
NECESSARY AND SUFFICIENT CONDITIONS FOR THE EXISTENCE OF AN LU FACTORIZATION FOR GENERAL RANK DEFICIENT MATRICES*

TECHNICAL REPORT

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ABSTRACT

We establish necessary and sufficient conditions for the existence of an LU factorization $A = LU$ for an arbitrary square matrix A , including singular and rank-deficient cases, without the use of row or column permutations. We prove that such a factorization exists if and only if the nullity of every leading principal submatrix is bounded by the sum of the nullities of the corresponding leading column and row blocks. While building upon the work of Okunev and Johnson, we present simpler, constructive proofs. Furthermore, we extend these results to characterize rank-revealing factorizations, providing explicit sparsity bounds for the factors L and U . Finally, we derive analogous necessary and sufficient conditions for the existence of factorizations constrained to have unit lower or unit upper triangular factors.

Keywords LU factorization, Rank-deficient matrices, Singular matrices, Rank-revealing factorization, Nullity, Sparsity

It is well-known that for any square matrix A , there exists a permutation of rows (and potentially columns) such that an LU factorization exists. Specifically, the factorization $PA = LU$, where P is a permutation matrix, L is unit lower triangular, and U is upper triangular, is guaranteed to exist for any matrix A Higham [2011], Lu [2021].

However, the existence of an LU factorization for a matrix A *without* permutations (that is, $A = LU$) is not guaranteed. A classical result states that for a non-singular matrix, such a factorization exists if and only if all its leading principal minors are non-zero. When the matrix is singular or when leading principal minors vanish, the situation becomes significantly more complex. The standard conditions involving determinants are no longer sufficient to characterize the existence of the factorization.

This paper addresses the necessary and sufficient conditions for the existence of an LU factorization for an arbitrary matrix A , without imposing restrictions on its rank or invertibility. We extend the work of Okunev and Johnson Okunev and Johnson [2005], who established rank-based conditions for this problem. See also Dopico et al. [2006] for a discussion on multiple factorizations of singular matrices. Other perspectives on factorizations and their existence in general algebraic structures or specific contexts can be found in Nagarajan et al. [1999], Johnson et al. [1989], Jeffrey [2010], Higham [2011].

The contributions of this paper are threefold. First, we formulate the necessary and sufficient condition using the *nullity* of the leading principal submatrices relative to the nullity of the corresponding column and row blocks. Specifically, we prove that an LU factorization exists if and only if for all k (this condition is equivalent to Okunev and Johnson [2005]):

$$\text{null}(A[1 : k, 1 : k]) \leq \text{null}(A[:, 1 : k]) + \text{null}(A[1 : k, :]^T)$$

*Code is available at <https://doi.org/10.5281/zenodo.18224816>

Note that, in this paper, null is the dimension of the null space of a matrix (see Table 1).

Second, we provide new, simpler proofs of these results. Our proofs are constructive and rely on induction, explicitly building the factorization by handling the singular cases while preserving the triangular structure. Finally, we extend these results to characterize rank-revealing factorizations, providing tight sparsity bounds for the factors. We also derive analogous conditions for factorizations requiring unit lower or unit upper triangular factors.

$\text{rank}(A)$	Rank of matrix A
$\text{null}(A)$	Dimension of the right null space of matrix A
A^T	Transpose of matrix A
a_{ij}	Entry (i, j) of matrix A
$A[:, i]$	Column i of matrix A
$A[i, :]$	Row i of matrix A
$A[i : j, k : l]$	Submatrix of A with rows from i to j and columns from k to l
$A[i : j, k :]$	Submatrix of A with rows from i to j and columns from k to the end
e_i	i -th vector of the standard basis
I_n	Identity matrix of size n

Table 1: Notations used in the paper.

Triangular factorizations and causal systems. Before presenting the technical results, we motivate the study of LU factorizations without permutations by considering their interpretation in causal systems and their computational advantages.

In some applications, the index ordering carries physical significance, such as time in dynamic systems. A lower triangular matrix L represents a causal operator where the current state i depends only on past states $j \leq i$. Similarly, U can be interpreted as capturing reverse-flow dependencies. When $A = LU$, the system respects this intrinsic ordering. However, introducing permutations (as in $PAQ = LU$) destroys this structure: P scrambles the equations (rows) and Q scrambles the variables (columns), breaking the link between the matrix indices and the causal dependencies. Consequently, in contexts where the ordering is immutable (e.g., autoregressive time series, structural equation modeling, or causal signal processing), standard pivoting strategies are inapplicable. This necessitates a theory for the existence of LU factorizations that strictly preserves the original indexing.

Moreover, the choice of the LU factorization over other decompositions like QR or SVD is often driven by computational efficiency and sparsity. While the QR decomposition always exists for any matrix, the orthogonal factor Q is typically dense. In contrast, the triangular factors L and U often preserve the sparsity of A to a much greater extent, leading to significant savings in storage and computational cost. This cost advantage may also extend to physical limitations, such as data transport or logistical constraints when they are represented by the matrix entries. These reasons lead us to the question of determining exactly when an LU factorization exists without permutations.

We finally summarize the contributions of this paper, which include:

- A Nullity-Based Characterization: We prove that factorization exists if and only if $\text{null}(A_{11}) \leq \text{null}(\text{Col}) + \text{null}(\text{Row})$ for all k . The proofs are original.
- Rank-Revealing Structure: we show that we obtain a rank-revealing factorization when the LU factorization exists.
- Sparsity: we provide tight sparsity bounds for the L and U factors.
- Constructive Proof: we provide a constructive proof by induction. We include a Python implementation in the appendix to fully characterize the algorithm and allow independent verification of our results.
- Unit Triangular Factors: we provide a characterization of the conditions for the existence of unit triangular factors.

Organization of paper. The remainder of the paper is organized as follows. Section 1 reviews classical results regarding factorizations with permutations. Section 2 presents the main theorem and the derivation of the nullity condition. Theorem 2.6 strengthens this result by characterizing rank-revealing factorizations. Finally, Section 3 discusses the specific requirements for unit triangular factors.

We begin with a few classical results that will serve as reference for the later sections.

1 Classical results

We begin by recalling standard existence results involving permutations. These theorems correspond to Gaussian elimination with partial and full pivoting.

Theorem 1.1 (Partial Pivoting). *For any square matrix A of size n , there exists a permutation matrix P such that $PA = LU$, where L is unit lower triangular and U is upper triangular.*

Proof. This is a classical result. We can prove it by induction on n . The result is true for $n = 1$.

