

LU decomposition

$$\boxed{A}x = \boxed{b}$$

$$x = A^{-1}b$$

bad idea in practice!

Let  $A \in \mathbb{R}^{n \times n}$ . Suppose we can decompose (or factorise)

$$P A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} = \underbrace{\begin{bmatrix} * & & & & \\ * & * & & & \\ * & * & * & & \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \\ & & & & * \end{bmatrix}}_{U} = \underbrace{LU}_{\sim} \quad x = \underbrace{A^{-1}b}_{\text{(great)}}$$

$L$ : lower triangular,  $U$ : upper triangular. How to find  $L, U$ ?

$$\underbrace{L}_{\sim} \underbrace{L_1 \dots L_n}_{(n \times n)} \underbrace{A}_{\sim} \rightarrow \underbrace{U}_{\sim} \Leftrightarrow A = \underbrace{L^{-1}U}_{L}$$

$$L^{-1} = (\text{low. triag.}) \quad \left( \begin{array}{ccccc} 1 & & & & \\ -l_{21} & 1 & & & \\ -l_{31} & -l_{32} & 1 & & \\ \vdots & \vdots & \ddots & 1 & \\ -l_{n1} & -l_{n2} & \cdots & -l_{n,n-1} & 1 \end{array} \right)$$

## LU decomposition

Let  $A \in \mathbb{R}^{n \times n}$ . Suppose we can decompose (or factorise)

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} = \begin{bmatrix} * & & & & \\ * & * & & & \\ * & * & * & & \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} = LU$$

$L$ : lower triangular,  $U$ : upper triangular. How to find  $L, U$ ?

equal to A's.

$$A = \underbrace{\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix}}_{L_1 U_1} + \underbrace{\begin{bmatrix} 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * \\ 0 & 0 & 0 & 0 & * \end{bmatrix}}_{L_2 U_2} + \dots$$

$\left[ \begin{array}{c} * \\ \vdots \\ * \end{array} \right] \not\models L_n U_n$

## LU decomposition cont'd

First step:

$$A = \underbrace{\begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix}}_{L_1 U_1} + \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}$$

algorithm:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} \\ A_{31} \\ A_{41} \\ A_{51} \end{bmatrix} = \begin{bmatrix} L_{11} \\ L_{21} \\ L_{31} \\ L_{41} \\ L_{51} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} & U_{13} & U_{14} & U_{15} \end{bmatrix} + \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ A_{21}/a \\ A_{31}/a \\ A_{41}/a \\ A_{51}/a \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \end{bmatrix} + \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}$$

$a = A_{11}$

$= L_1 U_1$

## LU decomposition cont'd 2

$$\begin{aligned}
 A &= \underbrace{\left[ \begin{array}{c|ccccc} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{array} \right]}_{L_1 U_1} + \underbrace{\left[ \begin{array}{c|ccccc} 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \end{array} \right]}_{L_2 U_2} + \underbrace{\left[ \begin{array}{c|ccccc} 0 & 0 & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & * & * & * & * \end{array} \right]}_{L_3 U_3} + \underbrace{\left[ \begin{array}{c|ccccc} 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * & * \end{array} \right]}_{L_4 U_4} + \underbrace{\left[ \begin{array}{c|ccccc} 0 & 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * \end{array} \right]}_{L_5 U_5} \\
 &= [L_1, L_2, \dots, L_5] \left[ \begin{array}{c} U_1 \\ U_2 \\ \vdots \\ U_5 \end{array} \right] = \left[ \begin{array}{ccccc} * & & & & \\ * & * & & & \\ * & * & * & & \\ * & * & * & * & \\ * & * & * & * & * \\ * & * & * & * & * \end{array} \right]
 \end{aligned}$$

# Solving $Ax = b$ via LU

$$\boxed{L} \quad \boxed{U} + \boxed{I} \sim \boxed{A}$$

$$\boxed{A} = \boxed{LU} \in \mathbb{R}^{n \times n}$$

$L$ : lower triangular,  $U$ : upper triangular

- ▶ Cost  $\frac{2}{3}n^3$  flops
- ▶ For  $\boxed{Ax = b}$ ,

$$Ax = b \Rightarrow \boxed{L} \boxed{U} \boxed{x} = b$$

▶ first solve  $Ly = b$ , then  $Ux = y$ .

▶ triangular solve is always backward stable: e.g.  $(L + \Delta L)\hat{y} = b$  (see Higham's book)

- ▶ **Pivoting** crucial for numerical stability:  $PA = LU$ , where  $P$ : permutation matrix

Then stability means  $\hat{L}\hat{U} = PA + \Delta A$

▶ Even with pivoting, unstable examples exist, but still always stable in practice and used everywhere!

- ▶ Special case where  $A \succ 0$  positive definite:  $A = R^T R$ , **Cholesky factorization**, ALWAYS stable,  $\frac{1}{3}n^3$  flops

$$\begin{aligned} & \text{Symmetric} \\ & \Leftrightarrow x^T Ax \geq 0 \quad \forall x \neq 0 \\ & \Leftrightarrow C-F \text{ minmax} \end{aligned}$$

$$\boxed{\begin{array}{l} L \\ U \end{array}} \boxed{y} = \boxed{b}$$

easy to solve!

