$B = D \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ & \ell_{32} & \ddots & & \\ & & \ddots & \ddots & \\ & & & \ell_{n,n-1} & 1 \end{bmatrix} \equiv DL. \tag{5.2}$$

Since D is clearly totally nonnegative, by Theorem 5.1 it suffices to show that L is totally nonnegative.

For $n = 4$ we have

$$L = \begin{bmatrix} 1 & & & \\ \ell_{21} & 1 & & \\ & \ell_{32} & 1 & \\ & & \ell_{43} & 1 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ \ell_{21} & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & \ell_{32} & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & \ell_{43} & 1 \end{bmatrix},$$

and this factorization clearly generalizes to

$$L = L_1(\ell_{21}) L_2(\ell_{32}) \dots L_{n-1}(\ell_{n,n-1}), \tag{5.3}$$

where $L_k(\ell_{k+1,k})$ is the elementary lower bidiagonal matrix (5.1). It is easy to see that $L_k(\ell_{k+1,k})$ is totally nonnegative for all k, so L is totally nonnegative by Theorem 5.1.

If B is singular then consider the bidiagonal matrix $B(\epsilon) = B + \epsilon I$, which is nonsingular for $\epsilon > 0$. By the argument above, $B(\epsilon)$ is totally nonnegative for $\epsilon > 0$. Any minor of $B(\epsilon)$

is the determinant of a submatrix of $B(\epsilon)$, which is a polynomial in ϵ, so it is continuous in ϵ. This minor is nonnegative for all $\epsilon > 0$ and so must remain nonnegative in the limit as $\epsilon \to 0$. Therefore $B = B(0)$ is totally nonnegative. □

Even if B is not totally nonnegative, there is a an associated totally nonnegative matrix.

Theorem 5.3. *If $B \in \mathbb{R}^{n\times n}$ is nonsingular and bidiagonal then $M(B)^{-1}$ is totally nonnegative.*

Proof. Assuming that $B = L$ is lower bidiagonal, by (5.2) and (5.3),

$$M(B) = M(DL) = |D|M(L) = |D|L_1(-|\ell_{21}|)L_2(-|\ell_{32}|)\ldots L_{n-1}(-|\ell_{n,n-1}|)$$

and $L_k(-|\ell_{k+1,k}|)^{-1} = L_k(|\ell_{k+1,k}|)$, so $M(B)^{-1} = L_{n-1}(|\ell_{n,n-1}|)L_{n-2}(|\ell_{n-1,n-2|})\ldots L_1(|\ell_{21}|)\times |D|^{-1}$, which is a product of totally nonnegative matrices and hence is totally nonnegative. □

The next result shows that any nonsingular totally nonnegative matrix can be written as a product of nonnegative bidiagonal matrices.

Theorem 5.4. *A nonsingular matrix $A \in \mathbb{R}^{n\times n}$ is totally nonnegative if and only if it can be factorized as*

$$A = L_{n-1}L_{n-2}\ldots L_1 D U_1 U_2 \ldots U_{n-1}, \tag{5.4}$$

where D is a diagonal matrix with positive diagonal entries and L_i and U_i are unit lower and unit upper bidiagonal matrices, respectively, with the first $i-1$ entries along the subdiagonal of L_i and U_i^T zero and the rest nonnegative.

The factorization (5.4) is essentially an LU factorization in which L and U have been factorized into a product of specially structured nonnegative bidiagonal matrices.

Theorem 5.4 is from Gasca and Peña [21, Thm. 4.2]. Fallat and Johnson [19, sec. 2.0] summarize the history of different forms of this factorization.

Since the bidiagonal matrices in the factorization (5.4) are all nonnegative, by (3.9) we have

$$\|A^{-1}\|_\infty = \|M(U_{n-1})^{-1}\ldots\ M(U_1)^{-1}D^{-1}M(L_1)^{-1}\ldots\ M(L_{n-1})^{-1}e\|_\infty, \tag{5.5}$$

and so we can compute $\|A^{-1}\|_\infty$ by $2(n-1)$ substitutions in $O(n^2)$ flops for any nonsingular totally nonnegative matrix given the factorization (5.4).

