

# 2072U Computational Science I

## Winter 2022

Week	Topic
1	Introduction
1–2	Solving nonlinear equations in one variable
3–4	Solving systems of (non)linear equations
5–6	Computational complexity
6–8	Interpolation and least squares
8–10	Integration & differentiation
10–12	Additional Topics

1. Central questions
2. LU decomposition with partial pivoting
3. Using LU decompositions to solve linear systems

## Central questions:

- ▶ For any square  $A \in \mathbb{R}^{n \times n}$ , does a decomposition  $A = LU$  exist?
- ▶ What is (partial) pivoting?
- ▶ What is a permutation matrix? How can it be represented?
- ▶ How is an LU decomposition  $PA = LU$  computed?
- ▶ How do LU decompositions  $A = LU$  or  $PA = LU$  relate to solving linear systems of equations?
- ▶ How can LU decompositions be computed and used in PYTHON?

Existence of LU decomposition  $A = LU$ .

## Proposition

For a given nonsingular matrix  $A \in \mathbb{R}^{n \times n}$ , the LU decomposition  $A = LU$  exists and is unique iff all the leading principal submatrices of  $A$  are nonsingular.

Note: a *leading submatrix* is obtained from a matrix  $A$  by extracting its first  $k$  rows and columns:  $A(1 : k, 1 : k)$ .

- ▶ LU decomposition  $A = LU$  has  $L$  unit lower triangular and  $U$  upper triangular
- ▶ Not always possible to find  $A = LU$  for  $A$  nonsingular
- ▶ When  $A$  nonsingular, **always** possible to find permutation  $P$  such that  $PA = LU$ , i.e., so that  $PA$  has a Gauss (LU) factorisation

Permutation matrices:

### Definition (Permutation matrix)

A **permutation matrix** is any matrix obtained from interchanging the rows or columns of the identity matrix.

▶ e.g.,  $P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$   $P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$ ,  $P = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix}$

- ▶ For any permutation matrix,  $P^{-1} = P^T$
- ▶  $PA$  permutes **rows** of matrix  $A$
- ▶  $AP^T$  permutes **columns** of matrix  $A$
- ▶ Permutation matrices can be stored as single vector

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- ▶  $PA$  permutes **rows** of matrix  $A$
- ▶  $AP^T$  permutes **columns** of matrix  $A$
- ▶ Permutation matrices can be stored as single vector

**Example:** left multiplication by permutation matrix permutes rows

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

**Example:** right multiplication by transpose of permutation matrix permutes rows

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

An example of the need for pivoting:

- ▶ Not every invertible matrix  $A$  has LU decomposition  
 $A = LU$



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- ▶  $A = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \Rightarrow a_{1,1} = 0$  prevents direct elimination
- ▶ Instead, use permutation matrix to swap rows 1 & 2

$$PA = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \quad \text{if} \quad P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

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$$PA = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \quad \text{if} \quad P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- ▶  $PA$  is upper triangular, so LU decomposition is  $PA = LU$   
 with  $P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ ,  $L = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$  and  $U = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$

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Example (Pivoting numerically useful)

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► Let  $A = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 1 \end{bmatrix}$ , so exact LU factors are

$$A = LU = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix} \begin{bmatrix} 10^{-20} & 1 \\ 0 & 1 - 10^{20} \end{bmatrix}$$

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- ▶ In finite precision arithmetic,  $1 - 10^{20} \simeq -10^{20}$ , so

$$\tilde{L} = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix} \text{ and } \tilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{bmatrix}$$

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$$\tilde{L} = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix} \text{ and } \tilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{bmatrix}$$

- ▶ Notice  $\tilde{L} = L$  and  $\tilde{U} \simeq U$  but  $\tilde{L}\tilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 1 & \textcolor{red}{0} \end{bmatrix} \neq A$

We want to find  $P$ ,  $L$ ,  $U$ , such that  $PA = LU$ .

→ Use  $LU$  with partial pivoting.

