

# Lecture 5: LU factorization, Cholesky factorization, Gaussian elimination with pivoting



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## 1. LU factorization

- **Definition:** Given  $\mathbf{A} \in \mathbb{C}^{m \times m}$ , an *LU factorization* (if it exists) of  $\mathbf{A}$  is a factorization

$$\mathbf{A} = \mathbf{L}\mathbf{U},$$

where  $\mathbf{L} \in \mathbb{C}^{m \times m}$  is *unit lower-triangular* and  $\mathbf{U} \in \mathbb{C}^{m \times m}$  is *upper-triangular*.

- An approach: find a sequence of unit lower-triangular matrices  $\mathbf{L}_k$  such that

$$\mathbf{L}_{m-1} \cdots \mathbf{L}_2 \mathbf{L}_1 \mathbf{A} = \mathbf{U}$$

and set

$$\mathbf{L} = \mathbf{L}_1^{-1} \mathbf{L}_2^{-1} \cdots \mathbf{L}_{m-1}^{-1}.$$

- A  $4 \times 4$  example

$$\begin{array}{c} \begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{bmatrix} \xrightarrow{\mathbf{L}_1} \begin{bmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{bmatrix} \xrightarrow{\mathbf{L}_2} \begin{bmatrix} \times & \times & \times & \times \\ & \times & \times & \times \\ & 0 & \times & \times \\ & 0 & \times & \times \end{bmatrix} \xrightarrow{\mathbf{L}_3} \begin{bmatrix} \times & \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times \\ & & 0 & \times \end{bmatrix} \\ \mathbf{A} \qquad \qquad \mathbf{L}_1 \mathbf{A} \qquad \qquad \mathbf{L}_2 \mathbf{L}_1 \mathbf{A} \qquad \qquad \mathbf{L}_3 \mathbf{L}_2 \mathbf{L}_1 \mathbf{A} \end{array}$$

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$$

$$\mathbf{L}_1 \mathbf{A} = \begin{bmatrix} 1 & & & \\ -2 & 1 & & \\ -4 & & 1 & \\ -3 & & & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & 3 & 5 & 5 \\ & 4 & 6 & 8 \end{bmatrix}$$

$$\mathbf{L}_2 \mathbf{L}_1 \mathbf{A} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ -3 & & 1 & \\ -4 & & & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & 3 & 5 & 5 \\ & 4 & 6 & 8 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & 2 & 4 \end{bmatrix}$$

$$\mathbf{L}_3 \mathbf{L}_2 \mathbf{L}_1 \mathbf{A} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & 2 & 4 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & & 2 \end{bmatrix} = \mathbf{U}.$$

$$\begin{bmatrix} 1 & & & \\ -2 & 1 & & \\ -4 & & 1 & \\ -3 & & & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & & & \\ 2 & 1 & & \\ 4 & & 1 & \\ 3 & & & 1 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ 2 & 1 & & \\ 4 & 3 & 1 & \\ 3 & 4 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & & 2 \end{bmatrix}$$

$\mathbf{A} \qquad \qquad \mathbf{L} \qquad \qquad \mathbf{U}$

## 1.1. General formulas for LU factorization

- Let  $\mathbf{u}_k$  denote the  $k$ th column of the matrix at the beginning of step  $k$  (which matrix?  $\mathbf{L}_{k-1} \cdots \mathbf{L}_2 \mathbf{L}_1 \mathbf{A}$ ).
- The purpose is to eliminate the entries below  $u_{kk}$ . To do this we construct the matrix  $\mathbf{L}_k$ :

$$\mathbf{L}_k = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -\ell_{k+1,k} & 1 & \\ & & \vdots & & \ddots \\ & & -\ell_{mk} & & 1 \end{bmatrix} = \begin{bmatrix} \mathbf{I}_{k-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 1 & \mathbf{0} \\ \mathbf{0} & -\widehat{\ell}_k & \mathbf{I}_{m-k} \end{bmatrix},$$

where  $\widehat{\ell}_k = [\ell_{k+1,k} \ \ell_{k+2,k} \ \cdots \ \ell_{mk}]^\top$  with the *multiplier*

$$\ell_{jk} = \frac{u_{jk}}{u_{kk}}, \quad k+1 \leq j \leq m.$$

## Proposition 1

The matrix  $\mathbf{L}_k$  can be inverted by negating its subdiagonal entries. We have

$$\mathbf{L}_k^{-1} = \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & \ell_{k+1,k} & 1 & & \\ & & \vdots & & \ddots & \\ & & \ell_{mk} & & & 1 \end{bmatrix} = \begin{bmatrix} \mathbf{I}_{k-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 1 & \mathbf{0} \\ \mathbf{0} & \widehat{\ell}_k & \mathbf{I}_{m-k} \end{bmatrix}.$$

