Factorizations for some classes of matrices related to positivity

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***Abstract*— We descrtibe factorizations for some classes of matrices related to positivity and important in applications. The classes of matrices considered include nonsingular M-matrices (matrices with nonpositive off-diagonal entries with positive inverse) and totally nonnegative matrices (matrices with all minors nonnegative). The considered factorizations include rank revealing factorizations, LDU-factorization, QR-factorization and symmetric-triangular factorization. Applications of these factorizations are presented.**

I. INTRODUCTION

We present some recent factorizations for some classes of matrices related to positivity and important in applications. The considered factorizations include rank revealing factorizations, LDU-factorization, QR-factorization and symmetric-triangular factorization. An important advance performed during the last years constis of finding some classes of matrices for which relevant computations (such us computing singular values or solving linear systems) can be carried out with high relative accuracy. These classes of matrices are formed either by sign-regular matrices or by M-matrices diagonally dominant. Section 2 is devoted to factorizations of sign-regular matrices and its important subclasses and Section 3 are devoted to factorizations of M-matrices diagonally dominant.

Let us recall the definitions of the classes of matrices considered in this paper. An $n \times n$ matrix A is *strictly sign regular* (SSR) if, for each k ($1 \leq k \leq n$), all $k \times k$ submatrices of A have determinant with the same strict sign. These matrices are characterizated as variation-diminishing linear maps: the maximum number of sign changes in the consecutive components of the image of a nonzero vector is bounded above by the minimum number of sign changes in the consecutive components of the vector (see Theorem 5.3 of [1]). These matrices appear in many fields: see, for instance, [1], and the books [26], [20] and [38] (for applications to computer aided geometric design). A very important subclass of the strictly sign regular matrices is formed by the totally positive matrices. A matrix is *totally positive* (TP) if all its minors are positive. If all its minors are nonnegative, then we say that the matrix is *totally nonnegative*. This terminology is more frequent nowadays in the context of Linear Algebra, although TP matrices and totally nonnegative matrices also have been called strictly totally positive matrices and totally positive matrices, respectively. Finally, a matrix is totally negative (TN) if all its minors are negative. Totally negative matrices belong to the class of N-matrices (matrices with all principal minors negative), which play an important role in Economy (see [3], [35] and [43]). Other aspects of totally negative matrices have been considered in [2], [13], [5] and [18].

Section 3 includes some factorizations and applications of M-matrices. Let us recall that if a matrix whose off-diagonal entries are nonpositive can be expressed as

$$A = sI - B, \quad B \geq 0, \quad s \geq \rho(B)$$

(where $\rho(B)$ is the spectral radius of B), then it is called an M-matrix. M-matrices have important applications, for instance, in iterative methods in numerical analysis, in the analysis of dynamical systems, in economics and in mathematical programming.

II. FACTORIZATIONS OF TOTALLY POSITIVE MATRICES AND RELATED CLASSES OF MATRICES

A. Basic notations

Let us start with some basic notations Following [1], for $k, n \in N$, $1 \leq k \leq n$, $Q_{k,n}$ will denote the set of all increasing sequences of k natural numbers not greater than n. For each $\alpha \in Q_{k,n}$, its dispersion number $d(\alpha)$ is defined by $d(\alpha) := \sum_{i=1}^{k-1}(\alpha_{i+1} - \alpha_i - 1) = \alpha_k - \alpha_1 - (k-1)$, with the convention $d(\alpha) = 0$ for $\alpha \in Q_{1,n}$. Let us observe that $d(\alpha) = 0$ means that α consists of k consecutive integers.

For $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_k)$, $\beta = (\beta_1, \beta_2, \ldots, \beta_k) \in Q_{k,n}$ and A an $n \times n$ matrix, we denote by $A[\alpha|\beta]$ the $k \times k$ submatrix of A containing rows $\alpha_1, \alpha_2, \ldots, \alpha_k$ and columns $\beta_1, \beta_2, \ldots, \beta_k$ of A. If $\alpha = \beta$, we denote by $A[\alpha] := A[\alpha|\alpha]$ the corresponding principal minor. Let A be an $n \times n$ lower (resp., upper) triangular matrix. Following [9], the minors $\det A[\alpha|\beta]$ with $\alpha_k \geq \beta_k$ (resp., $\alpha_k \leq \beta_k$ $\forall k$) are called nontrivial minors of A because all the remaining minors are obviously equal to zero. A triangular matrix A is called ΔTP if its nontrivial minors are all positive. We remark that these matrices are also called ΔSTP in other papers (see [19]).

