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LDU DECOMPOSITIONS WITH L AND U WELL CONDITIONED *

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Abstract. We present, for some classes of matrices, LDU-decompositions whose unit triangular factors L and U are simultaneously very well conditioned. Our examples include diagonally dominant matrices by rows and columns and their inverses, Stieljes matrices and M-matrices diagonally dominant by rows or columns. We also show a construction of an accurate computation of the LDU-decomposition for any M-matrix diagonally dominant by rows or columns, which in turn can be applied to obtain an accurate singular value decomposition.

Key words. conditioning, diagonal dominance, pivoting strategies, accuracy, singular value decomposition.

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1. Introduction. A pivoting strategy that interchanges the rows and/or columns of an $n \times n$ matrix A is associated with permutation matrices P, Q such that $PAQ = LV$, where L is a unit lower triangular matrix (i.e., a lower triangular matrix with diagonal entries equal to one) and V the upper triangular matrix which appears after the elimination phase. If A is nonsingular, then (see also Section 4.1 of [8]), after obtaining the factorization $V = DU$ and so $A = LDU$ (with D a diagonal matrix and U a unit upper triangular), the solution to $Ax = b$ may be found by solving $Ly = b$ (forward substitution), $Dz = y$ and $Ux = z$ (backward substitution). Clearly, the well conditioning of both triangular matrices L, U is convenient for controlling the errors of the computed solution because then the forward and backward substitutions can be performed in a stable way (see [15] and the other references of the same authors included there).

The traditional condition number of a matrix A with respect to the norm $\|\cdot\|_\infty$ is given by $\kappa_\infty(A) := \|A\|_\infty \, \|A^{-1}\|_\infty$.

Examples of pivoting strategies which simultaneously control the conditioning of both triangular matrices L, U are the complete pivoting (of a computational cost of $\mathcal{O}(n^3)$ comparisons beyond the cost of Gauss elimination with no pivoting) and the rook pivoting (see [7], [15] and [9]), of lower computational cost (in the worst case, $\mathcal{O}(n^3)$ comparisons beyond the cost of Gauss elimination with no pivoting). Both pivoting strategies get triangular matrices such that the off-diagonal elements have absolute value bounded above by 1 (the absolute value of the diagonal elements). As we recall in Section 2, an $n \times n$ lower matrix with unit diagonal whose off-diagonal elements have absolute value bounded above by 1 can have $\kappa_\infty(L) = n2^{n-1}$, although it is usually much smaller. Let us also recall that there are problems where the conditioning of the lower and upper triangular matrices can have different importance: this happens, for instance, in the backward stability of Gauss-Jordan elimination, where the conditioning of the upper triangular matrix is crucial (see [10], [13] and [14]).

In addition to the problem of solving linear systems, another problem where the simultaneous well conditioning of both triangular matrices L, U is needed, corresponds to rank revealing decompositions, which in turn can be used to obtain accurate singular value decompositions, as we shall recall in Section 4 (see [4]).

In this paper we present, for some classes of matrices, pivoting strategies leading to LDU-decompositions such that $\min\{\kappa_\infty(L), \kappa_\infty(U)\} \le 2n$ and $\max\{\kappa_\infty(L), \kappa_\infty(U)\} \le n^2$. Besides, the corresponding pivoting strategies associated to such decompositions have

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low computational cost: in the worst case, $\mathcal{O}(n^2)$ elementary operations beyond the cost of Gauss elimination with no pivoting. We start by showing in Section 2 that diagonal dominance implies very well conditioning of both unit triangular matrices L, U. In Section 2 we also prove that if either a nonsingular matrix or its inverse is diagonally dominant by rows and columns, then we can assure an LDU-decomposition of A (without row or column exchanges) with L and U diagonally dominant by columns and rows, respectively.

In Section 3, we find LDU-decompositions with L and U diagonally dominant by columns and rows, respectively, in the cases of Stieljes matrices or M-matrices diagonally dominant by rows or columns. As for this last class of matrices, we show in Section 4 how to construct an accurate LDU-decomposition (i.e., with small relative error in each entry of L, D and U) satisfying the previous properties and with $\mathcal{O}(n^3)$ elementary operations beyond the cost of Gauss elimination with no pivoting.

In [5], Demmel and Koev also present a method to compute accurately an LDU-decomposition of an $n \times n$ M-matrix diagonally dominant by rows. They use symmetric complete pivoting and so they can guarantee that one of the obtained triangular matrices is diagonally dominant and the other one has the off-diagonal elements with absolute value bounded above by the diagonal elements, in contrast to our method, where we can guarantee that both triangular matrices are diagonally dominant. Our pivoting strategy needs to increase the computational cost of Gauss elimination in $\mathcal{O}(n^2)$ elementary operations, and this cost is greater than that of the symmetric complete pivoting (which only needs $\mathcal{O}(n^2)$ comparisons).

