

CHARACTERIZATIONS AND DECOMPOSITIONS OF ALMOST STRICTLY POSITIVE MATRICES*

M. GASCA[†] AND J. M. PEÑA[†]

Abstract. A nonsingular matrix is called almost strictly totally positive when all its minors are nonnegative, and furthermore these minors are positive if and only if their diagonal entries are positive. In this paper we give a characterization of these matrices in terms of the positivity of a very reduced number of their minors (which are called boundary minors), improving previous characterizations that have appeared in the literature. We show the role of boundary minors in accurate computations with almost strictly totally positive matrices. Moreover, we analyze the QR factorization of these matrices, showing the differences and analogies with that of totally positive matrices.

Key words. total positivity, QR factorization, almost strictly totally positive matrices

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1. Introduction and basic notation. Matrices with all minors nonnegative (in particular, all positive) have attracted much interest in several branches of mathematics and their applications, including computer aided geometric design, combinatorics, and economics. Unfortunately there is not an agreement to use a unified terminology for them. On one hand, the American school, following Schoenberg and especially Karlin and his book [16] *Total Positivity*, used to call totally positive matrices those matrices with all minors nonnegative and strictly totally positive matrices the ones with all minors positive. Many authors, including Ando, de Boor, and Pinkus, have followed these names in the second half of the last century, and so have we in our papers on this subject. On the other hand, the German school used the terms “totally nonnegative” and “totally positive” matrices instead of the above ones, respectively. These last terms have become more accepted in the recent literature. Due to all of this, the term “totally positive matrix” has become ambiguous because it is used in two slightly (but significantly) different senses.

As we have said above, in the last decade we have used Karlin’s terminology in our papers, and so it would be even more confusing to change to the other terminology in the present paper because, as we explain below, it improves some of our previous results and we make frequent references to these results. Consequently, in this paper, we continue calling *totally positive (TP) matrices* those matrices with all minors nonnegative and *strictly totally positive (STP) matrices* those with all minors positive and hope this will cause no confusion to the reader. In any case, it would be good to unify terminology in the future.

For some important applications, for example, B-splines [2], interpolation [4], Hurwitz matrices [7, 17], or interval mathematics [8], the most important class of TP matrices is that which we called in [9] *almost strictly totally positive matrices* (referred to as ASTP matrices in the rest of this paper). This class is formed by TP

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[†]Departamento de Matemática Aplicada, Universidad de Zaragoza, 50009 Zaragoza, Spain (gasca@unizar.es, jmpena@unizar.es).

matrices whose minors are positive if and only if they do not contain a zero element in the diagonal. This class is intermediate between TP and STP matrices. The most interesting ASTP matrices are the nonsingular ones, and therefore, in the rest of the paper, we deal with these matrices. They have been called in [15] *inner totally positive matrices*. Matrices called in some papers [1] Δ -STP matrices are examples of triangular ASTP matrices.

From the beginning of the study of TP matrices it has been known that it is not necessary to check the sign of all minors of a matrix to decide whether or not it is totally positive and analogously for strict total positivity. Some of our efforts in the last decade have been devoted to getting criteria which decrease the number of minors to be checked and other characterizations in terms of bidiagonal factorizations [10, 11, 12, 14]. So we did this with ASTP matrices too. The nonzero pattern of these matrices [9, 13, 15] always has a staircase form. Roughly speaking (it will be explained more precisely in section 2) we proved [13, Theorem 3.1] that for a nonnegative matrix to be nonsingular ASTP we have to check only that minors formed with consecutive rows and columns, with the first row or column of the minor being the first row or column of a stair (of the nonzero pattern), are nonnegative and that they are positive if and only if the diagonal entries of the minor are all positive. These minors form a subclass of those called in [15, Theorem 2.1] inner minors with consecutive rows and columns, which are the minors to be checked in that paper. See also Theorem 3.1 of [9].