Assume it is true for $n - 1$. If $a_{11} \neq 0$, then consider:

$$A = LDU$$

where

$$L = \begin{pmatrix} 1 & 0 \\ a_{11}^{-1} A_{21} & I \end{pmatrix}, \quad D = \begin{pmatrix} 1 & 0 \\ 0 & S \end{pmatrix}, \quad U = \begin{pmatrix} a_{11} & A_{12} \\ 0 & I \end{pmatrix}$$

We can apply the induction hypothesis to S . The result for A follows.

If $a_{11} = 0$, we have two cases.

Case 1: column 1 of A is non-zero. We can find the smallest i such that $A[i, 1] \neq 0$. Pivot row 1 and i . Denote by $B = \Pi_i A$ the permuted matrix (with $\Pi_i^2 = I$). Since $b_{11} \neq 0$, B has an LU factorization. This proves the result for A .

Case 2: column 1 of A is zero. We choose:

$$A = IDU$$

where

$$D = \begin{pmatrix} 1 & 0 \\ 0 & S \end{pmatrix}, \quad U = \begin{pmatrix} 0 & A_{12} \\ 0 & I \end{pmatrix}$$

and $S = A_{22}$. We can apply the induction hypothesis to S . The result for A follows. \square

Corollary 1.2. *For any square matrix A of size n , there exists a permutation matrix Q such that $AQ = LU$, where L is lower triangular and U is unit upper triangular.*

Proof. Apply Theorem 1.1 to A^T . \square

Definition 1.3. A matrix A of size $m \times n$ is said to have a rank revealing LU factorization if it can be written as $A = LU$, where L is a lower triangular matrix of size $m \times r$, U is an upper triangular matrix of size $r \times n$, and $r = \text{rank}(A)$.

If we allow both row and column permutations, we can always obtain such a factorization.

Theorem 1.4 (Full Pivoting). *For any matrix A of size $m \times n$, there exist a row permutation matrix P and a column permutation matrix Q such that $PAQ = LU$ is a rank revealing LU factorization.*

Proof. This is also a classical result. We can prove it by induction on n . The result is true for $n = 1$.

Assume it is true for $n - 1$. If $a_{11} \neq 0$, then consider:

$$A = LDU$$

where

$$L = \begin{pmatrix} a_{11} & 0 \\ A_{21} & I \end{pmatrix}, \quad D = \begin{pmatrix} a_{11}^{-1} & 0 \\ 0 & S \end{pmatrix}, \quad U = \begin{pmatrix} a_{11} & A_{12} \\ 0 & I \end{pmatrix}$$

S has rank $r - 1$ if $r = \text{rank}(A)$. We can apply the induction hypothesis to S . The result for A then follows.

If $a_{11} = 0$, we have two cases. If A is 0, we pick $L = U = 0$. Otherwise we have some i and j such that $a_{ij} \neq 0$. We can permute row 1 and i and column 1 and j . Denote by $B = \Pi_i A \Pi_j$ the permuted matrix. Since $b_{11} \neq 0$, B has a rank revealing LU factorization. This proves the result for A .

We have also proved that this process must terminate after r steps where $r = \text{rank}(A)$. So the LU factorization of B is rank revealing.

From Theorem A.3 (see Section A in the Appendix), we can also prove that the remaining Schur complement is zero after r steps of the LU factorization. \square

We now consider LU factorizations without permutations. The fundamental result states that factorization is possible if and only if the matrix is *strongly non-singular* (i.e., all leading principal minors are non-zero).

Proposition 1.5. *Let A be a non-singular matrix of size n . A has an LU factorization if and only if all its leading principal submatrices are non-singular:*

$$\text{rank}(A[1:k, 1:k]) = k, \quad k = 1, \dots, n$$

Proof. We prove that the condition is necessary. Assume $A = LU$:

$$\det(A) = \prod_{i=1}^n l_{ii} u_{ii}$$

and $\det(A) \neq 0$. So, $l_{ii} \neq 0$ and $u_{ii} \neq 0$ for all i . Therefore: $\text{rank}(A[1:k, 1:k]) = k, k = 1, \dots, n$.

We prove that the condition is sufficient. We prove the result by induction on n . The result is true for $n = 1$.

Assume it is true for $n - 1$. By assumption, $a_{11} \neq 0$. We then have the factorization:

$$A = LDU$$

where

$$L = \begin{pmatrix} a_{11} & 0 \\ A_{21} & I \end{pmatrix}, \quad D = \begin{pmatrix} a_{11}^{-1} & 0 \\ 0 & S \end{pmatrix}, \quad U = \begin{pmatrix} a_{11} & A_{12} \\ 0 & I \end{pmatrix}$$

and $S = A_{22} - A_{21}a_{11}^{-1}A_{12}$ is the Schur complement. L and U are full rank. So D satisfies the condition of the theorem. Consequently, S also satisfies the condition of the theorem and is of size $n - 1$. By the induction hypothesis, S has an LU factorization. Therefore A also has an LU factorization. \square

2 General necessary and sufficient condition for the existence of an LU factorization

We now address the central question of this paper: determining the necessary and sufficient conditions for the existence of an LU factorization without permutations. We begin with two illustrative examples that motivate the general result.

Consider the matrix:

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

This matrix does not admit an LU factorization. We prove this by contradiction. Suppose $A = LU$. Then the diagonal entry satisfies $a_{11} = l_{11}u_{11} = 0$. This implies that either $l_{11} = 0$ or $u_{11} = 0$.

- If $l_{11} = 0$, then $a_{12} = l_{11}u_{12} = 0$, which contradicts $a_{12} = 1$.
- If $u_{11} = 0$, then $a_{21} = l_{21}u_{11} = 0$, which contradicts $a_{21} = 1$.

In this special case, we have $A^2 = I$ and A is a permutation matrix. So we note that $AA = I \cdot I$ is the factorization of Theorem 1.1 with $P = A$, $L = I$, and $U = I$.

However, a zero pivot does not always preclude factorization. Consider the singular matrix:

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

Despite the zero principal minors, this matrix *does* have an LU factorization. We can derive it by permuting A into a factorizable form and then reversing the permutations. Apply a cyclic row shift $(1, 2, 3) \rightarrow (2, 3, 1)$ via P and swap columns 1 and 3 via Q :

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

We can recover a factorization for A by writing $A = P^{-1}(PAQ)Q^{-1}$:

$$A = P^{-1} \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] Q^{-1} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

This yields a valid, rank-revealing LU factorization with no pivoting. Another valid LU factorization is:

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

We can generalize this result using block matrices. Let 0_n denote the $n \times n$ zero matrix. If B is a factorizable matrix such that $B = LU$, we can construct larger factorizable matrices A as follows:

$$A = \begin{pmatrix} 0_n & 0_n & 0_n \\ 0_n & 0_n & C \\ 0_n & B & D \end{pmatrix} = \begin{pmatrix} 0_n & 0_n \\ C & 0_n \\ D & L \end{pmatrix} \begin{pmatrix} 0_n & 0_n & I_n \\ 0_n & U & 0_n \end{pmatrix} = \begin{pmatrix} 0_n & 0_n \\ CX & 0_n \\ DX & L \end{pmatrix} \begin{pmatrix} 0_n & 0_n & X^{-1} \\ 0_n & U & 0_n \end{pmatrix}$$

for any invertible matrix X .

