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

$$\mathbf{A} = \mathbf{LU}$$

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

$$\begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{bmatrix} \overset{\mathbf{L}_1}{\longrightarrow} \begin{bmatrix} \times & \times & \times & \times \\ 0 & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ 0 & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ 0 & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \end{bmatrix} \overset{\mathbf{L}_2}{\longrightarrow} \begin{bmatrix} \times & \times & \times & \times \\ & \times & \times & \times \\ & 0 & \mathbf{\times} & \mathbf{\times} \\ & 0 & \mathbf{\times} & \mathbf{\times} \end{bmatrix} \overset{\mathbf{L}_3}{\longrightarrow} \begin{bmatrix} \times & \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times \\ & & 0 & \mathbf{\times} \end{bmatrix}$$

$$\quad \mathbf{A} \qquad\qquad \mathbf{L}_1\mathbf{A} \qquad\qquad \mathbf{L}_2\mathbf{L}_1\mathbf{A} \qquad\qquad \mathbf{L}_3\mathbf{L}_2\mathbf{L}_1\mathbf{A}$$

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

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

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

$$\mathbf{L_3 L_2 L_1 A} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & 2 & 4 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & & 2 \end{bmatrix} = \mathbf{U}.$$

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

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

1.1. General formulas for LU factorization

- Let $\mathbf{x}_k$ denote the kth 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 x_{kk}. To do this we construct the matrix $\mathbf{L}_k$:

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

where the *multiplier*

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

> ### Proposition 1
>
> *The matrix $\mathbf{L}_k$ can be inverted by negating its subdiagonal entries. We have*
>
> $$\mathbf{L}_k^{-1} = \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & \ell_{k+1,k} & 1 & & \\ & & \vdots & & \ddots & \\ & & \ell_{mk} & & & 1 \end{bmatrix} = \begin{bmatrix} \mathbf{I}_{k-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 1 & \mathbf{0} \\ \mathbf{0} & -\bigstar & \mathbf{I}_{m-k} \end{bmatrix}.$$

Proof. Define the vector

$$\boldsymbol{\ell}_k = \begin{bmatrix} 0 & \cdots & 0 & \ell_{k+1,k} & \cdots & \ell_{mk} \end{bmatrix}^\top.$$

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

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

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,

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

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

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

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

    end

end

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

- $\mathbf{A} = \mathbf{LU}, \quad \mathbf{Ly} = \mathbf{b}, \quad \mathbf{Ux} = \mathbf{y}$

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

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

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

$\quad$ **end**

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

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

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

$\quad$ **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

$$
\mathbf{A} = \begin{bmatrix} a_{11} & \mathbf{w}^* \\ \mathbf{w} & \mathbf{K} \end{bmatrix} = \begin{bmatrix} \alpha & \mathbf{0} \\ \mathbf{w}/\alpha & \mathbf{I} \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{K} - \mathbf{w}\mathbf{w}^*/a_{11} \end{bmatrix} \begin{bmatrix} \alpha & \mathbf{w}^*/\alpha \\ \mathbf{0} & \mathbf{I} \end{bmatrix}
$$

$$
= \begin{bmatrix} \alpha & \mathbf{0} \\ \mathbf{w}/\alpha & \mathbf{I} \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \widehat{\mathbf{R}}^*\widehat{\mathbf{R}} \end{bmatrix} \begin{bmatrix} \alpha & \mathbf{w}^*/\alpha \\ \mathbf{0} & \mathbf{I} \end{bmatrix}
$$

(by $\mathbf{K} - \mathbf{w}\mathbf{w}^*/a_{11}$ is HPD and the induction hypothesis)

$$
= \begin{bmatrix} \alpha & \mathbf{0} \\ \mathbf{w}/\alpha & \widehat{\mathbf{R}}^* \end{bmatrix} \begin{bmatrix} \alpha & \mathbf{w}^*/\alpha \\ \mathbf{0} & \widehat{\mathbf{R}} \end{bmatrix} = \mathbf{R}^*\mathbf{R}.
$$

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 $\widehat{\mathbf{R}}$ is unique. $\qquad\square$

2.1. A 4×4 example:

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

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

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

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

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

Row 4: $9 = 3 \times 1 \times 3$

- 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
$\quad$ **R=triu(A)**
$\quad$ **for** $k = 1$ **to** m
$\qquad$ **for** $j = k+1$ **to** m
$\qquad\quad$ $r_{j,j:m} = r_{j,j:m} - r_{k,j:m}\overline{r}_{kj}/r_{kk}$
$\qquad$ **end**
$\qquad$ $r_{k,k:m} = r_{k,k:m}/\sqrt{r_{kk}}$
$\quad$ **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? HPSD case?)

3. Gaussian elimination with partial pivoting (GEPP):

- Only rows are interchanged.

$$
\begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & x_{ik} & \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \\ & \times & \times & \times & \times \end{bmatrix} \xrightarrow{\mathbf{P}_k} \begin{bmatrix} \times & \times & \times & \times & \times \\ & x_{ik} & \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \\ & \times & \times & \times & \times \\ & \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \\ & \times & \times & \times & \times \end{bmatrix} \xrightarrow{\mathbf{L}_k} \begin{bmatrix} \times & \times & \times & \times & \times \\ & x_{ik} & \times & \times & \times \\ & \mathbf{0} & \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \\ & \mathbf{0} & \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \\ & \mathbf{0} & \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \end{bmatrix}
$$

$$
\text{Pivot selection} \qquad\qquad \text{Row interchange} \qquad\qquad \text{Elimination}
$$

- 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 pivoting)

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

3.1. A 4×4 Example

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

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

- 2: First elimination by $\mathbf{L}_1$

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

- 3: Interchange the second and fourth rows by $\mathbf{P}_2$

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

- 4: Second elimination by $\mathbf{L}_2$

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

- 5: Interchange the third and fourth rows by $\mathbf{P}_3$

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

- 6: Final elimination by $\mathbf{L}_3$

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

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

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

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

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

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

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

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

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

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

Remark 7

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

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

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

Remark 8

By Proposition 1, $\widehat{\mathbf{L}}_k^{-1}$ has the same sparsity pattern as that of $\widehat{\mathbf{L}}_k$. Thus, 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 ℓ_{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 $Ax = b$

- $PA = LU, \quad Ly = Pb, \quad Ux = y$

Algorithm: LU factorization $PA = LU$ in GEPP

$U = A, \ L = I, \ P = I$
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

3.4. Growth factor

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

Proposition 12

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

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 $\mathbf{P} = \mathbf{P}_{m-1}\cdots\mathbf{P}_2\mathbf{P}_1, \quad \mathbf{Q} = \mathbf{Q}_1\mathbf{Q}_2\cdots\mathbf{Q}_{m-1},$ *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 $Ax = b$

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

Algorithm: LU factorization $PAQ = LU$ in GECP

The details are left as an exercise.

- 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