2. Auxiliary results and diagonal dominance. As we have commented above, the triangular factors of the LDU-decomposition appearing when we apply complete pivoting to an $n \times n$ nonsingular matrix have off-diagonal elements with absolute value bounded above by 1 and then their condition numbers are bounded in terms of n. It is well known that this bound is exponential. In fact, consider the unit lower triangular matrix L with -1 at each entry (i, j) with $i > j$. Then the corresponding entry of L^{-1} is 2^{j-i-1} and so $\kappa_\infty(L) = n2^{n-1}$. However, usually, small values for the condition numbers of L and U appear. This phenomenon is similar to that of the backward error in Gauss elimination with partial pivoting, which is usually much smaller than the theoretical exponential bound.

The following result shows that unit triangular matrices diagonally dominant by rows or columns are always very well conditioned.

PROPOSITION 2.1. *Let $T = (t_{ij})_{1 \le i,j \le n}$ be a unit triangular matrix diagonally dominant by columns (resp., rows). Then the elements of T^{-1} have absolute value bounded above by 1 and $\kappa_\infty(T) \le n^2$ (resp., $\kappa_\infty(T) \le 2n$).*

Proof. Let us assume that T is a unit lower triangular matrix diagonally dominant by columns. If we compute T^{-1} by a procedure similar to Gauss-Jordan elimination, but using column elementary operations instead of row elementary operations and starting from the last row, we can easily obtain the following bound for the absolute value of $(T^{-1})_{ij}$ for any $i \in \{1, \ldots, n\}$ and $i \ge j$:

$$
\begin{gathered}
|(T^{-1})_{ij}| \le \\
|t_{ij}| + |t_{i-1,j}|\,|(T^{-1})_{i,i-1}| + |t_{i-2,j}|\,|(T^{-1})_{i,i-2}| + \cdots + |t_{j+1,j}|\,|(T^{-1})_{i,j+1}|.
\end{gathered} \tag{2.1}
$$

Let us first prove that $|(T^{-1})_{ij}| \le 1$ when $i > j$ by induction on $i - j$. It holds when $i - j = 0$ because $|(T^{-1})_{ii}| = 1$ and when $i - j = 1$ because $|(T^{-1})_{j+1,j}| = |t_{j+1,j}| \le 1$. Let us assume that it holds when $i - j \le k$ and let us prove it when $i - j = k + 1$. In this case, if we apply the induction hypothesis to (2.1) we derive

$$|(T^{-1})_{ij}| \le \sum_{s \ne j} |t_{sj}| \le 1.$$

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Then $\|T^{-1}\|_\infty \leq n$ and so $\kappa_\infty(T) \leq n^2$.

If T is a unit upper triangular matrix diagonally dominant by columns, a similar proof for the bound of the absolute value of the elements of its inverse can be derived and then we get the same bounds for $\kappa_\infty(T)$. For the cases when T is diagonally dominant by rows, analogous proofs can also be derived for the absolute value of the elements of their inverse matrices and the bound for $\kappa_\infty(T)$ holds because in these cases $\|T\|_\infty \leq 2$. $\square$

Remark 2.1. When T is a unit triangular matrix diagonally dominant by columns and using $\kappa_1(A) := \|A\|_1 \|A^{-1}\|_1$ instead of κ_∞, we can deduce, from $\|T\|_1 \leq 2$ and the information provided in Proposition 2.1 on the elements of its inverse, that $\kappa_1(T) \leq 2n$.

By Proposition 2.1, we know that unit triangular matrices diagonally dominant by rows or columns are very well conditioned. So our next goal will be finding LDU factorizations with L and U very well conditioned. Let us start by showing in the next result a first example, where pivoting is not necessary.

PROPOSITION 2.2. *If A (resp., A^{-1}) is an $n \times n$ ($n \geq 2$) nonsingular matrix diagonally dominant by rows and columns, then the LDU-decomposition of A satisfies $\kappa_\infty(L) \leq n^2$ (resp., $\kappa_\infty(L) \leq 2n$) and $\kappa_\infty(U) \leq 2n$ (resp., $\kappa_\infty(U) \leq n^2$).*

Proof. Let us first assume that A is diagonally dominant by rows and columns. It is well known (cf. [16]) that diagonal dominance by rows or columns is inherited by the Schur complements obtained when performing Gauss elimination. So, the LDU-decomposition of A satisfies that L diagonally dominant by columns and U diagonally dominant by rows and, by Proposition 2.1, $\kappa_\infty(L) \leq n^2$ and $\kappa_\infty(U) \leq 2n$.