Proof. Define the vector

$$\ell_k = [0 \quad \cdots \quad 0 \quad \ell_{k+1,k} \quad \cdots \quad \ell_{mk}]^\top.$$

The matrix  $\mathbf{L}_k = \mathbf{I} - \ell_k \mathbf{e}_k^*$ , where  $\mathbf{e}_k$  is the  $k$ th column of the identity matrix  $\mathbf{I}$ . Obviously,  $\mathbf{e}_k^* \ell_k = 0$ . Therefore, the statement follows from

$$(\mathbf{I} - \ell_k \mathbf{e}_k^*)(\mathbf{I} + \ell_k \mathbf{e}_k^*) = \mathbf{I} - \ell_k \mathbf{e}_k^* \ell_k \mathbf{e}_k^* = \mathbf{I}. \quad \square$$

## Proposition 2

The product  $\mathbf{L}_1^{-1}\mathbf{L}_2^{-1}\cdots\mathbf{L}_{m-1}^{-1}$ , i.e., the L factor  $\mathbf{L}$ , can be formed by collecting the entries  $\ell_{jk}$  in the appropriate places. We have

$$\mathbf{L} = \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & \vdots & \ddots & \ddots & \\ \ell_{m1} & \ell_{m2} & \cdots & \ell_{m,m-1} & 1 \end{bmatrix}.$$

Proof. It follows from  $\mathbf{L}_k^{-1} = \mathbf{I} + \boldsymbol{\ell}_k \mathbf{e}_k^*$  and  $\mathbf{e}_k^* \boldsymbol{\ell}_j = 0$  ( $\forall j \geq k$ ) that

$$\mathbf{L}_k^{-1} \mathbf{L}_{k+1}^{-1} = \mathbf{I} + \boldsymbol{\ell}_k \mathbf{e}_k^* + \boldsymbol{\ell}_{k+1} \mathbf{e}_{k+1}^*.$$

Therefore,

$$\mathbf{L} = \mathbf{L}_1^{-1} \mathbf{L}_2^{-1} \cdots \mathbf{L}_{m-1}^{-1} = \mathbf{I} + \boldsymbol{\ell}_1 \mathbf{e}_1^* + \boldsymbol{\ell}_2 \mathbf{e}_2^* + \cdots + \boldsymbol{\ell}_{m-1} \mathbf{e}_{m-1}^*. \quad \square$$

### Remark 3

- The matrices  $\mathbf{L}_k^{-1}$  are never formed and multiplied explicitly.
- The multipliers  $\ell_{jk}$  are computed and stored directly into  $\mathbf{L}$ .

## 1.2. LU factorization algorithm

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**Algorithm:** LU factorization  $\mathbf{A} = \mathbf{LU}$

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$\mathbf{U} = \mathbf{A}, \quad \mathbf{L} = \mathbf{I}$

**for**  $k = 1$  **to**  $m - 1$

**for**  $j = k + 1$  **to**  $m$

$$\ell_{jk} = u_{jk}/u_{kk}$$

$$u_{j,k:m} = u_{j,k:m} - \ell_{jk}u_{k,k:m}$$

**end**

**end**

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### 1.3. Gaussian elimination for $Ax = b$

- $A = LU$ ,  $Ly = b$ ,  $Ux = y$

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**Algorithm:** Forward elimination solving  $Ly = b$

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**for**  $k = 1$  **to**  $m$

$$y_k = b_k - \sum_{j=1}^{k-1} \ell_{kj} y_j$$

**end**

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**Algorithm:** Back substitution solving  $Ux = y$

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**for**  $k = m$  **downto**  $1$

$$x_k = \left( y_k - \sum_{j=k+1}^m u_{kj} x_j \right) / u_{kk}$$

**end**

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## 2. Cholesky factorization

- Every Hermitian positive definite matrix  $\mathbf{A}$  has a factorization

$$\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{L}^*,$$

where  $\mathbf{L}$  is the unit lower-triangular matrix in its LU factorization  $\mathbf{A} = \mathbf{L}\mathbf{U}$  and  $\mathbf{D}$  is a diagonal matrix with diagonal entries  $d_{ii} > 0$ .