In this paper we improve our characterization of nonsingular ASTP matrices of [13] in the sense that the number of minors to be checked can be decreased. We introduce in section 2 the concept of boundary minor, which has special interest in matrices with staircase nonzero pattern, and prove that only these minors should be checked. Since they are a subclass of the ones used in [13], we decrease considerably the number with respect to [9, 15]. Moreover, we show how boundary minors can play a role in accurate computations with nonsingular ASTP matrices.

In the process of proving these results we have realized that in Theorem 3.1 of [13] the assumption of nonnegativity of the matrix can be suppressed: it is a consequence of any of the two equivalent properties of the theorem. So we have taken into account this fact in Theorem 2.4 of section 2 which is the new, improved version of that theorem.

After getting some results on the LU factorization of TP matrices we studied their QR factorization in [11]. In [13] we provided a bidiagonal factorization of nonsingular ASTP matrices and also the result that a nonsingular matrix A is ASTP if and only if it can be factorized LU with L and U ASTP matrices. It seems natural to study now the QR factorization of ASTP matrices to know if it has some peculiarities with respect to the general class of TP matrices. In section 3 we show the differences and analogies of the QR factorization of nonsingular ASTP matrices with respect to that of nonsingular TP and STP matrices. Boundary minors play again a crucial role in the proofs of that section.

2. Boundary submatrices of ASTP matrices. For k, n positive integers, $1 \leq k \leq n$, $Q_{k,n}$ will denote the set of all increasing sequences of k natural numbers less than or equal to n . For $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_k)$, $\beta = (\beta_1, \beta_2, \dots, \beta_k) \in Q_{k,n}$, and A an $n \times n$ real matrix, we denote by $A[\alpha|\beta]$ the $k \times k$ submatrix of A containing rows $\alpha_1, \dots, \alpha_k$ and columns β_1, \dots, β_k of A . $Q_{k,n}^0$ will denote the set of sequences of k consecutive natural numbers less than or equal to n .

By the *shadow lemma* (see [3, Lemma A]), a nonsingular ASTP matrix $A =$

$(a_{ij})_{1 \leq i, j \leq n}$ satisfies

$$(2.1) \quad \begin{aligned} a_{ij} = 0, i > j &\Rightarrow a_{hk} = 0 \quad \forall h \geq i, k \leq j, \\ a_{ij} = 0, i < j &\Rightarrow a_{hk} = 0 \quad \forall h \leq i, k \geq j. \end{aligned}$$

Moreover, it cannot have zero diagonal entries due to its nonsingularity (cf. [1, Corollary 3.8]):

$$(2.2) \quad a_{ii} \neq 0, \quad i = 1, \dots, n.$$

Properties (2.1) and (2.2) produce a staircase form for the zero pattern of A , which will be made precise in the following notation, as in [13].

For an $n \times n$ matrix A let us denote

$$\begin{aligned} i_0 &= 1, \quad j_0 = 1; \\ \text{for } t &= 1, \dots, l : \\ i_t &= \max\{i | a_{i, j_{t-1}} \neq 0\} + 1 \quad (\leq n + 1), \\ j_t &= \max\{j | a_{i_t, j} = 0\} + 1 \quad (\leq n + 1), \end{aligned}$$

where l is given in this recurrent definition by $i_l = n + 1$. Analogously we denote

$$\begin{aligned} \hat{j}_0 &= 1, \quad \hat{i}_0 = 1; \\ \text{for } t &= 1, \dots, r : \\ \hat{j}_t &= \max\{j | a_{\hat{i}_{t-1}, j} \neq 0\} + 1, \\ \hat{i}_t &= \max\{i | a_{i, \hat{j}_t} = 0\} + 1, \end{aligned}$$

where $\hat{j}_r = n + 1$. In other words, the entries below the places $(i_1 - 1, j)$ with $j_0 \leq j < j_1$, $(i_2 - 1, j)$ with $j_1 \leq j < j_2$, \dots , $(i_{l-1} - 1, j)$ with $j_{l-2} \leq j < j_{l-1}$ are zero. So are the entries to the right of the places $(i, \hat{j}_1 - 1)$ with $\hat{i}_0 \leq i < \hat{i}_1$, $(i, \hat{j}_2 - 1)$ with $\hat{i}_1 \leq i < \hat{i}_2$, \dots , $(i, \hat{j}_{r-1} - 1)$ with $\hat{i}_{r-2} \leq i < \hat{i}_{r-1}$.