By a *signature sequence* we mean an (infinite) real sequence $\varepsilon = (\varepsilon_i)$ with $|\varepsilon_i| = 1$, $i = 1, 2, \ldots$. An $n \times n$ matrix A verifying $\varepsilon_k \det A[\alpha|\beta] > 0$ for all $\alpha, \beta \in Q_{k,n}$ and $k = 1, \ldots, n$ is called *strictly sign regular* with signature $\varepsilon_1, \ldots, \varepsilon_n$, and will be denoted by SSR.

B. LDU-factorizations

An LDU-factorization of a matrix A is the decomposition $A = LDU$ where L (resp., U) is a lower (resp., upper) triangular, unit diagonal matrix (i.e., with all diagonal entries

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equal to 1), and D is a diagonal matrix. From now on, $A = LDU$ will refer to this decomposition.

Let us start analyzing the LDU-factorization of SSR matrices. Let us recall the following result, which will be used in the following sections. The proof can be seen in Proposition 2.1 of [18].

Theorem 2.1. *If A is SSR, then $A = LDU$ with L (resp., U) a ΔTP and lower (resp., upper) triangular, unit diagonal matrix and D a diagonal nonsingular matrix.*

In the case of TP and TN matrices, we have the following characterizations. The characterization of TP matrices was obtained by Cryer in Theorem 1.1 of [9] and the characterization of TP matrices was obtained in Remark 3.6 (iv) of [18].

Theorem 2.2. An $n \times n$ matrix $A = (a_{ij})_{1\leq i,j\leq n}$ is TP (resp., TN) if and only if it can be decomposed in the form LDU with L a lower triangular, unit diagonal ΔSTP matrix and U an upper triangular, unit diagonal ΔSTP matrix and D a diagonal matrix with positive diagonal entries (resp., with first positive diagonal entry and negative remaing diagonal entries, and $a_{nn} < 0$).

The previous LDU-factorization are closely rerlated to the bidiagonal factorizations that will be presented in the next subsection and that have many useful applications.

C. Bidiagonal factorizations

Square totally nonnegative matrices of order n form a multiplicative semigroup S_n, and the nonsingular matrices of S_n form a semigroup s_n of the group of all real nonsingular square matrices of order n. In [31], Loewner used some notions from the theory of Lie groups which we briefly recall for the study of S_n and s_n. If $U(t)$ is a differentiable matrix function of the real parameter t in an interval $[0, t_0]$, representing for each t an element of s_n, and $U(0)$ is the identity matrix I (which belongs to s_n), then the matrix $(\frac{dU(t)}{dt})_{t=0}$ is called an *infinitesimal element* of s_n. The first task in [31] was to prove that the set σ_n of all infinitesimal elements of s_n consists of the Jacobi (i.e., tridiagonal) matrices with nonnegative off-diagonal elements. As in Lie-group theory, it can be shown that if $\Omega(t)$ $(0 \leq t \leq t_0)$ is any one-parameter family of elements of σ_n which is piecewise continuous in t, the differential equation

$$\frac{dU(t)}{dt} = \Omega(t)U(t)$$

has a unique continuous solution $U(t)$ in s_n satisfying $U(0) = I$. In this case we say that $U(t_0)$ is generated by the infinitesimal elements $\Omega(t)$ $(0 \leq t \leq t_0)$. In general, a semigroup cannot be completely generated by its infinitesimal elements. However, Loewner proved in [31] that this is not the case for s_n. He used a reformulation of a result due to Whitney [44]. The conclusion of [31] is that, by using infinitesimal generators, any nonsingular totally nonnegative matrix of order n can be generated from the identity by the solutions of the above differential equation.

In 1979 Frydman and Singer ([14], Theorem 1) showed that the class of transition matrices for the finite state time-inhomogeneous birth and death processes coincides with the class of nonsingular totally nonnegative stochastic matrices. This result was based upon a factorization of nonsingular totally nonnegative stochastic matrices in terms of bidiagonal matrices ([14],Theorem 1') similar to the previous one mentioned above. The fact that those transition matrices for birth and death processes are totally positive had been pointed out in 1959 by Karlin and Mc Gregor ([27], [28]) with probabilistic arguments. All these results had been surveyed in 1986 by G. Goodman [23], who extended them to compound matrices, that is matrices whose elements are the values of the minors of a certain order m of a given matrix A.