Let us now assume that A^{-1} is diagonally dominant by rows and columns. Given a matrix B, let $B^\#$ be the matrix obtained from B by reversing the order of its rows and columns (that is, $B^\# = PBP$, where P is the backward identity matrix). Besides, since $P^{-1} = P$, it can be proved that $\kappa_\infty(B^\#) = \kappa_\infty(B)$. Clearly, $(A^{-1})^\#$ is also diagonally dominant by rows and columns. Then, by the previous paragraph,

$$(A^{-1})^\# = LDU \tag{2.2}$$

with L unit lower triangular diagonally dominant by columns and U unit upper triangular diagonally dominant by rows. Premultiplicating and postmultiplicating (2.2) by P, we can deduce from (2.2) that

$$A^{-1} = L^\# D^\# U^\#$$

and so

$$A = (U^\#)^{-1}(D^\#)^{-1}(L^\#)^{-1}. \tag{2.3}$$

Let us observe that $L^\#$ (and so its inverse) is unit upper triangular and that $U^\#$ (and so its inverse) is unit lower triangular. Therefore, (2.3) gives the LDU-decomposition of A. Since, by Proposition 2.1, $\kappa_\infty((U^\#)^{-1}) = \kappa_\infty(U^\#) = \kappa_\infty(U) \leq 2n$ and $\kappa_\infty((L^\#)^{-1}) = \kappa_\infty(L^\#) = \kappa_\infty(L) \leq n^2$, the result follows. $\square$

3. Decompositions for Stieljes matrices and M-matrices diagonally dominant. 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 [3] appear fifty equivalent definitions. In particular, given a Z-matrix, the following three properties are equivalent: A is a nonsingular M-matrix, A^{-1} is nonnegative and all leading principal minors of A are strictly positive. A *Stieljes matrix* is a symmetric nonsingular M-matrix (see [3]). Taking into account the previous equivalences for M-matrices, we can also define a Stieljes matrix as a positive definite symmetric Z-matrix. In this section, we shall consider factorizations of Stieljes matrices and factorizations of M-matrices diagonally dominant by rows or columns. As we have commented in the introduction, we are interested in LDU-factorizations and so, in the context of symmetric matrices, in LDL^T-factorizations. Moreover, LDL^T is also sometimes preferred over the Cholesky factorization: with tridiagonal matrices or when it is convenient to avoid the calculation of square roots.

Given $k \in \{1, 2, \dots, n\}$, let α, β be two increasing sequence of k positive integers less than or equal to n. Then we denote by $A[\alpha|\beta]$ the $k \times k$ submatrix of A containing rows numbered by α and columns numbered by β. For principal submatrices, we use the notation $A[\alpha] := A[\alpha|\alpha]$. 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:

$$A = A^{(1)} \longrightarrow \tilde{A}^{(1)} \longrightarrow A^{(2)} \longrightarrow \tilde{A}^{(2)} \longrightarrow \cdots \longrightarrow A^{(n)} = \tilde{A}^{(n)} = DU, \tag{3.1}$$

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 $\tilde{a}_{tt}^{(t)} \neq 0$. 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.

In [12] 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 ($1 \le t \le n-1$) a row $i_t (\ge t)$ satisfying

$$|a_{i_t i_t}^{(t)}| - \sum_{j\ge t, j\ne i_t} |a_{i_t j}^{(t)}| = \max_{t\le i\le n} \{|a_{ii}^{(t)}| - \sum_{j\ge t, j\ne i} |a_{ij}^{(t)}|\}.$$

In order to determine uniquely the strategy, we suppose that we choose the first index $i_t (\ge t)$ 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.

Remark 3.1. By applying Theorem 2 of [1] to A^T, a nonsingular M-matrix A always has a diagonal element a_{ii} such that $(a_{ii} =)|a_{ii}| > \sum_{j\ne i} |a_{ij}|$ and so this property is satisfied by the pivot chosen by the symmetric m.a.d.d. pivoting strategy. Performing the corresponding row and column permutation of the matrix $A = A^{(1)}$ produces again a nonsingular M-matrix $\tilde{A}^{(1)}$. By [6], the Schur complement of an M-matrix is also an M-matrix. So, we can iterate the previous argument to the nonsingular M-matrices $A^{(t)}[t, \dots, n]$ and show that, if A is a nonsingular M-matrix, then the resulting upper triangular matrix DU is strictly diagonally dominant by rows.

