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Multiple LU factorizations of a singular matrix ☆

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Abstract

A singular matrix A may have more than one LU factorizations. In this work the set of all LU factorizations of A is explicitly described when the lower triangular matrix L is nonsingular. To this purpose, a canonical form of A under left multiplication by unit lower triangular matrices is introduced. This canonical form allows us to characterize the matrices that have an LU factorization and to parametrize all possible LU factorizations. Formulae in terms of quotient of minors of A are presented for the entries of this canonical form.

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1. Introduction

An m-by-n matrix $A = (A_{ij})$ is called lower (upper) triangular if $A_{ij} = 0$ whenever $i < (>)\, j$. A general m-by-n matrix A over the complex field $\mathbb{C}$ has an LU factorization if it can be written as

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$A = LU$ with L m-by-m lower triangular and U m-by-n upper triangular. The results we present remain valid for a general field $\mathbb{K}$. We restrict ourselves to $\mathbb{C}$ for the sake of simplicity.

For a variety of uses, it is convenient to have a matrix factored (implicitly or explicitly) as $A = LU$, especially if L may be taken to be nonsingular. Unfortunately, not every matrix has an LU factorization and fewer still have one with L nonsingular. It is known which matrices have an LU factorization [4] and which have one with L nonsingular [6] (see also Theorem 4 below). A nonsingular L can be normalized to have 1's on the diagonal; a lower triangular matrix normalized in such way will be called *unit lower triangular*. We shall henceforth assume that all the lower triangular matrices L in this work are nonsingular unit lower triangular.

If an n-by-n matrix A is nonsingular and has an LU factorization L and U will be unique [3]. The latter remains true if only the leading $n-1$ principal minors of A are nonzero [2] (see also Corollary 2 below). However, in all other cases in which an LU factorization exists with L unit lower triangular, there is ambiguity in the pair L, U. For example

$$\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ a & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 1-a \end{bmatrix},$$

with a free. Of course, $U = L^{-1}A$, so that any ambiguity is fully described among the factors L.

Our purpose here is to fully describe the collection of all LU factorizations, with L unit lower triangular, of any matrix A for which such a factorization exists. In particular, all the L's that occur are parametrically described, so that the degrees of freedom in L may be counted. Of course, all the U's that occur may and will be described as $U = L^{-1}A$. The key tool will be another factorization (it will be called `RRMCF` factorization) achievable for any matrix A under left multiplication by unit lower triangular matrices. This will introduce a new canonical form (whose entries can be determined in terms of quotients of minors of A), by which it will be easy to characterize the matrices having an LU factorization. Besides, previous characterizations of existence follow from the work herein. Finally, formulae, in terms of quotients of minors of A, the denominators of which are nonzero, are given for those entries of L and U that are uniquely determined.

We frequently appeal to submatrices. To refer to them, we will use ordered set of indices.

Notation 1. The ordered p-tuple $\alpha = [i_1, i_2, \ldots, i_p]$ is the ordered set of natural numbers that has i_1 as its first element, i_2 as its second element, ..., and i_p as its pth element. Given two ordered sets, $\alpha = [i_1, i_2, \ldots, i_p]$ and $\beta = [j_1, j_2, \ldots, j_q]$, we will also use $[\alpha, \beta] \equiv [i_1, i_2, \ldots, i_p, j_1, j_2, \ldots, j_q]$.

Observe that, contrary to the usual convention, these sets of indices, referring to rows or columns of a matrix, are not necessarily in increasing order. Many times we will have to use consecutive sets of indices. In these cases we will adopt the following MATLAB™ [7] style notation.

Notation 2. For any pair of natural numbers p, q, we denote

$$p : q = \begin{cases} [p, p+1, \ldots, q], & \text{if } p < q; \\ p, & \text{if } p = q; \\ \emptyset, & \text{if } p > q. \end{cases}$$

In a similar way we will use the notation $r_{1:q} \equiv [r_1, r_2, \ldots, r_q]$.

The set of all complex m-by-n matrices will be denoted by $\mathbb{C}^{m\times n}$. The different submatrices of a given matrix will be referred to as follows.

Notation 3. For any matrix $A \in \mathbb{C}^{m\times n}$

1. $A(\alpha, \beta)$, where α and β are ordered subsets of, respectively, $\{1, \dots, m\}$ and $\{1, \dots, n\}$, is the submatrix of A with row indices α and column indices β.
2. $A(k, j)$, where $k \in \{1, \dots, m\}$, $j \in \{1, \dots, n\}$, is the (k, j) entry of A. For single entries we will also use the conventional subscript notation A_{kj}.
3. $A(k, 1 : n)$, where $k \in \{1, \dots, m\}$, is the kth row of A.
4. $A(1 : m, j)$, where $j \in \{1, \dots, n\}$, is the jth column of A.

The identity matrix of order n will be denoted by $\mathbb{I}_n \in \mathbb{R}^{n\times n}$. According to what was said above, we use throughout the rest of this work the following definition.

Definition 1. $A \in \mathbb{C}^{m\times n}$ has an LU factorization if it can be written as

$$A = LU,$$

with $L \in \mathbb{C}^{m\times m}$ unit lower triangular and $U \in \mathbb{C}^{m\times n}$ upper triangular.

Finally, the row space of any matrix B, i.e., the subspace spanned by the rows of B, will be denoted by $\mathrm{Row}\{B\}$.

2. Rank revealing minimal canonical form (`RRMCF`)

A primary tool that we use throughout this work is a simple canonical form associated with a matrix. This is achievable through row reduction but using only downward row substitutions *without* permutation or scaling of rows. This is a variation upon the usual `Row Reduced Echelon Form` used in Gaussian Elimination [3,5].