Alternatively, if $C = LU$:

$$A = \begin{pmatrix} 0_n & 0_n \\ 0_n & L \\ I_n & 0_n \end{pmatrix} \begin{pmatrix} 0_n & B & D \\ 0_n & 0_n & U \end{pmatrix} = \begin{pmatrix} 0_n & 0_n \\ 0_n & L \\ X & 0_n \end{pmatrix} \begin{pmatrix} 0_n & X^{-1}B & X^{-1}D \\ 0_n & 0_n & U \end{pmatrix}$$

These examples demonstrate that the existence of a factorization is linked to the relationship between the ranks (or nullities) of specific sub-blocks. We formalize this observation in Theorem 2.1. We will show that Theorem 2.1 below is a necessary and sufficient condition for the existence of an LU factorization.

Property 2.1. *Matrix A is square of size n . For all $k = 1, \dots, n$:*

$$\text{null}(A[1 : k, 1 : k]) \leq \text{null}(A[:, 1 : k]) + \text{null}(A[1 : k, :]^T) \quad (1)$$

We informally describe the main strategy before stating the results formally. The primary obstacle to constructing an LU factorization is the occurrence of a zero pivot. Standard Gaussian elimination resolves this by permuting rows (partial pivoting) or both rows and columns (full pivoting) to bring a non-zero entry to the diagonal.

However, arbitrary permutations destroy the triangular structure required for the specific factorization $A = LU$. If we write the permuted factorization as $PAQ = LU$, recovering A yields $A = (P^{-1}L)(UQ^{-1})$. In general, $P^{-1}L$ is not lower triangular and UQ^{-1} is not upper triangular.

To maintain the triangular factors of A , we must restrict our pivoting strategy. We rely on the observation (detailed in Section A) that a zero column (or row) in the Schur complement corresponds to a column (or row) in the original matrix that is linearly dependent on the preceding columns (or rows).

Our constructive proof effectively “sorts” the matrix indices. Whenever we encounter a zero pivot, the condition in Theorem 2.1 guarantees that at least one of the following two scenarios must hold:

1. The current column in the Schur complement is zero (the column is linearly dependent). We permute this column rightward.
2. The current row in the Schur complement is zero (the row is linearly dependent). We permute this row downward.

Crucially, because we only permute *zero* columns or rows (relative to the active Schur complement), the triangular structure of the resulting factors is preserved. When we reverse these permutations, the factor $P^{-1}L$ remains lower triangular and UQ^{-1} remains upper triangular.

Condition (1) is the precise safeguard that ensures we never reach a “dead end” where the pivot is zero but neither the column nor the row can be safely permuted away (i.e., a case where the rank has not been exhausted, but the leading block is rank-deficient in a way that blocks factorization).

Consequently, this process produces a rank-revealing factorization where the indices are partitioned based on linear independence:

- **Linearly Independent Vectors:** If a column j_0 of A is linearly independent of the previous columns, it is retained (or moved) into the leading rank- r block ($j \leq r$).
- **Linearly Dependent Vectors:** If a column j_0 of A is linearly dependent on the previous columns, it is deferred to the trailing block ($j > r$).

A symmetric logic applies to the rows of A .

The main existence results are summarized in Table 2.

Factorization Type	Equation	Conditions for Existence	Limitations
Non-singular LU	$A = LU$	Strongly non-singular (all leading minors $\neq 0$).	Does not apply to singular matrices.
Partial Pivoting	$PA = LU$	Always exists for any square A .	Permutates rows, altering row-index meaning.
Full Pivoting	$PAQ = LU$	Always exists; rank-revealing.	Permutates rows and columns, destroying all index structure.
Generalized LU	$A = LU$	Subject of this work.	Handles singular/rank-deficient cases without P, Q .

Table 2: Summary of the main factorization types and their conditions for existence.

Informal description: producer-sensor duality

We can form a mental model of Theorem 2.1 by considering the following scenario which represents the class of matrices that have an LU factorization. Assume the columns of A correspond to producer points j and the rows of A correspond to sensor points i .

We say the producer j is *observable* by the current sensor network $1 : i$ if $A[1 : i, j]$ adds new information (is linearly independent) relative to previous producers $A[1 : i, 1 : j - 1]$. Conversely, we say the sensor i is *informative* regarding the current producers $1 : j$ if its measurement $A[i, 1 : j]$ is linearly independent of previous measurements $A[1 : i - 1, 1 : j]$.

The existence of an LU factorization implies a compatibility between observability and informativeness. A admits a factorization if and only if every “blind spot” (rank deficiency) in a leading block corresponds to a global redundancy. Specifically, if the interaction between the first k sensors and k producers is rank-deficient, this deficiency must be fully accounted for by producers that are globally redundant (dependent on previous columns) or sensors that are globally redundant (dependent on previous rows). The factorization is impossible only in the “crossed” scenario, or “deadlock”: where producer k carries a novel signal that current sensors miss (but future sensors see), while sensor k performs a novel measurement that misses current signals (but sees future ones).

We now provide the formal proof of the main results, Theorems 2.5 and 2.6.

2.1 Rank theorems

We recall rank theorems that will be useful in the proof of Theorem 2.5.

Theorem 2.2. *The rank-nullity theorem states that for any matrix A of size $m \times n$:*

$$\text{rank}(A) + \text{null}(A) = n$$

We now state Sylvester’s inequality for the rank of a product of matrices.

Lemma 2.3. *Consider $A = BC$. Then:*

$$\text{rank}(A) \leq \min(\text{rank}(B), \text{rank}(C)), \quad \text{rank}(B) + \text{rank}(C) - k \leq \text{rank}(A)$$

where k is the number of columns of B and rows of C .

Corollary 2.4. *If A , B , and C are square matrices then:*

$$\text{null}(A) \leq \text{null}(B) + \text{null}(C)$$

Proof. Assume $A = BC$ where A, B, C are $n \times n$ matrices. From Theorem 2.3:

$$\text{rank}(A) \geq \text{rank}(B) + \text{rank}(C) - n$$

Using Theorem 2.2, $\text{rank}(M) = n - \text{null}(M)$:

$$n - \text{null}(A) \geq (n - \text{null}(B)) + (n - \text{null}(C)) - n$$

Simplifying: $\text{null}(A) \leq \text{null}(B) + \text{null}(C)$. □

2.2 Necessary condition

We show that Theorem 2.1 is a necessary condition for the existence of an LU factorization.

