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)

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

Gaussian Elimination With No Pivoting (GENP)

$A \longrightarrow A^{(1)} \longrightarrow \cdots \longrightarrow A^{(n-1)} =: U$ (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 $A^{(k-1)}$:

$$
A^{(k-1)} = \left[\begin{array}{cccc|ccc}
a_{11} & \cdots & \cdots & a_{1k} & a_{1,k+1} & \cdots & a_{1k} \\
 & a_{22}^{(1)} & \cdots & a_{2k}^{(1)} & a_{2,k+1}^{(1)} & \cdots & a_{2n}^{(1)} \\
 & & \ddots & \vdots & \vdots & \cdots & \vdots \\
 & 0 & \approx & a_{kk}^{(k-1)} & a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\
\hline
 & & & a_{k+1,k}^{(k-1)} & a_{k+1,k+1}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\
 & & & \vdots & \vdots & & \vdots \\
 & & & a_{n,k}^{(k-1)} & a_{n,k+1}^{(k-1)} & \cdots & a_{nn}^{(k-1)}
\end{array}\right]
$$

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

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 $A^{(n-2)}$:

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

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

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

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

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

- 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

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

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

Let

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

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 $A = LU$.

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

Let

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

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,

$$U = A^{(n-1)} = M_{n-1}\underbrace{\left(M_{n-2}\cdots\underbrace{\left(M_k\cdots\underbrace{\left(M_2\underbrace{(M_1A)}_{=A^{(1)}}\right)}_{=A^{(2)}}\right)}_{=A^{(k)}}\right)}_{=A^{(n-2)}}$$

