Gaussian Elimination & LU Decompositions

Square System of Equations

Consider

$$Ax = b$$

where

$$A = [a_{ij}] \longleftarrow n \times n \text{ matrix}$$

$$b \longleftarrow n \times 1 \text{ vector.}$$

In expanded form,

$$\begin{aligned}
a_{11}x_1 + \cdots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + \cdots + a_{2n}x_n &= b_2 \\
&\vdots \\
a_{n1}x_1 + \cdots + a_{nn}x_n &= b_n
\end{aligned}$$

Gaussian Elimination

Carl Friedrich Gauss
(1777-1855)

A Summary of the Evolution of Gaussian Elimination

Gaussian Elimination With No Pivoting (GENP)

$$A \longrightarrow A^{(1)} \longrightarrow \cdots \longrightarrow A^{(n-1)} =: U \text{ (upper triangular).}$$
$$b \longrightarrow b^{(1)} \longrightarrow \cdots \longrightarrow b^{(n-1)}.$$

Gaussian Elimination With No Pivoting (GENP)

$$A \longrightarrow A^{(1)} \longrightarrow \cdots \longrightarrow A^{(n-1)} =: U \text{ (upper triangular).}$$
$$b \longrightarrow b^{(1)} \longrightarrow \cdots \longrightarrow b^{(n-1)}.$$

Step 1: Create zeros in the first column of A:

$$A \longrightarrow \underbrace{\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)} \end{bmatrix}}_{=:A^{(1)}}; \quad b \longrightarrow \underbrace{\begin{bmatrix} b_1 \\ b_2^{(1)} \\ \vdots \\ b_n^{(1)} \end{bmatrix}}_{=:b^{(1)}}$$

where

$$a_{ij}^{(1)} = a_{ij} - \underbrace{\frac{a_{i1}}{a_{11}}}_{=:m_{i1}} a_{1j}; \quad b_i^{(1)} = b_i - \frac{a_{i1}}{a_{11}} b_1; \quad i = 2:n, j = 2:n.$$

Here $a_{11} \longleftarrow$ pivot (assumed non zero); $m_{i1} \longleftarrow$ multipliers;

GENP

Step k: Create zeros in column k of $A^{(k-1)}$:

$$
A^{(k-1)} = \left[\begin{array}{cccc|ccc}
a_{11} & \cdots & \cdots & a_{1k} & a_{1,k+1} & \cdots & a_{1k} \\
 & a_{22}^{(1)} & \cdots & a_{2k}^{(1)} & a_{2,k+1}^{(1)} & \cdots & a_{2n}^{(1)} \\
 & & \ddots & \vdots & \vdots & \cdots & \vdots \\
 & & & a_{kk}^{(k-1)} & a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\
\hline
 & & & a_{k+1,k}^{(k-1)} & a_{k+1,k+1}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\
 & & & \vdots & \vdots & & \vdots \\
 & & & a_{n,k}^{(k-1)} & a_{n,k+1}^{(k-1)} & \cdots & a_{nn}^{(k-1)}
\end{array}\right]
$$

$$
\longrightarrow \left[\begin{array}{cccc|ccc}
a_{11} & \cdots & \cdots & a_{1k} & a_{1,k+1} & \cdots & a_{1k} \\
 & a_{22}^{(1)} & \cdots & a_{2k}^{(1)} & a_{2,k+1}^{(1)} & \cdots & a_{2n}^{(1)} \\
 & & \ddots & \vdots & \vdots & \cdots & \vdots \\
 & & & a_{kk}^{(k-1)} & a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\
\hline
 & & & & a_{k+1,k+1}^{(k)} & \cdots & a_{k+1,n}^{(k)} \\
 & & & & \vdots & & \vdots \\
 & & & & a_{n,k+1}^{(k)} & \cdots & a_{nn}^{(k)}
\end{array}\right] =: A^{(k)};
$$