- **Definition:** Given  $\mathbf{A} \in \mathbb{C}^{m \times m}$ , a *Cholesky factorization* (if it exists) of  $\mathbf{A}$  is a factorization

$$\mathbf{A} = \mathbf{R}^*\mathbf{R}$$

where  $\mathbf{R} \in \mathbb{C}^{m \times m}$  is *upper-triangular*.

### Theorem 4

*Every Hermitian positive definite matrix  $\mathbf{A} \in \mathbb{C}^{m \times m}$  has a unique Cholesky factorization*

$$\mathbf{A} = \mathbf{R}^*\mathbf{R},$$

*where  $\mathbf{R} \in \mathbb{C}^{m \times m}$  is upper-triangular and  $r_{jj} > 0$ .*

Proof. (By induction on the dimension).

It is easy for the case of dimension 1. Assume it is true for the case of dimension  $m - 1$ . We prove the case of dimension  $m$ . Let  $\alpha = \sqrt{a_{11}}$ . We have

$$\begin{aligned}\mathbf{A} &= \begin{bmatrix} a_{11} & \mathbf{w}^* \\ \mathbf{w} & \mathbf{K} \end{bmatrix} = \begin{bmatrix} \alpha & \mathbf{0} \\ \mathbf{w}/\alpha & \mathbf{I} \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{K} - \mathbf{w}\mathbf{w}^*/a_{11} \end{bmatrix} \begin{bmatrix} \alpha & \mathbf{w}^*/\alpha \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \\ &= \begin{bmatrix} \alpha & \mathbf{0} \\ \mathbf{w}/\alpha & \mathbf{I} \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{R}}^*\hat{\mathbf{R}} \end{bmatrix} \begin{bmatrix} \alpha & \mathbf{w}^*/\alpha \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \\ &\quad (\text{by } \mathbf{K} - \mathbf{w}\mathbf{w}^*/a_{11} \text{ is HPD and the induction hypothesis}) \\ &= \begin{bmatrix} \alpha & \mathbf{0} \\ \mathbf{w}/\alpha & \hat{\mathbf{R}}^* \end{bmatrix} \begin{bmatrix} \alpha & \mathbf{w}^*/\alpha \\ \mathbf{0} & \hat{\mathbf{R}} \end{bmatrix} = \mathbf{R}^*\mathbf{R}.\end{aligned}$$

The first row of  $\mathbf{R}$  is uniquely determined by  $r_{11} > 0$  and the factorization itself. The uniqueness of  $\mathbf{R}$  follows from the induction hypothesis that  $\hat{\mathbf{R}}$  is unique. □

## 2.1. A $4 \times 4$ example

$$\mathbf{A} = \begin{bmatrix} 4 & 4i & 6 & 2 \\ -4i & 5 & -4i & 5 - 2i \\ 6 & 4i & 17 & 3 - 8i \\ 2 & 5 + 2i & 3 + 8i & 36 \end{bmatrix}$$

- Compute the upper triangular matrix  $\mathbf{R}$  row by row

$$\text{Step 1: } \begin{bmatrix} 2 & & & \\ -2i & 1 & & \\ 3 & & 1 & \\ 1 & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & 2i & 5 \\ & \times & 8 & -8i \\ & \times & \times & 35 \end{bmatrix} \begin{bmatrix} 2 & 2i & 3 & 1 \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

$$\text{Step 2: } \begin{bmatrix} 1 & 2i & 5 \\ \times & 8 & -8i \\ \times & \times & 35 \end{bmatrix} = \begin{bmatrix} 1 & & \\ -2i & 1 & \\ 5 & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 4 & 2i \\ & \times & 10 \end{bmatrix} \begin{bmatrix} 1 & 2i & 5 \\ & 1 & \\ & & 1 \end{bmatrix}$$