Assume that A , a square matrix of size n , has an LU factorization:

$$A = LU$$

Then:

$$\begin{aligned} A[1:k,:] &= L[1:k, 1:k]U[1:k,:], \\ A[:, 1:k] &= L[:, 1:k]U[1:k, 1:k], \\ A[1:k, 1:k] &= L[1:k, 1:k]U[1:k, 1:k] \end{aligned}$$

Using Theorem 2.3 and Theorem 2.4, we have:

$$\begin{aligned} \text{rank}(A[1:k,:]) &\leq \text{rank}(L[1:k, 1:k]), \\ \text{rank}(A[:, 1:k]) &\leq \text{rank}(U[1:k, 1:k]), \\ \text{null}(A[1:k, 1:k]) &\leq \text{null}(L[1:k, 1:k]) + \text{null}(U[1:k, 1:k]) \end{aligned}$$

Using Theorem 2.2, we get:

$$\text{null}(A[1:k, 1:k]) \leq \text{null}(A[:, 1:k]) + \text{null}(A[1:k,:]^T)$$

So Theorem 2.1 is a necessary condition for the existence of an LU factorization.

2.3 Sufficient condition

We will now prove the main theorem:

Theorem 2.5. *Matrix A satisfies Theorem 2.1 if and only if it has an LU factorization.*

Proof. We prove the result by induction on the size of A . The result is true for $n = 1$.

Assume it is true for size $n - 1$.

Assume $a_{11} \neq 0$. We have the factorization:

$$A = LDU$$

where

$$L = \begin{pmatrix} a_{11} & 0 \\ A_{21} & I \end{pmatrix}, \quad D = \begin{pmatrix} a_{11}^{-1} & 0 \\ 0 & S \end{pmatrix}, \quad U = \begin{pmatrix} a_{11} & A_{12} \\ 0 & I \end{pmatrix}$$

Since L and U are triangular and full rank, D satisfies Theorem 2.1 if and only if A does. Consequently, S also satisfies Theorem 2.1 and is of size $n - 1$. Moreover S has rank $r - 1$ if $r = \text{rank}(A)$. By the induction hypothesis, S has an LU factorization. The result for A follows.

Assume $a_{11} = 0$. From Theorem 2.1, we have either:

1. $A[:, 1] = 0, A[1, :] \neq 0$, or
2. $A[1, :] = 0, A[:, 1] \neq 0$, or
3. $A[:, 1] = 0, A[1, :] = 0$.

Case 1: $A[:, 1] = 0$. We can find the smallest j such that $A[1, j] \neq 0$. Pivot column 1 and j . Denote by $B = A\Pi_j$ the permuted matrix (with $\Pi_j^2 = I$). We prove that B satisfies Theorem 2.1.

Consider $k < j$. We have

$$\text{null}(A[1:k, 1:k]) \leq \text{null}(A[:, 1:k]) + \text{null}(A[1:k, :]^T) \tag{2}$$

Since column 1 of A is zero, we have:

$$\text{null}(A[1:k, 1:k]) = \text{null}(A[1:k, 2:k]) + 1$$

We have

$$\text{null}(B[1:k, 2:k]) = \text{null}(A[1:k, 2:k])$$

Since the only non-zero entry in row 1 of $B[1 : k, 1 : k]$ is in column 1, $B[1 : k, 1]$ is linearly independent of $B[1 : k, 2 : k]$. Therefore, we have

$$\text{null}(B[1 : k, 1 : k]) = \text{null}(B[1 : k, 2 : k]) = \text{null}(A[1 : k, 2 : k]) = \text{null}(A[1 : k, 1 : k]) - 1$$

By a similar reasoning, we have

$$\text{null}(B[:, 1 : k]) = \text{null}(A[:, 1 : k]) - 1$$

The column pivoting does not affect the rank of the rows, so

$$\text{null}(B[1 : k, :]^T) = \text{null}(A[1 : k, :]^T)$$

Therefore B satisfies Theorem 2.1 for $k < j$.

For $k \geq j$, the pivoting does not affect the ranks in Equation (2), so B also satisfies Theorem 2.1 for $k \geq j$.

So B satisfies Theorem 2.1.

Since $b_{11} \neq 0$, B has an LU factorization: $B = LU$. Column j of B is zero. If column j of U is non-zero, we can zero it out without affecting any column in LU . So we can always choose U such that column j is zero. We have:

$$A = B\Pi_j = L U \Pi_j$$

and $U\Pi_j$ is still upper triangular because Π_j only permutes column 1 and j . Therefore A has an LU factorization.

Case 2: $A[1, :] = 0$. Consider $B = A^T$. B corresponds to Case 1, so B has an LU factorization: $B = LU$. Therefore:

$$A = B^T = U^T L^T$$

is an LU factorization of A .

Case 3: If A is 0, it has an LU factorization with $L = U = 0$. Otherwise, if $A \neq 0$, let's denote by j the smallest index such that column j is non zero. Let's denote by $i > 1$ the smallest index such that $a_{ij} \neq 0$. Let's pivot column 1 and j and denote by $B = A\Pi_j$ the permuted matrix. B satisfies Case 2, so it has an LU factorization: $B = LU$. Column j of U is zero. Therefore:

$$A = B\Pi_j = L U \Pi_j$$

is an LU factorization of A .

We have also proved that this process must terminate after r steps where $r = \text{rank}(A)$. So the LU factorization of B is rank revealing. \square

We now prove a stronger theorem. Please compare this result with Theorem 1.4.

Theorem 2.6. *Let A be a matrix of size n with rank $r \leq n$. If A satisfies Theorem 2.1, then there exist a row permutation P_r and a column permutation P_c such that the matrix*

$$B = P_r^{-1} A P_c^{-1}$$

has strongly non-singular leading principal submatrices $B[1 : k, 1 : k]$ for $1 \leq k \leq r$. Consequently, the leading principal block admits an LU factorization $B[1 : r, 1 : r] = L_r U_r$.

Define the rank-revealing factors of B as:

$$L_B = \begin{pmatrix} L_r \\ B[r+1 : n, 1 : r] U_r^{-1} \end{pmatrix} \quad \text{and} \quad U_B = \begin{pmatrix} U_r & L_r^{-1} B[1 : r, r+1 : n] \end{pmatrix}$$

Then $B = L_B U_B$. Furthermore, A admits a rank-revealing factorization

$$A = LU$$

where $L = P_r L_B$ is lower triangular and $U = U_B P_c$ is upper triangular.