Definition 2. For any $A \in \mathbb{C}^{m\times n}$,

1. A zero row is a row in which all entries are zero.
2. A leading entry of a nonzero row is the leftmost nonzero entry in that row.
3. A is in Rank Revealing Minimal Canonical Form (`RRMCF`) if all the entries below each leading entry are zero. The set $\{(r_k, c_k)\}_{k=1}^{q}$, where $r_1 < r_2 < \cdots < r_q$, indicates the positions of the leading entries in the nonzero rows. Notice that $\operatorname{rank}(A) = q$.

That is, $A \in \mathbb{C}^{m\times n}$, with $\operatorname{rank}(A) = q$, is in `RRMCF` if:

$$\begin{cases} A(r_k, c_k) \neq 0, & \text{for } k \in \{1, \dots, q\}; \\ A(i, j) = 0, & \text{if } i \notin \{r_1, \dots, r_q\}, \text{ for } j \in \{1, \dots, n\}; \\ A(r_k, j) = 0, & \text{if } j < c_k, \text{ for } k \in \{1, \dots, q\}; \\ A(i, c_k) = 0, & \text{if } i > r_k, \text{ for } k \in \{1, \dots, q\}. \end{cases}$$

We illustrate this key definition with an example.

Example 1. The following matrix is in RRMCF.

$$A = \begin{bmatrix} 0 & 0 & 0 & \boxed{4} & 2 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \boxed{6} & 1 & 0 & 4 & 0 \\ \boxed{-8} & 0 & -1 & 0 & 1 & 5 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{-1} & 1 \end{bmatrix}.$$

The leading entries are boxed:

$$\{(r_k, c_k)\}_{k=1}^4 = \{(1, 4), (3, 2), (4, 1), (6, 5)\}.$$

Observe that after some elementary row operations (including permutations and scalings) a matrix in RRMCF can be reduced to the `Row Reduced Echelon Form`, but the position of the pivot columns in the latter are fixed by the column positions of the leading entries in the RRMCF, i.e., $\{c_1, \dots, c_q\}$. We call the RRMCF minimal in the sense that any matrix can be transformed to another matrix in RRMCF through the use of only one type of elementary row operation, more precisely, downward row substitutions; this is the same as saying that any matrix can be transformed to another matrix in RRMCF through left multiplication by a unit lower triangular matrix. Observe also that the positions of the rows containing the leading entries are ordered, $r_1 < r_2 < \cdots < r_q$, while the positions of the columns containing the leading entries in general are not.

A simple algorithm to transform a general matrix A into RRMCF form, denoted $\mathscr{U}(A) = \mathscr{U}$, is given by the following pseudo-code:

Algorithm 1. RRMCF

Input: $A \in \mathbb{C}^{m \times n}$
Output: $L \in \mathbb{C}^{m \times m}$ unit lower triangular and $\mathscr{U} \in \mathbb{C}^{m \times n}$ in RRMCF such that $A = L\mathscr{U}$
$L = \mathbb{I}_m$;
$k = 0$;
for $i = 1 : m$
  if row i of A is nonzero **then**
    $k = k + 1$; $r_k = i$;
    c_k is the column of the leading entry in row i;
    for $j = r_k + 1 : m$
      do an elementary row substitution to make $A(j, c_k) = 0$, using $A(r_k, c_k)$ as pivot;
      store the multiplier used in $L(j, r_k) = A(j, c_k)/A(r_k, c_k)$;
    end for
  end if
end for
$\mathscr{U} = A$.

Definition 3. Given $A \in \mathbb{C}^{m \times n}$ we will say that $A = L\mathscr{U}$ is an RRMCF decomposition of A if $\mathscr{U} \in \mathbb{C}^{m \times n}$ is in RRMCF and $L \in \mathbb{C}^{m \times m}$ is unit lower triangular. It will be said that $\mathscr{U}$ is the RRMCF of A.

The following is an example of an RRMCF decomposition obtained with Algorithm 1.

Example 2. Let $A \in \mathbb{R}^{8\times 7}$ be

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 1 & -1 & 2 \\ 0 & -2 & 1 & 6 & 6 & -2 & 5 \\ 0 & 4 & -2 & 6 & -6 & -2 & 2 \\ 2 & 4 & -3 & -6 & -9 & 5 & -5 \\ 0 & 2 & -1 & -9 & -7 & 3 & -7 \\ -4 & -2 & 3 & -3 & 3 & -4 & -4 \\ 2 & 4 & -3 & -3 & -10 & 3 & -2 \end{bmatrix}.$$

Algorithm 1 gives $A = L\mathcal{U}$ with

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & -2 & -2 & 0 & 1 & 0 & 0 & 0 \\ 0 & -3 & -1 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & -2 & 0 & 1 & 0 \\ 0 & -1 & -2 & 0 & 1 & 0 & -1 & 1 \end{bmatrix},$$

$$\mathcal{U} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \boxed{3} & 1 & -1 & 2 \\ 0 & \boxed{-2} & 1 & 0 & 4 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \boxed{2} & 0 & -1 & 0 & 1 & 3 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \boxed{2} & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The positions of the leading entries are

$$\{(r_k, c_k)\}_{k=1}^{4} = \{(2, 4), (3, 2), (5, 1), (7, 5)\}.$$

Observe that Algorithm 1 shows that any matrix has at least one RRMCF decomposition. Our next theorem shows that the $\mathcal{U}$ factor is unique, so it is appropriate to call $\mathcal{U}$ *the* RRMCF of A, and precisely in this sense $\mathcal{U}$ is the *canonical* form of A under left multiplication by unit lower triangular matrices.