On the other hand, factorizations of totally nonnegative matrices as product of bidiagonal matrices are important in Computer Aided Geometric Design and, in particular, in corner cutting algorithms. In[24], Goodman and Micchelli showed that the existence of a corner cutting algorithm transforming a control polygon of a curve into another one with the same number of vertices was equivalent to the fact that both polygons were related by a nonsingular stochastic matrix. The key tool to obtain this result was again (see [24], Theorem 1) the characterization of a nonsingular totally nonnegative stochastic matrix of order n as the product of $n-1$ bidiagonal lower triangular stochastic matrices by other $n-1$ matrices which are bidiagonal upper triangular. In [34], Theorem 3.1, Micchelli and Pinkus obtained a factorization theorem for rectangular totally nonnegative matrices as a product of bidiagonal matrices in order to extend the previous interpretation to general corner cutting algorithms. For more details related with this matter and for concrete factorizations associated with corner cutting algorithms to the Bezier polygon, see [25] and [6]. The use of an elimination procedure called Neville elimination was crucial to prove the results on optimality obtained in these last two papers.

We now include a result illustrating bidiagonal factorizations in the case of TP matrices. The following charaterization of a TP matrix in terms of bidiagonal factors was presented in Theorem 4.3 of [20] and provides the uniqueness of the factorization.

Theorem 2.3. A nonsingular $n \times n$ matrix $A = (a_{ij})_{1\leq i,j\leq n}$ is TP if and only if it can be factorized in the form

$$A = F_{n-1}F_{n-2}\cdots F_1 D G_1 \cdots G_{n-2}G_{n-1}, \qquad (1)$$

with D a diagonal matrix with positive diagonal entries,

$$F_i = \begin{pmatrix} 1 & & & & & & \\ 0 & 1 & & & & & \\ & \ddots & \ddots & & & & \\ & & 0 & 1 & & & \\ & & & m_{i+1,1} & 1 & & \\ & & & & \ddots & \ddots & \\ & & & & & m_{n,n-i} & 1 \end{pmatrix},$$

$$G_i = \begin{pmatrix} 1 & 0 & & & & & & \\ & \ddots & \ddots & & & & & \\ & & 1 & 0 & & & & \\ & & & 1 & m_{1,i+1} & & & \\ & & & & \ddots & \ddots & & \\ & & & & & 1 & m_{n-i,n} \\ & & & & & & 1 \end{pmatrix} \quad (2)$$

and the $m_{i,j}$'s positive numbers. This factorization is unique.

In the more general case of nonsingular totally nonnegative matrices, characterizations through a factorization with bidiagonal factors with uniqueness were presented in [19]. Let us mention that these factorizations with bidiagonal factors have been recently used to derive algorithms with high relative accuracy to solve linear systems or calculate the singular values or the eigenvalues of these matrices (see [11], [29], [30], [32], [33]).

Let us also mention that an important subclass of totally nonnegative matrices is formed by the almost TP matrices (or almost strictly totally positive matrices), which are totally nonnegative matrices whose minors are nonzero if and only if all their diagonal entries are nonzero. Bidiagonal factorizations of these matrices can be seen in [21].

D. Other factorizations

We conclude this serction with other factorizations, such as QR-factorization or the symmetric-triangular factorization.

We first need some new definitions.

Definitions 2.3. A nonsingular matrix A is said to be *lowerly signed with signature* $\varepsilon_1, \dots, \varepsilon_n$ if it can be decomposed in the form $A = LDU$ and $LD\Sigma$ is ΔTP, where Σ is a diagonal matrix with diagonal entries $\varepsilon_1, \varepsilon_1\varepsilon_2, \dots, \varepsilon_{n-1}\varepsilon_n$. If, in addition, U^{-1} satisfies that $\Sigma U^{-1}\Sigma$ is ΔTP, then the matrix is called *strictly signed γ-matrix with signature* $\varepsilon_1, \dots, \varepsilon_n$. If $\varepsilon_i = +1$ for all $i = 1, \dots, n$, the previous definitions coincide with the definitions introduced in [17] of lowerly STP matrix and strict γ-matrix, and, if Σ is a diagonal matrix with diagonal entries $-1, +1, \dots, +1$, they coincide with the definitions introduced in [8] of lowerly TN matrix and strict γ^--matrix.

The following theorem gives a characterization of SSR matrices by their QR factorization and corresponds to Theorem 3.4 of [7].