Moreover, we have the following sparsity results for L . Let i_0 be the row index in A corresponding to the logical row index i in B (i.e., $e_{i_0} = P_r e_i$). Then:

- If $i \leq r$, then $i_0 \geq i$ and $L[i_0, i+1 :] = 0$. Row i_0 of A is linearly independent of the previous rows.
- If $i > r$, then $i_0 \leq i$; if $i_0 \leq r$, then $L[i_0, i_0 :] = 0$. Row i_0 of A is a linear combination of the previous rows.

Similarly for U , let j_0 be the column index in A corresponding to the logical column index j in B (i.e., $e_{j_0} = P_c^T e_j$). Then:

- If $j \leq r$, then $j_0 \geq j$ and $U[j+1 : , j_0] = 0$. Column j_0 of A is linearly independent of the previous columns.
- If $j > r$, then $j_0 \leq j$; if $j_0 \leq r$, then $U[j_0 : , j_0] = 0$. Column j_0 of A is a linear combination of the previous columns.

Proof. We follow a proof similar to the one for Theorem 2.5.

We do an induction on the size of A . The result is true for $n = 1$.

Assume it is true for size $n - 1$. If $a_{11} \neq 0$, we have the factorization:

$$A = LDU$$

where

$$L = \begin{pmatrix} a_{11} & 0 \\ A_{21} & I \end{pmatrix}, \quad D = \begin{pmatrix} a_{11}^{-1} & 0 \\ 0 & S \end{pmatrix}, \quad U = \begin{pmatrix} a_{11} & A_{12} \\ 0 & I \end{pmatrix}$$

We apply the induction hypothesis to S . We can define P_r and P_c in terms of the permutations for S :

$$P_r = \begin{pmatrix} 1 & 0 \\ 0 & P_{r,S} \end{pmatrix}, \quad P_c = \begin{pmatrix} 1 & 0 \\ 0 & P_{c,S} \end{pmatrix}$$

The sparsity results follow directly from the induction hypothesis.

Assume $a_{11} = 0$. From Theorem 2.1, we have:

1. $A[:, 1] = 0, A[1, :] \neq 0$, or
2. $A[1, :] = 0, A[:, 1] \neq 0$, or
3. $A[:, 1] = 0, A[1, :] = 0$.

Case 1: $A[:, 1] = 0$. As for Theorem 2.5, we can find the smallest j such that $A[1, j] \neq 0$. We pivot column 1 and j .

We need to prove that column j cannot be a linear combination of the previous columns. Assume it is. Then there exists x such that:

$$A[:, j] = A[:, 1:j-1]x$$

So:

$$A[1, j] = A[1, 1:j-1]x = 0$$

Since $A[1, j] \neq 0$, we have a contradiction. So column j is linearly independent of the previous columns.

Denote by $B = A\Pi_j$ the permuted matrix. B satisfies Theorem 2.1 and $b_{11} \neq 0$. So B has an LU factorization with the sparsity pattern of Theorem 2.6. Since column j of B is zero, column j of U_B is zero. We define

$$P_c = P_{c,B}\Pi_j, \quad U = U_B\Pi_j$$

Π_j swaps columns 1 and j of U_B . We have $e_1 = \Pi_j^T e_j$ and column j of U_B is zero. We also have a j_0 such that $e_j = P_{c,B}^T e_{j_0}$ and $e_1 = P_c^T e_{j_0}$. Note that since column j of B (which is column 1 of A) is zero, we are beyond the rank-revealing part and $j_0 > r$. Since column 1 of U is zero and the other columns of U have the sparsity pattern of Theorem 2.6, U also satisfies the sparsity pattern of Theorem 2.6.

Case 2: $A[1, :] = 0$. Consider $B = A^T$. B corresponds to Case 1 and satisfies the sparsity pattern of Theorem 2.6. So A also satisfies the sparsity pattern of Theorem 2.6.

Case 3: If $A = 0$, it has an LU factorization. In that case we pick $L = U = 0$ as the factors. If $A \neq 0$, let's denote by j the smallest index such that column j is non zero. Let's denote by $i > 1$ the smallest index such that $a_{ij} \neq 0$. Let's pivot column 1 and j and denote by $B = A\Pi_j$ the permuted matrix. B satisfies Case 2, so it has an LU factorization: $B = LU$ with the sparsity pattern of Theorem 2.6. Following a reasoning analogous to Case 1, we can show that A also satisfies the sparsity pattern of Theorem 2.6.

As in Theorem 2.5, we have also proved that this process must terminate after r steps where $r = \text{rank}(A)$. So the LU factorization of B is rank revealing.

Following Theorem A.3, any column j_0 in A that is a linear combination of the previous columns will become 0 at step $\min(r, j_0 - 1)$. If $j_0 \leq r$, this column will be moved rightward to position j with $j > r$. Any column j_0 that is a linearly independent of the previous columns will never become zero. If $j_0 > r$, it will be moved leftward to position j with $j \leq r$.

A similar result applies to the rows of A . □

2.4 Python implementation

In Section A.1, we provide a Python implementation of the algorithm. The algorithm returns L and U such that $A = L \otimes U$.

Please compare against the algorithm with full pivoting in Section A.2, which returns P, Q, L, and U such that $P \otimes A \otimes Q = L \otimes U$. Full pivoting selects the largest pivot for maximum stability. Our algorithm selects the pivot to ensure that the factors L and U remain triangular.

Algorithm 1 is vectorized for performance. The internal permutations are done implicitly. For example, line 34 moves column j to column k . Line 36 zeros out column j of A in exact arithmetic.

This algorithm is not backward stable as we do not control the size of the pivot. Finding a backward stable algorithm will be the topic of future work.

The pseudo-code in Okunev and Johnson [2005] (Algorithm 1, p. 12) does not consider the case where the factorization does not exist.

3 Unit triangular factors

We now discuss results where we require one of the factors to be unit triangular. Classical results consider the factorization with partial pivoting $PA = LU$ (Theorem 1.1). The row permutation P allows us to obtain a unit lower triangular factor L . When a zero pivot is encountered, we perform a row pivoting to get a non zero pivot. If the entire column is equal to zero, we set the diagonal entry of L to 1, the entries below to 0, and continue the factorization with the next column.

We are interested in conditions for the existence of $A = LU$ where L is unit lower triangular. As before, this requires internal permutations, but this time they can only be applied to the columns. The triangular unit structure of L prevents row permutations. The condition on A is more stringent than in the general LU case and we require

$$\text{null}(A[1 : k, 1 : k]) = \text{null}(A[:, 1 : k])$$

for all k .

We note that, for a general matrix A , column pivoting in general is not sufficient to get a unit lower triangular factor. For example, consider the matrix

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

No column pivoting works. However, row pivoting is sufficient to get a unit lower triangular factor.