1st:  $L_{11}y_1 = b_1 \quad y_1 = \frac{b_1}{L_{11}}$   
 2nd:  $L_{12}y_1 + L_{22}y_2 = b_2 \quad y_2 = \boxed{0}$

forward subst.

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

$$U_{nn}x_n = y_n$$

$$+ \frac{U_{n-1,n}x_n}{U_{n-1,n}}$$

$$O(n^2) \quad \frac{1}{x_1}$$

## LU decomposition with pivots

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & \dots & \dots & \dots & \dots \\ A_{31} & \dots & \dots & \dots & \dots \\ A_{41} & \dots & \dots & \dots & \dots \\ A_{51} & \dots & \dots & \dots & \dots \end{bmatrix} = \begin{bmatrix} 1 & & & & \\ A_{21}/a & 1 & & & \\ A_{31}/a & & 1 & & \\ A_{41}/a & & & 1 & \\ A_{51}/a & & & & 1 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & \dots & \dots & \dots & \dots \\ A_{31} & \dots & \dots & \dots & \dots \\ A_{41} & \dots & \dots & \dots & \dots \\ A_{51} & \dots & \dots & \dots & \dots \end{bmatrix} + \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix}$$

Trouble if  $a = A_{11} = 0$ ! e.g. no LU for

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

solution: **pivot**, permute rows s.t.

largest entry of first (active) column is at top.  $\Rightarrow PA = LU$ ,  $P$ : permutation matrix

- $PA = LU$  exists for any nonsingular  $A$  (exercise)
- for  $Ax = b$ , solve  $LUX = Pb$
- cost still  $\frac{2}{3}n^3 + O(n^2)$

$$PA \xrightarrow{\text{sub}} Pb \xrightarrow{\text{sub}} LUx \xrightarrow{\text{sub}} Pb$$

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ b \end{bmatrix}$$

permutation  $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

# Cholesky factorisation for $A \succ 0$

SPSD  $\lambda_i(A) \geq 0$

If  $A \succ 0$  (symmetric positive definite (S)PD  $\Leftrightarrow \lambda_i(A) > 0$ ), two simplifications:

- We can take  $U_i = L_i^T =: R_i$  by symmetry  $\Rightarrow \frac{1}{3}n^3$  flops
- No pivot needed

$$A = LU = R^T R$$

not 's.

Suppose

$$A_2 V = \lambda V$$

$$\lambda \leq 0$$

$$\sqrt{\lambda} A_2 V = \sqrt{\lambda} V^T V < 0$$

$$A = \underbrace{\begin{bmatrix} * & * & \dots & * \\ * & * & \dots & * \\ \vdots & \vdots & \ddots & \vdots \\ * & * & \dots & * \end{bmatrix}}_{R_1 R_1^T} + \underbrace{\begin{bmatrix} 0 & & & \\ & * & * & * \\ & * & * & * \\ & * & * & * \end{bmatrix}}_{A_2}$$

also PSD

$$D = \begin{bmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{bmatrix} \in \mathbb{R}^{n \times n}$$

Notes:

$$\triangleright \text{diag}(R) \text{ no longer 1's} \quad \text{consider} \quad = \begin{bmatrix} 1 & 1 & \dots & 1 \end{bmatrix} = R^T R$$

$$[\alpha \ \alpha^T] \cdot A \begin{bmatrix} \alpha \\ \alpha^T \end{bmatrix} = [\alpha \ \alpha^T] \begin{bmatrix} 1 & \alpha^T \alpha \\ \alpha^T \alpha & 1 \end{bmatrix} \begin{bmatrix} \alpha \\ \alpha^T \end{bmatrix} = \alpha^T \alpha + \alpha^T A_2 \alpha < 0$$

$$\begin{bmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \alpha^T \end{bmatrix} \begin{bmatrix} 0 & A_2 & 0 \\ A_2 & 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \alpha^T \end{bmatrix} = \alpha^T A_2 \alpha < 0$$

$\triangleright A$  can be written as  $A = R^T R$  for some  $R \in \mathbb{R}^{n \times n}$  iff  $A \succeq 0$  ( $\lambda_i(A) \geq 0$ )

$\triangleright$  Indefinite case: when  $A = A^*$  but  $A$  not PSD,  $\exists A = LDL^*$  where  $D$  diagonal (when  $A \in \mathbb{R}^{n \times n}$ ,  $D$  can have  $2 \times 2$  diagonal blocks),  $L$  has 1's on diagonal

$$A = LDL^* \quad \text{cont. } \begin{bmatrix} x \\ x^T \end{bmatrix}^T A \begin{bmatrix} x \\ x^T \end{bmatrix} > 0 \iff A \text{ PD} \quad x = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad x^T A x = A_{11} > 0.$$