

Inverse matrices

- ▶ A square matrix $A \in \mathbf{R}^{n \times n}$ is **non-singular** if a matrix $B \in \mathbf{R}^{n \times n}$ such that

$$AB = BA = I.$$

$B \stackrel{\text{def}}{=} A^{-1}$ is **inverse** of A .

- ▶ A matrix without an inverse is **singular**.

examples



$$A = \begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}, \quad A^{-1} = \frac{1}{5} \begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix}, \quad A \text{ is non-singular.}$$



$$C = \begin{pmatrix} 2 & -1 \\ 0 & 0 \end{pmatrix}, \quad C \text{ is singular.}$$

Solving $A\mathbf{x} = \mathbf{b}$ with Inverse

- ▶ If A^{-1} is available,

$$\mathbf{x} = I\mathbf{x} = (A^{-1}A)\mathbf{x} = A^{-1}(A\mathbf{x}) = A^{-1}\mathbf{b}.$$

- ▶ example

$$A = \begin{pmatrix} 1 & 2 & -1 \\ 2 & 1 & 0 \\ -1 & 1 & 2 \end{pmatrix}, \quad A^{-1} = \frac{1}{9} \begin{pmatrix} -2 & 5 & -1 \\ 4 & -1 & 2 \\ -3 & 3 & 3 \end{pmatrix}, \quad \mathbf{b} \in \mathbf{R}^3,$$

$$\text{solution } \mathbf{x} = \frac{1}{9} \begin{pmatrix} -2 & 5 & -1 \\ 4 & -1 & 2 \\ -3 & 3 & 3 \end{pmatrix} \mathbf{b}.$$

Catch: A^{-1} rarely available, harder to compute than \mathbf{x}

Facts about A^{-1}

Assume A^{-1} exists.

- ▶ A^{-1} is unique.
- ▶ $(A^{-1})^{-1} = A$.
- ▶ If B^{-1} exists, $A, B \in \mathbf{R}^{n \times n}$, then

$$(AB)^{-1} = B^{-1}A^{-1}.$$

What if I have to compute A^{-1} anyway?

- ▶ A^{-1} is solution to

$$AX = I, \quad X \in \mathbf{R}^{n \times n}.$$

- ▶ Partition

$$X = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \end{pmatrix}, \quad I = \begin{pmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \cdots & \mathbf{e}_n \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & \ddots & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}.$$

$$AX = I \Leftrightarrow A \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \end{pmatrix} = \begin{pmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \cdots & \mathbf{e}_n \end{pmatrix} \Leftrightarrow A\mathbf{x}_j = \mathbf{e}_j, \\ \text{for } j = 1, \dots, n.$$

computing A^{-1} is to solve n systems of equations with same A

Review: GEPP for $A\mathbf{x} = \mathbf{b}$

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}.$$

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$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}.$$

- ▶ for $s = 1, 2, \dots, n - 1$:
 - ▶ **pivoting**: choose largest entry in absolute value:

$$\mathbf{piv} \stackrel{\text{def}}{=} \operatorname{argmax}_{s \leq j \leq n} |a_{js}|, \quad E_s \leftrightarrow E_{\mathbf{piv}}.$$

Review: GEPP for $Ax = b$

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}.$$

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► **eliminating** x_s from E_{s+1} through E_n :

$$\mathbf{a}_{jk} = a_{jk} - \frac{a_{js}}{a_{ss}} a_{sk} \stackrel{\text{overwrite}}{=} a_{jk}, \quad s + 1 \leq j \leq n, \quad s + 1 \leq k \leq n,$$

$$\mathbf{b}_j = b_j - \frac{a_{js}}{a_{ss}} b_s \stackrel{\text{overwrite}}{=} b_j, \quad s + 1 \leq j \leq n.$$

Review: backward substitution after GEPP

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}.$$

Review: backward substitution after GEPP

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}.$$

► for $s = n, n-1, \dots, 1$:

$$x_s = \frac{b_s - \sum_{k=s+1}^n a_{sk} x_k}{a_{ss}}.$$

GEPP for $\mathbf{AX} = \mathbf{B} \in \mathbf{R}^{n \times n}$

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nn} \end{pmatrix}.$$

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▶ for $s = 1, 2, \dots, n - 1$:

▶ **pivoting**: choose largest entry in absolute value:

$$\mathbf{piv} \stackrel{\text{def}}{=} \operatorname{argmax}_{s \leq j \leq n} |a_{js}|, \quad E_s \leftrightarrow E_{\mathbf{piv}}.$$

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$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nn} \end{pmatrix}.$$

► for $s = 1, 2, \dots, n-1$:

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► **eliminating** x_s from E_{s+1} through E_n :

$$\mathbf{a}_{jk} = a_{jk} - \frac{a_{js}}{a_{ss}} a_{sk} \xrightarrow{\text{overwrite}} a_{jk}, \quad s+1 \leq j \leq n, \quad s+1 \leq k \leq n,$$

$$\mathbf{b}_{jk} = b_{jk} - \frac{a_{js}}{a_{ss}} b_{sk} \xrightarrow{\text{overwrite}} b_{jk}, \quad s+1 \leq j \leq n, \quad 1 \leq k \leq n.$$

total cost: $\frac{5}{3} n^3$ operations

Backward substitution

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nn} \end{pmatrix}.$$

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$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nn} \end{pmatrix}.$$

- ▶ for $s = n, n-1, \dots, 1$:

$$x_{sj} = \frac{b_{sj} - \sum_{k=s+1}^n a_{sk} x_{kj}}{a_{ss}}, \quad j = 1, \dots, n.$$

- ▶ total cost for backward substitution: n^3 operations.
- ▶ total cost for computing A^{-1} : $\frac{8}{3} n^3$ operations.
- ▶ computing A^{-1} is 4 times as expensive as solving $A\mathbf{x} = \mathbf{b}$.

Matrix transpose: A^T (I)

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix} \in \mathbf{R}^{m \times n},$$

$$A^T = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{m1} \\ a_{12} & a_{22} & \cdots & a_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{mn} \end{pmatrix} \in \mathbf{R}^{n \times m}.$$

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example

$$A = \begin{pmatrix} 2 & 4 & 7 & 1 \\ 2 & -9 & -1 & 2 \end{pmatrix} \in \mathbf{R}^{2 \times 4}, \quad A^T = \begin{pmatrix} 2 & 2 \\ 4 & -9 \\ 7 & -1 \\ 1 & 2 \end{pmatrix} \in \mathbf{R}^{4 \times 2}.$$

Matrix transpose: A^T (II)

Theorem:

$$\left(A^T\right)^T = A, \quad (AB)^T = B^T A^T.$$

If A^{-1} exists, then

$$\left(A^{-1}\right)^T = \left(A^T\right)^{-1} \quad \square$$

The Determinant of a Matrix



$$\text{for } A = a, \quad \mathbf{det}(A) \stackrel{\text{def}}{=} a.$$



$$\text{for } A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad \mathbf{det}(A) \stackrel{\text{def}}{=} a_{11} a_{22} - a_{12} a_{21}.$$

- ▶ **definition: minor** M_{ij} is determinant of $(n-1) \times (n-1)$ submatrix of A without row i and column j .