Table 3 summarizes the constraints on the factorization, the condition (for all k), and the stringency of the condition.

Constraint	Condition (for all k)	Stringency
General LU	$\text{null}(A_{11}) \leq \text{null}(\text{Col}) + \text{null}(\text{Row})$	Least stringent (allows mixed dependencies)
Unit Lower L	$\text{null}(A_{11}) = \text{null}(\text{Col})$	Moderate (requires column dependencies)
Unit Upper U	$\text{null}(A_{11}) = \text{null}(\text{Row})$	Moderate (requires row dependencies)
Unit L and Unit U	Only possible if A is strongly non-singular	Most stringent (impossible for singular A)

Table 3: Constraints on factorization, condition (for all k), and stringency of condition.

The theorem below should be compared with Theorem 1.1.

Theorem 3.1. *Let A be a matrix of size n and rank $r \leq n$. A has an LU factorization $A = LU$ where L is square unit lower triangular if and only if for all $k = 1, \dots, n$:*

$$\text{null}(A[1 : k, 1 : k]) = \text{null}(A[:, 1 : k]) \tag{3}$$

Construction: *If A satisfies Equation (3), there exists a column permutation P_c such that the matrix $B = AP_c^{-1}$ admits a factorization $B = L_B U_B$ where L_B is unit lower triangular. Consequently,*

$$A = L_B(U_B P_c) = LU$$

is a valid factorization of A with $L = L_B$ unit lower triangular and U upper triangular.

Structure: For the matrix B constructed above, row j is a linear combination of the previous rows if and only if column j is a linear combination of the previous columns.

Sparsity: Let j_0 be the column index in A corresponding to the logical column index j in B (i.e., $e_{j_0} = P_c^T e_j$). The factors exhibit the following sparsity patterns:

- **Dependent Case:** If row j of B is a linear combination of the previous rows, then $j_0 \leq j$. Furthermore:

$$L[:, j] = e_j, \quad U[j, :] = 0, \quad \text{and} \quad U[j_0 :, j_0] = 0$$

- **Independent Case:** If row j of B is linearly independent of the previous rows, then $j_0 \geq j$. Furthermore:

$$U[j+1 :, j_0] = 0$$

Proof. **Condition is necessary.** Short proof: U trivially satisfies Equation (3) since it is upper triangular. Since $L[1 : k, 1 : k]$ is full rank, A also satisfies Equation (3).

Direct proof: Assume that the matrix A admits a factorization $A = LU$, where L is a unit lower triangular matrix and U is an upper triangular matrix.

We analyze the structure of the matrices for an arbitrary $k \in \{1, \dots, n\}$. Because U is upper triangular, the first k columns of A depend only on the first k columns of U . Specifically, we can write the submatrices of A as:

- Leading principal submatrix

$$A[1 : k, 1 : k] = L[1 : k, 1 : k] U[1 : k, 1 : k]$$

- Leading column block

$$A[:, 1 : k] = L[:, 1 : k] U[1 : k, 1 : k]$$

Since L is **unit** lower triangular, its diagonal entries are all 1. This implies that any leading principal submatrix of L is invertible.

- Let $L_{kk} = L[1 : k, 1 : k]$. Because $\det(L_{kk}) = 1$, L_{kk} is non-singular (full rank).
- Let $L_{col} = L[:, 1 : k]$. The top block of L_{col} is L_{kk} . Since L_{kk} is non-singular, the larger matrix L_{col} must have full column rank (rank k).

We now compute the ranks of the submatrices of A using the properties of L :

- For the principal submatrix: since L_{kk} is non-singular, multiplying by it does not change the rank:

$$\text{rank}(A[1 : k, 1 : k]) = \text{rank}(L_{kk} \cdot U[1 : k, 1 : k]) = \text{rank}(U[1 : k, 1 : k])$$

- For the column block: since L_{col} has full column rank, multiplying by it on the left preserves the rank of the matrix on the right:

$$\text{rank}(A[:, 1 : k]) = \text{rank}(L_{col} \cdot U[1 : k, 1 : k]) = \text{rank}(U[1 : k, 1 : k])$$

Comparing the results, we see that the ranks are identical:

$$\text{rank}(A[1 : k, 1 : k]) = \text{rank}(A[:, 1 : k])$$

By the Rank-Nullity Theorem, for any matrix M with k columns, $\text{null}(M) = k - \text{rank}(M)$. Since both $A[1 : k, 1 : k]$ and $A[:, 1 : k]$ have exactly k columns:

$$\begin{aligned} \text{null}(A[1 : k, 1 : k]) &= k - \text{rank}(A[1 : k, 1 : k]) \\ \text{null}(A[:, 1 : k]) &= k - \text{rank}(A[:, 1 : k]) \end{aligned}$$

Therefore:

$$\text{null}(A[1 : k, 1 : k]) = \text{null}(A[:, 1 : k])$$

This completes the proof that the condition is necessary.

Condition is sufficient. We follow a proof similar to the one for Theorem 2.6. We do an induction on the size of A . The result is true for $n = 1$.

Assume it is true for size $n - 1$. If $a_{11} \neq 0$, we verify that the result is true by the induction hypothesis.

Assume $a_{11} = 0$. From Equation (3), we have $A[:, 1] = 0$.

Case 1: If row 1 of A is non-zero, we can use the same steps as in the proof as Theorem 2.6 with a column permutation to prove the result by induction. In addition, this shows that if $e_{j_0} = P_c^T e_j$ and if row j of B is linearly independent of the previous rows then $j_0 \geq j$ and $U[j + 1 :, j_0] = 0$.

Case 2: If row 1 of A is zero, we cannot use the same proof as Theorem 2.6 because we can no longer permute rows. However, since row 1 of A is zero, we can define:

$$A = IDU$$

with

$$D = \begin{pmatrix} 1 & 0 \\ 0 & S \end{pmatrix}, \quad U = \begin{pmatrix} 0 & A[1, 2 : n] \\ 0 & I \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}$$

and $S = A_{22}$. D satisfies

$$\text{null}(D[1 : k, 1 : k]) = \text{null}(A[1 : k, 1 : k]) - 1 = \text{null}(A[:, 1 : k]) - 1 = \text{null}(D[:, 1 : k])$$

D satisfies Equation (3). By the induction hypothesis, we can find a column permutation $P_{c,S}$ such that $SP_{c,S}^{-1}$ has an LU factorization with unit lower triangular factor.

This also proves that row j of B is a linear combination of the previous rows if and only if column j of B is a linear combination of the previous columns. Moreover, if $e_{j_0} = P_c^T e_j$ and row j of B is a linear combination of the previous rows, then $j_0 \leq j$. We have $L[:, j] = e_j$, $U[j, :] = 0$, and $U[j_0 :, j_0] = 0$.