Let $\widehat{c} = \mathrm{fl}(\|A^{-1}\|_\infty)$. Taking ∞-norms in (4.5) with $b = e$ gives, using the triangle inequality,

$$\frac{|\widehat{c} - \|A^{-1}\|_\infty|}{\|A^{-1}\|_\infty} \le dn^2u \tag{5.6}$$

for a modest constant d. Therefore $\widehat{c}$ is highly accurate, essentially because there is no cancellation in evaluating (5.5): all additions are of nonnegative quantities. Standard methods for evaluating $\|A^{-1}\|_\infty$ for general A only satisfy $|\widehat{c} - \|A^{-1}\|_\infty|/\|A^{-1}\|_\infty \le cn^3\kappa_\infty(A)u$, which is the best that can be expected in general because the condition number of $\kappa_\infty(A)$ is $\kappa_\infty(A)$ [24].

To obtain $\kappa_\infty(A)$ we need $\|A\|_\infty$, which can either be computed from A if it is explicitly known, or from $\|A\|_\infty = \|L_{n-1}L_{n-2}\ldots L_1DU_1U_2\ldots U_{n-1}e\|_\infty$ otherwise. We summarize the computations in an algorithm.

Algorithm 5.5. *This algorithm computes $c = \kappa_\infty(A)$ for a totally nonnegative matrix A given the factorization (5.4).*

Table 5.1: Condition numbers and relative errors for the Hilbert matrix.

n	$\kappa_\infty(H_n)$	Relative error for Algorithm 5.5
4	2.84e4	1.28e-16
8	3.39e10	2.25e-16
16	5.06e22	3.67e-17
32	1.36e47	1.75e-15
64	1.10e96	1.77e-15

If A is explicitly known
  $\alpha = \|A\|_\infty$
else
  $\alpha = \|L_{n-1}L_{n-2}\dots L_1 D U_1 U_2 \dots U_{n-1} e\|_\infty$
end
Compute $\beta = \|M(U_{n-1})^{-1} \dots\ M(U_1)^{-1} D^{-1} M(L_1)^{-1} \dots\ M(L_{n-1})^{-1} e\|_\infty$
  by substitutions.
$c = \alpha\beta$

How do we obtain the parameters in the factorization (5.4)? In some cases they are known from the construction of the matrix. Formulas are known for totally positive Vandermonde matrices and Cauchy matrices [34, eqs. (3.5), (3.6)] and a variety of Vandermonde-type matrices [9]. For totally positive matrices determinantal formulas for the parameters are available [34, Prop. 3.1]. Assuming the determinants can be computed accurately, in all these cases the parameters can be evaluated to high relative accuracy. and so in view of Theorem 2.3 the errors in the evaluation of the parameters do not affect the form of the bound (5.6).

We give two numerical experiments in MATLAB to illustrate the accuracy of the condition number evaluation. We take as the exact condition number the one computed at a precision of 500 decimal digits using the Multiprecision Computing Toolbox [39] and then rounded to double precision.

First, in Table 5.1 we show the relative errors in computing the ∞-norm condition number of the Hilbert matrix H_n, which has (i, j) element $1/(i + j - 1)$ and is totally positive. The parameters in the bidiagonal factorization (5.4) are computed using the function `TNCauchyBD` from the TNTool toolbox.[1] We see that even extremely large condition numbers are obtained to high accuracy.

Next we consider the Pascal matrix (4.10), which is totally positive [19, Ex. 0.1.6]. Since this matrix is exactly representable at the working precision for n up to around 25, we can compare Algorithm 5.5 with the MATLAB `cond` function. We see from the results in Table 5.2 that the MATLAB function loses accuracy as n increases while Algorithm 5.5 returns a result correct to the working precision.