$$\mathbf{det}(A) = \sum_{j=1}^n (-1)^{i+j} a_{ij} M_{ij}, \quad 1 \leq i \leq n.$$

The Determinant of a Matrix: example

$$B = \begin{pmatrix} 2 & 1 \\ 2 & -1 \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 1 & 1 \\ 2 & 2 & 1 \\ 1 & 2 & -1 \end{pmatrix}.$$



$$\det(B) = 2 * (-1) - 2 * 1 = -4.$$



$$\begin{aligned} \det(A) &= (-1)^{1+1} * 1 * \det \begin{pmatrix} 2 & 1 \\ 2 & -1 \end{pmatrix} + (-1)^{1+2} * 2 * \det \begin{pmatrix} 1 & 1 \\ 2 & -1 \end{pmatrix} \\ &\quad + (-1)^{1+3} * 1 * \det \begin{pmatrix} 1 & 1 \\ 2 & 1 \end{pmatrix} \\ &= (2 * (-1) - 2 * 1) - 2 * (1 * (-1) - 2 * 1) + (1 * 1 - 2 * 1) \\ &= -4 + 6 - 1 = 1. \end{aligned}$$

How to calculate **det** quickly? What does it do?

Properties of $\det(A)$, $A \in \mathbf{R}^{n \times n}$ (I)

- ▶ If \tilde{A} is obtained from A with elementary operation $(E_i) \leftrightarrow (E_j)$ for $i \neq j$, then $\det(\tilde{A}) = -\det(A)$.
(ROW SWAPS CHANGE SIGN IN $\det(A)$.)
- ▶ If \tilde{A} is obtained from A with elementary operation $(E_i + \lambda E_j) \rightarrow (E_i)$ for $i \neq j$, then $\det(\tilde{A}) = \det(A)$.
(ELIMINATION DOES NOT CHANGE $\det(A)$.)
- ▶ If A is upper-triangular, then

$$\det(A) = \prod_{j=1}^n a_{jj}$$

GEPP can be used to compute $\det(A)$

Properties of $\det(A)$, $A \in \mathbf{R}^{n \times n}$ (II)

- ▶ $\det(A^T) = \det(A)$.
- ▶ If A has two identical rows, then $\det(A) = 0$.
- ▶ If $B \in \mathbf{R}^{n \times n}$, then $\det(AB) = \det(A) \det(B)$.
- ▶ If A^{-1} exists, then $\det(A^{-1}) = (\det(A))^{-1}$.

Properties of $\det(A)$, $A \in \mathbf{R}^{n \times n}$ (III)

$$\det(A) \neq 0$$

$\Leftrightarrow A^{-1}$ exists

$\Leftrightarrow A\mathbf{x} = \mathbf{b}$ has a unique solution for any $b \in \mathbf{R}^n$.

\Leftrightarrow GEPP can be performed on $A\mathbf{x} = \mathbf{b}$ for any $b \in \mathbf{R}^n$.

GEPP works for $\det(A)$ (I)

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}.$$

- ▶ **pivoting**: choose largest entry in absolute value:

$$\mathbf{piv} \stackrel{\text{def}}{=} \operatorname{argmax}_{1 \leq j \leq n} |a_{j1}|, \quad (|a_{\mathbf{piv},1}| = \max_{1 \leq j \leq n} |a_{j1}|)$$

- ▶ exchange rows E_1 and $E_{\mathbf{piv}}$ ($E_1 \leftrightarrow E_{\mathbf{piv}}$)
($\det(A)$ CHANGES SIGN IF $\mathbf{piv} \neq 1$; $\det(A) = 0$ IF $a_{11} = 0$.)
- ▶ elimination of x_1 from E_2 through E_n :

$$\left(E_j - \frac{a_{j1}}{a_{11}} E_1 \right) \rightarrow (E_j), \quad 2 \leq j \leq n.$$

($\det(A)$ DOES NOT CHANGE)

GEPP works for $\det(A)$ (II)

$$\text{new } A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} \xrightarrow{\text{overwrite}} A,$$

$$\text{where } \mathbf{a}_{jk} = a_{jk} - \frac{a_{j1}}{a_{11}} a_{1k}, \quad 2 \leq j \leq n, \quad 2 \leq k \leq n.$$

- ▶ repeat same process til A becomes upper triangular

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix}.$$

- ▶ determinant of the original matrix A is

$$(-1)^{\# \text{ of row swaps}} \prod_{1 \leq j \leq n} a_{jj}.$$

General linear equations

$$E_1 : \quad a_{11}x_1 + a_{12}x_2 \cdots + a_{1n}x_n = b_1,$$

$$E_2 : \quad a_{21}x_1 + a_{22}x_2 \cdots + a_{2n}x_n = b_2,$$

$$\vdots \qquad \qquad \qquad \vdots \qquad \qquad \qquad \qquad \qquad \vdots$$

$$E_n : \quad a_{n1}x_1 + a_{n2}x_2 \cdots + a_{nn}x_n = b_n,$$

$$A \stackrel{\text{def}}{=} \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{b} \stackrel{\text{def}}{=} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}, \quad \mathbf{x} \stackrel{\text{def}}{=} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}.$$

General linear equations

$$E_1 : a_{11}x_1 + a_{12}x_2 \cdots + a_{1n}x_n = b_1,$$

$$E_2 : a_{21}x_1 + a_{22}x_2 \cdots + a_{2n}x_n = b_2,$$

$$\vdots \qquad \qquad \qquad \vdots \qquad \qquad \qquad \qquad \qquad \vdots$$

$$E_n : a_{n1}x_1 + a_{n2}x_2 \cdots + a_{nn}x_n = b_n,$$

$$A \stackrel{\text{def}}{=} \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{b} \stackrel{\text{def}}{=} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}, \quad \mathbf{x} \stackrel{\text{def}}{=} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}.$$

▶ equation E_j maps to **row** j of A : $(a_{j1}, a_{j2}, \dots, a_{jn})$, $1 \leq j \leq n$.

▶ variable x_k relates to **column** k of A : $\begin{pmatrix} a_{1k} \\ a_{2k} \\ \vdots \\ a_{nk} \end{pmatrix}$, $1 \leq k \leq n$.

▶ will concentrate on A for now.

Gifts from Math God in GE (I), assuming $a_{11} \neq 0$

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \text{first column} = \begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{pmatrix}.$$

- ▶ elimination in rows E_2 through E_n , on first column:

$$l_{j1} \stackrel{\text{def}}{=} \frac{a_{j1}}{a_{11}}, \quad (E_j - l_{j1}E_1) \rightarrow (E_j), \quad 2 \leq j \leq n.$$

$$\text{new } A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix},$$

$$\text{where } \mathbf{a}_{jk} = a_{jk} - \frac{a_{j1}}{a_{11}} a_{1k}, \quad 2 \leq j \leq n, \quad 2 \leq k \leq n.$$

Gifts from Math God in GE (II), assuming $a_{11} \neq 0$

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \mathbf{new} \quad A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix},$$

where $\mathbf{a}_{jk} = a_{jk} - l_{j1} a_{1k}$, $l_{j1} = \frac{a_{j1}}{a_{11}}$, $2 \leq j \leq n$, $2 \leq k \leq n$.