GENP

The same operations are performed on $b^{(k-1)}$:

$$b^{(k-1)} \longrightarrow \begin{bmatrix} b_1 \\ b_2^{(1)} \\ \vdots \\ b_k^{(k-1)} \\ b_{k+1}^{(k)} \\ \vdots \\ b_n^{(k)} \end{bmatrix} =: b^{(k)}$$

where for $i = k+1 : n, j = k+1 : n$,

$$a_{ij}^{(k)} = a_{ij}^{(k-1)} - \underbrace{\frac{a_{ik}^{(k-1)}}{a_{kk}^{(k-1)}}}_{=:m_{ik}} a_{kj}^{(k-1)}; \quad b_i^{(k)} = b_i^{(k-1)} - \frac{a_{ik}^{(k-1)}}{a_{kk}^{(k-1)}} b_k^{(k-1)};$$

Here $a_{kk}^{(k-1)} \longleftarrow$ pivot (assumed non zero); $m_{ik} \longleftarrow$ multipliers;

GENP

Step $n-1$**:** Create a zero in the $(n, n-1)$ of $A^{(n-2)}$:

$$A^{(n-2)} \longrightarrow \underbrace{\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \\ & & \ddots & \vdots \\ & & & a_{nn}^{(n-1)} \end{bmatrix}}_{=:A^{(n-1)} \text{ (also called } U\text{)}}; \quad b^{(n-2)} \longrightarrow b^{(n-1)};$$

where assuming pivot $a_{n-1,n-1}^{(n-2)} \neq 0$ and using multiplier $m_{n,n-1} := \frac{a_{n,n-1}^{(n-2)}}{a_{n-1,n-1}^{(n-2)}}$,

$$a_{nn}^{(n-1)} = a_{nn}^{(n-2)} - m_{n,n-1} a_{n-1,n}^{(n-2)}; \quad b_n^{(n-1)} = b_n^{(n-2)} - m_{n,n-1} b_{n-1}^{(n-2)}.$$

GENP

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where assuming pivot $a_{n-1,n-1}^{(n-2)} \neq 0$ and using multiplier

$m_{n,n-1} := \frac{a_{n,n-1}^{(n-2)}}{a_{n-1,n-1}^{(n-2)}}$,

$$a_{nn}^{(n-1)} = a_{nn}^{(n-2)} - m_{n,n-1} a_{n-1,n}^{(n-2)}; \quad b_n^{(n-1)} = b_n^{(n-2)} - m_{n,n-1} b_{n-1}^{(n-2)}.$$

- The system is transformed to $Ux = b^{(n-1)}$.
- The pivots at each step are on the diagonal of U!
- All steps have to be repeated to solve any new system $Ax = c$ if the multipliers used in the GENP are not saved.

GENP $\equiv$ *LU* decomposition of *A*

Let

$$L = \begin{bmatrix} 1 & & & & & & & \\ m_{21} & 1 & & & & & & \\ m_{31} & m_{32} & \ddots & & & & & \\ \vdots & \vdots & & \ddots & & & & \\ m_{k1} & m_{k2} & \cdots & \cdots & 1 & & & \\ m_{k+1,1} & m_{k+1,2} & \cdots & \cdots & m_{k+1,k} & \ddots & & \\ \vdots & \vdots & & & \vdots & & 1 & \\ m_{n1} & m_{n2} & \cdots & \cdots & m_{nk} & \cdots & m_{n,n-1} & 1 \end{bmatrix}.$$

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Then $A = LU$!

***LU* decomposition:** A square matrix A is said to have an LU decomposition if there exists a unit lower triangular matrix L and an upper triangular matrix U such that $A = LU$.

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Then $A = LU$! This needs a proof!

LU **decomposition:** A square matrix A is said to have an LU decomposition if there exists a unit lower triangular matrix L and an upper triangular matrix U such that $A = LU$.