When the matrix A is nonsingular ASTP, by (2.1), the remaining elements of A are nonzero. We shall express this by saying that the matrix A has a zero pattern given by $I = \{i_0, i_1, \dots, i_l\}$, $J = \{j_0, j_1, \dots, j_l\}$, $\hat{I} = \{\hat{i}_0, \hat{i}_1, \dots, \hat{i}_r\}$, and $\hat{J} = \{\hat{j}_0, \hat{j}_1, \dots, \hat{j}_r\}$. Only matrices with these patterns of zeros and all the other entries positive can be nonsingular ASTP.

Observe that, for a nonsingular ASTP matrix, by (2.2) we have necessarily

$$(2.3) \quad \begin{aligned} i_t &\geq j_t, \quad t = 1, \dots, l - 1, \\ \hat{j}_t &\geq \hat{i}_t, \quad t = 1, \dots, r - 1. \end{aligned}$$

In formula (3.2) of [13], the previous inequalities appeared strict, but in fact the equalities can also appear.

Remark 2.1. Given any matrix $A = (a_{ij})_{1 \leq i, j \leq n}$, it is easy to deduce that the following properties are equivalent:

- (i) A satisfies (2.1) and (2.2).
- (ii) A has a zero pattern given by I, J, \hat{I}, \hat{J} as above satisfying (2.3).

The submatrices introduced in the following definition are relevant in the context of matrices with a staircase zero pattern and will play a key role in this paper.

DEFINITION 2.2. *Given an $n \times n$ matrix A , let $B := A[\alpha|\beta]$ with $\alpha, \beta \in Q_{k,n}^0$ and $a_{\alpha_1, \beta_1} \cdots a_{\alpha_k, \beta_k} \neq 0$. Then B is a column boundary submatrix if either $\beta_1 = 1$ or*

$\beta_1 > 1$ and $A[\alpha|\beta_1 - 1] = 0$. Analogously, B is a row boundary submatrix if either $\alpha_1 = 1$ or $\alpha_1 > 1$ and $A[\alpha_1 - 1|\beta] = 0$.

Minors corresponding to column or row boundary submatrices are called, respectively, column or row boundary minors.

Remark 2.3. Using staircase notation, we can easily identify the boundary submatrices for matrices satisfying the zero pattern described above. Let $A = (a_{ij})_{1 \leq i, j \leq n}$ be an $n \times n$ matrix with a zero pattern given by I, J, \hat{I}, \hat{J} satisfying (2.3). Let $B := A[\alpha|\beta]$ with $\alpha, \beta \in Q_{k,n}^0$ and $a_{\alpha_1, \beta_1} \cdots a_{\alpha_k, \beta_k} \neq 0$. Then B is a column boundary submatrix if there exists $k \geq 1$ such that $\beta_1 = \hat{j}_k$ and $\alpha_1 \geq i_k$. B is a row boundary submatrix if there exists $k \geq 1$ such that $\alpha_1 = \hat{j}_k$ and $\beta_1 \geq \hat{i}_k$. The leading principal minors of A are column and row boundary minors of it.

Let us consider an example of a 5×5 matrix A with $l = 2, r = 1, \{i_0, i_1, i_2\} = \{1, 4, 6\}, \{j_0, j_1, j_2\} = \{1, 3, 6\}, \{\hat{j}_0, \hat{j}_1\} = \{1, 6\}$, and $\{\hat{i}_0, \hat{i}_1\} = \{1, 6\}$. Entries represented by the symbol $*$ are nonzero. The row boundary minors of the matrix

$$(2.4) \quad A = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & * & * & * \end{pmatrix}$$

are the minors using initial consecutive rows and consecutive columns. The column boundary minors of A are its leading principal minors, the entries $a_{21}, a_{31}, a_{43}, a_{53}$, the minors

$$(2.5) \quad \det A[2, 3|1, 2], \quad \det A[4, 5|3, 4],$$

and the following minors which can be obtained from the previous ones: the minor $\det A[2, 3, 4|1, 2, 3]$ (which is equal to $a_{43} \det A[2, 3|1, 2]$) and $\det A[2, 3, 4, 5|1, 2, 3, 4]$ (which coincides with $\det A[2, 3|1, 2] \det A[4, 5|3, 4]$).