- ▶ *Gift #1*: Matrix-matrix product connection

$$A = L_1 \cdot (\mathbf{new} \quad A), \quad \text{where} \quad L_1 = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix}.$$

Gifts from Math God in GE (III), assuming $a_{11} \neq 0$

$$A = L_1 \cdot (\text{new } A) = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix},$$

Gifts from Math God in GE (III), assuming $a_{11} \neq 0$

$$A = L_1 \cdot (\text{new } A) = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix},$$

► new step of elimination, assuming $\mathbf{a}_{22} \neq 0$,

$$\begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} \stackrel{\text{def}}{=} \begin{pmatrix} 1 & & & \\ l_{32} & 1 & & \\ \vdots & & \ddots & \\ l_{n2} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{a}_{22} & \mathbf{a}_{23} & \cdots & \mathbf{a}_{2n} \\ 0 & \widehat{a}_{33} & \cdots & \widehat{a}_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \widehat{a}_{n3} & \cdots & \widehat{a}_{nn} \end{pmatrix}$$

Gifts from Math God in GE (III), assuming $a_{11} \neq 0$

$$A = L_1 \cdot (\text{new } A) = \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ \vdots & & \ddots & & \\ l_{n1} & & & 1 & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix},$$

- ▶ new step of elimination, assuming $\mathbf{a}_{22} \neq 0$,

$$\begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} \stackrel{\text{def}}{=} \begin{pmatrix} 1 & & & & \\ l_{32} & 1 & & & \\ \vdots & & \ddots & & \\ l_{n2} & & & 1 & \end{pmatrix} \cdot \begin{pmatrix} \mathbf{a}_{22} & \mathbf{a}_{23} & \cdots & \mathbf{a}_{2n} \\ 0 & \hat{\mathbf{a}}_{33} & \cdots & \hat{\mathbf{a}}_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \hat{\mathbf{a}}_{n3} & \cdots & \hat{\mathbf{a}}_{nn} \end{pmatrix}$$

- ▶ Gift #2: "free" matrix-matrix product

$$A = \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ l_{31} & l_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ l_{n1} & l_{n2} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \mathbf{a}_{23} & \cdots & \mathbf{a}_{2n} \\ 0 & 0 & \hat{\mathbf{a}}_{33} & \cdots & \hat{\mathbf{a}}_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \hat{\mathbf{a}}_{n3} & \cdots & \hat{\mathbf{a}}_{nn} \end{pmatrix}.$$

Gifts from Math God in GE (IV), GE=LU factorization

- ▶ GE for $n = 2$:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} 1 & \\ l_{21} & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} \\ 0 & \mathbf{a}_{22} \end{pmatrix}$$

$$\stackrel{\text{def}}{=} L \cdot U = \begin{pmatrix} \triangle \\ \square \end{pmatrix} \cdot \begin{pmatrix} \triangle \\ \square \end{pmatrix},$$

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- ▶ GE for $n \geq 3$:

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & & & \\ \mathbf{l} & I_{n-1} & & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \quad \left(\mathbf{l} \stackrel{\text{def}}{=} \begin{pmatrix} l_{21} \\ \vdots \\ l_{n1} \end{pmatrix} \right).$$

Gifts from Math God in GE (V), GE=LU factorization

- ▶ Induction hypothesis:

$$\begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} = \mathbf{L} \cdot \mathbf{U} = \begin{pmatrix} \triangleleft \\ \square \\ \square \end{pmatrix} \cdot \begin{pmatrix} \triangleleft \\ \square \\ \square \end{pmatrix}$$

Gifts from Math God in GE (V), GE=LU factorization

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- ▶ Gift #3: LU factorization

$$\begin{aligned} A &= \begin{pmatrix} 1 & & & \\ \mathbf{I} & I_{n-1} & & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & (a_{12} & \cdots & a_{1n}) \\ \mathbf{0} & & \mathbf{LU} & \end{pmatrix}, \\ &= \begin{pmatrix} 1 & & & \\ \mathbf{I} & \mathbf{L} & & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & (a_{12} & \cdots & a_{1n}) \\ \mathbf{0} & & \mathbf{U} & \end{pmatrix} \\ &\stackrel{\text{def}}{=} \mathbf{L} \cdot \mathbf{U} = \begin{pmatrix} \triangle \end{pmatrix} \cdot \begin{pmatrix} \nabla \end{pmatrix} \end{aligned}$$

Gaussian Elimination as LU factorization

- ▶ In Gaussian Elimination: for $s = 1, \dots, n - 1$,

$$l_{js} = \frac{a_{js}}{a_{ss}}, \quad 1 + s \leq j \leq n,$$

$$a_{jk} \xrightarrow{\text{overwrite}} a_{jk} - l_{js} a_{sk}, \quad 1 + s \leq j, k \leq n.$$

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- ▶ A becomes upper-triangular after GE:

$$A \xrightarrow{GE} \left(\begin{array}{c|ccc} & & & \\ \hline & \diagdown & & \\ & & & \\ & & & \end{array} \right) \stackrel{\text{def}}{=} U \stackrel{\text{notation}}{=} \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \vdots \\ & & & u_{nn} \end{pmatrix}.$$

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- ▶ LU factorization

$$A = L \cdot U, \quad \text{where } L \stackrel{\text{def}}{=} \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & 1 \end{pmatrix} = \left(\begin{array}{c|ccc} & & & \\ \hline & & & \\ & & & \\ & & & \end{array} \right).$$

Gaussian Elimination as LU factorization, example

$$A = \begin{pmatrix} 1 & 1 & 0 & 3 \\ 2 & 1 & -1 & 1 \\ 3 & -1 & -1 & 2 \\ -1 & 2 & 3 & -1 \end{pmatrix} \in \mathbf{R}^{4 \times 4}$$

$$\begin{aligned} A &= \begin{pmatrix} 1 & & & \\ 2 & 1 & & \\ 3 & & 1 & \\ -1 & & & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 3 \\ & -1 & -1 & -5 \\ & -4 & -1 & -7 \\ & 3 & 3 & 2 \end{pmatrix} \\ &= \begin{pmatrix} 1 & & & \\ 2 & 1 & & \\ 3 & 4 & 1 & \\ -1 & -3 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 3 \\ & -1 & -1 & -5 \\ & & 3 & 13 \\ & & & -13 \end{pmatrix}. \end{aligned}$$

Row interchange vs. Permutation Matrix

- ▶ **definition:** A permutation matrix $P = (p_{ij})$ is a matrix obtained by rearranging the rows of the identity matrix I_n .

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$$P_{2,3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}.$$

- ▶ $P_{2,3} \cdot A$ is A with interchanged rows:

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- ▶ Let $P_{k,s}$ be permutation interchanging rows k and s of I_n .
For any $A = (a_{ij}) \in \mathbf{R}^{n \times n}$,
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For any $A = (a_{ij}) \in \mathbf{R}^{n \times n}$,
 $P_{k,s} \cdot A$ is A with rows k and s interchanged.
- ▶ Let P be a permutation, then $P P_{k,s}$ is also a permutation.