Theorem 1. *Let $A \in \mathbb{C}^{m\times n}$, then there is a unique matrix $\mathcal{U} \in \mathbb{C}^{m\times n}$ in* RRMCF *such that*

$$A = L\mathcal{U}$$

being $L \in \mathbb{C}^{m\times m}$ unit lower triangular.

Proof. Let $A = L\mathcal{U} = L'\mathcal{U}'$ be two different RRMCF decompositions. Then $L'^{-1}L\mathcal{U} \equiv \widetilde{L}\mathcal{U} = \mathcal{U}'$ with $\widetilde{L}$ unit lower triangular. This implies that $\mathrm{Row}\{\mathcal{U}'(1 : p, 1 : n)\} = \mathrm{Row}\{\mathcal{U}(1 : p, 1 : n)\}$, for

$p \in \{1, \dots, m\}$, that $\mathscr{U}'$ and $\mathscr{U}$ have the same rank, and the same number of zero rows. Besides, both are in RRMCF, and therefore the nonzero rows are linearly independent in each matrix. All this implies that the zero rows are the same in each matrix: if $\mathscr{U}(p, 1:n) = 0$ and $\mathscr{U}'(p, 1:n) \neq 0$ for some $p \in \{1, \dots, m\}$, this would imply that $\dim \mathrm{Row}\{\mathscr{U}(1:p, 1:n)\} = \dim \mathrm{Row}\{\mathscr{U}(1:p-1, 1:n)\} = \dim \mathrm{Row}\{\mathscr{U}'(1:p-1, 1:n)\} = \dim \mathrm{Row}\{\mathscr{U}'(1:p, 1:n)\} - 1$, that is $0 = -1$, which is impossible.

Let us pay attention to the nonzero rows. We have that for the first nonzero row

$$\mathscr{U}'(r_1, 1:n) = \widetilde{L}(r_1, 1:m)\mathscr{U}(1:m, 1:n) = \widetilde{L}(r_1, r_1)\mathscr{U}(r_1, 1:n) = \mathscr{U}(r_1, 1:n)$$

because $\widetilde{L}$ is unit lower triangular. Let us now suppose that

$$\mathscr{U}'(r_i, 1:n) = \mathscr{U}(r_i, 1:n) \quad \text{for } i = 1, \dots, s \tag{1}$$

and let us show that $\mathscr{U}'(r_{s+1}, 1:n) = \mathscr{U}(r_{s+1}, 1:n)$.

From (1) we conclude that

$$\mathscr{U}'(k, c_i) = \mathscr{U}(k, c_i) = 0 \quad \text{for } k > r_i \text{ and } i = 1, \dots, s. \tag{2}$$

Let us write

$$\mathscr{U}'(r_{s+1}, 1:n) = \widetilde{L}(r_{s+1}, 1:m)\mathscr{U}(1:m, 1:n) = \widetilde{L}(r_{s+1}, r_{1:s+1})\mathscr{U}(r_{1:s+1}, 1:n). \tag{3}$$

From (2) and (3) we have

$$0 = \mathscr{U}'(r_{s+1}, c_1) = \widetilde{L}(r_{s+1}, r_1)\mathscr{U}(r_1, c_1),$$

and, because $\mathscr{U}(r_1, c_1) \neq 0$ we have that

$$\widetilde{L}(r_{s+1}, r_1) = 0.$$

Now, we can use induction to prove that $\widetilde{L}(r_{s+1}, r_{1:s}) = 0$. Supposing that $\widetilde{L}(r_{s+1}, r_{1:p}) = 0$ for a given $p < s$, we get from (3) that

$$\mathscr{U}'(r_{s+1}, c_{p+1}) = \widetilde{L}(r_{s+1}, r_{p+1:s+1})\mathscr{U}(r_{p+1:s+1}, c_{p+1})$$

but $\mathscr{U}'(r_{s+1}, c_{p+1}) = 0$ and $\mathscr{U}(r_{p+2:s+1}, c_{p+1}) = 0$ because of (2), what implies

$$0 = \widetilde{L}(r_{s+1}, r_{p+1})\mathscr{U}(r_{p+1}, c_{p+1})$$

and finally $\widetilde{L}(r_{s+1}, r_{p+1}) = 0$, because $\mathscr{U}(r_{p+1}, c_{p+1}) \neq 0$. As a consequence of $\widetilde{L}(r_{s+1}, r_{1:s}) = 0$ we have finally from (3) that

$$\mathscr{U}'(r_{s+1}, 1:n) = \mathscr{U}(r_{s+1}, 1:n)$$

and all the nonzero rows are the same in $\mathscr{U}'$ and $\mathscr{U}$. Because the zero rows are also in the same position we have that $\mathscr{U}' = \mathscr{U}$. □

Observe that though the matrix $\mathscr{U}$ produced by Algorithm 1 is unique, if $\mathscr{U}$ has zero rows there are many unit lower triangular matrices $L(\alpha)$ such that $A = L(\alpha)\mathscr{U}$, in which the parameters α denote the entries below the diagonal in the columns of L corresponding to the zero rows of $\mathscr{U}$. In Example 2 it can be seen that the entries below the diagonal in the columns 1, 4 and 6 of L are arbitrary because they correspond to the zero rows in $\mathscr{U}$. When we get to the LU factorization (Theorem 5), in which case $\mathscr{U}$ has to be upper triangular, those free parameters in L will still be present, but this will not be the full multiplicity existing in the L. We will show in Lemma 1 that there are more free parameters in the factor L than those due to the zero rows in $\mathscr{U}$. Those new parameters will come from the possibility of changing $\mathscr{U}$ while keeping it upper triangular.