Partial pivoting refers to swapping rows, not columns:

- ▶ Initialise  $U = A$ ,  $L = I$ , and  $P = I$
- ▶ Loop through pivot columns ( $k = 1 : n - 1$ ):
  - ▶ Find **largest entry** in pivot column  $k$ , say  $U_{\ell,k}$ ,  $\ell \geq k$
  - ▶ Interchange rows  $k \leftrightarrow \ell$  in  $P$  and  $U$
  - ▶ Interchange rows  $k \leftrightarrow \ell$  in  $L$  **up to (not including) pivot column**, i.e. just the first  $k - 1$  columns
  - ▶ Eliminate rows below row  $k$  as usual (Gaussian elimination)
- ▶ End result is three matrices  $P$ ,  $L$ , and  $U$  such that  $PA = LU$



## Pseudo-code for LU decomposition with partial pivoting

**Input:**  $A \in \mathbb{R}^{n \times n}$

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

(initialise matrices)

**for**  $k = 1 : n - 1$

(loop through pivot columns)

    Select  $\ell \geq k$  to maximise  $|U_{\ell,k}|$

(choose pivot element)

$U_{k,k:n} \leftrightarrow U_{\ell,k:n}$

(swap rows of  $U$ )

$L_{k,1:k-1} \leftrightarrow L_{\ell,1:k-1}$

(swap rows of  $L$  up to pivot)

$P_{k,:} \leftrightarrow P_{\ell,:}$

(swap rows of  $P$ )

**for**  $j = k + 1 : n$

(loop through rows under pivot)

$L_{j,k} \leftarrow U_{j,k} / U_{k,k}$

(store multiplier in  $L$  matrix)

$U_{j,k:n} \leftarrow U_{j,k:n} - L_{j,k} U_{k,k:n}$

(update row  $j$  of  $U$  matrix)

**end for**

**end for**

**Output:** Matrices  $L, U$  and  $P$

Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition with partial pivoting, i.e. find  $PA = LU$ .

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$$U = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$$

$$P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Initialise matrices; pivot column  $k = 1$

Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition with partial pivoting, i.e. find  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ 1 & 1 & 3 \\ 2 & 2 & 2 \end{bmatrix}$$

$$R_1 \leftrightarrow R_2$$

$$P = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$R_1 \leftrightarrow R_2$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Swap rows 1 and 2 in  $U$  and  $P$

Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition with partial pivoting, i.e. find  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ -1 & \frac{5}{3} & \frac{2}{3} \\ -2 & -\frac{2}{3} & \frac{2}{3} \end{bmatrix} \quad P = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{3} & 1 & 0 \\ \frac{2}{3} & 0 & 1 \end{bmatrix}$$

$$R_2 \leftarrow R_2 - \frac{1}{3}R_1$$

$$R_3 \leftarrow R_3 - \frac{2}{3}R_1$$

$$L_{2,1} \leftarrow \frac{1}{3}$$

$$L_{3,1} \leftarrow \frac{2}{3}$$

Eliminate beneath pivot column  $k = 1$  in  $U$ , store multipliers in  $L$

Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition with partial pivoting, i.e. find  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ -2 & -\frac{2}{3} \\ -1 & \frac{5}{3} \end{bmatrix}$$

$R_2 \leftrightarrow R_3$

$$P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

$R_2 \leftrightarrow R_3$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{2}{3} & 1 & 0 \\ \frac{1}{3} & 0 & 1 \end{bmatrix}$$

$R_2 \leftrightarrow R_3$

Swap rows 2 and 3 in  $U$  and  $P$ ; swap up to pivot column  $k = 2$  in  $L$

Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition with partial pivoting, i.e. find  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ & -2 & -\frac{2}{3} \\ & & \color{red}{2} \end{bmatrix} \quad P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \quad L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{2}{3} & 1 & 0 \\ \frac{1}{3} & \color{red}{\frac{1}{2}} & 1 \end{bmatrix}$$

$$R_3 \leftarrow R_3 - \frac{1}{2}R_2 \quad L_{3,2} \leftarrow \frac{1}{2}$$

Eliminate beneath pivot column  $k = 2$  in  $U$ , store multiplier in  $L$

Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition with partial pivoting, i.e. find  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ & -2 & -\frac{2}{3} \\ & & 2 \end{bmatrix} \quad P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \quad L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{2}{3} & 1 & 0 \\ \frac{1}{3} & \frac{1}{2} & 1 \end{bmatrix}$$

We arrive at the decomposition  $PA = LU$ .



Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$$PA = LU.$$

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

Initialise matrices; pivot column  $k = 1$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$$PA = LU.$$

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

$R_1 \leftrightarrow R_3 \qquad R_1 \leftrightarrow R_3$

Swap rows 1 and 3 in  $U$  and  $P$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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

$$R_2 \leftarrow R_2 - \frac{1}{2}R_1$$

$$R_3 \leftarrow R_3 - \frac{3}{4}R_1$$

$$R_4 \leftarrow R_4 - \frac{3}{4}R_1$$

$$L_{2,1} \leftarrow \frac{1}{2}$$

$$L_{3,1} \leftarrow \frac{3}{4}$$

$$L_{4,1} \leftarrow \frac{3}{4}$$

Eliminate beneath pivot column  $k = 1$  in  $U$ , store multipliers in  $L$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

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$R_2 \leftrightarrow R_4$                        $R_2 \leftrightarrow R_4$                        $R_2 \leftrightarrow R_4$

Swap rows 2 and 4 in  $U$  and  $P$ ; swap up to pivot column  $k = 2$  in  $L$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$$PA = LU.$$

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

$$R_3 \leftarrow R_3 + \frac{3}{7}R_2$$

$$R_4 \leftarrow R_4 + \frac{2}{7}R_2$$

$$L_{3,2} \leftarrow -\frac{3}{7}$$

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Eliminate beneath pivot column  $k = 2$  in  $U$ , store multipliers in  $L$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

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$R_3 \leftrightarrow R_4 \qquad R_3 \leftrightarrow R_4 \qquad R_3 \leftrightarrow R_4$

Swap rows 3 and 4 in  $U$  and  $P$ ; swap up to pivot column  $k = 3$  in  $L$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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

$R_4 \leftarrow R_4 - \frac{1}{3}R_3$ 
 $L_{4,3} \leftarrow \frac{1}{3}$

Eliminate beneath pivot column  $k = 3$  in  $U$ , store multiplier in  $L$



Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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We arrive at the decomposition  $PA = LU$

## Solving $A\mathbf{x} = \mathbf{b}$ from $PA = LU$

- ▶ Multiply by  $P$ :

$$PA\mathbf{x} = P\mathbf{b}$$

- ▶ Replace  $PA$  by  $LU$ :

$$LU\mathbf{x} = P\mathbf{b}$$

- ▶ Define  $\mathbf{y} = U\mathbf{x}$  and solve

$$L\mathbf{y} = P\mathbf{b}$$

for  $\mathbf{y}$  by forward substitution.

- ▶ Solve

$$U\mathbf{x} = \mathbf{y}$$

for  $\mathbf{x}$  by backward substitution.

## Using `scipy.linalg`:

```
import scipy

A = np.array([[0.2, 1.4, -0.4, 12.3],
              [-2.3, 4.2, 1.1, -0.9],
              [9.2, -2.3, -0.1, 2.2],
              [3.4, 3.3, -10.1, 4.0]])
b = np.array([[0.2], [-1.2], [3.3], [0.2]])
Pt, L, U = scipy.linalg.lu(A)
Pb = scipy.dot(Pt.T, b)
y = scipy.linalg.solve_triangular(L, Pb, lower=True)
x = scipy.linalg.solve_triangular(U, y, lower=False)
```

- ▶ `scipy.linalg.solve` computes solution directly.
- ▶ Better to compute LU decomposition first if you have many systems to solve with different right hand sides.

# Remarks

- ▶ **Partial pivoting**: interchanging rows to use small multipliers.
- ▶ Partial pivoting: multipliers  $L_{k,\ell}$  satisfy  $|L_{k,\ell}| \leq 1$ .
- ▶ Pivoting stabilises differences in elimination.
- ▶ Complete pivoting: swapping rows **and** columns.
- ▶  $PA = LU$  decomposition is the default way to solve linear systems.