Another use of the factorization of Theorem 5.4 is to construct totally nonnegative matrices by choosing the n^2 parameters that make up the L_i, D, and the U_i. The function call

```
A = anymatrix('core/totally_nonneg',X)
```

in the Anymatrix toolbox [30] constructs an $n \times n$ totally nonnegative matrix A from parameters given in the $n \times n$ matrix X, whose format is as suggested in [34, sec. 4]. The Pascal matrix is generated when `X = ones(n)`. In a call

[1] http://www.math.sjsu.edu/~koev/software/TNTool.html

Table 5.2: Condition numbers and relative errors for the Pascal matrix.

n	$\kappa_\infty(P_n)$	Relative errors	
		Algorithm 5.5	`cond(P_n,inf)`
5	1.56e4	0.00	0.00
10	8.13e9	0.00	1.49e-11
15	5.77e15	0.00	2.19e-8
20	4.50e21	4.66e-17	3.41e-4
25	3.81e27	1.70e-17	3.17e-2

```
A = anymatrix('core/totally_nonneg',n)
```

the parameters are chosen randomly, and this is a convenient way to generate random totally nonnegative matrices.

Koev [34, sec. 7], [35] shows that small relative changes in the parameters in the factorization (5.4) produce small relative changes in the the determinant, the eigenvalues, and the singular values. In [34] he develops algorithms for accurate computation of eigenvalues and the SVD of nonsingular totally nonnegative matrices, given an accurate bidiagonal factorization, by carrying out transformations on the bidiagonal factorization in such a way that no subtractions occur.

For later use, we note a useful theorem about the eigenvalues of a totally nonnegative matrix [18, Thm. 3.3].

Theorem 5.6. *If $A \in \mathbb{R}^{n\times n}$ is totally nonnegative and irreducible then its eigenvalues are real and nonnegative and the positive eigenvalues are distinct.*

Note that the irreducibility requirement in the theorem means that it cannot be applied to triangular matrices, so there is no contradiction to the fact that the totally nonnegative matrix $\left[\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right]$ (for example) has repeated nonzero eigenvalues.

6. Matrix Functions and Polynomial Evaluation and Interpolation. Bidiagonal matrices are intimately connected with polynomial evaluation and interpolation. Horner's method for evaluating a polynomial at a point α can be expressed as the solution of a linear system with coefficient matrix $T_n(-\alpha)$ [28, sec. 5.2], where T_n is defined in (1.2). Premultiplying a vector by $T_n(-1)^T$ corresponds to forming a backward difference, and a subsequent multiplication by a diagonal matrix yields divided differences [28, sec. 5.3]. In fact, an explicit formula for a function of a bidiagonal matrix is available in terms of divided differences. Recall that divided differences of a function f at points x_k are defined recursively by (see, e.g. [7, Chap. 2] or [29, sec. B.16])

$$f[x_k] = f(x_k),$$

$$f[x_0, x_1, \dots, x_{k+1}] = \begin{cases} \dfrac{f[x_1, x_2, \dots, x_{k+1}] - f[x_0, x_1, \dots, x_k]}{x_{k+1} - x_0}, & x_0 \ne x_{k+1}, \\[2ex] \dfrac{f^{(k+1)}(x_{k+1})}{(k+1)!}, & x_0 = x_{k+1}, \end{cases} \tag{6.1}$$

where, since $f[x_1, x_2, \dots, x_{k+1}]$ does not depend on the order of its arguments, we assume without loss of geniality that equal points are contiguous.

Theorem 6.1. *If $B \in \mathbb{C}^{n\times n}$ is upper bidiagonal then $F = f(B)$ is upper triangular with $f_{ii} = f(t_{ii})$ and*

$$f_{ij} = b_{i,i+1}b_{i+1,i+2}\dots b_{j-1,j}\, f[b_{ii}, b_{i+1,i+1}, \dots, b_{jj}], \quad j > i. \tag{6.2}$$

Proof. The formula (6.2) is a special case of the formula for $f(T)$, where T is upper triangular, given in Davis [8], Descloux [11], and Van Loan [45]. ∎