Theorem 1 says that the matrix $\mathscr{U}$, the RRMCF of any matrix A, is unique. The next two theorems show that every entry of $\mathscr{U}$ can be given explicitly in term of minors of A. First, Theorem 2 shows that the set of indices $\{(r_k, c_k)\}_{k=1}^{q}$ that determines the positions of the leading entries in the RRMCF can be characterized using the value of some nonzero minors of A. The entire set can be obtained recursively.

Theorem 2. *Let* $A \in \mathbb{C}^{m\times n}$ *have* $\operatorname{rank}(A) = q$ *and let* $\mathscr{U}$ *be its unique* RRMCF *with leading entries in positions* $\{(r_k, c_k)\}_{k=1}^{q}$. *Then*

1. *The first pair* (r_1, c_1) *is the position of the leading entry of the first nonzero row of* A.
2. *If the first* s *leading entries* $\{(r_k, c_k)\}_{k=1}^{s}$, $s < q$, *are known*, (r_{s+1}, c_{s+1}) *is determined by*
$$(r_{s+1}, c_{s+1}) = \min_{1\leqslant j\leqslant n, r_s<i\leqslant m} \{(i, j) : \det A([r_{1:s}, i], [c_{1:s}, j]) \neq 0\},$$
where the minimum is to be understood with respect to the lexicographical order in the set $\{(i, j)\}_{i=1,j=1}^{i=m,j=n}$.
3. *The zero rows of* $\mathscr{U}$, i, *between* r_s *and* r_{s+1} *are those for which* $\det A([r_{1:s}, i], [c_{1:s}, j]) = 0$ *for all* $1 \leqslant j \leqslant n$.

Proof. Let us assume that $A = L\mathscr{U}$ with $\mathscr{U} \in \mathbb{C}^{m\times n}$ its unique RRMCF and $L \in \mathbb{C}^{m\times m}$ unit lower triangular. Then, for $s \in \{1, \ldots, q\}$,

$$\begin{aligned}A(r_{1:s}, c_{1:s}) &= L(r_{1:s}, 1 : m)\mathscr{U}(1 : m, c_{1:s})\\ &= L(r_{1:s}, r_{1:q})\mathscr{U}(r_{1:q}, c_{1:s}) = L(r_{1:s}, r_{1:s})\mathscr{U}(r_{1:s}, c_{1:s}),\end{aligned}$$

and

$$\det A(r_{1:s}, c_{1:s}) = \det \mathscr{U}(r_{1:s}, c_{1:s}) = \prod_{i=1}^{s} \mathscr{U}(r_i, c_i) \neq 0$$

so $\operatorname{rank}(A(r_{1:s}, c_{1:s})) = s$. If $r_s < i < r_{s+1}$ and $1 \leqslant j \leqslant n$

$$\begin{aligned}A([r_{1:s}, i], [c_{1:s}, j]) &= L([r_{1:s}, i], r_{1:q})\mathscr{U}(r_{1:q}, [c_{1:s}, j])\\ &= L([r_{1:s}, i], r_{1:s})\mathscr{U}(r_{1:s}, [c_{1:s}, j]).\end{aligned}$$

The last equality follows from the fact that $L(i, r_{s+1:q}) = 0$. Therefore $\det A([r_{1:s}, i], [c_{1:s}, j]) = 0$ because it is the product of two rank s matrices.

Now let us consider:

$$\begin{aligned}A(r_{1:s+1}, [c_{1:s}, j]) &= L(r_{1:s+1}, r_{1:q})\mathscr{U}(r_{1:q}, [c_{1:s}, j])\\ &= L(r_{1:s+1}, r_{1:s+1})\mathscr{U}(r_{1:s+1}, [c_{1:s}, j])\end{aligned}$$

and

$$\det A(r_{1:s+1}, [c_{1:s}, j]) = \det \mathscr{U}(r_{1:s+1}, [c_{1:s}, j]). \tag{4}$$

The minimum j for which the right hand side is nonzero is $j = c_{s+1}$ and therefore the lemma is proved. □

It has already been noted that some of the entries in the matrix L in an RRMCF decomposition of $A = L\mathscr{U}$ are arbitrary; however the rest of entries below the diagonal of L (those not corresponding to zero rows of $\mathscr{U}$) and all the entries in $\mathscr{U}$ that are not zero can be obtained in terms of quotient of minors of A. This result, resembling a similar one for the LU factorization (see [1, Theorem 1, II §4, vol. 1]), is given in Theorem 3.

Theorem 3. *Let $A \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A) = q$ and let $\mathscr{U} \in \mathbb{C}^{m\times n}$ be its unique* RRMCF *and $L \in \mathbb{C}^{m\times m}$ a unit lower triangular matrix such that $A = L\mathscr{U}$. Let $\{(r_k, c_k)\}_{k=1}^{q}$ be the set of indices that determines the position of the leading entries in the nonzero rows of $\mathscr{U}$. Then, for $k \in \{1, \ldots, q\}$*

$$\mathscr{U}_{r_k c_k} = \frac{\det A(r_{1:k}, c_{1:k})}{\det A(r_{1:k-1}, c_{1:k-1})}, \tag{5}$$

$$\mathscr{U}_{r_k g} = \frac{\det A(r_{1:k}, [c_{1:k-1}, g])}{\det A(r_{1:k-1}, c_{1:k-1})}, \quad g \notin \{c_1, \ldots, c_k\}, \tag{6}$$

$$L_{f r_k} = \frac{\det A([r_{1:k-1}, f], c_{1:k})}{\det A(r_{1:k}, c_{1:k})}, \quad f \in \{r_k + 1, \ldots, m\}. \tag{7}$$

Observe that (5) and (6) are expressions for all, zero and nonzero entries of $\mathscr{U}$ in the nonzero rows. However (7) gives all the entries of L below the diagonal that are not arbitrary. The entries $L(f, h)$ for $f > h$ and $h \notin \{r_1, \ldots, r_k\}$ are arbitrary because they correspond to the zero rows of $\mathscr{U}$.

