

# 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,

$$a_{11}x_1 + \cdots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + \cdots + a_{2n}x_n = b_2$$

$$\vdots$$

$$a_{n1}x_1 + \cdots + a_{nn}x_n = b_n$$

# Gaussian Elimination



**Carl Friedrich Gauss**  
**(1777-1855)**

## A Summary of the Evolution of Gaussian Elimination

# Gaussian Elimination With No Pivoting (GENP)

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

$b \longrightarrow b^{(1)} \longrightarrow \dots \longrightarrow b^{(n-1)}.$

# Gaussian Elimination With No Pivoting (GENP)

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

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

# GENP

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

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

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

# 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;

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

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- ▶ 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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This needs a proof!

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

**Proof:** In step  $k$  of GENP

$$A^{(k)} = \left[ \begin{array}{ccccccc} 1 & & & & & & \\ & \ddots & & & & & \\ & & \ddots & & & & \\ & & & 1 & & & \\ & & & -m_{k+1,k} & \ddots & & \\ & & & \vdots & & \ddots & \\ 0 & \cdots & -m_{nk} & \cdots & & & 1 \end{array} \right] A^{(k-1)}$$

$\underbrace{\hspace{10em}}_{=:M_k}$

Then

$$U = A^{(n-1)} = M_{n-1}M_{n-2}\cdots M_k\cdots M_2M_1A$$

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

**Exercise:**  $b^{(n-1)} = M_{n-1}M_{n-2}\cdots M_1b$ .

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

Note that,

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

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

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

$\blacktriangleright$  For  $i_1 < \dots < i_p$ ,

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

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

So  $U = M_{n-1}M_{n-2} \cdots M_2M_1A$  implies,

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

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



# Algorithm for GENP/LU

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

$L \longrightarrow I_n +$  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  $k$ ,

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

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

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

# Rank one updates in GENP

Now

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

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

# Rank one updates in GENP

Now

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

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

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  $\hat{M}_k$  is

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

# Rank one updates in GENP

Therefore,

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

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

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

where

$$\begin{aligned} A_{11}^{(k-1)} &\rightarrow k \times k; & A_{21}^{(k-1)} &\rightarrow k \times (n-k); \\ A_{21}^{(k-1)} &\rightarrow (n-k) \times k; & A_{22}^{(k-1)} &\rightarrow (n-k) \times (n-k). \end{aligned}$$

# Rank one updates in GENP

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

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

where

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

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



# Algorithm for GENP/LU with higher level BLAS

```
for k = 1:n-1
    if A(k,k)  $\neq$  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  $A$ .  $(\frac{2}{3}n^3 + O(n^2)$  flops)
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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**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.