Lemma 2.1 is the special case of Theorem 6.1 with $f(x) = 1/x$. Since $f[\lambda, \lambda, \dots, \lambda] = f^{(n-1)}(\lambda)/(n-1)!$, another special case is the formula for a function of an $m \times m$ Jordan block [29, sec. 1.2]

$$f\left(\begin{bmatrix} \lambda & 1 & & \\ & \lambda & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{bmatrix}\right) = \begin{bmatrix} f(\lambda) & f'(\lambda) & \dots & \dfrac{f^{(m-1)}(\lambda)}{(m-1)!} \\ & f(\lambda) & \ddots & \vdots \\ & & \ddots & f'(\lambda) \\ & & & f(\lambda) \end{bmatrix}. \tag{6.3}$$

Yet another special case is

$$f\left(\begin{bmatrix} \lambda_1 & 1 & & \\ & \lambda_2 & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_n \end{bmatrix}\right)_{1n} = f[\lambda_1, \lambda_2, \dots, \lambda_n],$$

which is a result of Opitz [40] and is used in computing divided differences of the exponential by McCurdy, Ng, and Parlett [37].

A natural question is whether a function of a nonnegative bidiagonal matrix is totally nonnegative. For the exponential, the answer is yes.

Theorem 6.2. *If $B \in \mathbb{R}^{n\times n}$ is a nonnegative bidiagonal matrix then e^B is totally nonnegative.*

Proof. Consider the formula [29, sec. 10.1] $\mathrm{e}^A = \lim_{m\to\infty}(I + A/m)^m$, valid for any A, where $m \in \mathbb{Z}$. For nonnegative bidiagonal B, $I + B/m \geq 0$ for all $m > 0$, so by Theorem 5.2 $I + B/m$ is totally nonnegative and therefore $X_m = (I + B/m)^m$ is totally nonnegative for all $m > 0$ by Theorem 5.1. Suppose that $\lim_{m\to\infty} X_m$ is not totally nonnegative, so that some submatrix with indices (α, β) has negative determinant. Let $x_m = \det(X_m(\alpha, \beta))$. Then $\lim_{m\to\infty} x_m < 0$ but $x_m > 0$ for all m, which is a contradiction, so e^B is totally nonnegative. ∎

Note that Theorem 6.2 does not generalize to wider bandwidths, as the example

$$\exp\left(\begin{bmatrix} 1 & 1 & 1 \\ & 1 & 1 \\ & & 1 \end{bmatrix}\right) = \begin{bmatrix} \mathrm{e} & \mathrm{e} & 3\mathrm{e}/2 \\ & \mathrm{e} & \mathrm{e} \\ & & \mathrm{e} \end{bmatrix}$$

shows, since the $(1\colon 2, 3\colon 4)$ submatrix has negative determinant.

7. Upper Triangular Toeplitz matrices. Upper triangular Toeplitz matrices $T \in \mathbb{C}^{n\times n}$ can be written in the form

$$T = \begin{bmatrix} t_0 & t_1 & \dots & t_{n-1} \\ & t_0 & \ddots & \vdots \\ & & \ddots & t_1 \\ & & & t_0 \end{bmatrix} = \sum_{j=1}^{n} t_{j-1} N^{j-1},$$

where N is upper bidiagonal with a superdiagonal of ones:

$$N = \begin{bmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{bmatrix},$$

Note that $N^n = 0$. It follows that the product of two upper triangular Toeplitz matrices is again upper triangular Toeplitz and that upper triangular Toeplitz matrices commute. Furthermore, since $f(T)$ is a polynomial in T, it follows that $f(T)$ is also upper triangular and Toeplitz. Note that as a special case, if B is a Toeplitz bidiagonal matrix with $b_{ii} = b$ and $b_{i,i+1} = c$ then Theorem 6.1 gives $f(B)_{ij} = c^{j-i} f[b, b, \ldots, b] = c^{j-i} f^{(j-i)}(b)/(j-i)!$, of which (6.3) is a special case.

8. Exploiting Factorizations Into Products of Bidiagonal Matrices. In this section we show how factorizations involving bidiagonal matrices or their inverses can provide valuable information about particular matrices.