Proof. The proof is based upon expression (4) in Theorem 2:

$$\det A(r_{1:k+1}, [c_{1:k}, j]) = \det \mathscr{U}(r_{1:k+1}, [c_{1:k}, j])$$

for $k \in \{1, \ldots, q - 1\}$ and $j \in \{1, \ldots, n\}$. Using that $\mathscr{U}(r_{1:k+1}, [c_{1:k}, j])$ is upper triangular we have that

$$\det \mathscr{U}(r_{1:k+1}, [c_{1:k}, j]) = \mathscr{U}(r_{k+1}, j) \prod_{j=1}^{k} \mathscr{U}(r_j, c_j) = \mathscr{U}(r_{k+1}, j) \det \mathscr{U}(r_{1:k}, c_{1:k}).$$

Taking $j = c_{k+1}$ (5) follows, and for $j = g \notin \{c_1, \ldots, c_k\}$ (6) is obtained.

To get (7) we consider the submatrix, for $k \in \{1, \ldots, q\}$ and $f \in \{r_k + 1, \ldots, m\}$,

$$A([r_{1:k-1}, f], c_{1:k}) = L([r_{1:k-1}, f], r_{1:q})\mathscr{U}(r_{1:q}, c_{1:k}) = L([r_{1:k-1}, f], r_{1:k})\mathscr{U}(r_{1:k}, c_{1:k}),$$

because $\mathscr{U}(r_{k+1:q}, c_{1:k}) = 0$. $L([r_{1:k-1}, f], r_{1:k})$ is unit lower triangular except for the entry (k, k) that is $L(f, r_k)$, therefore if we take determinants:

$$\begin{aligned}\det A([r_{1:k-1}, f], c_{1:k}) &= \det L([r_{1:k-1}, f], r_{1:k}) \det \mathscr{U}(r_{1:k}, c_{1:k})\\ &= L(f, r_k) \det A(r_{1:k}, c_{1:k}),\end{aligned}$$

which is (7). □

Some observations on Theorems 2 and 3 are in order:

1. Minors of A whose columns (some or all) correspond to a subset of the set of indices $\{c_1, \ldots, c_q\}$ appear, as for example in $\det A([r_{1:k}, i], [c_{1:k}, j])$ or in $\det A(r_{1:k}, c_{1:k})$. The columns are to be taken in the order that they are written: $c_1, c_2, \ldots, c_q$, even if they are not in increasing order.

2. Formula (5) is presented separately from (6) because it is similar to the well known formula for the pivots of the LU factorization. However it is easy to see that (6) becomes (5) when $g = c_k$. A more concise statement of the Theorem would have been to replace (5) and (6) by
$$\mathcal{U}_{r_k g} = \frac{\det A(r_{1:k}, [c_{1:k-1}, g])}{\det A(r_{1:k-1}, c_{1:k-1})}, \quad g \in \{1, \ldots, n\}. \tag{8}$$
3. In fact, using the information in Theorem 2 together with (8), we can write a concise expression for any entry of $\mathcal{U}$ that, at the same time, gives the position of the leading entry (r_k, c_k), if $\{r_1, \ldots, r_{k-1}\}$ is known:
$$\mathcal{U}_{fg} = \frac{\det A([r_{1:k-1}, f], [c_{1:k-1}, g])}{\det A(r_{1:k-1}, c_{1:k-1})}, \quad r_{k-1} < f \leqslant r_k,\ g \in \{1, \ldots, n\}. \tag{9}$$
Observe that (9) becomes (8) when $f = r_k$. Observe also that c_k is the minimum index of the column for which the minor in the numerator is not zero, if it exists for that f (in this case $r_k = f$). If for a given f all the minors in the numerator are zero then f is a zero row of $\mathcal{U}$.
4. Observe that the only entries below the diagonal of the unit lower triangular matrix L that are determined by (7) are the ones in columns corresponding to the nonzero rows in $\mathcal{U}$. The entries in the columns corresponding to the zero rows in $\mathcal{U}$ are arbitrary (see the paragraph after the proof of Theorem 1). If these columns are taken to be the corresponding columns of the identity matrix $\mathbb{I}_m$, the unit lower triangular matrix L obtained using (7) will be the one given by Algorithm 1.

3. Multiple LU factorizations

In this section we fully describe the collection of all possible LU factorization s of any matrix for which such a factorization exists. The basic tool is going to be the unique RRMCF, $\mathcal{U}$, in Theorem 1. First we will identify the matrices that have an LU factorization as those whose RRMCF is upper triangular (Theorem 4). When a matrix A has an LU factorization all other possible LU factorization s will be obtained from the RRMCF factorization, the multiplicity will be parametrized in terms of the different unit lower triangular matrices L that can be used (Theorem 5) and, given any L, the upper triangular matrix U such that $A = LU$ is uniquely determined: $U = L^{-1}A$.

The first step will be to relate the RRMCF with the existence of the LU factorization. In the next theorem we do that, and furthermore we will characterize the existence in a variety of ways, some already known ([6], item 4), and some not (items 2 and 3).