Let us now focus on Stieljes matrices. Although Gauss elimination without pivoting of a positive definite symmetric matrix is stable, it does not guarantee the well conditioning of

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the triangular factors. So, we have to admit pivoting strategies and, in order to preserve the symmetry, symmetric pivoting strategies. For positive definite symmetric matrices, it is well known that we can perform symmetric complete pivoting (which increases in $\mathcal{O}(n^2)$ comparisons the computational cost) and obtaining the triangular matrix L with elements of absolute value bounded above by 1. However, if we have a Stieljes matrix and we apply the symmetric m.a.d.d. pivoting strategy, we get with a computational effort of $\mathcal{O}(n^2)$ elementary operations (as we shall recall at the end of the section) that the triangular factors are strictly diagonally dominant, and they can be much better conditioned than those obtained with symmetric complete pivoting, as shown in Example 3.1. In fact, if we have a Stieljes matrix and apply symmetric m.a.d.d. pivoting, then DL^T (and so L^T) is strictly diagonally dominant by rows by Remark 3.1. Therefore L is strictly diagonally dominant by columns. So, we have the following result.

PROPOSITION 3.1. *If A is an Stieljes matrix and P is the permutation matrix associated to the symmetric m.a.d.d. pivoting strategy, then $PAP^T = LDL^T$, where L is a unit lower triangular matrix strictly diagonally dominant by columns.*

The following example shows that applying symmetric complete pivoting to a Stieljes matrix does not guarantee that the triangular factors are diagonally dominant. In fact, we show a 3×3 matrix for which the symmetric complete pivoting produces triangular factors worse conditioned than those obtained by the symmetric m.a.d.d. pivoting. Moreover, the condition numbers of the triangular factors associated to the symmetric complete pivoting do not satisfy the bounds of Proposition 2.1 (which, in turn, are always satisfied by the triangular factors associated to the symmetric m.a.d.d. pivoting by Proposition 3.1).

Example 3.1. Given the Stieljes matrix

$$A = \begin{bmatrix} 100 & -70 & -70 \\ -70 & 199/2 & -1 \\ -70 & -1 & 99 \end{bmatrix},$$

then the permutation matrix associated to the symmetric complete pivoting is the identity and $A = LDL^T$, where

$$L = \begin{bmatrix} 1 & 0 & 0 \\ -7/10 & 1 & 0 \\ -7/10 & -100/101 & 1 \end{bmatrix}.$$

It can be checked that $\kappa_\infty(L) \approx 9.1$ and $\kappa_\infty(L^T) \approx 7.42$. However, the symmetric m.a.d.d. pivoting interchanges the first and second rows and columns in the first step of Gauss elimination and it still produces another row and column exchange in the second step. If P is the permutation matrix associated to the symmetric m.a.d.d. pivoting, then $PAP^T = LDL^T$, where

$$P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 1 & 0 & 0 \\ -2/199 & 1 & 0 \\ -140/199 & -14070/19699 & 1 \end{bmatrix},$$

and so $\kappa_\infty(L) \approx 5.86$ and $\kappa_\infty(L^T) \approx 2.95$.

The following remark shows that the symmetric m.a.d.d. pivoting also can be applied to an $n \times n$ M-matrix A of rank $r < n$ diagonally dominant by columns in order to obtain an upper triangular matrix $A^{(r+1)} = DU$, whose r first diagonal entries are nonzero.

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Remark 3.2. Let A be a nonzero $n \times n$ M-matrix A of rank $r < n$ diagonally dominant by columns. Since by Theorem 1 of [1], an M-matrix A always has a diagonal element a_{ii} such that