8.1. The Frank Matrix. In 1958 Frank [20] reported that his algorithms had difficulty computing accurately the smaller eigenvalues of the $n \times n$ upper Hessenberg matrix

$$F_n = \begin{bmatrix} n & n-1 & n-2 & \ldots & 2 & 1 \\ n-1 & n-1 & n-2 & \ldots & 2 & 1 \\ 0 & n-2 & n-2 & \ldots & 2 & 1 \\ \vdots & 0 & \ddots & \ddots & \vdots & 1 \\ \vdots & \vdots & \ldots & 2 & 2 & 1 \\ 0 & 0 & \ldots & 0 & 1 & 1 \end{bmatrix}.$$

Wilkinson [47, sec. 8] [48, pp. 92–93] showed that the difficulties are caused by the sensitivity of the eigenvalues to perturbations in the matrix, which can be measured by the condition number of a simple eigenvalue λ: $\kappa_2(\lambda) = \|y\|_2 \|x\|_2 / |y^* x|$, where x and y are right and left eigenvectors, respectively, corresponding to λ. The eigenvalues are known to be real and positive, and they can be expressed in terms of the zeros of Hermite polynomials [13], [46]. However, in none of these references is it shown that the eigenvalues are distinct, which is necessary for the eigenvalue condition numbers to be defined.

If we subtract row $k+1$ from row k for $k = 1\colon n-1$, we obtain a lower bidiagonal matrix. For $n = 4$ this transformation can be written

$$\begin{bmatrix} 1 & -1 & & \\ & 1 & -1 & \\ & & 1 & -1 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 4 & 3 & 2 & 1 \\ 3 & 3 & 2 & 1 \\ & 2 & 2 & 1 \\ & & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ 3 & 1 & & \\ & 2 & 1 & \\ & & 1 & 1 \end{bmatrix},$$

and in general we have

$$F_n = T_n(-1)^{-1} \begin{bmatrix} 1 & & & & \\ n-1 & 1 & & & \\ & n-2 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 1 \end{bmatrix} \equiv T_n(-1)^{-1} L, \qquad (8.1)$$

where T_n is defined in (1.2). This is equivalent to a factorization noted by Rutishauser [43, sec. 9]. Note that this is a UL factorization, not an LU factorization, and it takes advantage of the rank-1 nature of the upper triangle of F_n. This factorization shows that the inverse $F_n^{-1} = L^{-1}T_n(-1)$ is lower Hessenberg with integer entries and that $\det(F_n) = 1$. Furthermore, L is totally nonnegative by Theorem 5.2 and $T_n(-1)^{-1} = M(T_n(-1))^{-1}$ is totally nonnegative by Theorem 5.3, so F_n is the product of two totally nonnegative matrices and so is totally nonnegative by Theorem 5.1—a property that to our knowledge has not previously been noted. Since F_n is nonsingular, irreducible (being upper Hessenberg with nonzero subdiagonal), and totally nonnegative it follows from by Theorem 5.6 that F_n has distinct eigenvalues. The distinctness of the eigenvalues also follows from some rather lengthy analysis of the characteristic polynomial in [38, Thm. 2.5].

Frank discussed two matrices in his paper. The other matrix is obtained from $A_n = (\min(i,j)) \in \mathbb{R}^{n\times n}$ by taking the rows and columns in reverse order. We will focus on A_n. For example,

$$A_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix}.$$

The determinant, the inverse, and the eigenvalues of A_n can all be easily found by constructing a factorization involving a bidiagonal matrix. Consider subtracting row $k-1$ from row k for $k = n : -1 : 2$. For A_4 this yields

$$\begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & -1 & 1 & \\ & & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ & 1 & 1 & 1 \\ & & 1 & 1 \\ & & & 1 \end{bmatrix}.$$