Gaussian Elimination with partial pivoting: review

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}.$$

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- ▶ for $s = 1, 2, \dots, n - 1$:
 - ▶ **pivoting**: choose largest entry in absolute value:

$$\mathbf{piv}_s \stackrel{\text{def}}{=} \mathbf{argmax}_{s \leq j \leq n} |a_{js}|, \quad E_s \leftrightarrow E_{\mathbf{piv}_s}$$

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► **eliminating** x_s from E_{s+1} through E_n :

$$l_{js} = \frac{a_{js}}{a_{ss}}, \quad s + 1 \leq j \leq n,$$
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GEPP as LU factorization, example

$$A = \begin{pmatrix} 0 & 0 & -1 & 1 \\ 1 & 1 & -1 & 2 \\ -1 & -1 & 2 & 0 \\ 1 & 2 & 0 & 2 \end{pmatrix} \in \mathbf{R}^{4 \times 4}$$

$$\begin{aligned} P_{1,2} \cdot A &= \begin{pmatrix} & 1 & & \\ 1 & & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \cdot \begin{pmatrix} 0 & 0 & -1 & 1 \\ 1 & 1 & -1 & 2 \\ -1 & -1 & 2 & 0 \\ 1 & 2 & 0 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & -1 & 2 \\ 0 & 0 & -1 & 1 \\ -1 & -1 & 2 & 0 \\ 1 & 2 & 0 & 2 \end{pmatrix} \\ &= \begin{pmatrix} 1 & & & \\ 0 & 1 & & \\ -1 & & 1 & \\ 1 & & & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & -1 & 2 \\ 0 & -1 & 1 & \\ 0 & 1 & 2 & \\ 1 & 1 & 0 & \end{pmatrix}. \end{aligned}$$

$$P_{1,2} \cdot A = \begin{pmatrix} 1 & & & \\ 0 & 1 & & \\ -1 & & 1 & \\ 1 & & & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & -1 & 2 \\ 0 & -1 & 1 & \\ 0 & 1 & 2 & \\ 1 & 1 & 0 & \end{pmatrix}.$$

$$\begin{aligned} P_{1,3} \cdot \begin{pmatrix} 0 & -1 & 1 \\ 0 & 1 & 2 \\ 1 & 1 & 0 \end{pmatrix} &= \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 2 \\ 0 & -1 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & & \\ 0 & 1 & \\ 0 & & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 & 0 \\ & 1 & 2 \\ & -1 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & & \\ 0 & 1 & \\ 0 & -1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 & 0 \\ & 1 & 2 \\ & & 3 \end{pmatrix}. \end{aligned}$$

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$$P_{1,3} \cdot \begin{pmatrix} 0 & -1 & 1 \\ 0 & 1 & 2 \\ 1 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & & \\ 0 & 1 & \\ 0 & -1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 & 0 \\ & 1 & 2 \\ & & 3 \end{pmatrix}.$$

► Permutation

$$\begin{aligned} P &= \begin{pmatrix} 1 & & \\ & P_{1,3} & \\ & & 1 \end{pmatrix} \cdot P_{1,2} = \begin{pmatrix} 1 & & \\ & 1 & 1 \\ & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & & \\ & 1 & 1 \\ 1 & & 1 \end{pmatrix}. \end{aligned}$$

$$P_{1,2} \cdot A = \begin{pmatrix} 1 & & & \\ 0 & 1 & & \\ -1 & & 1 & \\ 1 & & & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & -1 & 2 \\ 0 & -1 & 1 & \\ 0 & 1 & 2 & \\ 1 & 1 & 0 & \end{pmatrix},$$

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► LU factorization

$$P \cdot A = \begin{pmatrix} 1 & & & \\ P_{1,3} \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix} & & & \\ & P_{1,3} & & \end{pmatrix} \cdot \begin{pmatrix} 1 & \begin{pmatrix} 1 & -1 & 2 \\ 0 & -1 & 1 \\ 0 & 1 & 2 \\ 1 & 1 & 0 \end{pmatrix} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & & & \\ 1 & 1 & & \\ -1 & & 1 & \\ 0 & & & 1 \end{pmatrix} \begin{pmatrix} 1 & \begin{pmatrix} 1 & -1 & 2 \\ 0 & -1 & 1 \\ 0 & 1 & 2 \\ 1 & 1 & 0 \end{pmatrix} \\ P_{1,3} & & & \end{pmatrix}.$$

$$A = \begin{pmatrix} 0 & 0 & -1 & 1 \\ 1 & 1 & -1 & 2 \\ -1 & -1 & 2 & 0 \\ 1 & 2 & 0 & 2 \end{pmatrix}, \quad P = \begin{pmatrix} & 1 & & \\ & & 1 & \\ & & & 1 \\ 1 & & & \end{pmatrix}.$$

$$\begin{aligned} P \cdot A &= \begin{pmatrix} 1 & & & \\ 1 & 1 & & \\ -1 & & 1 & \\ 0 & & & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & & (1 & -1 & 2) \\ & \begin{pmatrix} 1 & & \\ 0 & 1 & \\ 0 & -1 & 1 \end{pmatrix} & \cdot \begin{pmatrix} 1 & 1 & 0 \\ & 1 & 2 \\ & & 3 \end{pmatrix} \end{pmatrix} \\ &= \begin{pmatrix} 1 & & & \\ 1 & 1 & & \\ -1 & 0 & 1 & \\ 0 & 0 & -1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 & -1 & 2 \\ & 1 & 1 & 0 \\ & & 1 & 2 \\ & & & 3 \end{pmatrix} \stackrel{\text{def}}{=} L \cdot U. \end{aligned}$$

GEPP as LU factorization

Theorem: Let $A = (a_{ij}) \in \mathbf{R}^{n \times n}$ be non-singular. Then GEPP computes an LU factorization with permutation matrix P such that

$$P \cdot A = L \cdot U = \begin{pmatrix} \triangleleft \\ \text{---} \\ \text{---} \end{pmatrix} \cdot \begin{pmatrix} \triangleleft \\ \text{---} \\ \text{---} \end{pmatrix}.$$

$P \cdot A = L \cdot U$, Proof by Induction

▶ GEPP for $n = 2$, $A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$.

▶ **pivoting:**

$$\mathbf{piv}_1 \stackrel{\text{def}}{=} \operatorname{argmax}_{1 \leq j \leq 2} |a_{j1}|, \quad P = \begin{cases} I, & \text{if } \mathbf{piv}_1 = 1, \\ P_{1,2} & \text{if } \mathbf{piv}_1 = 2. \end{cases}$$

▶ **elimination:**

$$P \cdot A = L \cdot U.$$

$P \cdot A = L \cdot U$, Proof by Induction

▶ GEPP for $n \geq 3$, $A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$:

▶ **pivoting:**

$$\mathbf{piv}_1 \stackrel{\text{def}}{=} \mathbf{argmax}_{1 \leq j \leq n} |a_{j1}|, \quad \bar{P} = \begin{cases} I, & \text{if } \mathbf{piv}_1 = 1, \\ P_{1, \mathbf{piv}_1} & \text{if } \mathbf{piv}_1 \geq 2. \end{cases}$$

▶ **elimination:**

$$\bar{P} \cdot A = \begin{pmatrix} 1 & & & \\ & I_{n-1} & & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \quad \left(I \stackrel{\text{def}}{=} \begin{pmatrix} l_{21} \\ \vdots \\ l_{n1} \end{pmatrix} \right).$$