GENP $\equiv$ *LU* decomposition of *A*

Proof: In step k of GENP

$$A^{(k)} = \underbrace{\begin{bmatrix} 1 & & & & & \\ 0 & \ddots & & & & \\ \vdots & \cdots & 1 & & & \\ 0 & & -m_{k+1,k} & \ddots & & \\ \vdots & & \vdots & & \ddots & \\ 0 & \cdots & -m_{nk} & \cdots & & 1 \end{bmatrix}}_{=:M_k} A^{(k-1)}$$

Then

$$U = A^{(n-1)} = M_{n-1} M_{n-2} \cdots M_k \cdots M_2 M_1 A$$

where M_k, $k = 1, \ldots, n-1$ are the *multiplier* matrices or *Gauss transforms* of Gaussian Elimination.

Exercise: $b^{(n-1)} = M_{n-1} M_{n-2} \cdots M_1 b.$

GENP $\equiv$ LU decomposition of A

Note that,

$$U = A^{(n-1)} = \underbrace{M_{n-1}\left(M_{n-2}\cdots\underbrace{\left(M_k\cdots\underbrace{\left(M_2\underbrace{(M_1 A)}_{=A^{(1)}}\right)}_{=A^{(2)}}\right)}_{=A^{(k)}}\right)}_{=A^{(n-2)}}$$

and

$$M_k = I_n - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} e_k^T, \quad k = 1 : n-1,$$

are rank one updates of I_n. Here e_k is column k of I_n.

GENP $\equiv$ *LU* decomposition of *A*

Observe that

- $$M_k^{-1} = I_n + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{kn} \end{bmatrix} e_k^T, \quad k = 1 : n-1,$$ (Prove this!)
- For $i_1 < \cdots < i_p$,

$$M_{i_1}^{-1} \cdots M_{i_p}^{-1} = I_n + \sum_{i=i_1}^{i_p} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{i+1,i} \\ \vdots \\ m_{ni} \end{bmatrix} e_i^T,$$ (Prove this!)

GENP $\equiv$ LU decomposition of A

So $U = M_{n-1}M_{n-2}\cdots M_2 M_1 A$ implies,

$$A = M_1^{-1}M_2^{-1}\cdots M_{n-1}^{-1}U = \left(I_n + \sum_{k=1}^{n-1}\left(\begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} e_k^T \right)\right) U$$

$$= \begin{bmatrix} 1 & & & & & & & \\ m_{21} & 1 & & & & & & \\ m_{31} & m_{32} & \ddots & & & & & \\ \vdots & \vdots & & \ddots & & & & \\ m_{k1} & m_{k2} & \cdots & \cdots & 1 & & & \\ m_{k+1,1} & m_{k+1,2} & \cdots & \cdots & m_{k+1,k} & \ddots & & \\ \vdots & \vdots & & & \vdots & & 1 & \\ m_{n1} & m_{n2} & \cdots & \cdots & m_{nk} & \cdots & m_{n,n-1} & 1 \end{bmatrix} U = LU.$$

Rank one updates in GENP

In Step k,

$$A^{(k)} = M_k A^{(k-1)}$$

$$= \left(I_n - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} e_k^T \right) A^{(k-1)} = A^{(k-1)} - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \underbrace{e_k^T A^{(k-1)}}_{\text{row } k \text{ of } A^{(k-1)}}$$

$$\underbrace{= A^{(k-1)} - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} 0 & \cdots & 0 & a_{kk}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix}}_{\text{rank one update of } A^{(k-1)}}$$

Rank one updates in GENP

Now

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} 0 & \cdots & 0 & a_{kk}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix} = \left[\begin{array}{c|c} \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \widehat{M}_k \end{array}\right],$$

where $\widehat{M}_k = \begin{bmatrix} m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} a_{kk}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix}$.