In general, $T_n(-1)^T A_n = U$, where U is the upper triangular matrix of 1s. Hence $A_n = T_n(-1)^{-T}U$, which is a Cholesky factorization $A_n = U^TU$ since $T_n(-1)^{-1} = U$, which shows that A_n is symmetric positive definite. Furthermore, $\det(A) = \det(U)^2 = 1$ and $A_n^{-1} = U^{-1}U^{-T} = T_n(-1)T_n(-1)^T$, which is tridiagonal since T_n is upper bidiagonal. Now $T_n(-1)^{-1}$ is totally nonnegative, as noted above; hence A_n is the product of two totally nonnegative matrices and therefore is totally nonnegative. By Theorem 5.6, the eigenvalues of A_n are distinct. In fact, A_n^{-1} is the almost-Toeplitz tridiagonal matrix

$$A_n^{-1} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & \ddots & \ddots & \\ & & \ddots & 2 & -1 \\ & & & -1 & 1 \end{bmatrix},$$

and its eigenvalues are [16], [23, Chap. 7] (and as given by Frank)

$$\mu_k = 2\left(1 + \cos\left(\frac{2k\pi}{2n+1}\right)\right), \quad k = 1 : n.$$

The eigenvalues of A_n are the reciprocals of the μ_k.

8.2. The Kac–Murdock–Szegö Matrix. The Kac–Murdock–Szegö matrix is the symmetric Toeplitz matrix, depending on a single parameter $\rho \in \mathbb{R}$,

$$A_n(\rho) = \begin{bmatrix} 1 & \rho & \rho^2 & \dots & \rho^{n-1} \\ \rho & 1 & \rho & \dots & \rho^{n-2} \\ \rho^2 & \rho & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \rho \\ \rho^{n-1} & \rho^{n-2} & \dots & \rho & 1 \end{bmatrix} \in \mathbb{R}^{n\times n}. \tag{8.2}$$

It was considered by Kac, Murdock, and Szegö [33, p. 784 ff.], who investigated its spectral properties. It arises in the autoregressive AR(1) model in statistics and signal processing.

It is straightforward to verify that A_n has a factorization $A_n = LDL^T$ with

$$L = T_n(-\rho)^{-T}, \qquad D = \operatorname{diag}(1, 1-\rho^2, 1-\rho^2, \dots, 1-\rho^2). \tag{8.3}$$

This factorization reveals several properties.

(1) $\det(A_n(\rho)) = (1-\rho^2)^{n-1}$.

(2) For $\rho \neq \pm 1$, A_n is nonsingular and $A_n(\rho)^{-1} = T_n(-\rho)D^{-1}T_n(-\rho)^T$ is the tridiagonal (but not Toeplitz) matrix

$$A_n(\rho)^{-1} = \frac{1}{1-\rho^2} \begin{bmatrix} 1 & -\rho & & & & \\ -\rho & 1+\rho^2 & -\rho & & & \\ & -\rho & 1+\rho^2 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\rho & 1+\rho^2 & -\rho \\ & & & & -\rho & 1 \end{bmatrix}. \tag{8.4}$$

(3) For $0 \le \rho \le 1$, $T_n(-\rho) = M(T_n(-\rho))$ and so by Theorem 5.3 $M(T_n(-\rho))^{-1} = T_n(-\rho)^{-1} = L^T$ is totally nonnegative, so $A_n(\rho)$ is the product of three totally nonnegative matrices and is therefore totally nonnegative. For $0 < \rho < 1$, $A_n(\rho)$ is also nonsingular and irreducible, so the eigenvalues are distinct by Theorem 5.6. Since $A_n(\rho) = \Sigma A_n(-\rho)\Sigma$ for Σ in (3.4), $A_n(\rho)$ is similar to $A_n(-\rho)$ and therefore $A_n(\rho)$ has distinct eigenvalues for $0 \neq \rho \in (-1, 1)$.

8.3. The Pascal Matrix. The Pascal matrix $P_n \in \mathbb{R}^{n\times n}$, defined in (4.10), contains the rows of Pascal's triangle along the antidiagonals. For example:

$$P_5 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 6 & 10 & 15 \\ 1 & 4 & 10 & 20 & 35 \\ 1 & 5 & 15 & 35 & 70 \end{bmatrix}.$$

This matrix is much-studied and most analyses involve the use of combinatorial identities. A number of key properties can be obtained from a factorization of P_n into a product of bidiagonal matrices.