► Induction hypothesis:

$$\mathbf{P} \cdot \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} = \mathbf{L} \cdot \mathbf{U}.$$

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► putting it together,

$$\begin{aligned} \begin{pmatrix} 1 & \\ & \mathbf{P} \end{pmatrix} \cdot \bar{\mathbf{P}} \cdot \mathbf{A} &= \begin{pmatrix} 1 & \\ & \mathbf{P} \end{pmatrix} \cdot \begin{pmatrix} 1 & \\ & \mathbf{I}_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} \\ &= \begin{pmatrix} 1 & \\ & \mathbf{P} \cdot \mathbf{I} & \mathbf{P} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & \begin{pmatrix} a_{12} & \cdots & a_{1n} \\ \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} \end{pmatrix} \\ &= \begin{pmatrix} 1 & \\ & \mathbf{P} \cdot \mathbf{I} & \mathbf{I}_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & \begin{pmatrix} a_{12} & \cdots & a_{1n} \\ \mathbf{P} \cdot \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} \end{pmatrix} \end{pmatrix} \end{aligned}$$

$$\text{Let } P \stackrel{\text{def}}{=} \begin{pmatrix} 1 & \\ & \mathbf{P} \end{pmatrix} \cdot \bar{P}.$$

► LU magic:

$$\begin{aligned} P \cdot A &= \begin{pmatrix} 1 & \\ \mathbf{P} \cdot \mathbf{I} & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & (a_{12} & \cdots & a_{1n}) \\ & \mathbf{L} \cdot \mathbf{U} \end{pmatrix} \\ &= \begin{pmatrix} 1 & \\ \mathbf{P} \cdot \mathbf{I} & \mathbf{L} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & (a_{12} & \cdots & a_{1n}) \\ & \mathbf{U} \end{pmatrix} \\ &\stackrel{\text{def}}{=} L \cdot U = \begin{pmatrix} \triangle & \\ & \triangle \\ & & \triangle \end{pmatrix} \cdot \begin{pmatrix} \triangle & \\ & \triangle \\ & & \triangle \end{pmatrix}. \end{aligned}$$

Solving general linear equations with GEPP

$$A\mathbf{x} = \mathbf{b}, \quad P \cdot A = L \cdot U$$

- ▶ interchanging components in \mathbf{b}

$$P \cdot (A\mathbf{x}) = (P \cdot \mathbf{b}), \quad (L \cdot U)\mathbf{x} = (P \cdot \mathbf{b}).$$

- ▶ solving for \mathbf{b} with forward and backward substitution

$$\begin{aligned}\mathbf{x} &= (L \cdot U)^{-1} (P \cdot \mathbf{b}) \\ &= (U^{-1} (L^{-1} (P \cdot \mathbf{b}))).\end{aligned}$$

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Cost Analysis

- ▶ computing $P \cdot A = L \cdot U$: about $2/3n^3$ operations.
- ▶ forward and backward substitution: about $2n^2$ operations.
- ▶ most important to compute $P \cdot A = L \cdot U$ **efficiently**

Strictly Diagonally Dominant (**SDD**) Matrices

- ▶ **Definition:** Matrix $A = (a_{ij}) \in \mathbf{R}^{n \times n}$ is **SDD** if

$$|a_{ii}| > \sum_{j=1, j \neq i}^n |a_{ij}| \quad \text{holds for each } i = 1, 2, \dots, n.$$

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- ▶ Example I: matrix $A = \begin{pmatrix} 7 & 2 & 0 \\ 3 & 5 & -1 \\ 0 & 5 & -6 \end{pmatrix}$ is **SDD**.

$$|7| > |2| + |0|, \quad |5| > |3| + |-1|, \quad |-6| > |0| + |5|.$$

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$$|7| > |2| + |0|, \quad |5| > |3| + |-1|, \quad |-6| > |0| + |5|.$$

- ▶ Example II: matrix $B = \begin{pmatrix} 7 & 5 & 0 \\ 3 & 5 & -1 \\ 0 & -3 & 3 \end{pmatrix}$ is **NOT SDD**.

$$|3| \leq |0| + |-3|.$$

GE on **SDD**: succeeds without pivoting (I)

- ▶ Let $A = (a_{ij}) \in \mathbf{R}^{n \times n}$ be **SDD**, so

$$|a_{11}| > \sum_{j=1, j \neq 1}^n |a_{1j}| \geq 0.$$

GE on **SDD**: succeeds without pivoting (I)

- ▶ Let $A = (a_{ij}) \in \mathbf{R}^{n \times n}$ be **SDD**, so

$$|a_{11}| > \sum_{j=1, j \neq 1}^n |a_{1j}| \geq 0.$$

- ▶ elimination with $a_{11} \neq 0$:

$$\begin{aligned} A &= L_1 \cdot (\text{new } A) \\ &= \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \\ l_{j1} &= \frac{a_{j1}}{a_{11}}, \quad \mathbf{a}_{jk} = a_{jk} - \frac{a_{j1}}{a_{11}} a_{1k}, \quad 2 \leq j \leq n, \quad 2 \leq k \leq n. \end{aligned}$$

GE on **SDD**: succeeds without pivoting (I)

- ▶ Let $A = (a_{ij}) \in \mathbf{R}^{n \times n}$ be **SDD**, so

$$|a_{11}| > \sum_{j=1, j \neq 1}^n |a_{1j}| \geq 0.$$

- ▶ elimination with $a_{11} \neq 0$:

$$\begin{aligned} A &= L_1 \cdot (\text{new } A) \\ &= \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \\ l_{j1} &= \frac{a_{j1}}{a_{11}}, \quad \mathbf{a}_{jk} = a_{jk} - \frac{a_{j1}}{a_{11}} a_{1k}, \quad 2 \leq j \leq n, \quad 2 \leq k \leq n. \end{aligned}$$

- ▶ **only do**: show $\mathbf{A} \stackrel{\text{def}}{=} \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}$ remains **SDD**.

GE on **SDD**: only need to show **A** remains **SDD**

$$|a_{11}| > \sum_{j=1, j \neq 1}^n |a_{1j}|, \quad |a_{ii}| > \sum_{j=1, j \neq i}^n |a_{ij}|, \quad i = 2, \dots, n,$$

$$\mathbf{A} = \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \quad \mathbf{a}_{ij} = a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j}.$$

GE on **SDD**: only need to show **A** remains **SDD**

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► for $i = 2, \dots, n$,

$$\sum_{j=2, j \neq i}^n |\mathbf{a}_{ij}| = \sum_{j=2, j \neq i}^n \left| a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j} \right| \leq \left(\sum_{j=2, j \neq i}^n |a_{ij}| \right) + \left| \frac{a_{i1}}{a_{11}} \right| \left(\sum_{j=2, j \neq i}^n |a_{1j}| \right)$$

GE on **SDD**: only need to show **A** remains **SDD**

$$|a_{11}| > \sum_{j=1, j \neq 1}^n |a_{1j}|, \quad |a_{ii}| > \sum_{j=1, j \neq i}^n |a_{ij}|, \quad i = 2, \dots, n,$$

$$\mathbf{A} = \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \quad \mathbf{a}_{ij} = a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j}.$$