$$(a_{ii} =)|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|, \tag{3.2}$$

this property is satisfied by the pivot chosen by the symmetric m.a.d.d. pivoting strategy. Let $\{i_1, \dots, i_s\}$ be the set of row indices for which the corresponding diagonal element satisfies (3.2). Let us see that we can find a nonzero pivot satisfying (3.2). For this purpose, let us assume that $a_{i_1 i_1} = \cdots = a_{i_s i_s} = 0$ and we shall get a contradiction. From (3.2) we deduce that all off-diagonal elements of rows $i_1, \dots, i_s$ are also null. Since A is diagonally dominant by columns, all off-diagonal elements of columns $i_1, \dots, i_s$ are also null. Then we form the submatrix C obtained from A by deleting rows and columns $i_1, \dots, i_s$, which are null. It is well known that the principal submatrices of an M-matrix are also M-matrices (cf. Theorem 4.3 of Chapter 6 of [11]). Hence C is an M-matrix and, again by Theorem 2 of [1], there exists a diagonal element of C (and so of A) satisfying (3.2), contradiction which proves that we can find a nonzero pivot satisfying (3.2). Performing the corresponding row and column permutation of the matrix $A = A^{(1)}$ produces again an M-matrix diagonally dominant by columns $\tilde{A}^{(1)}$. By [6], the Schur complement of an M-matrix is also an M-matrix. So, we can iterate the previous argument to the nonzero M-matrices diagonally dominant by columns $A^{(t)}[t, \dots, n]$, $1 \leq t \leq r$. The matrix $A^{(r+1)}[r+1, \dots, n]$ is null. In conclusion, the symmetric m.a.d.d. pivoting applied to an $n \times n$ M-matrix A of rank $r < n$ diagonally dominant by columns has produced the following sequence of matrices (instead of (3.1)):

$$A = A^{(1)} \longrightarrow \tilde{A}^{(1)} \longrightarrow A^{(2)} \longrightarrow \tilde{A}^{(2)} \longrightarrow \cdots \longrightarrow A^{(r+1)} = DU, \tag{3.3}$$

where DU is an upper triangular matrix with its diagonal formed by the r nonzero pivots and $n - r$ zeros.

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 well conditioned as the following result shows.

PROPOSITION 3.2. *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.*

Proof. Let us assume that A is diagonally dominant by columns. By Remark 3.2, $PAP^T = LDU$, where the upper triangular matrix DU (and so U) is diagonally dominant by rows. As we have recalled in Section 2, diagonal dominance by columns is inherited by the Schur complements and hence L is diagonally dominant by columns.

If A is diagonally dominant by rows, we apply Gauss elimination with the symmetric m.a.d.d. pivoting to A^T (which is an M-matrix diagonally dominant by columns) and so, by the previous paragraph, there exists a permutation matrix P such that $PA^TP^T = LDU$, with L a lower triangular matrix diagonally dominant by columns and U an upper triangular matrix diagonally dominant by rows. So, $PAP^T = U^TD^TL^T$, where U^T is a lower triangular matrix diagonally dominant by columns and L^T is an upper triangular matrix diagonally dominant by rows. $\square$

Remark 3.3. If A is a nonsingular M-matrix strictly diagonally dominant by rows or columns, since strict diagonal dominance by columns is inherited by the Schur complements, one can deduce from the proof of the previous proposition and Remark 3.1 that in this case L is strictly diagonally dominant by columns and U is strictly diagonally dominant by rows.

As shown in Remark 4.6 and Proposition 4.7 of [12], if A is a nonsingular $n \times n$ M-matrix, the symmetric m.a.d.d. pivoting strategy consists of choosing as pivot row in each step the row whose elements give a maximal sum and it can be implemented in such a way that it costs $\mathcal{O}(n^2)$ elementary operations beyond the cost of Gauss elimination with no pivoting. Taking into account Remark 3.2, these properties also hold for singular M-matrices diagonally dominant by columns. In fact, following the notations of Proposition 4.7 of [12], let $e := (1, \ldots, 1)^T$ and $b_1 := Ae$, and let us assume that A is an $n \times n$ nonsingular M-matrix (resp., an M-matrix A of rank $r < n$ diagonally dominant by columns). The symmetric m.a.d.d. pivoting strategy produces the sequence of matrices (3.1) (resp., (3.3)) and the calculation of the corresponding sequence of vectors

$$b_1 = b_1^{(1)} \longrightarrow \tilde{b_1}^{(1)} \longrightarrow b_1^{(2)} \longrightarrow \tilde{b_1}^{(2)} \longrightarrow \cdots \longrightarrow b_1^{(m)} = \tilde{b_1}^{(m)},$$

where $m = n$ (resp., $m = r + 1$) increases in $\mathcal{O}(n^2)$ elementary operations the computational cost of Gaussian elimination. Then the maximal component among the last $n - k + 1$ components of $b_1^{(k)}$ gives the kth pivot of the symmetric m.a.d.d. pivoting strategy (take into account that each of those components of $b_1^{(k)}$ gives the sum of the elements of the corresponding row of the submatrix of $A^{(k)}[k \ldots, n]$, which is also an M-matrix and so it has nonnegative diagonal entries and nonpositive off-diagonal entries).