## Representing permutation matrices by a vector:

- ▶ Unnecessary to store entire matrix  $P$ ; single vector suffices
- ▶ Represent permutation matrix  $P$  by column vector  $\mathbf{p}$
- ▶ Initialise  $\mathbf{p} = (1 : n)^T$
- ▶ Swap rows of  $\mathbf{p}$  at each pivot step of Gaussian elimination
- ▶ End result: vector  $\mathbf{p}$  with order of rows of identity matrix to give  $P$

$$P = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \rightarrow \mathbf{p} = \begin{bmatrix} 3 \\ 4 \\ 2 \\ 1 \end{bmatrix}$$

Exercise: Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition  $PA = LU$ .

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$$U = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$$

$$\mathbf{p} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Initialise matrices; pivot column  $k = 1$

Exercise: Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ 1 & 1 & 3 \\ 2 & 2 & 2 \end{bmatrix}$$

$$R_1 \leftrightarrow R_2$$

$$\mathbf{p} = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$$

$$R_1 \leftrightarrow R_2$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Swap rows 1 and 2 in  $U$  and  $\mathbf{p}$



Exercise: Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ & -1 & \frac{5}{3} \\ & -2 & -\frac{2}{3} \end{bmatrix} \quad \mathbf{p} = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \quad L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{3} & 1 & 0 \\ \frac{2}{3} & 0 & 1 \end{bmatrix}$$

$$R_2 \leftarrow R_2 - \frac{1}{3}R_1$$

$$R_3 \leftarrow R_3 - \frac{2}{3}R_1$$

$$L_{2,1} \leftarrow \frac{1}{3}$$

$$L_{3,1} \leftarrow \frac{2}{3}$$

Eliminate beneath pivot column  $k = 1$  in  $U$ , store multipliers in  $L$

Exercise: Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ -2 & -\frac{2}{3} \\ -1 & \frac{5}{3} \end{bmatrix}$$

$R_2 \leftrightarrow R_3$

$$\mathbf{p} = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}$$

$R_2 \leftrightarrow R_3$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{2}{3} & 1 & 0 \\ \frac{1}{3} & 0 & 1 \end{bmatrix}$$

$R_2 \leftrightarrow R_3$

Swap rows 2 and 3 in  $U$  and  $\mathbf{p}$ ; swap up to pivot column  $k = 2$  in  $L$

Exercise: Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ & -2 & -\frac{2}{3} \\ & & \textcolor{red}{2} \end{bmatrix}$$

$$R_3 \leftarrow R_3 - \frac{1}{2}R_2$$

$$\mathbf{p} = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{2}{3} & 1 & 0 \\ \frac{1}{3} & \textcolor{red}{\frac{1}{2}} & 1 \end{bmatrix}$$

$$L_{3,2} \leftarrow \frac{1}{2}$$

Eliminate beneath pivot column  $k = 2$  in  $U$ , store multiplier in  $L$

Exercise: Given  $A = \begin{bmatrix} 1 & 1 & 3 \\ 3 & 6 & 4 \\ 2 & 2 & 2 \end{bmatrix}$ , construct the LU decomposition  $PA = LU$ .

$$U = \begin{bmatrix} 3 & 6 & 4 \\ & -2 & -\frac{2}{3} \\ & & 2 \end{bmatrix} \quad \mathbf{p} = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix} \quad L = \begin{bmatrix} 1 & 0 & 0 \\ \frac{2}{3} & 1 & 0 \\ \frac{1}{3} & \frac{1}{2} & 1 \end{bmatrix}$$

We arrive at the decomposition  $PA = LU$ .

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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

$$\mathbf{p} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Initialise matrices; pivot column  $k = 1$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$$PA = LU.$$