$$\text{Step 3: } \begin{bmatrix} 4 & 2i \\ \times & 10 \end{bmatrix} = \begin{bmatrix} 2 & \\ -1i & 1 \end{bmatrix} \begin{bmatrix} 1 & \\ & 9 \end{bmatrix} \begin{bmatrix} 2 & 1i \\ & 1 \end{bmatrix}$$

$$\text{Step 4: } 9 = 3 \times 3$$

$$\text{The Cholesky factor } \mathbf{R} = \begin{bmatrix} 2 & 2i & 3 & 1 \\ & 1 & 2i & 5 \\ & & 2 & 1i \\ & & & 3 \end{bmatrix}.$$

## 2.2. Algorithm for Cholesky factorization

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**Algorithm:** Cholesky factorization

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**R**=triu(**A**)

**for**  $k = 1$  **to**  $m$

**for**  $j = k + 1$  **to**  $m$

$$r_{j,j:m} = r_{j,j:m} - \bar{r}_{kj} r_{k,j:m} / r_{kk}$$

**end**

$$r_{k,k:m} = r_{k,k:m} / \sqrt{r_{kk}}$$

**end**

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- **Exercise:** Design an algorithm to compute  $\mathbf{R}^*$  column by column.

## 2.3. Other factorization of HPD matrix

- For any HPD matrix  $\mathbf{A}$ , there exists a unique HPD matrix  $\mathbf{B}$  satisfying

$$\mathbf{A} = \mathbf{B}^2.$$

$\mathbf{B}$  is called the *square root* of  $\mathbf{A}$ . (Proof? HPD case?)

### 3. Gaussian elimination with partial pivoting (GEPP)

- Partial pivoting:  $|u_{ik}| = \max_{k \leq j \leq m} |u_{jk}|$ , rows are interchanged.

$$\begin{array}{ccc}
 \begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & u_{ik} & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix} & \xrightarrow{\mathbf{P}_k} & \begin{bmatrix} \times & \times & \times & \times & \times \\ & u_{ik} & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix} & \xrightarrow{\mathbf{L}_k} & \begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & 0 & \times & \times & \times \\ & 0 & \times & \times & \times \\ & 0 & \times & \times & \times \end{bmatrix} \\
 \text{Pivot selection} & & \text{Row interchange} & & \text{Elimination}
 \end{array}$$

- After  $m - 1$  steps,  $\mathbf{A}$  becomes an upper-triangular matrix  $\mathbf{U}$ :

$$\mathbf{L}_{m-1} \mathbf{P}_{m-1} \cdots \mathbf{L}_2 \mathbf{P}_2 \mathbf{L}_1 \mathbf{P}_1 \mathbf{A} = \mathbf{U},$$

where  $\mathbf{P}_k$  is an elementary permutation matrix ( $\mathbf{P}_k = \mathbf{P}_k^\top = \mathbf{P}_k^{-1}$ ).

#### Remark 5

*Absolute values of all the entries of  $\mathbf{L}_k$  in GEPP are  $\leq 1$  due to the property at step  $k$  (after pivoting)*

$$|u_{kk}| = \max_{k \leq j \leq m} |u_{jk}|.$$

### 3.1. A $4 \times 4$ Example

- **Step 1.** Interchange the first and third rows by  $\mathbf{P}_1$

$$\begin{bmatrix} & & 1 & \\ & 1 & & \\ 1 & & & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ 4 & 3 & 3 & 1 \\ 2 & 1 & 1 & 0 \\ 6 & 7 & 9 & 8 \end{bmatrix}$$

First elimination by  $\mathbf{L}_1$

$$\begin{bmatrix} 1 & & & \\ -\frac{1}{2} & 1 & & \\ -\frac{1}{4} & & 1 & \\ -\frac{3}{4} & & & 1 \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ 4 & 3 & 3 & 1 \\ 2 & 1 & 1 & 0 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ -\frac{1}{2} & -\frac{3}{2} & -\frac{3}{2} & \\ -\frac{3}{4} & -\frac{5}{4} & -\frac{5}{4} & \\ \frac{7}{4} & \frac{9}{4} & \frac{17}{4} & \end{bmatrix}$$