The next example shows that applying symmetric complete pivoting to an M-matrix diagonally dominant by columns does not guarantee that the upper triangular factor is diagonally dominant, in contrast to the symmetric m.a.d.d. pivoting, where both triangular factors are diagonally dominant. In fact, the condition number of the upper triangular factor corresponding to the symmetric complete pivoting is considerably larger than the condition number of the upper triangular factor corresponding to the symmetric m.a.d.d. pivoting.

Example 3.2. Given the M-matrix diagonally dominant by columns

$$A = \begin{bmatrix} 10 & -20/3 & -20/3 & -20/3 \\ -2 & 59/6 & -35/12 & -19/24 \\ -3 & -5/2 & 79/8 & -31/16 \\ -5 & -2/3 & -1/6 & 19/2 \end{bmatrix},$$

then the permutation matrix associated to the symmetric complete pivoting is the identity and $A = L_1 D_1 U_1$, where

$$L_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1/5 & 1 & 0 & 0 \\ -3/10 & -9/17 & 1 & 0 \\ -1/2 & -8/17 & -44/45 & 1 \end{bmatrix}, \quad U_1 = \begin{bmatrix} 1 & -2/3 & -2/3 & -2/3 \\ 0 & 1 & -1/2 & -1/4 \\ 0 & 0 & 1 & -9/10 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

If P is the permutation matrix associated to the symmetric m.a.d.d. pivoting, then $PAP^T = L_2 D_2 U_2$, where

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad L_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -4/59 & 1 & 0 & 0 \\ -15/59 & -6057/26752 & 1 & 0 \\ -40/59 & -1275/1672 & -4080/4139 & 1 \end{bmatrix}$$

and

$$U_2 = \begin{bmatrix} 1 & -19/236 & -35/118 & -12/59 \\ 0 & 1 & -301/17936 & -909/1672 \\ 0 & 0 & 1 & -27770/53807 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

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Both lower triangular matrices inherit the diagonal dominance by columns and so their condition numbers satisfy the corresponding bound of Proposition 2.1: $\kappa_\infty(L_1) \approx 11.67$ and $\kappa_\infty(L_2) \approx 13.59$. On the other hand, the upper triangular matrix U_2 obtained by the symmetric m.a.d.d. pivoting is diagonally dominant by rows and satisfies $\kappa_\infty(U_2) \approx 2.81$. In contrast, the upper triangular matrix U_1 obtained by the symmetric complete pivoting is not diagonally dominant by rows and its condition number does not satisfy the corresponding bound of Proposition 2.1 and is considerably greater than that of U_2: $\kappa_\infty(U_1) = 13.2$.

4. An efficient and accurate algorithm for the LDU-decomposition of diagonally dominant M-matrices. A *rank revealing decomposition* of a matrix A is defined in [4] 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. Given an M-matrix diagonally dominant by rows or columns, by Proposition 3.2 and Proposition 2.1 the LDU-factorization associated to symmetric m.a.d.d. pivoting is a rank revealing decomposition. In this section, we show that we can compute accurately this LDU-factorization. For this purpose, we shall assume that we have an $n \times n$ M-matrix A of rank r diagonally dominant by columns (if it is diagonally dominant by rows we can apply the construction to A^T). In [2] it is shown that, 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.

Let us consider the sequences of matrices (3.1) (if $r = n$) or (3.3) (if $r < n$) obtained when applying symmetric m.a.d.d. pivoting to $A = A^{(1)}$. Since $A^{(1)}$ is an M-matrix, it has nonnegative diagonal entries and nonpositive off-diagonal entries and since $A^{(1)}$ is diagonally dominant by columns, the vector $c^{(1)} := e^T A^{(1)}$ provided by the column sums of $A^{(1)}$ is nonnegative. When applying symmetric m.a.d.d. pivoting, we can calculate the corresponding sequence of vectors:

$$c^{(1)} \longrightarrow \tilde{c}^{(1)} \longrightarrow c^{(2)} \longrightarrow \tilde{c}^{(2)} \longrightarrow \cdots \longrightarrow c^{(m)} = \tilde{c}^{(m)},$$

(where $m = n$ if $r = n$ and $m = r+1$ if $r < n$), giving $c^{(k)}$ and $\tilde{c}^{(k)}$ the column sums of the corresponding matrices $A^{(k)}[k, \ldots, n]$ and $\tilde{A}^{(k)}[k, \ldots, n]$, respectively. If A is a singular M-matrix of rank $r < n$ diagonally dominant by columns, then there will be r nonzero pivots and the Schur complement $A^{r+1)}[r+1, \ldots, n]$ will be null.