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

$$R_1 \leftrightarrow R_3$$

$$\mathbf{p} = \begin{bmatrix} 3 \\ 2 \\ 1 \\ 4 \end{bmatrix}$$

$$R_1 \leftrightarrow R_3$$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Swap rows 1 and 3 in  $U$  and  $\mathbf{p}$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

$$U = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & -\frac{1}{2} & -\frac{3}{2} & -\frac{3}{2} \\ & -\frac{3}{4} & -\frac{5}{4} & -\frac{5}{4} \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \end{bmatrix} \quad \mathbf{p} = \begin{bmatrix} 3 \\ 2 \\ 1 \\ 4 \end{bmatrix} \quad L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{2} & 1 & 0 & 0 \\ \frac{1}{4} & 0 & 1 & 0 \\ \frac{3}{4} & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{aligned} R_2 &\leftarrow R_2 - \frac{1}{2}R_1 \\ R_3 &\leftarrow R_3 - \frac{1}{4}R_1 \\ R_4 &\leftarrow R_4 - \frac{3}{4}R_1 \end{aligned} \quad \begin{aligned} L_{2,1} &\leftarrow \frac{1}{2} \\ L_{3,1} &\leftarrow \frac{1}{4} \\ L_{4,1} &\leftarrow \frac{3}{4} \end{aligned}$$

Eliminate beneath pivot column  $k = 1$  in  $U$ , store multipliers in  $L$



Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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

$R_2 \leftrightarrow R_4$

$$\mathbf{p} = \begin{bmatrix} 3 \\ 4 \\ 1 \\ 2 \end{bmatrix}$$

$R_2 \leftrightarrow R_4$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{3}{4} & 1 & 0 & 0 \\ \frac{1}{4} & 0 & 1 & 0 \\ \frac{1}{2} & 0 & 0 & 1 \end{bmatrix}$$

$R_2 \leftrightarrow R_4$

Swap rows 2 and 4 in  $U$  and  $\mathbf{p}$ ; swap up to pivot column  $k = 2$  in  $L$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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

$$R_3 \leftarrow R_3 + \frac{3}{7}R_2$$

$$R_4 \leftarrow R_4 + \frac{2}{7}R_2$$

$$p = \begin{bmatrix} 3 \\ 4 \\ 1 \\ 2 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{3}{4} & 1 & 0 & 0 \\ \frac{1}{4} & -\frac{3}{7} & 1 & 0 \\ \frac{1}{2} & -\frac{2}{7} & 0 & 1 \end{bmatrix}$$

$$L_{3,2} \leftarrow -\frac{3}{7}$$

$$L_{4,2} \leftarrow -\frac{2}{7}$$

Eliminate beneath pivot column  $k = 2$  in  $U$ , store multipliers in  $L$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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

$R_3 \leftrightarrow R_4$

$$\mathbf{p} = \begin{bmatrix} 3 \\ 4 \\ 2 \\ 1 \end{bmatrix}$$

$R_3 \leftrightarrow R_4$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{3}{4} & 1 & 0 & 0 \\ \frac{1}{2} & -\frac{2}{7} & 1 & 0 \\ \frac{1}{4} & -\frac{3}{7} & 0 & 1 \end{bmatrix}$$

$R_3 \leftrightarrow R_4$

Swap rows 3 and 4 in  $U$  and  $\mathbf{p}$ ; swap up to pivot column  $k = 3$  in  $L$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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

$$R_4 \leftarrow R_4 - \frac{1}{3}R_3$$

$$\mathbf{p} = \begin{bmatrix} 3 \\ 4 \\ 2 \\ 1 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{3}{4} & 1 & 0 & 0 \\ \frac{1}{2} & -\frac{2}{7} & 1 & 0 \\ \frac{1}{4} & -\frac{3}{7} & \frac{1}{3} & 1 \end{bmatrix}$$

$$L_{4,3} \leftarrow \frac{1}{3}$$

Eliminate beneath pivot column  $k = 3$  in  $U$ , store multiplier in  $L$

Exercise:

Given  $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$ , construct the LU decomposition

$PA = LU$ .

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

We arrive at the decomposition  $PA = LU$

# Summary

- ▶ Diagonal & triangular systems are simple to solve
- ▶ Gaussian elimination: converting square matrix to triangular form
- ▶ Gauss factorisation: finding  $L$ ,  $U$  such that  $A = LU$
- ▶ Permutation matrices (representation as matrices and vectors)
- ▶ Gaussian elimination with partial pivoting always possible
- ▶ Pivoting reduces magnitude of multipliers, stabilising elimination
- ▶ Decomposition  $PA = LU$  useful for repeated solves