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Now

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} 0 & \cdots & 0 & a_{kk}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix} = \left[\begin{array}{c|c} \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \widehat{M}_k \end{array}\right],$$

where $\widehat{M}_k = \begin{bmatrix} m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} a_{kk}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix}.$

As

$$m_{ik} a_{kk}^{(k-1)} = \left(a_{ik}^{(k-1)} / a_{kk}^{(k-1)} \right) a_{kk}^{(k-1)} = a_{ik}^{(k-1)}, \quad i = k+1 : n,$$

the first column of $\widehat{M}_k$ is

$$\begin{bmatrix} a_{k+1,k}^{(k-1)} \\ \vdots \\ a_{nk}^{(k-1)} \end{bmatrix}.$$

Rank one updates in GENP

Therefore,

$$A^{(k)} = A^{(k-1)} - \left[\begin{array}{c|c} \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \widehat{M}_k \end{array}\right]$$

$$= \left[\begin{array}{c|c} A_{11}^{(k-1)} & A_{12}^{(k-1)} \\ \hline A_{21}^{(k-1)} & A_{22}^{(k-1)} \end{array}\right]$$

$$- \left[\begin{array}{cccc|ccc} 0 & & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \cdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & & 0 & 0 & 0 & \cdots & 0 \\ \hline 0 & & 0 & a_{k+1,k}^{(k-1)} & \multicolumn{3}{c}{\multirow{3}{*}{$\begin{bmatrix} m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix}$}} \\ \vdots & \cdots & \vdots & \vdots & & & \\ 0 & & 0 & a_{nk}^{(k-1)} & & & \end{array}\right]$$

where

$$A_{11}^{(k-1)} \to k \times k; \quad A_{21}^{(k-1)} \to k \times (n-k);$$

$$A_{21}^{(k-1)} \to (n-k) \times k; \quad A_{22}^{(k-1)} \to (n-k) \times (n-k).$$

Rank one updates in GENP

As $A_{21}^{(k-1)} = \begin{bmatrix} 0 & & 0 & a_{k+1,k}^{(k-1)} \\ \vdots & \cdots & \vdots & \vdots \\ 0 & & 0 & a_{nk}^{(k-1)} \end{bmatrix}$, therefore,

$$A^{(k)} = \left[\begin{array}{c|c} A_{11}^{(k-1)} & A_{12}^{(k-1)} \\ \hline & A_{22}^{(k)} \end{array}\right],$$

where

$$A_{22}^{(k)} = \underbrace{A_{22}^{(k-1)} - \begin{bmatrix} m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} \begin{bmatrix} a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix}}_{\text{rank one update of } A_{22}^{(k-1)}}$$

$$= \begin{bmatrix} a_{k+1,k}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\ \vdots & \ddots & \vdots \\ a_{nk}^{(k-1)} & \cdots & a_{nn}^{(k-1)} \end{bmatrix} - \begin{bmatrix} \frac{a_{k+1,k}^{(k-1)}}{a_{kk}^{(k-1)}} \\ \vdots \\ \frac{a_{nk}^{(k-1)}}{a_{kk}^{(k-1)}} \end{bmatrix} \begin{bmatrix} a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \end{bmatrix}$$

Algorithm for GENP/LU

```
for k = 1 : n − 1
    if a_kk ≠ 0          (multiplier computation begins)
        for i = k + 1 : n
            a_ik = a_ik / a_kk;
        end
    else
            exit {'zero pivot encountered'}
    end      (multiplier computation ends)
    for i = k + 1 : n (matrix update begins)
        for j = k + 1 : n
            a_ij = a_ij − a_ik a_kj
        end
    end      (matrix update ends)
end
```

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```

$L \longrightarrow I_n +$ strictly lower triangular part of output A.
$U \longrightarrow$ upper triangular part of output A.

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    for $i = k + 1 : n$ (matrix update begins)
        for $j = k + 1 : n$
            $a_{ij} = a_{ij} - a_{ik} a_{kj}$
        end
    end (matrix update ends)
end

$L \longrightarrow I_n +$ strictly lower triangular part of output A.
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Exercise: Show that the flop count of LU decomposition of an $n \times n$ matrix is $\frac{2}{3}n^3 + O(n^2)$ flops.

