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?

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$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} = \color{red}{\begin{bmatrix} * & & & & \\ * & * & & & \\ * & * & * & & \\ * & * & * & * & \\ * & * & * & * & * \end{bmatrix}} \color{blue}{\begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \\ & & & & * \end{bmatrix}} \color{black}{=} \color{red}{L}\color{blue}{U}$$

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

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

$$= \underbrace{\begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix}}_{L_1U_1} + \underbrace{\begin{bmatrix} 0 \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} 0 & * & * & * & * \end{bmatrix}}_{L_2U_2} + \begin{bmatrix} & & & & \\ & & & & \\ & & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix} = \cdots$$

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:

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

$$= \underbrace{\begin{bmatrix} 1 & & & & \\ A_{21}/a & & & & \\ A_{31}/a & & & & \\ A_{41}/a & & & & \\ A_{51}/a & & & & \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix}}_{=L_1 U_1} + \begin{bmatrix} & & & & \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}$$

LU decomposition cont'd 2

$$A = \begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix} + \begin{bmatrix} 0 \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} 0 & * & * & * & * \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} 0 & 0 & * & * & * \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ * \\ * \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & * & * \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ * \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 & * \end{bmatrix}$$

$$= L_1U_1 + L_2U_2 + L_3U_3 + L_4U_4 + L_5U_5$$

$$= [L_1, L_2, \ldots, L_5] \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_5 \end{bmatrix} = \begin{bmatrix} * & & & & \\ * & * & & & \\ * & * & * & & \\ * & * & * & * & \\ * & * & * & * & * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \\ & & & & * \end{bmatrix}$$

Solving $Ax = b$ via LU

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

L: lower triangular, U: upper triangular

- Cost $\frac{2}{3}n^3$ flops (floating-point operations)
- For $Ax = b$,
  - 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

LU decomposition with pivots

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

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 $LUx = P^T b$
- cost still $\frac{2}{3}n^3 + O(n^2)$

Cholesky factorisation for $A \succ 0$

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

$$A = \underbrace{\begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \begin{bmatrix} * & * & * & * & * \end{bmatrix}}_{R_1 R_1^T} + \underbrace{\begin{bmatrix} & & & & \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}}_{\text{also PSD}}$$

Notes:

- $\mathrm{diag}(R)$ no longer 1's
- A can be written as $A = R^T R$ for some $R \in \mathbb{R}^{n \times n}$ iff $A \succeq 0$ ($\lambda_i(A) \geq 0$)
- 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 2×2 diagonal blocks), L has 1's on diagonal