Theorem 2.4. Let $A = (a_{ij})_{1\le i,j\le n}$ be an $n \times n$ matrix. Then A is SSR with signature $\varepsilon_1, \dots, \varepsilon_n$ if and only if for each $i = 1, \dots, n$,

$$A[i, \dots, n] = Q_i R_i, \quad (A[i, \dots, n])^T = \tilde{Q}_i \tilde{R}_i. \quad (3)$$

where $Q_i, \tilde{Q}_i$ are orthogonal strictly signed γ-matrices with signature $\varepsilon_1, \dots, \varepsilon_{n-i+1}$, and $R_i, \tilde{R}_i$ are nonsingular and upper triangular ΔTP matrices.

In the case of TP and TN matrices the characterization can be considerably simplified as the following result shows. It is a consequence of Theorem 4.7 of [17] and Theorem 3.1 of [8].

Theorem 2.5. Let $A = (a_{ij})_{1\le i,j\le n}$ be an $n \times n$ matrix. A is TP (resp., TN) if and only if

$$A = QR, \quad A^T = \tilde{Q}\tilde{R}, \quad (4)$$

where R and $\tilde{R}$ are upper triangular and ΔTP matrices and Q and $\tilde{Q}$ are orthogonal and strict γ-matrices (resp., γ^--matrices and $a_{nn} < 0$).

Golub and Yuan have introduced in [22] a symmetric-triangular decomposition of a nonsingular matrix. We now characterize SSR matrices in terms of this decomposition and corresponds to Theorem 5.1 of [7].

Theorem 2.6. Let $A = (a_{ij})_{1\le i,j\le n}$ be an $n \times n$ matrix. Then A is SSR with signature $\varepsilon_1, \dots, \varepsilon_n$ if and only if for each $i = 1, \dots, n$,

$$A[i, \dots, n] = S_i R_i, \quad (A[i, \dots, n])^T = \tilde{S}_i \tilde{R}_i \quad i = 1, \dots, n,$$

where S_i and $\tilde{S}_i$ are symmetric and lowerly signed matrices with signature $\varepsilon_1, \dots, \varepsilon_{n-i+1}$ and R_i and $\tilde{R}_i$ are upper triangular, unit diagonal matrices.

Taking into account that the symmetric and lowerly signed matrices S_i and $\tilde{S}_i$ of Theorem **??** can be written through their LDU-factorization as $S_i = L_{S_i} D_{S_i} L_{S_i}^T$ and $\tilde{S}_i = L_{\tilde{S}_i} D_{\tilde{S}_i} L_{\tilde{S}_i}^T$, we conclude that they are also upperly signed with the same signature $\varepsilon_1, \dots, \varepsilon_n$.

Again, in the case of TP and TN matrices the characterization can be considerably simplified as the following result shows. It is a consequence of Theorem 4.2 of [41] and Theorem 4.1 of [8].

Theorem 2.7. Let $A = (a_{ij})_{1\le i,j\le n}$ be an $n \times n$ matrix. A is TP (resp., TN) if and only if

$$A = SR, \quad A^T = \tilde{S}\tilde{R}, \quad (5)$$

where R and $\tilde{R}$ are upper triangular matrices with unit diagonal and S and $\tilde{S}$ are symmetric and lowerly TP matrices (resp., lowerly TN matrices and $a_{nn} < 0$).

Characterizations of TP matrices with other factorizations, such as Schur or singular value decompositions, can be found in [36].

III. FACTORIZATIONS OF M-MATRICES AND DIAGONALLY DOMINANT MATRICES

We start this section with some basic notation of Gaussian elimination. Gaussian elimination with a given pivoting strategy, for nonsingular matrices $A = (a_{ij})_{1\le i,j\le n}$, consists of a succession of at most $n-1$ major steps resulting in a sequence of matrices as follows:

$$A = A^{(1)} \longrightarrow \tilde{A}^{(1)} \longrightarrow \cdots \longrightarrow A^{(n)} = \tilde{A}^{(n)} = DU, \quad (6)$$

where $A^{(t)} = (a_{ij}^{(t)})_{1\le i,j\le n}$ has zeros below its main diagonal in the first $t-1$ columns and DU is upper triangular with the pivots on its main diagonal. The matrix $\tilde{A}^{(t)} = (\tilde{a}_{ij}^{(t)})_{1\le i,j\le n}$ is obtained from the matrix $A^{(t)}$ by reordering the rows and/or columns $t, t+1, \dots, n$ of $A^{(t)}$ according to the given pivoting strategy and satisfying $\tilde{a}_{tt}^{(t)} \ne 0$. To obtain $A^{(t+1)}$ from $\tilde{A}^{(t)}$ we produce zeros in column t below the *pivot element* $\tilde{a}_{tt}^{(t)}$ by subtracting multiples of row t from the rows beneath it. We say that we carry out a *symmetric pivoting strategy* when we perform the same row and column exchanges, that is, $PAP^T = LDU$, where P is the associated permutation matrix. A real matrix with nonpositive off-diagonal elements is called a Z-matrix. Let us recall that if a Z-matrix can be expressed as