Now we shall prove that, for a matrix A , being nonsingular ASTP depends only on the sign of the boundary minors, improving the characterization of Theorem 3.1 of [13]. In addition, as said in section 1, we point out that the hypothesis of nonnegativity of A used in that theorem is not necessary because it is a consequence of any of the two equivalent properties of the theorem.

THEOREM 2.4. *Let $A = (a_{ij})_{1 \leq i, j \leq n}$ be a real matrix satisfying (2.1) and (2.2). Then the following properties are equivalent:*

- (i) *A is a nonsingular ASTP matrix.*
- (ii) *All boundary minors of A are positive.*

Proof. By definition of nonsingular ASTP matrices, (i) implies (ii). For the converse, take into account that, by definition, A is a (trivial) boundary submatrix of itself, and consequently it is nonsingular. Now, the arguments of the proof of the converse part of Theorem 3.1 of [13] can be applied. Let us sketch the main points of that proof. It consists of showing that the Neville elimination of A and A^T can be performed without row or column exchanges and with nonnegative pivots which are zero if and only if they lie in the zero pattern of A , which by Remark 2.1 is given by I, J, \hat{I}, \hat{J} as above. If we take a column j with $j_{t-1} \leq j < j_t$, the crucial point of the proof of Theorem 3.1 of [13] is to show the positivity of the quotients

$$(2.6) \quad \frac{\det A[i - j + j_k, \dots, i - 1, i|j_k, \dots, j - 1, j]}{\det A[i - j + j_k, \dots, i - 1|j_k, \dots, j - 1]}, \quad i = j, j + 1, \dots, i_t - 1,$$

where

$$(2.7) \quad j_k = \max\{j_s \leq j \mid 0 \leq s \leq t-1, j - j_s \leq i - i_s\}.$$

In fact, in that proof it is shown that the numerator and denominator of (2.6) are positive. Observe that for $j = j_{t-1}$ and $i = i_{t-1}, \dots, i_t - 1$ we have $j_k = j_{t-1}$, and the quotient above becomes simply a_{ij} . Let us also point out that, by (2.3), in (2.6) one has $i_t \geq j_t$.

Coming back to our present theorem, the same arguments lead us to consider the quotients (2.6). Now, taking into account that, by (2.7), $j - j_k \leq i - i_k$, we have

$$i - j + j_k = i - (j - j_k) \geq i - (i - i_k) = i_k.$$

So, the submatrices of the numerator and denominator of (2.6) are of the form $A[\alpha|\beta]$ with $\alpha, \beta \in Q_{k,n}^0$, $\beta_1 = j_k$, and $\alpha_1 \geq i_k$, and, consequently, they are column boundary submatrices by Remark 2.3. Then (ii) implies that these minors are positive and the arguments of Theorem 3.1 of [13] to prove their positivity are not needed.

Since similar reasoning can be applied to A^T , the positivity of the row boundary minors is also involved.

In summary, the proof of Theorem 3.1 of [13] has been simplified, pointing out that the positivity of all boundary minors of A implies that A is a nonsingular ASTP matrix. \square

If we apply the previous theorem to the matrix A of (2.4) in order to know if it is nonsingular ASTP, we have to check the positivity of the minors using initial consecutive rows and consecutive columns (row boundary minors), the elements $a_{21}, a_{31}, a_{43}, a_{53}$, and the two minors given by (2.5). If we apply Theorem 3.1 of [13], we should also check, in addition to all the above minors, the positivity of the entries a_{13}, a_{23}, a_{33} and of the following four minors:

$$\det A[2, 3|3, 4], \det A[3, 4], \det A[2, 3, 4|3, 4, 5], \det A[3, 4, 5].$$

Finally, if we apply the characterization given in [15, Theorem 2.1] and [9], we should check the positivity of the remaining nonzero entries of A and of the following six minors, in addition to all of the previous ones: $\det A[2, 3]$, $\det A[2, 3, 4]$, $\det A[2, 3, 4, 5|2, 3, 4, 5]$, $\det A[2, 3|4, 5]$, $\det A[3, 4|4, 5]$, $\det A[4, 5]$. In larger matrices, the differences in the number of minors to be checked easily increase.