- **Step 2.** Interchange the second and fourth rows by  $\mathbf{P}_2$

$$\begin{bmatrix} 1 & & & \\ & & & 1 \\ & 1 & & \\ & & 1 & \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ -\frac{1}{2} & -\frac{3}{2} & -\frac{3}{2} & \\ -\frac{3}{4} & -\frac{5}{4} & -\frac{5}{4} & \\ \frac{7}{4} & \frac{9}{4} & \frac{17}{4} & \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ \frac{7}{4} & \frac{9}{4} & \frac{17}{4} & \\ -\frac{3}{4} & -\frac{5}{4} & -\frac{5}{4} & \\ -\frac{1}{2} & -\frac{3}{2} & -\frac{3}{2} & \end{bmatrix}$$

Second elimination by  $\mathbf{L}_2$

$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & \frac{3}{7} & 1 & \\ & \frac{2}{7} & & 1 \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & -\frac{3}{4} & -\frac{5}{4} & -\frac{5}{4} \\ & -\frac{1}{2} & -\frac{3}{2} & -\frac{3}{2} \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{2}{7} & \frac{4}{7} \\ & & -\frac{6}{7} & -\frac{2}{7} \end{bmatrix}$$

• **Step 3.** Interchange the third and fourth rows by  $\mathbf{P}_3$

$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{2}{7} & \frac{4}{7} \\ & & -\frac{6}{7} & -\frac{2}{7} \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{6}{7} & -\frac{2}{7} \\ & & -\frac{2}{7} & \frac{4}{7} \end{bmatrix}$$

Final elimination by  $\mathbf{L}_3$

$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & -\frac{1}{3} & 1 \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{6}{7} & -\frac{2}{7} \\ & & -\frac{2}{7} & \frac{4}{7} \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{6}{7} & -\frac{2}{7} \\ & & & \frac{2}{3} \end{bmatrix}$$



$$\bullet \mathbf{A} = \mathbf{P}_1^{-1} \mathbf{L}_1^{-1} \mathbf{P}_2^{-1} \mathbf{L}_2^{-1} \mathbf{P}_3^{-1} \mathbf{L}_3^{-1} \mathbf{U}$$

$$\begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} \frac{1}{4} & -\frac{3}{7} & \frac{1}{3} & 1 \\ \frac{1}{2} & -\frac{2}{7} & 1 & \\ 1 & & & \\ \frac{3}{4} & 1 & & \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ \frac{7}{4} & \frac{9}{4} & \frac{17}{4} & \\ & -\frac{6}{7} & -\frac{2}{7} & \\ & & \frac{2}{3} & \end{bmatrix}$$

$$\mathbf{PA} = \mathbf{LU} \text{ with } \mathbf{P} = \mathbf{P}_3 \mathbf{P}_2 \mathbf{P}_1 \text{ and } \mathbf{L} = \mathbf{P}_3 \mathbf{P}_2 \mathbf{L}_1^{-1} \mathbf{P}_2^{-1} \mathbf{P}_3^{-1} \mathbf{P}_3 \mathbf{L}_2^{-1} \mathbf{P}_3^{-1} \mathbf{L}_3^{-1}$$

$$\begin{bmatrix} & & & 1 \\ & & & & 1 \\ & & 1 & & \\ 1 & & & & \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ \frac{3}{4} & 1 & & \\ \frac{1}{2} & -\frac{2}{7} & 1 & \\ \frac{1}{4} & -\frac{3}{7} & \frac{1}{3} & 1 \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ \frac{7}{4} & \frac{9}{4} & \frac{17}{4} & \\ & -\frac{6}{7} & -\frac{2}{7} & \\ & & \frac{2}{3} & \end{bmatrix}$$

$\mathbf{P} \qquad \qquad \mathbf{A} \qquad \qquad \mathbf{L} \qquad \qquad \mathbf{U}$