► for $i = 2, \dots, n$,

$$\begin{aligned} \sum_{j=2, j \neq i}^n |a_{ij}| &= \sum_{j=2, j \neq i}^n \left| a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j} \right| \leq \left(\sum_{j=2, j \neq i}^n |a_{ij}| \right) + \left| \frac{a_{i1}}{a_{11}} \right| \left(\sum_{j=2, j \neq i}^n |a_{1j}| \right) \\ &\stackrel{\text{SDD}}{<} (|a_{ii}| - |a_{i1}|) + \left| \frac{a_{i1}}{a_{11}} \right| (|a_{11}| - |a_{1i}|) = |a_{ij}| - \left| \frac{a_{i1}}{a_{11}} \right| |a_{1i}| \end{aligned}$$

GE on **SDD**: only need to show **A** remains **SDD**

$$|a_{11}| > \sum_{j=1, j \neq 1}^n |a_{1j}|, \quad |a_{ii}| > \sum_{j=1, j \neq i}^n |a_{ij}|, \quad i = 2, \dots, n,$$

$$\mathbf{A} = \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \quad \mathbf{a}_{ij} = a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j}.$$

► for $i = 2, \dots, n$,

$$\begin{aligned} \sum_{j=2, j \neq i}^n |a_{ij}| &= \sum_{j=2, j \neq i}^n \left| a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j} \right| \leq \left(\sum_{j=2, j \neq i}^n |a_{ij}| \right) + \left| \frac{a_{i1}}{a_{11}} \right| \left(\sum_{j=2, j \neq i}^n |a_{1j}| \right) \\ &\stackrel{\text{SDD}}{<} (|a_{ii}| - |a_{i1}|) + \left| \frac{a_{i1}}{a_{11}} \right| (|a_{11}| - |a_{1i}|) = |a_{ii}| - \left| \frac{a_{i1}}{a_{11}} \right| |a_{1i}| \\ &\leq \left| a_{ii} - \frac{a_{i1}}{a_{11}} a_{1i} \right| = |\mathbf{a}_{ii}|. \end{aligned}$$

GE on **SDD**: example

$$A = \begin{pmatrix} 7 & 2 & 0 \\ 3 & 5 & -1 \\ 0 & 5 & -6 \end{pmatrix} \text{ is } \mathbf{SDD}.$$

$$A = \begin{pmatrix} 1 & & \\ \frac{3}{7} & 1 & \\ 0 & & 1 \end{pmatrix} \cdot \begin{pmatrix} 7 & 2 & 0 \\ \frac{29}{7} & -1 & \\ 5 & -6 & \end{pmatrix} \left[\begin{pmatrix} \frac{29}{7} & -1 \\ 5 & -6 \end{pmatrix} \text{ is } \mathbf{SDD} \right]$$

GE on **SDD**: example

$$A = \begin{pmatrix} 7 & 2 & 0 \\ 3 & 5 & -1 \\ 0 & 5 & -6 \end{pmatrix} \text{ is } \mathbf{SDD}.$$

$$\begin{aligned} A &= \begin{pmatrix} 1 & & \\ \frac{3}{7} & 1 & \\ 0 & & 1 \end{pmatrix} \cdot \begin{pmatrix} 7 & 2 & 0 \\ & \frac{29}{7} & -1 \\ & 5 & -6 \end{pmatrix} \left[\begin{pmatrix} \frac{29}{7} & -1 \\ 5 & -6 \end{pmatrix} \text{ is } \mathbf{SDD} \right] \\ &= \begin{pmatrix} 1 & & \\ \frac{3}{7} & 1 & \\ 0 & \frac{35}{29} & 1 \end{pmatrix} \cdot \begin{pmatrix} 7 & 2 & 0 \\ & \frac{29}{7} & -1 \\ & & -\frac{139}{29} \end{pmatrix} \end{aligned}$$

Symmetric Positive Definite Matrices

- ▶ **Definition:** Matrix $A = (a_{ij}) \in \mathbf{R}^{n \times n}$ is **SPD** if

$$A = A^T, \quad \mathbf{x}^T A \mathbf{x} > 0 \quad \text{for any non-zero } \mathbf{x} \in \mathbf{R}^n.$$

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$$A = A^T, \quad \mathbf{x}^T A \mathbf{x} > 0 \quad \text{for any non-zero } \mathbf{x} \in \mathbf{R}^n.$$

- ▶ Example I: matrix $A = \begin{pmatrix} \mathbf{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = A^T$ is NOT **SPD**.

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}^T \begin{pmatrix} \mathbf{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \mathbf{0}.$$

Definition: $A = A^T$ is **SPD** if $\mathbf{x}^T A \mathbf{x} > 0$ for any $\mathbf{x} \neq 0$

▶ Example II: matrix $A = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = A^T$ is **SPD**.

▶ Let $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \in \mathbf{R}^3$.

Definition: $A = A^T$ is **SPD** if $\mathbf{x}^T A \mathbf{x} > 0$ for any $\mathbf{x} \neq 0$

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▶ Let $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \in \mathbf{R}^3$.

$$\begin{aligned} \mathbf{x}^T A \mathbf{x} &= \begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\ &= \begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} 2x_1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 \end{pmatrix} \\ &= 2x_1^2 - 2x_1 x_2 + 2x_2^2 - 2x_2 x_3 + 2x_3^2 \end{aligned}$$

Definition: $A = A^T$ is **SPD** if $\mathbf{x}^T A \mathbf{x} > 0$ for any $\mathbf{x} \neq 0$

▶ Example II: matrix $A = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = A^T$ is **SPD**.

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$$\begin{aligned} \mathbf{x}^T A \mathbf{x} &= \begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\ &= \begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} 2x_1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 \end{pmatrix} \\ &= 2x_1^2 - 2x_1 x_2 + 2x_2^2 - 2x_2 x_3 + 2x_3^2 \end{aligned}$$

$$\begin{aligned} &\underline{\underline{\text{rearranging}}} \quad x_1^2 + (x_1^2 - 2x_1 x_2 + x_2^2) + (x_2^2 - 2x_2 x_3 + x_3^2) + x_3^2 \\ &= x_1^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + x_3^2 > 0, \quad \text{unless } \mathbf{x} = 0. \end{aligned}$$

GE on **SPD**: succeeds without pivoting (I)

- ▶ Let $A = (a_{ij}) \in \mathbf{R}^{n \times n}$ be **SPD**, then

$$A^T = A, \quad \text{therefore } a_{jk} = a_{kj} \quad \text{for all } 1 \leq j, k \leq n$$

$$a_{11} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}^T \cdot A \cdot \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} > 0.$$

GE on **SPD**: succeeds without pivoting (I)

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- ▶ elimination without pivoting

$$A = L_1 \cdot (\mathbf{new} \ A)$$

$$= \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix},$$

$$l_{j1} = \frac{a_{j1}}{a_{11}}, \quad \mathbf{a}_{jk} = a_{jk} - \frac{a_{j1}}{a_{11}} a_{1k}, \quad 2 \leq j \leq n, \quad 2 \leq k \leq n.$$

$$A = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{a}_{11} & \mathbf{a}_{12} & \cdots & \mathbf{a}_{1n} \\ & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ & \vdots & \ddots & \vdots \\ & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix},$$