Given an algebraic expression defined by additions, subtractions, multiplications, and divisions and assuming that each initial real datum is known to high relative accuracy (see p. 52 of [5]), then it is well known that the algebraic expression can be computed accurately if it is defined by sums of numbers of the same sign, products, and quotients. In other words, the only ‘‘forbidden’’ operation is true subtraction, due to possible cancellation in leading digits. From now on, we will use the word *accurately* to mean *to high relative accuracy*. Let us recall that a nonsingular TP matrix admits a unique factorization as a product of nonnegative bidiagonal, unit diagonal matrices and a diagonal matrix (see [12] or [14]). This factorization has been called recently in [6] and [18] *bidiagonal decomposition* of A and is denoted by $\mathcal{BD}(A)$. Moreover, the property of A being nonsingular ASTP or not can be decided by $\mathcal{BD}(A)$ as can be seen in Theorem 4.1 of [13].

In [18] it is shown that an accurate bidiagonal decomposition of a nonsingular TP matrix A allows us to determine its eigenvalues and singular value decomposition to high relative accuracy. The following result proves that the accurate computation

of the boundary minors of A guarantees an accurate bidiagonal decomposition of a nonsingular ASTP matrix A . For the sake of brevity, we refer to [12] and [14] instead of introducing all notation related to Neville elimination.

PROPOSITION 2.5. *Let A be a nonsingular ASTP matrix. If we are able to compute all boundary minors of A accurately, then we can compute an accurate $\mathcal{BD}(A)$.*

Proof. As can be seen in [12] or in section 2 of [14], the diagonal entries of the diagonal factor of $\mathcal{BD}(A)$ are the diagonal pivots of the Neville elimination of A . The nonzero off-diagonal entries of the bidiagonal factors of $\mathcal{BD}(A)$ are the multipliers of the Neville elimination of A or of A^T (see p. 116 of [14]) and, by formula (2.7) of [12], they are quotients of pivots of the Neville elimination of A or A^T . Since the pivots of the Neville elimination of A are given by (2.6) (see (2.3) of [12]), they are quotients of column boundary minors of A , and, analogously, the pivots of the Neville elimination of A^T are quotients of row boundary minors of A . Then we conclude that all pivots and multipliers can be computed accurately and the result follows. \square

3. QR factorization of nonsingular ASTP matrices. In [11], nonsingular TP matrices and STP matrices were characterized in terms of their QR factorization. Now we are going to study that factorization for nonsingular ASTP matrices and show its peculiarity with respect to the other classes.

In this section, L (resp., U) represents a lower (upper) triangular, unit diagonal matrix, and D represents a diagonal matrix. Let us recall that, by Corollary 4.2 of [13], a nonsingular matrix A is ASTP if and only if it can be factorized as $A = LDU$ with L, U ASTP matrices and D a diagonal matrix with positive diagonal entries. Now we define a new class of matrices containing ASTP matrices.

DEFINITION 3.1. *A nonsingular matrix A is said to be lowerly ASTP if it can be decomposed in the form $A = LDU$ and LD is ASTP.*

The following proposition characterizes lowerly ASTP matrices.

PROPOSITION 3.2. *An $n \times n$ matrix A is lowerly ASTP if and only if all its column boundary minors are positive.*

Proof. If A is lowerly ASTP, then A can be factorized as $A = LDU$ with LD ASTP. Hence, all column boundary minors of LD are positive. Since U is an upper triangular matrix with unit diagonal, it is easy to see that rows and columns involved in the column boundary submatrices of A are the same as those of the column boundary submatrices of LD and that the column boundary minors of A have the same value as the corresponding column boundary minors of LD . So, all column boundary minors of A are positive.