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,

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

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

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
```

Algorithm for GENP/LU

for $k = 1 : n-1$
    if $a_{kk} \neq 0$ (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

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

Algorithm for GENP/LU

for $k = 1 : n - 1$
    if $a_{kk} \neq 0$ (multiplier computation begins)
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            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

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

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.

Rank one updates in GENP

In Step k,

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

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

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

As

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

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,

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

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

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

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

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

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

Algorithm for GENP/LU 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.

GENP for solving systems of equations

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

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

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

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

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

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

But the algorithm does not always work!

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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.

$\boxed{A \to \text{nonsingular.}}$

Suppose $A = LU \Rightarrow$

$$\begin{array}{cc} & \begin{array}{cc} k & n-k \end{array} \\ \begin{array}{c} k \\ n-k \end{array} & \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right] \end{array} = \begin{array}{cc} & \begin{array}{cc} k & n-k \end{array} \\ \begin{array}{c} k \\ n-k \end{array} & \left[\begin{array}{c|c} L_{11} & \\ \hline L_{12} & L_{22} \end{array}\right] \end{array} \begin{array}{c} \begin{array}{cc} k & n-k \end{array} \\ \left[\begin{array}{c|c} U_{11} & U_{12} \\ \hline & U_{22} \end{array}\right] \end{array}$$

$\Rightarrow A_{11} = L_{11} U_{11}$

$\therefore \det A_{11} = \det(L_{11} U_{11}) = \underbrace{\det L_{11}}_{=1} \det U_{11} = \det U_{11}$ — (1)

But $0 \neq \det A = \det(LU) = \underbrace{\det L}_{=1} \det U = \det U_{11} \det U_{22}$

$\Rightarrow \det U_{11} \neq 0$

$\therefore (1) \Rightarrow \det A_{11} \neq 0 \Rightarrow$ leading principal submatrices of A are nonsingular.

Conversely let all leading principal submatrices of A be nonsingular. For $n = 1$, $A = [a]$, $a \neq 0$.

& $A = [a] = \underbrace{[1]}_{=:L} \underbrace{[a]}_{=:U}$.

Suppose that A has an LU decomposition for sizes $< n$,

$$A = \begin{array}{c c} & \begin{array}{cc} n-1 & 1 \end{array} \\ \begin{array}{c} n-1 \\ 1 \end{array} & \left[\begin{array}{c|c} \hat{A} & b \\ \hline c^T & a_{nn} \end{array}\right] \end{array}.$$

So $\hat{A}$ has an LU decomposition say $\hat{A} = \hat{L}\hat{U}$.

$$= \left[\begin{array}{c|c} \hat{L}\hat{U} & b \\ \hline c^T & a_{nn} \end{array}\right] = \left[\begin{array}{c|c} \hat{L}\hat{U} & \hat{L}\hat{L}^{-1}b \\ \hline c^T & a_{nn} \end{array}\right]$$

$$= \left[\begin{array}{c|c} \hat{L} & \\ \hline l^T & 1 \end{array}\right] \left[\begin{array}{c|c} \hat{U} & \hat{L}^{-1}b \\ \hline & u_{nn} \end{array}\right]$$

where $l^T \hat{U} = c^T$ and $u_{nn} + l^T \hat{L}^{-1} b = a_{nn}$

i.e. $l = (\hat{U}^T)^{-1} c$ and $u_{nn} = a_{nn} - l^T(\hat{L}^{-1} b)$

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?

Gaussian Elimination With Partial Pivoting (GEPP)

1. Checking A for existence of LU decomposition is not possible in practice.

$PA = A(p,:) = LU$

2. Even if A has an LU decomposition, computing it is a numerically unstable process.

$P = I(p,:)$

Any remedies?

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

What is this?

$p = [1:n]$

For each $k = 1 : n-1$

$[r, m] = \max(\text{abs}(A(k:n,k)))$

1. Find $a_{pk}^{(k-1)}$ such that $|a_{pk}^{(k-1)}| = \max_{k \leq j \leq n} |a_{jk}^{(k-1)}|$.