Let us see a simple relation of the last $n-k$ components $c_j^{(k+1)}$ ($j = k+1, \ldots, n$) of the vector $c^{(k+1)}$ and the components of $\tilde{c}^{(k)}$. In fact,

$$c_j^{(k+1)} = \sum_{i=k+1}^{n} a_{ij}^{(k+1)} = \sum_{i=k+1}^{n} \left(\tilde{a}_{ij}^{(k)} - \frac{\tilde{a}_{ik}^{(k)}}{\tilde{a}_{kk}^{(k)}} \tilde{a}_{kj}^{(k)} \right) = \sum_{i=k+1}^{n} \tilde{a}_{ij}^{(k)} - \tilde{a}_{kj}^{(k)} \left(\sum_{i=k+1}^{n} \frac{\tilde{a}_{ik}^{(k)}}{\tilde{a}_{kk}^{(k)}} \right). \tag{4.1}$$

Taking into account that

$$\sum_{i=k+1}^{n} \frac{\tilde{a}_{ik}^{(k)}}{\tilde{a}_{kk}^{(k)}} = \frac{\tilde{c}_k^{(k)} - \tilde{a}_{kk}^{(k)}}{\tilde{a}_{kk}^{(k)}},$$

we deduce from (4.1) that

$$c_j^{(k+1)} = \sum_{i=k}^{n} \tilde{a}_{ij}^{(k)} - \frac{\tilde{a}_{kj}^{(k)}}{\tilde{a}_{kk}^{(k)}} \tilde{c}_k^{(k)}$$

and so

$$c_j^{(k+1)} = \tilde{c}_j^{(k)} - \frac{\tilde{a}_{kj}^{(k)}}{\tilde{a}_{kk}^{(k)}} \tilde{c}_k^{(k)}, \quad j = k+1, \ldots, n. \tag{4.2}$$

Remark 4.1. We have commented in previous sections that if a matrix $\tilde{A}^{(k)}$ is diagonally dominant by columns, then its Schur complement $A^{(k+1)}[k+1, \ldots, n]$ is also diagonally dominant by columns. If, in addition, the matrix $\tilde{A}^{(k)}$ is a nonsingular M-matrix, we can apply formula (4.2) and deduce that the diagonal dominance by columns is increased. In fact, since $\tilde{a}_{kj}^{(k)} \leq 0$, $\tilde{a}_{kk}^{(k)} > 0$ and $\tilde{c}_k^{(k)} > 0$, we derive from (4.2)

$$c_j^{(k+1)} \geq \tilde{c}_j^{(k)}. \tag{4.3}$$

Remark 4.2. Given a nonsingular $n \times n$ M-matrix A diagonally dominant by columns, (4.2) also shows that we can calculate the vectors $(c^{(k)})_{2 \leq k \leq n}$ from $c^{(1)}$ with an additional cost of $\mathcal{O}(n^2)$ elementary operations to that of Gauss elimination with symmetric m.a.d.d. pivoting. As we have commented above, we assume that we know the off-diagonal entries and the vector $c^{(1)}$ of column sums.

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 (cf. p. 52 of [4]). In other words, the only forbidden operation is true subtraction, due to possible cancellation in leading digits.

Let us see that we can can compute accurately the LDU-factorization associated to Gauss elimination with symmetric m.a.d.d. pivoting of an M-matrix $A = A^{(1)}$ diagonally dominant by columns *if we know the off-diagonal elements* $a_{ij}^{(1)} (\leq 0)$ $(i \neq j)$ *and the column sums* $c_j^{(1)} (\geq 0)$ $(j = 1, \ldots, n)$ of the matrix. Since we know the off-diagonal elements and all are nonpositive, then we can calculate accurately their column sums:

$$s_j^{(1)} = \sum_{i=1, i \neq j}^{n} a_{ij}^{(1)}, \quad j = 1, \ldots, n. \tag{4.4}$$

Clearly, calculating $s_j^{(1)}$, $j = 1, \ldots, n$, requires $n(n-2)$ sums. Again, when applying symmetric m.a.d.d. pivoting, we can calculate the corresponding sequence of vectors:

$$s^{(1)} \longrightarrow \tilde{s}^{(1)} \longrightarrow s^{(2)} \longrightarrow \tilde{s}^{(2)} \longrightarrow \cdots \longrightarrow s^{(m)} \longrightarrow \tilde{s}^{(m)},$$

(where $m = n-1$ if A is nonsingular and $m = r$ if rank$A = r < n$) giving $s^{(k)}$ and $\tilde{s}^{(k)}$ the column sums of the off-diagonal elements of the corresponding matrices $A^{(k)}[k, \ldots, n]$ and

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$\tilde{A}^{(k)}[k,\ldots,n]$, respectively (see (3.1) or (3.3)). Observe that

$$s_j^{(k+1)} = \sum_{i=k+1, i\neq j}^{n} a_{ij}^{(k+1)}, \quad j = k+1,\ldots,n. \tag{4.5}$$

We can calculate by (4.5) the column sums of the off-diagonal elements $s_j^{(k+1)}$ with an additional cost of $\mathcal{O}(n^3)$ elementary operations.