► symmetry in A implies for $2 \leq j, k \leq n$,

$$l_{j1} = \frac{a_{j1}}{a_{11}} = \frac{a_{1j}}{a_{11}}, \quad \mathbf{a}_{jk} = a_{jk} - \frac{a_{j1}}{a_{11}} a_{1k} = \mathbf{a}_{kj}.$$

$$A = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & & \ddots & \\ l_{n1} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{a}_{11} & \mathbf{a}_{12} & \cdots & \mathbf{a}_{1n} \\ & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ & \vdots & \ddots & \vdots \\ & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix},$$

- symmetry in A implies for $2 \leq j, k \leq n$,

$$l_{j1} = \frac{a_{j1}}{a_{11}} = \frac{a_{1j}}{a_{11}}, \quad \mathbf{a}_{jk} = a_{jk} - \frac{a_{j1}}{a_{11}} a_{1k} = \mathbf{a}_{kj}.$$



$$\mathbf{l}_1 \stackrel{\text{def}}{=} \begin{pmatrix} l_{21} \\ \vdots \\ l_{n1} \end{pmatrix}, \quad \mathbf{A} \stackrel{\text{def}}{=} \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \quad \text{and}$$

$$\begin{aligned} A &= \begin{pmatrix} 1 & & \\ \mathbf{l}_1 & I_{n-1} & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{11} \mathbf{l}_1^T \\ & \mathbf{A} \end{pmatrix} \\ &= \begin{pmatrix} 1 & & \\ \mathbf{l}_1 & I_{n-1} & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & \\ & \mathbf{A} \end{pmatrix} \begin{pmatrix} 1 & \mathbf{l}_1^T \\ & I_{n-1} \end{pmatrix} \end{aligned}$$

- ▶ symmetric matrix factorization

$$\begin{aligned}
 A &= \begin{pmatrix} 1 & & \\ \mathbf{l}_1 & I_{n-1} & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & \\ & \mathbf{A} \end{pmatrix} \begin{pmatrix} 1 & \mathbf{l}_1^T \\ & I_{n-1} \end{pmatrix} \\
 &= \begin{pmatrix} 1 & & \\ \mathbf{l}_1 & I_{n-1} & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & \\ & \mathbf{A} \end{pmatrix} \begin{pmatrix} 1 & & \\ \mathbf{l}_1 & I_{n-1} \end{pmatrix}^T,
 \end{aligned}$$

$$\mathbf{A} \stackrel{\text{def}}{=} \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix}, \quad \mathbf{a}_{jk} = a_{jk} - \frac{a_{j1} a_{1k}}{a_{11}} = \mathbf{a}_{kj},$$

Only need to compute \mathbf{a}_{jk} for $j \leq k$ due to symmetry

- ▶ **next step:** show \mathbf{A} remains **SPD**.

$$A = \begin{pmatrix} 1 & & \\ & \mathbf{I}_1 & \\ & & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & \\ & \mathbf{A} & \\ & & \end{pmatrix} \begin{pmatrix} 1 & & \\ & \mathbf{I}_1 & \\ & & I_{n-1} \end{pmatrix}^T,$$

- ▶ Let $\hat{\mathbf{x}} \in \mathbf{R}^{n-1}$ be any non-zero vector.
Must show $\hat{\mathbf{x}}^T \cdot \mathbf{A}\hat{\mathbf{x}} > 0$ for \mathbf{A} to be **SPD**.



Note $\mathbf{x} \stackrel{\text{def}}{=} \begin{pmatrix} -\hat{\mathbf{x}}^T \mathbf{I}_1 \\ \hat{\mathbf{x}} \end{pmatrix} \in \mathbf{R}^n$ is non-zero, therefore $\mathbf{x}^T \cdot A \cdot \mathbf{x} > 0$.

$$A = \begin{pmatrix} 1 & & \\ & \mathbf{I}_1 & \\ & & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & \\ & \mathbf{A} & \\ & & \end{pmatrix} \begin{pmatrix} 1 & & \\ & \mathbf{I}_1 & \\ & & I_{n-1} \end{pmatrix}^T,$$

- ▶ Let $\hat{\mathbf{x}} \in \mathbf{R}^{n-1}$ be any non-zero vector.
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▶

Note $\mathbf{x} \stackrel{\text{def}}{=} \begin{pmatrix} -\hat{\mathbf{x}}^T \mathbf{I}_1 \\ \hat{\mathbf{x}} \end{pmatrix} \in \mathbf{R}^n$ is non-zero, therefore $\mathbf{x}^T \cdot A \cdot \mathbf{x} > 0$.

- ▶ consequently,

$$\begin{aligned} 0 &< \mathbf{x}^T \cdot A \cdot \mathbf{x} \\ &= \begin{pmatrix} -\mathbf{I}_1^T \hat{\mathbf{x}} \\ \hat{\mathbf{x}} \end{pmatrix}^T \cdot \begin{pmatrix} 1 & & \\ & \mathbf{I}_1 & \\ & & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & \\ & \mathbf{A} & \\ & & \end{pmatrix} \begin{pmatrix} 1 & & \\ & \mathbf{I}_1 & \\ & & I_{n-1} \end{pmatrix}^T \cdot \begin{pmatrix} -\mathbf{I}_1^T \hat{\mathbf{x}} \\ \hat{\mathbf{x}} \end{pmatrix} \\ &= \begin{pmatrix} 0 & \hat{\mathbf{x}}^T \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & \\ & \mathbf{A} & \\ & & \end{pmatrix} \cdot \begin{pmatrix} 0 \\ \hat{\mathbf{x}} \end{pmatrix} \\ &= \hat{\mathbf{x}}^T \cdot \mathbf{A} \cdot \hat{\mathbf{x}}. \end{aligned}$$

Cholesky factorization for SPD matrix: $A = L D L^T$

- ▶ Cholesky for $n = 2$:

$$\begin{aligned} A &= \begin{pmatrix} a_{11} & a_{21} \\ a_{21} & a_{22} \end{pmatrix} \quad [A \text{ is symmetric}] \\ &= \begin{pmatrix} 1 & \\ l_{21} & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & \\ & \mathbf{a}_{22} \end{pmatrix} \cdot \begin{pmatrix} 1 & \\ l_{21} & 1 \end{pmatrix}^T, \quad \left[l_{21} = \frac{a_{21}}{a_{11}} \right] \\ \stackrel{\text{def}}{=} L \cdot D \cdot L^T &= \begin{pmatrix} \triangle & \\ & \square \end{pmatrix} \cdot \begin{pmatrix} \triangle & \\ & \square \end{pmatrix} \cdot \begin{pmatrix} \triangle & \\ & \square \end{pmatrix}^T, \end{aligned}$$

Cholesky factorization for SPD matrix: $A = LDL^T$

- ▶ Cholesky for $n \geq 3$:

$$A = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{21} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \quad [A \text{ is symmetric}]$$
$$= \begin{pmatrix} 1 & & & \\ \mathbf{l} & I_{n-1} & & \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & & \\ & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ & \vdots & \ddots & \vdots \\ & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} \cdot \begin{pmatrix} 1 & & & \\ \mathbf{l} & I_{n-1} & & \end{pmatrix}^T,$$

where $\mathbf{l} \stackrel{\text{def}}{=} \begin{pmatrix} l_{21} \\ \vdots \\ l_{n1} \end{pmatrix}$.