$r \to$ largest abs. entry
$m \to$ position where r occurs

2. If $p \neq k$ interchange rows k and p.
3. Perform the usual GE steps to create zeros in column k.

if $m \neq k$ $A([k,m],:) = A([m,k],:)$ end
$p([k,m],:) = p([m,k],:)$

GEPP

$$A^{(k-1)} = \left[\begin{array}{cccc|ccc}
a_{11} & \cdots & \cdots & a_{1k} & a_{1,k+1} & \cdots & a_{1k} \\
m_{21} & a_{22}^{(1)} & \cdots & a_{2k}^{(1)} & a_{2,k+1}^{(1)} & \cdots & a_{2n}^{(1)} \\
 & m_{32} & \ddots & \vdots & \vdots & \cdots & \vdots \\
\hline
\vdots & \vdots & & \color{red}{a_{kk}^{(k-1)}} & a_{k,k+1}^{(k-1)} & \cdots & a_{kn}^{(k-1)} \\
 & & & \color{red}{a_{k+1,k}^{(k-1)}} & a_{k+1,k+1}^{(k-1)} & \cdots & a_{k+1,n}^{(k-1)} \\
 & & & \color{red}{\vdots} & \vdots & & \vdots \\
m_{n1} & m_{n2} & & \color{red}{a_{n,k}^{(k-1)}} & a_{n,k+1}^{(k-1)} & \cdots & a_{nn}^{(k-1)}
\end{array}\right]$$

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. $P^T = P^{-1}$
2. Transpositions are symmetric matrices. $P^T = P$
3. Transpositions are there own inverses. $P^T = P = P^{-1}$

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3. Transpositions are there own inverses.
4. Every permutation is a finite product of transpositions.
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Theorem Given any $n \times n$ matrix A, there exists a permutation P such that PA has an LU decomposition.

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

Recall that GENP requires multiplier matrices $M_1, \ldots, M_{n-1}$ such that

$$U = M_{n-1} M_{n-2} \cdots M_1 A.$$

GEPP $\equiv LU$ decomposition of row permuted A

Recall that GENP requires multiplier matrices $M_1, \dots, M_{n-1}$ such that

$$U = M_{n-1}M_{n-2}\cdots M_1 A.$$

Now GEPP requires finding transpositions $P_1, \dots P_{n-1}$ and multipliers matrices $M_1, \dots, M_{n-1}$, such that

$$U = \underbrace{\left\{ M_{n-1}P_{n-1} \underbrace{\left(M_{n-2}P_{n-2}\cdots \underbrace{\left(M_kP_k \cdots \underbrace{\left(M_2P_2 \underbrace{(M_1P_1A)}_{=A^{(1)}}\right)}_{=A^{(2)}} \right)}_{=A^{(k)}} \right)}_{=A^{(n-2)}} \right\}}_{=A^{(n-1)}}$$

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

Here for $k = 1, \ldots, n-1$,

1. $P_k = \left[\begin{array}{c|c} I_{k-1} & \\ \hline & \widehat{P}_k \end{array}\right]$, $\widehat{P}_k$ being a $(n-k+1) \times (n-k+1)$ transposition.

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2. $M_k = I_n - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix} e_k^T$, with $m_{jk} = a_{jk}^{(k-1)} / a_{kk}^{(k-1)}$, $j = k+1 : n$.

GEPP $\equiv$ LU decomposition of row permuted A

1. Let $\mathcal{P}_k = P_{k+1} \cdots P_{n-1}$, $k = 1, \ldots, n-2$. Then,

$$\mathcal{P}_k = \left[\begin{array}{c|c} I_k & \\ \hline & \widetilde{P}_{k+1} \cdots \widetilde{P}_{n-1} \end{array} \right]$$

where for all $j = k+1, \ldots, n-1$, $\widetilde{P}_j$ are transpositions of size $n-k \times n-k$.

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where for all $j = k+1, \ldots, n-1$, $\widetilde{P}_j$ are transpositions of size $n-k \times n-k$.
2. Let $\widetilde{M}_k = \mathcal{P}_k^T M_k \mathcal{P}_k$, $k = 1, \ldots, n-2$. Then,
$$\widetilde{M}_k = I_n - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \widetilde{m}_{k+1,k} \\ \vdots \\ \widetilde{m}_{nk} \end{bmatrix} e_k^T,$$
where
$$\begin{bmatrix} \widetilde{m}_{k+1,k} \\ \vdots \\ \widetilde{m}_{nk} \end{bmatrix} = \widetilde{P}_{n-1} \cdots \widetilde{P}_{k+1} \begin{bmatrix} m_{k+1,k} \\ \vdots \\ m_{nk} \end{bmatrix}.$$

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3. $U = M_{n-1} \widetilde{M}_{n-2} \cdots \widetilde{M}_1 P_{n-1} P_{n-2} \cdots P_1 A.$

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

1. Let $\mathcal{P}_k = P_{k+1}\cdots P_{n-1}$, $k = 1,\dots,n-2$. Then,

   $\Rightarrow \mathcal{P}_k^T = (P_{k+1}\cdots P_{n-1})^T = P_{n-1}\cdots P_{k+1}$

   $$\mathcal{P}_k = \left[\begin{array}{c|c} I_k & \\ \hline & \widetilde{P}_{k+1}\cdots\widetilde{P}_{n-1}\end{array}\right]$$

   where for all $j = k+1,\dots,n-1$, $\widetilde{P}_j$ are transpositions of size $n-k\times n-k$. Prove this!

2. Let $\widetilde{M}_k = \mathcal{P}_k^T M_k \mathcal{P}_k$, $k = 1,\dots,n-2$. Then,

   $\Rightarrow \widetilde{M}_k \mathcal{P}_k^T = \mathcal{P}_k^T M_k$

   $\Rightarrow P_{n-1}\cdots P_{k+1} M_k = \widetilde{M}_k P_{n-1}\cdots P_{k+1}$

   $P_{n-1} M_{n-2} = \widetilde{M}_{n-2} P_{n-1}$ $(k = n-2)$

   $P_{n-1} P_{n-2} M_{n-3} = \widetilde{M}_{n-3} P_{n-1} P_{n-2}$ $(k = n-3)$

