

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 4×4 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 :

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

where $\mathbf{l}_k = [\ell_{k+1,k} \quad \ell_{k+2,k} \quad \cdots \quad \ell_{mk}]^\top$ with the *multipliers*

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

Proposition 1

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

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

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 ℓ_{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 ℓ_{jk} are computed and stored directly into \mathbf{L} .

1.2. LU factorization algorithm

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

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

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

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

$\ell_{jk} = u_{jk}/u_{kk}$ (compute multipliers)

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

end

end

- **Exercise.** For any $\mathbf{b} \in \mathbb{C}^m$, modify the above algorithm to obtain $\mathbf{y} = \mathbf{L}_{m-1} \cdots \mathbf{L}_2 \mathbf{L}_1 \mathbf{b}$.

1.3. Gaussian elimination for $\mathbf{Ax} = \mathbf{b}$

• $\mathbf{y} = \mathbf{L}_{m-1} \cdots \mathbf{L}_2 \mathbf{L}_1 \mathbf{b}, \quad \mathbf{U}\mathbf{x} = \mathbf{y}$

Algorithm: Back substitution solving $\mathbf{U}\mathbf{x} = \mathbf{y}$

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

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

end

1.4. Algorithm for general lower-triangular system $\mathbf{Ly} = \mathbf{b}$

Algorithm: Forward elimination solving $\mathbf{Ly} = \mathbf{b}$

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

$$y_k = \left(b_k - \sum_{j=1}^{k-1} \ell_{kj} y_j \right) / \ell_{kk}$$

end

2. Cholesky factorization

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

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

where \mathbf{L} is the unit lower-triangular matrix in its LU factorization $\mathbf{A} = \mathbf{LU}$ 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 4×4 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

Algorithm: Cholesky factorization $\mathbf{A} = \mathbf{R}^* \mathbf{R}$

$\mathbf{R} = \text{triu}(\mathbf{A})$

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

- **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 ≤ 1 due to the property at step k (after pivot selection and row interchange)

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

3.1. A 4×4 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

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

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

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

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

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

Is there a unit lower-triangular \mathbf{L} ? Yes! Let $\mathbf{P} = \mathbf{P}_3 \mathbf{P}_2 \mathbf{P}_1$. Then

$$\mathbf{L} = \mathbf{P}(\mathbf{L}_3 \mathbf{P}_3 \mathbf{L}_2 \mathbf{P}_2 \mathbf{L}_1 \mathbf{P}_1)^{-1} = \mathbf{P}_3 \mathbf{P}_2 \mathbf{L}_1^{-1} \mathbf{P}_2^{-1} \mathbf{P}_3^{-1} \mathbf{P}_3 \mathbf{L}_2^{-1} \mathbf{P}_3^{-1} \mathbf{L}_3^{-1}.$$

$$\begin{array}{ccc} \begin{bmatrix} & & 1 & \\ & & & 1 \\ & 1 & & \\ 1 & & & \end{bmatrix} & \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} & = & \begin{bmatrix} 1 & & & \\ \frac{3}{4} & 1 & & \\ \frac{1}{2} & -\frac{2}{7} & 1 & \\ \frac{1}{4} & -\frac{3}{7} & \frac{1}{3} & 1 \end{bmatrix} & \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{6}{7} & -\frac{2}{7} \\ & & & \frac{2}{3} \end{bmatrix} \\ \mathbf{P} & \mathbf{A} & & \mathbf{L} & \mathbf{U} \end{array}$$

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

$$\begin{aligned} \bullet \mathbf{U} &= \mathbf{L}_{m-1} \mathbf{P}_{m-1} \cdots \mathbf{L}_2 \mathbf{P}_2 \mathbf{L}_1 \mathbf{P}_1 \mathbf{A}, \quad \mathbf{P} = \mathbf{P}_{m-1} \cdots \mathbf{P}_2 \mathbf{P}_1, \\ \mathbf{L} &= \mathbf{P}(\mathbf{L}_{m-1} \mathbf{P}_{m-1} \cdots \mathbf{L}_2 \mathbf{P}_2 \mathbf{L}_1 \mathbf{P}_1)^{-1} = \hat{\mathbf{L}}_1^{-1} \hat{\mathbf{L}}_2^{-1} \cdots \hat{\mathbf{L}}_{m-2}^{-1} \mathbf{L}_{m-1}^{-1}, \\ \hat{\mathbf{L}}_k^{-1} &= \mathbf{P}_{m-1} \cdots \mathbf{P}_{k+2} \mathbf{P}_{k+1} \mathbf{L}_k^{-1} \mathbf{P}_{k+1}^{-1} \mathbf{P}_{k+2}^{-1} \cdots \mathbf{P}_{m-1}^{-1}, \quad k = 1 : m-2. \end{aligned}$$

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 $\hat{\mathbf{L}}_k^{-1}$ in GEPP has the same sparsity pattern as that of \mathbf{L}_k^{-1} . 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 $\hat{\mathbf{L}}_k^{-1}$ is equal to \mathbf{L}_k^{-1} but with the \star 's entries permuted.