### 3.2. General formulas for $\mathbf{PA} = \mathbf{LU}$

- The matrix  $\mathbf{L}_{m-1} \mathbf{P}_{m-1} \cdots \mathbf{L}_2 \mathbf{P}_2 \mathbf{L}_1 \mathbf{P}_1$  can be rewritten in the form

$$\mathbf{L}_{m-1} \mathbf{P}_{m-1} \cdots \mathbf{L}_2 \mathbf{P}_2 \mathbf{L}_1 \mathbf{P}_1 = \widehat{\mathbf{L}}_{m-1} \cdots \widehat{\mathbf{L}}_2 \widehat{\mathbf{L}}_1 \mathbf{P}_{m-1} \cdots \mathbf{P}_2 \mathbf{P}_1,$$

$$\text{where } \widehat{\mathbf{L}}_k = \mathbf{P}_{m-1} \cdots \mathbf{P}_{k+2} \mathbf{P}_{k+1} \mathbf{L}_k \mathbf{P}_{k+1}^{-1} \mathbf{P}_{k+2}^{-1} \cdots \mathbf{P}_{m-1}^{-1}.$$

## Remark 6

The elementary permutation matrix  $\mathbf{P}_k$  in GEPP has the form

$$\mathbf{P}_k = \begin{bmatrix} \mathbf{I}_{k-1} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{P}}_k \end{bmatrix},$$

where  $\hat{\mathbf{P}}_k \in \mathbb{R}^{(m-k+1) \times (m-k+1)}$  is an elementary permutation matrix.

## Remark 7

The unit lower triangular matrix  $\hat{\mathbf{L}}_k$  in GEPP has the same sparsity pattern as that of  $\mathbf{L}_k$ . The sparsity pattern is

$$\begin{bmatrix} \mathbf{I}_{k-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 1 & \mathbf{0} \\ \mathbf{0} & \star & \mathbf{I}_{m-k} \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \star & \mathbf{0} \end{bmatrix} + \mathbf{I}.$$

The matrix  $\hat{\mathbf{L}}_k$  is equal to  $\mathbf{L}_k$  but with the  $\star$ 's entries permuted.

## Remark 8

*By Proposition 1,  $\widehat{\mathbf{L}}_k^{-1}$  has the same sparsity pattern as that of  $\widehat{\mathbf{L}}_k$ . By Proposition 2, the product  $\widehat{\mathbf{L}}_1^{-1}\widehat{\mathbf{L}}_2^{-1}\cdots\widehat{\mathbf{L}}_{m-1}^{-1}$  is unit lower triangular.*

## Remark 9

*GEPP has the LU factorization  $\mathbf{PA} = \mathbf{LU}$  where*

$$\mathbf{P} = \mathbf{P}_{m-1} \cdots \mathbf{P}_2 \mathbf{P}_1, \quad \mathbf{U} = \mathbf{L}_{m-1} \mathbf{P}_{m-1} \cdots \mathbf{L}_2 \mathbf{P}_2 \mathbf{L}_1 \mathbf{P}_1 \mathbf{A},$$

$$\mathbf{L} = \widehat{\mathbf{L}}_1^{-1} \widehat{\mathbf{L}}_2^{-1} \cdots \widehat{\mathbf{L}}_{m-1}^{-1} = \mathbf{P}_{m-1} \cdots \mathbf{P}_3 \mathbf{P}_2 \mathbf{L}_1^{-1} \mathbf{P}_2^{-1} \mathbf{L}_2^{-1} \mathbf{P}_3^{-1} \cdots \mathbf{P}_{m-1}^{-1} \mathbf{L}_{m-1}^{-1}.$$

## Remark 10

*The matrices  $\widehat{\mathbf{L}}_k^{-1}$  are never formed and multiplied explicitly. The multipliers  $\ell_{jk}$  are computed and stored in the appropriate places.*

## Remark 11

*The permutation matrix  $\mathbf{P}$  is not known ahead of time.*

### 3.3. GEPP for $\mathbf{Ax} = \mathbf{b}$

- $\mathbf{PA} = \mathbf{LU}$ ,  $\mathbf{Ly} = \mathbf{Pb}$ ,  $\mathbf{Ux} = \mathbf{y}$

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**Algorithm:** LU factorization  $\mathbf{PA} = \mathbf{LU}$  in GEPP

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$\mathbf{U} = \mathbf{A}$ ,  $\mathbf{L} = \mathbf{I}$ ,  $\mathbf{P} = \mathbf{I}$