Theorem 4. *Let* $A \in \mathbb{C}^{m\times n}$ *have* $\operatorname{rank}(A) = q$, $\mathcal{U} \in \mathbb{C}^{m\times n}$ *be its unique* RRMCF, *and* $\{(r_j, c_j)\}_{j=1}^{q}$ *be the set of indices that determines the positions of the leading entries in the nonzero rows of* $\mathcal{U}$. *Then the following statements are equivalent*:

1. *A has an LU factorization.*
2. *$\mathcal{U}$ is upper triangular.*
3. $c_k \geqslant r_k$ *for* $k \in \{1, \ldots, q\}$.
4. $A(f, 1:k) \in \operatorname{Row}\{A(1:k, 1:k)\}$, *for* $k \in \{1, \ldots, \min\{m, n\}\}$ *and* $f \in \{k+1, \ldots, m\}$.

Proof

(1 ⇒ 4) $A = LU$ implies for any row $f \geqslant k+1$ that
$$A(f, 1:k) = L(f, 1:m)U(1:m, 1:k) = L(f, 1:k)U(1:k, 1:k)$$

and $A(f, 1:k) \in Row(U(1:k, 1:k))$. The result is proven because $Row(U(1:k, 1:k)) = Row(A(1:k, 1:k))$ since L is invertible and lower triangular.

($4 \Rightarrow 3$) Let $L \in \mathbb{C}^{m\times m}$ be unit lower triangular such that $A = L\mathscr{U}$. In the first place, (r_1, c_1) is the leading entry of the first nonzero row of A. $c_1 < r_1$ would imply that $A(r_1, 1:c_1) \notin \text{Row}\{A(1:c_1, 1:c_1)\} = \{0\}$, which would contradict 4. If $r_k > c_k$ for $k \in \{2, \ldots, q\}$ we would have that $A(r_k, 1:r_k-1) \notin \text{Row}\{A(1:r_k-1, 1:r_k-1)\}$, also in contradiction with 4. This is because $A(r_k, 1:r_k-1) = L(r_k, 1:r_k-1)\mathscr{U}(1:r_k-1, 1:r_k-1) + \mathscr{U}(r_k, 1:r_k-1)$ and $\mathscr{U}(r_k, 1:r_k-1) \notin \text{Row}\{\mathscr{U}(1:r_k-1, 1:r_k-1)\} = \text{Row}\{A(1:r_k-1, 1:r_k-1)\}$ because $\mathscr{U}(1:r_k, 1:r_k-1)$ is also in RRMCF, and its nonzero rows are linearly independent.

($3 \Rightarrow 2$) Obvious.

($2 \Rightarrow 1$) If $\mathscr{U}$ is upper triangular $A = L\mathscr{U}$ is an LU factorization of A with L given by Algorithm 1. □

Then if, given A, its unique RRMCF $\mathscr{U}(A)$ is upper triangular, A has at least one LU factorization. We already know that the entries below the diagonal of the columns of L corresponding to the zero rows of $\mathscr{U}$ are arbitrary. As mentioned in the paragraph after the proof of Theorem 1, these changes in L do not change $\mathscr{U}$. Our next lemma shows that there are more degrees of freedom in L compatible with keeping the LU factorization of A: those that change both L and $\mathscr{U}$ but keeping them, respectively, unit lower and upper triangular.

Lemma 1. *Let $\mathscr{U} \in \mathbb{C}^{m\times n}$ be an upper triangular matrix in* RRMCF, *with $\{(r_k, c_k)\}_{k=1}^{q}$ the set of indices that determines the positions of its leading entries ($r_k \leqslant c_k$), and $L \in \mathbb{C}^{m\times m}$ be an unit lower triangular matrix. Then*

$$L\mathscr{U} \text{ is upper triangular if and only if } \quad L(i, r_k) = 0, \quad i > c_k,\ k \in \{1, \ldots, q\}.$$

All the entries of L that are not defined above as zero, are arbitrary, i.e., they can take any value and $L\mathscr{U}$ will still be upper triangular. That is, if the jth *column of L is such that $j \notin \{r_1, \ldots, r_q\}$ then all its entries below the diagonal are arbitrary. The same happens if $j = r_k \in \{r_1, \ldots, r_q\}$ and $c_k \geqslant m$. If, on the other hand, $j = r_k \in \{r_1, \ldots, r_q\}$ and $c_k < m$ the* jth *column is of the form*

$$L(1:m, r_k) = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ \alpha_1 \\ \vdots \\ \alpha_{c_k-r_k} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \begin{matrix} 1 \\ \vdots \\ r_k-1 \\ r_k \\ r_k+1 \\ \vdots \\ c_k \\ c_k+1 \\ \vdots \\ m \end{matrix}$$

with $\alpha_1, \ldots, \alpha_{c_k-r_k}$ arbitrary.

Proof. If $L(i, r_k) = 0$, for $i > c_k$ and $k \in \{1, \ldots, q\}$, it is obvious by construction that $L\mathscr{U}$ is upper triangular. On the other hand if $U \equiv L\mathscr{U}$ is upper triangular, let us write the ith row of U:

$$U(i, 1:n) = L(i, 1:m)\mathscr{U}(1:m, 1:n). \tag{10}$$

The first $i-1$ entries of $U(i,1:n)$ and the last $m-i$ of $L(i,1:m)$ are zero. Then

$$U(i,1:i-1)=0=L(i,1:i)\mathscr{U}(1:i,1:i-1). \tag{11}$$

Because of the structure of $\mathscr{U}$, some of the rows of the submatrix $\mathscr{U}(1:i,1:i-1)$ are zero. The only nonzero are those in the subset of nonzero rows of $\mathscr{U}$, $\{r_1,\dots,r_q\}$, that have $c_j \leqslant i-1$. That is, $\mathscr{U}(r_j,1:i-1)$ is nonzero if and only if $r_j \in \mathscr{R}$ with $\mathscr{R}=\{r_j \in \{r_1,\dots,r_q\}$ such that $c_j \leqslant i-1\}$. Then (11) becomes

$$0=L(i,\mathscr{R})\mathscr{U}(\mathscr{R},1:i-1). \tag{12}$$

But the rows of $\mathscr{U}(\mathscr{R},1:i-1)$ are nonzero and linearly independent, so $L(i,r_j)=0$ if $c_j \leqslant i-1$. That is our result. □