   $$\widetilde{M}_k = I_n - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \widetilde{m}_{k+1,k} \\ \vdots \\ \widetilde{m}_{nk}\end{bmatrix} e_k^T,$$

   where $\begin{bmatrix} \widetilde{m}_{k+1,k} \\ \vdots \\ \widetilde{m}_{nk}\end{bmatrix} = \widetilde{P}_{n-1}\cdots\widetilde{P}_{k+1}\begin{bmatrix} m_{k+1,k} \\ \vdots \\ m_{nk}\end{bmatrix}$. Prove this!

3. $U = M_{n-1}\widetilde{M}_{n-2}\cdots\widetilde{M}_1 P_{n-1}P_{n-2}\cdots P_1 A$. Prove this!

GEPP $\equiv LU$ decomposition of row permuted A

Theorem Gaussian Elimination with Partial Pivoting (GEPP) on an $n \times n$ matrix A that transforms it to an upper triangular matrix U also finds a permutation matrix P and a lower triangular matrix L such that $PA = LU$. Moreover if P_k be the transposition used in step k, $1 \leq k \leq n-1$, then $P = P_{n-1} \cdots P_1$ and

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

where $\widetilde{m}_{ik}$, $k+1 \leq i \leq n$, $1 \leq k \leq n-2$ and $m_{n,n-1}$ are as described earlier.

GEPP

Exercise: Prove the theorem in the previous slide.

Use it to write a Matlab program `[L,U,P] = gepp(A)` that execute GEPP on A to find a permutation P, a unit lower triangular matrix L and an upper triangular matrix U such that $PA = LU$.

Your program should make only the most essential modifications to `[L,U] = genp(A)` and retain all major features essential for efficiency.

Exercise: The flop count of GEPP on an $n \times n$ matrix A, or equivalently the flop count of finding the permutation P such that $PA = LU$ is $\frac{2}{3}n^3 + O(n^2)$ flops.

Solving a system of equations via GEPP

Pseudocode for solving $Ax = b$ via GEPP:

1. Find a permutation P a unit lower triangular matrix L and an upper triangular matrix U via GEPP such that $PA = LU$. $(\frac{2}{3}n^3 + O(n^2)$ flops$)$
2. Solve $Ly = Pb$ for y. $(n^2$ flops$)$
3. Solve $Ux = y$ for x. $(n^2$ flops$)$

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

$PAx = Pb$

$\Leftrightarrow LUx = Pb$

Let $Ux = y$

Then $Ly = Pb$

& $Ux = y$

Gaussian Elimination with Complete pivoting (GECP)

The following alternative strategy may be used to find a largest possible pivot:

For each $k = 1 : n - 1$

1. Find $a_{pm}^{(k-1)}$ such that

$$|a_{pm}^{(k-1)}| = \max_{k \le j \le n} \max_{k \le i \le n} |a_{ij}^{(k-1)}|.$$

2. If $p \neq k$ interchange rows p and k and if $m \neq k$ interchange columns m and k.
3. Perform the usual GE steps to create zeros in column k.

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This is **Gaussian Elimination with Complete Pivoting (GECP).**

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This is **Gaussian Elimination with Complete Pivoting (GECP).**

Theorem GECP is equivalent to finding permutation matrices P and Q, a unit lower triangular matrix L and an upper triangular matrix U such that $PAQ = LU$.

GECP

Flop Count: Pivoting costs an additional $(n-k+1)^2-1$ comparisons in step k. This raises the total flop count by $n^3/3$. Thus GECP (or equivalently) finding $PAQ = LU$ costs $n^3 + O(n^2)$ flops.

Exercise: Find a pseudocode for solving an $n \times n$ system of equations $Ax = b$ via GECP.

Decompositions related to $A = LU$.

Exercise: Let A be an $n \times n$ nonsingular matrix with nonsingular leading principal submatrices. Prove the following:

1. There exists a unique unit lower triangular matrix L, a unique unit upper triangular matrix V and a unique diagonal matrix D such that $A = LDV$.

Decompositions related to $A = LU$.

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1. There exists a unique unit lower triangular matrix L, a unique unit upper triangular matrix V and a unique diagonal matrix D such that $A = LDV$.
2. If A is symmetric, then there exists a unique unit lower triangular matrix L, and a unique diagonal matrix D such that $A = LDL^T$.

$A = A^T = (LDV)^T = V^T D L^T$

$\therefore V^T = L$

Decompositions related to $A = LU$.

Exercise: Let A be an $n \times n$ nonsingular matrix with nonsingular leading principal submatrices. Prove the following:

1. There exists a unique unit lower triangular matrix L, a unique unit upper triangular matrix V and a unique diagonal matrix D such that $A = LDV$.
2. If A is symmetric, then there exists a unique unit lower triangular matrix L, and a unique diagonal matrix D such that $A = LDL^T$.
3. Additionally the decomposition $A = LDL^T$ in part 2 has the property that $x^T Ax > 0$ for all nonzero $x \in \mathbb{R}^n$ if and only if D has positive diagonal entries.