**for**  $k = 1$  **to**  $m - 1$

    Select  $i \geq k$  to maximize  $|u_{ik}|$

$u_{k,k:m} \leftrightarrow u_{i,k:m}$  (interchange two rows)

$\ell_{k,1:k-1} \leftrightarrow \ell_{i,1:k-1}$

$p_{k,:} \leftrightarrow p_{i,:}$

**for**  $j = k + 1$  **to**  $m$

$\ell_{jk} = u_{jk}/u_{kk}$

$u_{j,k:m} = u_{j,k:m} - \ell_{jk}u_{k,k:m}$

**end**

**end**

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### 3.4. Growth factor

- Define the *growth factor* for  $\mathbf{A}$  as the ratio  $\rho = \frac{\max_{ij} |u_{ij}|}{\max_{ij} |a_{ij}|}$ .

#### Proposition 12

*The growth factor  $\rho$  of Gaussian elimination with partial pivoting applied to any matrix  $\mathbf{A} \in \mathbb{C}^{m \times m}$  satisfies  $\rho \leq 2^{m-1}$ .*

Proof. Exercise 22.1. □

- Worst case of  $\rho$ :** Consider the  $5 \times 5$  matrix  $\mathbf{A}$ :

$$\mathbf{A} = \begin{bmatrix} 1 & & & & 1 \\ -1 & 1 & & & 1 \\ -1 & -1 & 1 & & 1 \\ -1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 \end{bmatrix}.$$

The L and U factors are given by

$$\mathbf{L} = \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ -1 & -1 & 1 & & \\ -1 & -1 & -1 & 1 & \\ -1 & -1 & -1 & -1 & 1 \end{bmatrix},$$

and

$$\mathbf{U} = \begin{bmatrix} 1 & & & 1 \\ & 1 & & 2 \\ & & 1 & 4 \\ & & & 1 & 8 \\ & & & & 16 \end{bmatrix}.$$

The growth factor  $\rho = 2^{m-1} = 16$ .

#### 4. Gaussian elimination with complete pivoting (GECP)

- Both rows and columns are interchanged
- After  $m - 1$  steps,  $\mathbf{A}$  becomes an upper-triangular matrix  $\mathbf{U}$ :

$$\mathbf{L}_{m-1}\mathbf{P}_{m-1}\cdots\mathbf{L}_2\mathbf{P}_2\mathbf{L}_1\mathbf{P}_1\mathbf{A}\mathbf{Q}_1\mathbf{Q}_2\cdots\mathbf{Q}_{m-1} = \mathbf{U}.$$

#### Remark 13

*GE with complete pivoting has the LU factorization*

$$\mathbf{PAQ} = \mathbf{LU},$$

*where  $\mathbf{P} = \mathbf{P}_{m-1}\cdots\mathbf{P}_2\mathbf{P}_1$ ,  $\mathbf{Q} = \mathbf{Q}_1\mathbf{Q}_2\cdots\mathbf{Q}_{m-1}$ , and*

$$\mathbf{L} = \widehat{\mathbf{L}}_1^{-1}\widehat{\mathbf{L}}_2^{-1}\cdots\widehat{\mathbf{L}}_{m-1}^{-1} = \mathbf{P}_{m-1}\cdots\mathbf{P}_3\mathbf{P}_2\mathbf{L}_1^{-1}\mathbf{P}_2^{-1}\mathbf{L}_2^{-1}\mathbf{P}_3^{-1}\cdots\mathbf{P}_{m-1}^{-1}\mathbf{L}_{m-1}^{-1}.$$

#### Remark 14

*The permutation matrices  $\mathbf{P}$  and  $\mathbf{Q}$  are not known ahead of time.*

## 4.1. GECP for $Ax = b$

- $PAQ = LU$ ,  $Ly = Pb$ ,  $Uz = y$ ,  $x = Qz$

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**Algorithm:** LU factorization  $PAQ = LU$  in GECP

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The details are left as an exercise.

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- [Exercise:](#)

Modify the pseudocode of the algorithms in this lecture to save storage.

- [Further reading:](#)

Shufang Xu, Li Gao, and Pingwen Zhang

[Numerical Linear Algebra](#).

Second Edition, Peking University Press, 2013