From Lemma 1 we can build the full parametric description of all possible L's in the LU factorizations of a given A. It starts from a particular RRMCF factorization $A=L_0\mathscr{U}$ and then builds all the unit lower triangular matrices L_* such that $L_*\mathscr{U}\equiv U$ is still upper triangular, in this way $A=L_0L_*^{-1}L_*\mathscr{U}$, with $L\equiv L_0L_*^{-1}$. This is presented in Theorem 5, the main theorem of this work, in which we fully describe all the LU factorization s that are associated with a matrix that at least has one.

Theorem 5. *Let $A\in\mathbb{C}^{m\times n}$ be a matrix of rank q that has an LU factorization. Without loss of generality it can be written in the form $A=L_0\mathscr{U}$, with $L_0\in\mathbb{C}^{m\times m}$ unit lower triangular given by Algorithm 1, and $\mathscr{U}\in\mathbb{C}^{m\times n}$ its unique upper triangular* RRMCF, *with $\{(r_k,c_k)\}_{k=1}^{q}$ the set of indices that determines the positions of the leading entries of $\mathscr{U}$. Then all unit lower triangular matrices L in the set*

$$S_L=\{L_0L_*^{-1}: L_* \text{ unit lower triangular such that } L_*(j,r_k)=0,\ j>c_k,\ k=1,\dots,q\}$$

are such that $A=LU$ with U upper triangular, and, viceversa, if $A=LU$ with L unit lower triangular and U upper triangular then $L\in S_L$. This characterizes all possible LU factorizations of A because $U=L^{-1}A$. Explicitly, the set of all possible U's is

$$S_U=\{L_*\mathscr{U}: L_*\in\mathbb{C}^{m\times m} \text{ unit lower triangular such that } L_*(j,r_k)=0,\\ j>c_k,\ k=1,\dots,q\}.$$

Proof. First, all the elements of S_L are valid factors of an LU factorization: given $L=L_0L_*^{-1}$ there exists $U\equiv L_*\mathscr{U}$ such that $LU=L_0\mathscr{U}=A$ is an LU factorization because $U=L_*\mathscr{U}$ is upper triangular by Lemma 1. On the other hand, if A has an LU factorization $A=LU=L_0\mathscr{U}$, then $U=L^{-1}L_0\mathscr{U}$ is upper triangular and because of Lemma 1, $L^{-1}L_0=L_*$, for some L_* of the stated form. □

Notice that the set S_U of all possible U factors is convex. Given $A\in\mathbb{C}^{m\times n}$ with an LU factorization and two upper triangular matrices $U_1,U_2\in S_U$ then $U_1=L_{*,1}\mathscr{U}$ and $U_2=L_{*,2}\mathscr{U}$. If we form a convex combination $U=tU_1+(1-t)U_2$, with $0\leqslant t\leqslant 1$, we have that

$$U=tL_{*,1}\mathscr{U}+(1-t)L_{*,2}\mathscr{U}=(tL_{*,1}+(1-t)L_{*,2})\mathscr{U}\equiv L_*\mathscr{U},$$

with $L_*=tL_{*,1}+(1-t)L_{*,2}$ unit lower triangular and such that $L_*(j,r_k)=0$ if $j>c_k$, for $k\in\{1,\dots,q\}$. Therefore U also belongs to S_U and S_U is convex.

We summarize here how to obtain and parametrize all the LU factorizations of a matrix $A \in \mathbb{C}^{m\times n}$.

1. Apply Algorithm 1 to A, $A = L_0\mathscr{U}$. If the RRMCF of A, $\mathscr{U}$, is upper triangular then A has at least one LU factorization. Let $\{(r_k, c_k)\}_{k=1}^{q}$ be the set of indices that determines the position of the leading entries of $\mathscr{U}$.
2. Let us denote $L = L_0L_*(\Lambda)^{-1}$, where $L_*(\Lambda)$ is any of the unit lower triangular matrices referred to in Theorem 5 and Λ are the free parameters that describe them. Following Lemma 1 the parameters in $L_*(\Lambda)$ can be separated, for the sake of clarity, into two parts $\Lambda = [\alpha, \omega]$:

   $$\alpha = [\alpha_1, \ldots, \alpha_{N_\alpha}], \quad \text{with } N_\alpha \equiv \sum_{k\in\{1,\ldots,q\}} (\min\{c_k, m\} - r_k),$$

   are the parameters coming from the columns of $L_*(\Lambda)$ corresponding to the nonzero rows of $\mathscr{U}$ and

   $$\omega = [\omega_1, \ldots, \omega_{N_\omega}], \quad \text{with } N_\omega \equiv \sum_{j\in\{1,\ldots,m\}-\{r_1,\ldots,r_q\}} (m - j),$$

   are the parameters coming from the columns of $L_*(\Lambda)$ corresponding to the zero rows of $\mathscr{U}$. Then all parametric LU factorization s of A are of the form

   $$A = LU \equiv [L_0L_*(\Lambda)^{-1}][L_*(\Lambda)\mathscr{U}].$$

   $L \equiv L_0L_*(\Lambda)^{-1}$ and $U \equiv L_*(\Lambda)\mathscr{U}$ parametrize, respectively, all the unit lower triangular and upper triangular LU factors of A.