Note that the step above with D is not a valid step in Theorem 2.6. Indeed:

$$\begin{aligned} \text{null}(D[1 : k, 1 : k]) &= \text{null}(A[1 : k, 1 : k]) - 1 \\ \text{null}(D[:, 1 : k]) &= \text{null}(A[:, 1 : k]) - 1 \\ \text{null}(D[1 : k, :]^T) &= \text{null}(A[1 : k, :]^T) - 1 \end{aligned}$$

So that Theorem 2.1 may not be satisfied by D . □

We now state the corresponding result where U is unit upper triangular. Please compare the result below with Theorem 1.2.

Corollary 3.2. *Let A be a matrix of size n and rank $r \leq n$. A has an LU factorization $A = LU$ where U is unit upper triangular if and only if for all $k = 1, \dots, n$:*

$$\text{null}(A[1 : k, 1 : k]) = \text{null}(A[1 : k, :]^T) \tag{4}$$

Construction: If A satisfies Equation (4), there exists a row permutation P_r such that the matrix $B = P_r^{-1}A$ admits a factorization $B = L_B U_B$ where U_B is unit upper triangular. Consequently,

$$A = (P_r L_B) U_B = LU$$

is a valid factorization of A with $U = U_B$ unit upper triangular and L lower triangular.

Structure: For the matrix B constructed above, column i is a linear combination of the previous columns if and only if row i is a linear combination of the previous rows.

Sparsity: Let i_0 be the row index in A corresponding to the logical row index i in B (i.e., $e_{i_0} = P_r e_i$). The factors exhibit the following sparsity patterns:

- **Dependent Case:** If column i of B is a linear combination of the previous columns, then $i_0 \leq i$. Furthermore:

$$U[i, :] = e_i, \quad L[:, i] = 0, \quad \text{and} \quad L[i_0, i_0 :] = 0$$

- **Independent Case:** If column i of B is linearly independent of the previous columns, then $i_0 \geq i$. Furthermore:

$$L[i_0, i + 1 :] = 0$$

Proof. Consider $B = A^T$. Apply Theorem 3.1. □

3.1 Python implementation

In Section A.3, we provide a Python implementation of the algorithm. This code is significantly simpler since we only do internal permutations on the columns of A . As previously, the internal permutations are done implicitly, and this algorithm is not backward stable.

4 Conclusion

In this paper, we have provided an analysis of the necessary and sufficient conditions for the existence of an LU factorization for arbitrary square matrices, without the use of pivoting. We established that the existence of such a factorization is determined by a specific inequality relating the nullity of the leading principal submatrices to the nullity of the corresponding leading column and row blocks. This condition generalizes the classical requirement for non-singular matrices (non-vanishing leading principal minors) to the general rank-deficient case.

Our approach utilizes a constructive proof based on induction. This method not only simplifies the theoretical derivation but also provides explicit insight into how singular blocks can be handled through internal permutations that preserve the overall triangular structure of the factors.

Furthermore, we defined and characterized rank-revealing LU factorizations without global pivoting. We derived tight sparsity bounds for the resulting factors L and U , linking the physical indices of the non-zero entries to the logical rank profile of the matrix. Finally, we examined the constrained cases where one factor is required to be unit triangular, identifying the specific rank conditions required and their duality with respect to row and column permutations. These results offer a unified framework for understanding matrix factorizations in the presence of singularity and rank deficiency.

A Appendix

We prove a few additional results that are helpful in the main proofs. For additional background on connections between the LU factorization, Schur complements, and oblique projections, please refer to Ouellette [1981], Zhang [2006], Householder [2013].

Lemma A.1. Denote by X and Y two matrices of size $n \times k$. Assume that X is full rank and that $Y^T X$ is non-singular. Define:

$$P = X(Y^T X)^{-1} Y^T$$

Then P is the oblique projection onto the range of X along the orthogonal complement of the range of Y .

Proof. We have:

$$PX = X(Y^T X)^{-1} Y^T X = X$$

So the range of P contains the range of X . Since $\text{rank}(P) \leq k$ and $\text{rank}(X) = k$, the range of P is exactly the range of X .

Consider v in the orthogonal complement of the range of Y (i.e., $Y^T v = 0$). We have:

$$Pv = X(Y^T X)^{-1} Y^T v = 0$$

Thus, the null space of P contains the orthogonal complement of the range of Y . By the rank-nullity theorem, the dimensions match, so the null space of P is exactly the orthogonal complement of the range of Y . \square

Lemma A.2. Denote by $X = [x_1, \dots, x_k]$ a rank k matrix. Consider the oblique projection $P_o(X)$ onto

$$S = \text{span}\{x_1, \dots, x_k\}$$

along the subspace of vectors with the first k entries equal to zero. Assume that $X[1:k,:]$ is non-singular. Then:

$$P_o(X) = X(X[1:k,:])^{-1} Y^T$$

where

$$Y = \begin{pmatrix} I_k \\ 0 \end{pmatrix}$$

Proof. In Theorem A.1, set Y as

$$Y = \begin{pmatrix} I_k \\ 0 \end{pmatrix}$$

The range of Y is the span of the first k standard basis vectors. Its orthogonal complement is exactly the subspace of vectors with the first k entries equal to zero. \square

Denote by $Q_o(X) = I - P_o(X)$ the oblique projection onto the subspace of vectors with the first k entries equal to zero along $S = \text{span}(X)$.

Consider the state of the matrix at the beginning of step k of the LU factorization algorithm (after $k - 1$ columns have been eliminated). The Schur complement can be interpreted in terms of the oblique projection Q_o . Specifically, from Theorem A.2 applied to the first $k - 1$ columns, we have:

$$S_k^o = A[:, k :] - A[:, 1:k-1]A[1:k-1, 1:k-1]^{-1}A[1:k-1, k :] = Q_o(A[:, 1:k-1])A[:, k :]$$

The standard Schur complement S_k corresponds to the bottom block of this projected matrix: $S_k = S_k^o[k :, :]$.