In conclusion, given the off-diagonal elements and the column sums, we have seen that we can calculate accurately $s_j^{(1)}(\leq 0)$ $(j = 1,\ldots,n)$ and then we can perform accurately the following steps:

1. Calculation of the diagonal elements of $A = A^{(1)}$: $a_{jj}^{(1)} = c_j^{(1)} - s_j^{(1)}$, $j = 1,\ldots,n$.

2. After applying the symmetric m.a.d.d. pivoting in order to choose the first pivot and forming the matrix $\tilde{A}^{(1)}$ (whose column sums $\tilde{c}_j^{(1)}$ coincide, up to the order, with those of $A^{(1)}$), we calculate the multipliers

$$l_{i1} = \frac{\tilde{a}_{i1}^{(1)}}{\tilde{a}_{11}^{(1)}}(\leq 0), \quad i = 2,\ldots,n.$$

3. Calculation of the off-diagonal elements of $A^{(2)}[2,\ldots,n]$: $a_{ij}^{(2)} = \tilde{a}_{ij}^{(1)} - l_{i1}\tilde{a}_{1j}^{(1)}$ (observe that $\tilde{a}_{ij}^{(1)}$ and $-l_{i1}\tilde{a}_{1j}^{(1)}$ are both nonpositive).

4. Calculation of the column sums of $A^{(2)}[2,\ldots,n]$ by (4.2) for $k = 1$ (observe that $\tilde{c}_j^{(1)}$ and $-\frac{\tilde{a}_{1j}^{(1)}}{\tilde{a}_{11}^{(1)}}\tilde{c}_1^{(1)}$ are both nonnegative).

5. Calculation of the column sums of the off-diagonal elements of $A^{(2)}[2,\ldots,n]$ by (4.5) (observe that all elements $a_{ij}^{(2)}$, $i \in \{2,\ldots,n\} - \{j\}$, are nonpositive).

Now we can iterate the previous procedure with the corresponding sequence of matrices $A^{(2)}[2,\ldots,n],\ldots,A^{(n-1)}[n-1,n]$, until obtaining DU from which we also can compute accurately D and U (if rank$A = r < n$, we can stop after calculating r matrices of the sequence because the matrix $A^{(r+1)}[r+1,\ldots,n]$ is null).

Remark 4.3. The computational cost of the previous procedure to compute accurately the LDU-factorization associated to Gauss elimination with symmetric m.a.d.d. pivoting of a nonsingular $n \times n$ M-matrix diagonally dominant by columns is $\mathcal{O}(n^3)$ elementary operations. This follows from the following facts: calculating $s_j^{(1)}$, $j = 1,\ldots,n$ requires $\mathcal{O}(n^2)$ elementary operations, the symmetric m.a.d.d. pivoting strategy can be implemented so that it adds $\mathcal{O}(n^2)$ elementary operations to the $\mathcal{O}(n^3)$ elementary operations of Gauss elimination (as shown at the end of the previous section), the iterated application of step 1 of the previous procedure increases a total cost of $\mathcal{O}(n^2)$ elementary operations, the iterated application of step 4 of the previous procedure increases a total cost of $\mathcal{O}(n^2)$ elementary operations (see Remark 4.2), the iterated application of step 5 of the previous procedure increases a total cost of $\mathcal{O}(n^3)$ elementary operations and obtaining D and U from DU adds $\mathcal{O}(n^2)$ elementary operations.

By Propositions 3.2 and 2.1, the LDU-factorization associated to symmetric m.a.d.d. pivoting of a nonsingular $n \times n$ M-matrix diagonally dominant by columns is a rank revealing decomposition and, by Remark 4.3, we can compute it accurately with $\mathcal{O}(n^3)$ elementary operations. Finally, let us take into account that the algorithm of [4] for computing an accurate singular value decomposition from a rank revealing decomposition has a complexity of $\mathcal{O}(n^3)$ elementary operations.

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