As a consequence the number of free parameters in the LU factorization is given in the following Corollary.

Corollary 1. *Let $A \in \mathbb{C}^{m\times n}$ be a matrix of rank q that has an LU factorization. Let $\{(r_k, c_k)\}_{k=1}^{q}$ be the set of indices that determines the positions of the leading entries of its unique upper triangular* RRMCF $\mathscr{U} \in \mathbb{C}^{m\times n}$. *Then the number of free parameters for the multiple LU factorization s of A is*:

$$N_{LU} = \sum_{j\in\{1,\ldots,m\}-\{r_1,\ldots,r_q\}} (m - j) + \sum_{k\in\{1,\ldots,q\}} (\min\{c_k, m\} - r_k). \tag{13}$$

Let us end this section by applying Theorem 5 to two special cases, in which we can easily gain precise information. First is the well known result about uniqueness of the LU factorization [2, Theorem 9.1]. Here we present a new proof based on the results in this work, its novelty residing in being completely algebraic. In addition, Corollary 2 covers also the case of rectangular matrices.

Corollary 2. *$A \in \mathbb{C}^{m\times n}$ with $m \leqslant n + 1$ has an unique LU factorization if and only if* $\det A(1 : k, 1 : k) \neq 0, k = 1, \ldots, m - 1$. *If $m > n + 1$ an LU factorization cannot be unique.*

Proof. Let $\mathscr{U} \in \mathbb{C}^{m\times n}$ be the unique RRMCF of A and $\{(r_k, c_k)\}_{k=1}^{q}$ be the set of indices that determines the position of its leading entries. Let us assume first that $m \leqslant n + 1$. If $A \in \mathbb{C}^{m\times n}$ has an unique LU factorization, then $\mathscr{U}$ is upper triangular (Theorem 4), and, as a consequence of Corollary 1, $N_{LU} = 0$. Therefore, $\{1, \ldots, m\} - \{r_1, \ldots, r_q\} = \emptyset$ (in this case $q = m$) or $\{1, \ldots, m\} - \{r_1, \ldots, r_q\} = \{m\}$ (in this case $q = m - 1$). In both cases $r_1 = 1, r_2 = 2, \ldots, r_{m-1} =$

$m-1$. Besides, $N_{LU}=0$ implies $r_k=\min\{c_k,m\}$ for $k\in\{1,\ldots,q\}$, and then $r_1=c_1=1, r_2=c_2=2,\ldots,r_{m-1}=c_{m-1}=m-1$. Therefore, for $k=1,\ldots,m-1$,

$$\det A(1:k,1:k)=\det \mathscr{U}(1:k,1:k)=\prod_{i=1}^{k}\mathscr{U}(r_i,c_i)\neq 0.$$

On the other hand, if $\det A(1:k,1:k)\neq 0$, $k=1,\ldots,m-1$, Theorems 4 and 2 imply, respectively, that A has an LU factorization and that $r_k=c_k=k$ for $k\in\{1,\ldots,m-1\}$. Finally, Corollary 1 implies that the LU factorization is unique, because in the case $q=m$ we have that $r_q=m$, $c_q\geqslant r_q$, and $\min\{c_q,m\}=m$.

In the case $m>n+1$, notice that the unique RRMCF $\mathscr{U}$ associated to A will have always at least two zero rows and therefore the LU factorization will never be unique. □

Our last result is another immediate consequence of Theorem 5.

Corollary 3. *Let $A\in\mathbb{C}^{m\times n}$ be a matrix of* $\operatorname{rank}(A)=q$ *and* $\operatorname{rank}(A_{11})=q$, *with $A_{11}=A(1:q,1:q)\in\mathbb{C}^{q\times q}$. Then if A_{11} has an (unique) LU factorization, $A_{11}=L_{11}U_{11}$, all the LU factorization s of A are of the form*

$$A=\begin{bmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{bmatrix}=\begin{bmatrix}L_{11} & 0\\ L_{21} & L_{22}\end{bmatrix}\begin{bmatrix}U_{11} & U_{12}\\ 0 & 0\end{bmatrix},$$

with $U_{12}=L_{11}^{-1}A_{12}$, $L_{21}=A_{21}U_{11}^{-1}$ and L_{22} unit lower triangular with all the entries below the diagonal arbitrary.

Proof. If $A_{11}=L_{11}U_{11}$ with $\operatorname{rank}(A)=\operatorname{rank}(A_{11})=q$ we have that $\det A(1:k,1:k)\neq 0$, for $k=1,\ldots,q$. Using Theorem 2 we know that $r_k=c_k=k$, for $k=1,\ldots,q$. Then $\mathscr{U}$ has the last $m-q$ rows zero. The result is then a simple consequence of Theorem 5. □

References

[1] F.R. Gantmacher, The Theory of Matrices, vol. I, AMS, Chelsea, Providence, RI, 1998.
[2] N.J. Higham, Accuracy and Stability of Numerical Algorithms, second ed., SIAM, Philadelphia, 2002.
[3] R.A. Horn, C.R. Johnson, Matrix Analysis, Cambridge University Press, Cambridge, 1985.
[4] C.R. Johnson et al., On the existence of LU factorizations, in preparation.
[5] D.C. Lay, Linear Algebra and Its Applications, second ed., Addison Wesley, Reading, Massachusetts, 1997.
[6] C.M. Lau, T.L. Markham, LU factorizations, Czech. Math. J. 29 (104) (1979) 546–550.
[7] The MathWorks, Inc., MATLAB Reference Guide, Natick, MA, 1992.