Lemma A.3. *If column j of A (where $j \geq k$) is linearly dependent on columns 1 to $k - 1$ of A , then column $j - k + 1$ of S_k^o is zero.*

Proof. Since column j of A is linearly dependent on columns 1 to $k - 1$, we have:

$$A[:, j] \in \text{span}\{A[:, 1], \dots, A[:, k-1]\}$$

Let $X = A[:, 1:k-1]$. Then $A[:, j] \in \text{span}(X)$. By definition of the projection $P_o(X)$:

$$P_o(X)A[:, j] = A[:, j]$$

Therefore:

$$Q_o(X)A[:, j] = (I - P_o(X))A[:, j] = 0$$

Since S_k^o is formed by applying $Q_o(X)$ to the columns $A[:, k :]$, the column corresponding to $A[:, j]$ is zero. \square

A.1 Python code for LU factorization

See Algorithm 1.

```

4 def lu_factorization(A_in):
5     A = A_in.astype(np.float64).copy()
6     n = A.shape[0]
7     L, U = np.zeros_like(A), np.zeros_like(A)
8     for k in range(n):
9         i, j = k, k
10        if np.isclose(A[i, j], 0.0):
11            # Search for the first shell 'i' (relative to k) that contains a non-zero element in either
12            # its row or column slice.
13            is_nz = ~np.isclose(A[k:, k:], 0.0)
14
15            # valid_rows[x] is True if Row x of A[k:, k:] (upper part, j>=x) has non-zero
16            valid_rows = np.any(np.triu(is_nz), axis=1)
17            # valid_cols[x] is True if Col x of A[k:, k:] (lower part, i>=x) has non-zero
18            valid_cols = np.any(np.tril(is_nz), axis=0)
19            valid_shells = valid_rows | valid_cols
20
21            if np.any(valid_shells):
22                l_rel = np.argmax(valid_shells) # First index where valid
23                l = k + l_rel
24                # Find k_row and k_col for this specific shell l
25                k_row = l + np.argmax(~np.isclose(A[l, 1:], 0.0)) if valid_rows[l_rel] else n + 1
26                k_col = l + np.argmax(~np.isclose(A[1:, l], 0.0)) if valid_cols[l_rel] else n + 1
27                use_row = k_row <= k_col
28                if l == k and np.any(~np.isclose(A[k:, k] if use_row else A[k, k:], 0.0)):
29                    # Factorization does not exist
30                    return None
31                i, j = (l, k_row) if use_row else (k_col, l)
32            else:
33                break
34
35            L[k:, k] = A[k:, j] / A[i, j] #
36            U[k, k:] = A[i, k:]
37            A[k+1:, k+1:] -= np.outer(L[k+1:, k], U[k, k+1:]) #

```

```
38     return L, U
```

Algorithm 1: Algorithm for LU factorization. Returns the LU factorization of a matrix $A = LU$ or None if the factorization does not exist. The algorithm is guaranteed to return None only when the factorization does not exist.

A.2 Python code for classical LU with full pivoting

See Algorithm 2.

```
4 def lu_pivoting(A_in):
5     A = A_in.astype(np.float64).copy()
6     n = A.shape[0]
7     L, U = np.zeros_like(A), np.zeros_like(A)
8     p, q = np.arange(n), np.arange(n)
9
10    def swap_rows(k, i):
11        A[[k, i], k:] = A[[i, k], k:]
12        p[[k, i]] = p[[i, k]]
13        L[[k, i], :k] = L[[i, k], :k]
14
15    def swap_cols(k, j):
16        A[:, [k, j]] = A[:, [j, k]]
17        q[[k, j]] = q[[j, k]]
18        U[:, [k, j]] = U[:, [j, k]]
19
20    for k in range(n):
21        idx_max = np.argmax(np.abs(A[:, k:]))
22        i_local, j_local = np.unravel_index(idx_max, A[:, k:].shape)
23        i_max, j_max = k + i_local, k + j_local
24        swap_rows(k, i_max)
25        swap_cols(k, j_max)
26        if np.isclose(A[k, k], 0.0): break
27
28        L[:, k] = A[:, k] / A[k, k]
29        U[:, k:] = A[:, k:]
30        A[k+1:, k+1:] -= np.outer(L[k+1:, k], U[k, k+1:])
31
32    P, Q = np.eye(n)[p], np.eye(n)[:, q]
33    return P, Q, L, U
```

Algorithm 2: Classical LU factorization with full pivoting. Returns a factorization of the form $PAQ = LU$.

A.3 Python code for unit lower triangular LU factorization

See Algorithm 3.

```
4 def unit_lower_lu_factorization(A_in):
5     A = A_in.astype(np.float64).copy()
6     n = A.shape[0]
7     L, U = np.eye(n), np.zeros_like(A)
8
9     for k in range(n):
10        j = k + np.argmax(~np.isclose(A[k, k:], 0.0))
11        if np.isclose(A[k, k], 0.0):
12            if not np.allclose(A[k+1:, k], 0.0):
13                # Factorization does not exist
14                return None
15            if np.isclose(A[k, j], 0.0): continue
16
17        L[k+1:, k] = A[k+1:, j] / A[k, j]
18        U[:, k:] = A[:, k:]
19        A[k+1:, k+1:] -= np.outer(L[k+1:, k], U[k, k+1:])
20
21    return L, U
```

Algorithm 3: Unit lower triangular LU factorization. Returns a factorization $A = LU$ where L is unit lower triangular or None if the factorization does not exist.

References

- Nicholas J. Higham. Gaussian elimination. *WIREs Computational Statistics*, 3(3):230–238, 2011. ISSN 1939-0068. doi:10.1002/wics.164.
- Jun Lu. Numerical matrix decomposition. *arXiv preprint arXiv:2107.02579*, 2021. doi:10.48550/arXiv.2107.02579.
- Pavel Okunev and Charles R. Johnson. Necessary and sufficient conditions for existence of the LU factorization of an arbitrary matrix, 2005.
- Froilán M. Dopico, Charles R. Johnson, and Juan M. Molera. Multiple LU factorizations of a singular matrix. *Linear Algebra and its Applications*, 419(1):24–36, 2006. ISSN 0024-3795. doi:10.1016/j.laa.2006.03.043.
- K. R. Nagarajan, M. Paul Devasahayam, and T. Soundararajan. Products of three triangular matrices. *Linear Algebra and its Applications*, 292(1):61–71, 1999. ISSN 0024-3795. doi:10.1016/S0024-3795(99)00003-8.
- Charles R. Johnson, D. D. Olesky, and P. van den Driessche. Inherited matrix entries: LU factorizations. *SIAM Journal on Matrix Analysis and Applications*, 10(1):94–104, 1989. ISSN 0895-4798. doi:10.1137/0610007.
- D. J. Jeffrey. LU factoring of non-invertible matrices. *ACM Commun. Comput. Algebra*, 44(1):1–8, 2010. ISSN 1932-2232. doi:10.1145/1838599.1838602.
- Diane Valérie Ouellette. Schur complements and statistics. *Linear Algebra and its Applications*, 36(1):187–295, 1981. ISSN 0024-3795. doi:10.1016/0024-3795(81)90232-9.
- Fuzhen Zhang. *The Schur complement and its applications*, volume 4. Springer Science & Business Media, 2006. doi:10.1007/b105056.
- Alston S. Householder. *The theory of matrices in numerical analysis*. Courier Corporation, 2013.