For the converse, if all column boundary minors of A are positive, in particular, the leading principal minors of A are positive. So A can be decomposed as $A = LDU$. Again the column boundary minors of LD have the same value as those of A , and so they are positive. The row boundary minors of the lower triangular matrix LD are principal minors of LD using consecutive rows and columns, that is, of the form $(LD)[k, k+1, \dots, k+r]$ ($1 \leq k \leq n$, $0 \leq r \leq n-k$). Using Schur complements, we have

$$(3.1) \quad \det(LD)[k, k+1, \dots, k+r] = \frac{\det A[1, 2, \dots, k+r]}{\det A[1, 2, \dots, k]}.$$

Since the numerator and the denominator of (3.1) are column boundary minors of A , they are positive, and so the row boundary minors of LD are positive. Then, by Theorem 2.4, LD is ASTP and A is lowerly ASTP. \square

The following definition will be used in the QR decomposition of nonsingular ASTP matrices.

DEFINITION 3.3. *A nonsingular matrix A is said to be an almost strict γ -matrix if it is lowerly ASTP and, in the factorization $A = LDU$, U^{-1} is ASTP.*

PROPOSITION 3.4. *If A and $(A^T)^{-1}$ are lowerly ASTP, then A is an almost strict γ -matrix.*

Proof. The proof is completely analogous to that of Proposition 4.6 of [11]. The only difference is that, in the factorization $A = LDU$, in order to see that the upper triangular matrix $(U^T)^{-1}$ is ASTP, we have to use the same reasoning as in the proof of the converse of Proposition 3.2 to show the almost strict total positivity of LD . \square

The following theorem characterizes ASTP matrices by means of their QR decompositions. This characterization is slightly different from those of nonsingular TP matrices and STP matrices given in Theorem 4.7 of [11], as we shall explain later.

THEOREM 3.5. *Let A be a nonsingular matrix. Then A is ASTP if and only if there exist two orthogonal almost strict γ -matrices Q_1, Q_2 and two nonsingular, upper triangular TP matrices R_1, R_2 , such that*

$$(3.2) \quad A = Q_1 R_1, \quad A^T = Q_2 R_2.$$

The proof is analogous to that of Theorem 4.7 of [11], replacing TP by ASTP until the step when we use that the product of TP matrices $A^T A$ is also TP, because the product of ASTP matrices is *not* necessarily ASTP. So, the reasoning leading to the total positivity of R_1 (R_2) in the proof of Theorem 4.7 of [11] does not lead to the almost strict total positivity of them but only to their total positivity.

In fact, the following counterexample shows that in the above theorem we cannot replace the total positivity of R_1, R_2 by almost strict total positivity. The ASTP matrix

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

can be decomposed as $A = Q_1 R_1$, where

$$Q_1 = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad R_1 = \begin{pmatrix} \sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 1 \end{pmatrix}.$$

The matrix R_1 is TP but not ASTP due to the minor $\det R_1[1, 2|2, 3] = 0$ in spite of the positivity of its diagonal elements. The essential uniqueness of the QR factorization implies that it is not possible to decompose $A = QR$ with Q orthogonal and R ASTP. Moreover, $A^T A$ illustrates that the property of being ASTP is not inherited under the product of matrices. In fact, $A^T A$ is not ASTP due to the minor $\det(A^T A)[1, 2|2, 3]$, which is zero and has positive diagonal elements.

Finally, let us recall that, in the particular case of A being STP, Theorem 4.7 of [11] shows that Q_1 and Q_2 are strict γ -matrices and R_1 and R_2 are Δ -STP matrices.

In summary, a matrix A is STP or nonsingular ASTP or nonsingular TP if and only if A and A^T can be decomposed as in (3.2) with Q_1, Q_2 orthogonal and R_1, R_2

nonsingular upper triangular, according to the following table.

A	Q_1, Q_2	R_1, R_2
STP	strict γ -matrices	Δ -STP
nonsingular ASTP	almost strict γ -matrices	TP
nonsingular TP	γ -matrices	TP

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