The key observation is that P_n can be reduced to upper triangular form by repeatedly subtracting a row from the row below. For $n = 5$, with $L_k(-1)$ denoting the unit lower bidiagonal matrix with -1s in subdiagonal elements $(k+1,k),\dots,(n-1,n)$,

$$L_4(-1)L_3(-1)L_2(-1)L_1(-1)P_5 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$
$$\times \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} P_5$$
$$= \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 \\ 0 & 0 & 1 & 3 & 6 \\ 0 & 0 & 0 & 1 & 4 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} = R.$$

In general, we have

$$P_n = L_1(-1)^{-1}L_2(-1)^{-1}\dots L_{n-1}(-1)^{-1}R_n = L_nR_n,$$

where L_n is unit lower triangular and R_n is unit upper triangular. By the uniqueness of the LU and Cholesky factorizations of a positive definite matrix we must have $L_n = R_n^T$, so $P_n = R_n^TR_n$, and it can be shown that $R_n = L_{n-1}(1)^TL_{n-2}(1)^T\dots L_1(1)^T$, which contains the binomial coefficients downs its columns.

This is the factorization (5.4) in Theorem 5.4: all the parameters are equal to 1.

We can make several deductions.

(1) P_n is symmetric positive definite.

(2) $\det(P_n) = 1$.

(3) P_n and R_n are both totally nonnegative, since they are products of bidiagonal matrices $L_i(1)$, each of which is totally nonnegative by Theorem 5.2. Hence the eigenvalues of P_n are distinct by Theorem 5.6.

(4) The matrix $S_n = \Sigma R_n$ (where Σ is defined in (3.4)) is involutory, that is, $S_n^2 = I$. This can be proved with the aid of the bidiagonal factorization but we omit the rather tedious details. Since $P_n = S_n^TS_n$, we have $P_n^{-1} = S_n^{-1}S_n^{-T} = S_nS_n^T = S_n^{-T}P_nS_n^T$, so P_n^{-1} is similar to P_n, which means that the eigenvalues of P_n occur in reciprocal pairs. It follows, in particular, that $\|P_n\|_2 = \|P_n^{-1}\|_2$ and so $\kappa_2(P_n) = \|P_n\|_2^2$.

It is also interesting to note that, as an instance of Theorem 6.2, the Cholesky factor R_n is the exponential of a bidiagonal matrix: $R_n = \mathrm{e}^{C_n}$, where [2], [14]

$$C_n = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 2 & & \\ & & \ddots & \ddots & \\ & & & 0 & n-1 \\ & & & & 0 \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

The matrix C_n is called the creation matrix in [1], [2] because of its role in generating matrix representations of polynomials and providing simple proofs of identities.

8.4. Tridiagonal Matrices from Partial Differential Equations. Consider a linear system $Ax = b$, where $A = D + L + U$ with $D = \mathrm{diag}(A)$ and L and U the strictly lower triangular and strictly upper triangular parts of A, respectively. The powers of the matrix $B = -(D + L)^{-1}U$ govern the convergence of the Gauss–Seidel iteration. Note that B is nonsymmetric and so in general can have complex eigenvalues.

Suppose A is tridiagonal with negative diagonal elements and nonnegative elements on the superdiagonal and subdiagonal, as is frequently the case in discretizations of partial differential equations, in which A is typically a Toeplitz matrix. For example,

$$A = \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & -2 & 1 \\ & & 1 & -2 \end{bmatrix} \quad \Rightarrow \quad B = \begin{bmatrix} 0 & 1/2 & 0 & 0 \\ 0 & 1/4 & 1/2 & 0 \\ 0 & 1/8 & 1/4 & 1/2 \\ 0 & 1/16 & 1/8 & 1/4 \end{bmatrix}.$$

The matrix $(-D-L)^{-1}$ is totally nonnegative by Theorem 5.3, because $-D-L = M(-D-L)$, and U is totally nonnegative by Theorem 5.2. Hence $B = (-D - L)^{-1}U$ is lower Hessenberg and totally nonnegative. Furthermore, B is irreducible if the subdiagonal of L and the superdiagonal of U are nonzero. Then Theorem 5.6 shows that the eigenvalues of B are real and nonnegative and the positive eigenvalues are distinct. The eigenvalues of B can be deduced from the analysis of Young [49], [50, Chap. 5].

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