Remark 8

By Proposition 2, the product $\widehat{\mathbf{L}}_1^{-1}\widehat{\mathbf{L}}_2^{-1}\cdots\widehat{\mathbf{L}}_{m-2}^{-1}\mathbf{L}_{m-1}^{-1}$ is unit lower triangular, and the matrices $\widehat{\mathbf{L}}_k^{-1}$ and \mathbf{L}_{m-1}^{-1} are never formed and multiplied explicitly.

Remark 9

The multipliers ℓ_{jk} are computed and stored in the appropriate places. It is not a one-step process, but a dynamic adjustment one.

Remark 10

We have the LU factorization of $\mathbf{PA} = \mathbf{LU}$ (note that the permutation matrix \mathbf{P} is not known ahead of time) where $\mathbf{P} = \mathbf{P}_{m-1}\cdots\mathbf{P}_2\mathbf{P}_1$,

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

$$\mathbf{L} = \mathbf{P}(\mathbf{L}_{m-1}\mathbf{P}_{m-1}\cdots\mathbf{L}_2\mathbf{P}_2\mathbf{L}_1\mathbf{P}_1)^{-1} = \widehat{\mathbf{L}}_1^{-1}\widehat{\mathbf{L}}_2^{-1}\cdots\widehat{\mathbf{L}}_{m-2}^{-1}\mathbf{L}_{m-1}^{-1},$$

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

3.3. Algorithm for $\mathbf{PA} = \mathbf{LU}$

Algorithm: LU factorization $\mathbf{PA} = \mathbf{LU}$ in GEPP for $\mathbf{Ax} = \mathbf{b}$

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

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

 Select $i \geq k$ to maximize $|u_{ik}|$ (select pivot)

$p_{k,:} \leftrightarrow p_{i,:}$ (update \mathbf{P})

$\ell_{k,1:k-1} \leftrightarrow \ell_{i,1:k-1}$ (update $\hat{\mathbf{L}}_1^{-1}, \hat{\mathbf{L}}_2^{-1}, \dots, \hat{\mathbf{L}}_{k-1}^{-1}$)

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

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

$\ell_{jk} = u_{jk}/u_{kk}$ (compute multipliers)

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

end

end

3.4. GEPP for $\mathbf{Ax} = \mathbf{b}$.

- $\mathbf{y} = \mathbf{L}_{m-1}\mathbf{P}_{m-1} \cdots \mathbf{L}_2\mathbf{P}_2\mathbf{L}_1\mathbf{P}_1\mathbf{b}$, $\mathbf{Ux} = \mathbf{y}$.
- [Exercise](#). Add a few lines to the above algorithm to obtain \mathbf{y} .

3.5. Growth factor of GEPP

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

Proposition 11

The growth factor ρ of GEPP applied to any matrix $\mathbf{A} \in \mathbb{C}^{m \times m}$ satisfies $\rho \leq 2^{m-1}$.

Proof. See Exercise 22.1. □

- The upper bound in the above proposition is sharp.

Consider the 5×5 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 $\rho = 2^{5-1} = 16$.

It is easy to construct an $m \times m$ matrix such that $\rho = 2^{m-1}$.

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 12

We have the LU factorization (note that the permutation matrices \mathbf{P} and \mathbf{Q} are not known ahead of time)

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

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

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

$$\mathbf{L} = \mathbf{P}(\mathbf{L}_{m-1}\mathbf{P}_{m-1}\cdots\mathbf{L}_2\mathbf{P}_2\mathbf{L}_1\mathbf{P}_1)^{-1} = \hat{\mathbf{L}}_1^{-1}\hat{\mathbf{L}}_2^{-1}\cdots\hat{\mathbf{L}}_{m-2}^{-1}\mathbf{L}_{m-1}^{-1},$$

$$\hat{\mathbf{L}}_k^{-1} = \mathbf{P}_{m-1}\cdots\mathbf{P}_{k+2}\mathbf{P}_{k+1}\mathbf{L}_k^{-1}\mathbf{P}_{k+1}^{-1}\mathbf{P}_{k+2}^{-1}\cdots\mathbf{P}_{m-1}^{-1}, \quad k = 1 : m - 2.$$

4.1. Algorithm for $\mathbf{PAQ} = \mathbf{LU}$

Algorithm: LU factorization $\mathbf{PAQ} = \mathbf{LU}$ in GECP

The details are left as an exercise.

4.2. GECP for $\mathbf{Ax} = \mathbf{b}$

- $\mathbf{y} = \mathbf{L}_{m-1}\mathbf{P}_{m-1} \cdots \mathbf{L}_2\mathbf{P}_2\mathbf{L}_1\mathbf{P}_1\mathbf{b}, \quad \mathbf{U}\mathbf{z} = \mathbf{y}, \quad \mathbf{x} = \mathbf{Q}\mathbf{z}$

5. Further reading

- Shufang Xu, Li Gao, and Pingwen Zhang

Numerical Linear Algebra.

Second Edition, Peking University Press, 2013

- **Exercise:** Try your best to modify the pseudocode of the algorithms in this lecture to save storage and to improve efficiency.