Cholesky factorization for SPD matrix: $A = LDL^T$

► induction hypothesis

$$\begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} = \mathbf{LDL}^T = \begin{pmatrix} \triangle \\ \square \end{pmatrix} \cdot \begin{pmatrix} \triangle \\ \square \end{pmatrix} \cdot \begin{pmatrix} \triangle \\ \square \end{pmatrix}^T$$

Cholesky factorization for SPD matrix: $A = LDL^T$

► induction hypothesis

$$\begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} = \mathbf{LDL}^T = \begin{pmatrix} \triangle \\ \square \end{pmatrix} \cdot \begin{pmatrix} \triangle \\ \square \end{pmatrix} \cdot \begin{pmatrix} \triangle \\ \square \end{pmatrix}^T$$

► Cholesky factorization

$$\begin{aligned} A &= \begin{pmatrix} 1 & \\ \mathbf{I} & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & \\ & \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} & \\ & & \end{pmatrix} \cdot \begin{pmatrix} 1 & \\ \mathbf{I} & I_{n-1} \end{pmatrix}^T, \\ &= \begin{pmatrix} 1 & \\ \mathbf{I} & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & \\ & \mathbf{LDL}^T & \\ & & \end{pmatrix} \cdot \begin{pmatrix} 1 & \\ \mathbf{I} & I_{n-1} \end{pmatrix}^T, \\ &= \begin{pmatrix} 1 & \\ \mathbf{I} & \mathbf{L} \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & \\ & \mathbf{D} & \\ & & \end{pmatrix} \cdot \begin{pmatrix} 1 & \\ \mathbf{I} & \mathbf{L} \end{pmatrix}^T = \begin{pmatrix} \triangle \\ \square \end{pmatrix} \cdot \begin{pmatrix} \triangle \\ \square \end{pmatrix} \cdot \begin{pmatrix} \triangle \\ \square \end{pmatrix}^T. \end{aligned}$$

Cholesky factorization $A = L D L^T$: example

$$A = \begin{pmatrix} 4 & -1 & 1 \\ -1 & 4.25 & 2.75 \\ 1 & 2.75 & 3.5 \end{pmatrix} = A^T.$$

$$A = \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & & \\ & 4 & 3 \\ & 3 & \frac{13}{4} \end{pmatrix} \cdot \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix}^T$$

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$$A = \begin{pmatrix} 4 & -1 & 1 \\ -1 & 4.25 & 2.75 \\ 1 & 2.75 & 3.5 \end{pmatrix} = A^T.$$

$$\begin{aligned} A &= \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & & \\ & 4 & 3 \\ & 3 & \frac{13}{4} \end{pmatrix} \cdot \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix}^T \\ &= \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & & \\ & \begin{pmatrix} 1 & \\ \frac{3}{4} & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & \\ & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & \\ \frac{3}{4} & 1 \end{pmatrix}^T \\ &\quad \cdot \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix}^T \end{pmatrix} \end{aligned}$$

Cholesky factorization $A = LDL^T$: example

$$A = \begin{pmatrix} 4 & -1 & 1 \\ -1 & 4.25 & 2.75 \\ 1 & 2.75 & 3.5 \end{pmatrix} = A^T.$$

$$\begin{aligned} A &= \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & & \\ & 4 & 3 \\ & 3 & \frac{13}{4} \end{pmatrix} \cdot \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix}^T \\ &= \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & & \\ & \begin{pmatrix} 1 & \\ \frac{3}{4} & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & \\ & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & \\ \frac{3}{4} & 1 \end{pmatrix}^T \\ &\quad \cdot \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix}^T \\ &= \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & \frac{3}{4} & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & & \\ & 4 & \\ & & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & \frac{3}{4} & 1 \end{pmatrix}^T. \end{aligned}$$

Cholesky factorization is a special LU factorization

- ▶ $A = LDL^T = LU$, with $U = DL^T = \begin{pmatrix} \triangle & & \\ & \triangle & \\ & & \triangle \end{pmatrix}$
- ▶ only L need to be computed, saving half of the work in factorization.
- ▶ total cost: about $\frac{1}{3}n^3$ operations.

Review on Natural Splines: equations in matrix form

Equations for spline coefficients $\{c_j\}_{j=1}^{n-1}$,

$$A \cdot \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_{n-2} \\ c_{n-1} \end{pmatrix} = \mathbf{rhs},$$

where

$$A \stackrel{\text{def}}{=} \begin{pmatrix} 2(h_0 + h_1) & h_1 & & & & & & \\ h_1 & 2(h_1 + h_2) & h_2 & & & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & & h_{n-3} & 2(h_{n-3} + h_{n-2}) & h_{n-2} & & \\ & & & & h_{n-2} & 2(h_{n-2} + h_{n-1}) & & \end{pmatrix}.$$

A is **SDD**, **SPD**, and **tri-diagonal**

Special matrix: **tri-diagonal** matrix

$A \in \mathbf{R}^{n \times n}$ is **tri-diagonal** if

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$
$$= \begin{pmatrix} a_{11} & a_{12} & & & & \\ a_{21} & a_{22} & a_{23} & & & \\ & \ddots & \ddots & \ddots & & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} & \\ & & & a_{n,n-1} & a_{n,n} & \end{pmatrix}.$$

LU should simplify since A has so many zero entries

tri-diagonal LU factorization

Let $l_{21} = \frac{a_{21}}{a_{11}}$ and $\mathbf{a}_{22} = a_{22} - l_{21} a_{12}$, then

$$A = \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{12} & & & \\ & \mathbf{a}_{22} & a_{23} & & \\ & & \ddots & \ddots & \\ & & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & & a_{n,n-1} & a_{n,n} \end{pmatrix}.$$

elimination only means computing l_{21} and \mathbf{a}_{22}

tri-diagonal LU factorization

Let $\mathbf{a}_{11} = a_{11}$, then

$$A = \begin{pmatrix} a_{11} & a_{12} & & & & \\ a_{21} & a_{22} & a_{23} & & & \\ & \ddots & \ddots & \ddots & & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} & \\ & & & a_{n,n-1} & a_{n,n} & \end{pmatrix}$$

tri-diagonal LU factorization

Let $\mathbf{a}_{11} = a_{11}$, then

$$A = \begin{pmatrix} a_{11} & a_{12} & & & \\ a_{21} & a_{22} & a_{23} & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & a_{n,n-1} & a_{n,n} \end{pmatrix}$$
$$= \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ & \ddots & \ddots & & \\ & & l_{n-1,n-2} & 1 & \\ & & & l_{n,n-1} & 1 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{a}_{11} & a_{12} & & & \\ & \mathbf{a}_{22} & a_{23} & & \\ & & \ddots & \ddots & \\ & & & \mathbf{a}_{n-1,n-1} & a_{n-1,n} \\ & & & & \mathbf{a}_{n,n} \end{pmatrix}$$

$$l_{j+1,j} = \frac{a_{j+1,j}}{\mathbf{a}_{jj}}, \quad \mathbf{a}_{j+1,j+1} = a_{j+1,j+1} - l_{j+1,j} a_{j,j+1}, \quad j = 1, \dots, n-1.$$

grand total: $3n$ operations. Pivoting at $O(n)$ additional operations