Algorithm for GENP/LU with higher level BLAS

```
for k = 1:n-1
        if A(k,k) ≠ 0          (multiplier computation begins)
                A(k+1:n,k) = A(k+1:n,k)/A(k,k);
        else
                        exit {'zero pivot encountered'}
        end          (multiplier computation ends)

        (matrix update)
        A(k+1:n,k+1:n) = A(k+1:n,k+1:n) - A(k+1:n,k)*A(k,k+1:n);
end
```

GENP for solving systems of equations

Pseudocode for solving $n \times n$ system $Ax = b$:

1. Find LU decomposition of A. $\left(\frac{2}{3}n^3 + O(n^2)\text{ flops}\right)$
2. Solve $Ly = b$ for y. (n^2 flops)
3. Solve $Ux = y$ for x. (n^2 flops)

Total flops: $\frac{2}{3}n^3 + O(n^2)$ flops.

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First step need NOT be repeated for solving other systems with same A.

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Total flops: $\frac{2}{3}n^3 + O(n^2)$ flops.

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But the algorithm does not always work!

Theorem: A nonsingular square matrix has an LU decomposition if and only if all its leading principal submatrices are nonsingular.

Additionally for such matrices, the LU decomposition is unique.

Gaussian Elimination With Partial Pivoting (GEPP)

1. Checking A for existence of LU decomposition is not possible in practice.
   (i) Numerically it is only possible to ascertain how close A and its leading principal submatrices are to being singular.
   (ii) Ascertaining the proximity of A and its leading principal submatrices to a singular matrix will cost more flops than finding the LU factors.

Gaussian Elimination With Partial Pivoting (GEPP)

1. Checking A for existence of LU decomposition is not possible in practice.
2. Even if A has an LU decomposition, computing it is a numerically unstable process.
   - Small pivots can lead to large multipliers and result in instability in finite precision arithmetic.

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Any remedies?

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Try Gaussian Elimination with row exchanges also called **Gaussian Elimination with Partial Pivoting (GEPP)**!

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What is this?

For each $k = 1 : n - 1$

1. Find $a_{pk}^{(k-1)}$ such that $|a_{pk}^{(k-1)}| = \max_{k \le j \le n} |a_{jk}^{(k-1)}|$.
2. If $p \neq k$ interchange rows k and p.
3. Perform the usual GE steps to create zeros in column k.

GEPP

$$
A^{(k-1)} = \left[\begin{array}{cccc|ccc}
a_{11} & \cdots & \cdots & a_{1k} & a_{1,k+1} & \cdots & a_{1k} \\
 & a^{(1)}_{22} & \cdots & a^{(1)}_{2k} & a^{(1)}_{2,k+1} & \cdots & a^{(1)}_{2n} \\
 & & \ddots & \vdots & \vdots & \cdots & \vdots \\
\hline
 & & & a^{(k-1)}_{kk} & a^{(k-1)}_{k,k+1} & \cdots & a^{(k-1)}_{kn} \\
 & & & & & & \\
 & & & a^{(k-1)}_{k+1,k} & a^{(k-1)}_{k+1,k+1} & \cdots & a^{(k-1)}_{k+1,n} \\
 & & & \vdots & \vdots & & \vdots \\
 & & & a^{(k-1)}_{n,k} & a^{(k-1)}_{n,k+1} & \cdots & a^{(k-1)}_{nn}
\end{array}\right]
$$

GEPP $\equiv$ LU decomposition of row permuted A

Permutation Matrices: An $n \times n$ permutation matrix P is obtained by interchanging rows and/or columns of I_n.

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Examples: $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$

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Transposition: A transposition is a permutation matrix obtained by interchanging only two rows or two columns of an identity matrix.

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Transposition: A transposition is a permutation matrix obtained by interchanging only two rows or two columns of an identity matrix.

1. Permutations are orthogonal matrices.

GEPP $\equiv$ *LU* decomposition of row permuted *A*

Permutation Matrices: An $n \times n$ permutation matrix P is obtained by interchanging rows and/or columns of I_n.

Examples: $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$

Transposition: A transposition is a permutation matrix obtained by interchanging only two rows or two columns of an identity matrix.

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Theorem Given any $n \times n$ matrix A, there exists a permutation P such that PA has an LU decomposition.