$$A = sI - B, \quad B \geq 0, \quad s \geq \rho(B)$$

(where $\rho(B)$ is the spectral radius of B), then it is called an M-matrix. Nonsingular M-matrices form a subclass of Z-matrices and have important applications, for instance, in iterative methods in numerical analysis, in the analysis of dynamical systems, in economics and in mathematical programming. Nonsingular M-matrices have many equivalent definitions. In fact, in Theorem 2.3 in Chapter 6 of [4] appear fifty equivalent definitions.

A *rank revealing decomposition* of a matrix A is defined in [10] as a decomposition $A = XDY^T$, where X, Y are well conditioned and D is a diagonal matrix. In that paper it is shown that if we can compute an accurate rank revealing decomposition then we also can compute (with an algorithm presented there) an accurate singular value decomposition.

We say that we compute an accurate LDU-decomposition if we compute with small relative error each entry of L, D and U, that is, the relative error of each mentioned entry is bounded by $\mathcal{O}(\varepsilon)$, where ε is the machine precision. Given an algebraic expression defined by additions, subtractions, multiplications and divisions and assuming that each initial real datum is known to high relative accuracy, 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.

Given an M-matrix A diagonally dominant by rows (resp., columns), the off-diagonal elements and the row sums (resp., column sums) are natural parameters in many applications and that small relative changes in those quantities produce small relative changes in the entries of A (and of A^{-1} if A is nonsingular). In conclusion, we assume that, if A is diagonally dominant by columns, we know the off-diagonal entries and the column sums. From now on, let us assume that these natural parameters are given. In [11], Demmel and Koev used complete pivoting to obtain an accurate LDU-decomposition of an M-matrix diagonally dominant by columns that is a rank revealing decomposition because L is diagonally dominant by columns (and so it is very well conditioned) and U has rows whose entry of maximal absolute value belongs to the main diagonal (and so it is well conditioned).

In [40] we provided , given an M-matrix diagonally dominant by columns and knowing the off-diagonal entries and the column sums, an accurate LDU-decomposition of an M-matrix diagonally dominant by columns that is a rank revealing decomposition because L is diagonally dominant by columns (and so it is very well conditioned) and U diagonally dominant by rows (and so it is also very well conditioned). For this purpose we used the pivoting strategy that we now present.

In [37] we defined a symmetric *maximal absolute diagonal dominance* (m.a.d.d.) pivoting as a symmetric pivoting which chooses as pivot at the tth step ($1 \leq t \leq n-1$) a row $i_t (\geq t)$ satisfying

$$|a_{i_t i_t}^{(t)}| - \sum_{j \geq t, j \neq i_t} |a_{i_t j}^{(t)}| = \max_{t \leq i \leq n} \{|a_{ii}^{(t)}| - \sum_{j \geq t, j \neq i} |a_{ij}^{(t)}|\}.$$

In order to determine uniquely the strategy, we suppose that we choose the first index $i_t (\geq t)$ satisfying the previous property and such that $a_{i_t i_t}^{(t)} \neq 0$, and then we interchange the row and column t by the row and column i_t.

If we have an M-matrix A diagonally dominant by rows or columns, the symmetric m.a.d.d. pivoting also provides an LDU-decomposition with L and U very well conditioned as the following result (corresponding to Proposition 3.5 of [40]) shows.

Theorem 3.1.. If A is an M-matrix diagonally dominant by rows or columns and P is the permutation matrix associated to the symmetric m.a.d.d. pivoting strategy of A or A^T, respectively, then $PAP^T = LDU$, where L is a lower triangular matrix diagonally dominant by columns and U is an upper triangular matrix diagonally dominant by rows.

The corresponding efficient and with high relative accuracy algorithm for the LDU-decomposition of diagonally dominant M-matrices of Theorem 3.1 was developed in Section 4 of [40].

Recently, Ye has obtained in [45] the extension to all diagonally dominant matrices the accurate algorithms for their LDU-decomposition, so that this factorization provides a rank revealing decomposition. For this purpose he proposes the use of complete pivoting (as in [11]) as well as the symmetric m.a.d.d. pivoting of [40], called in [45] column diagonally dominant pivoting strategy.

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