Review on 12:00-1:00PM, Friday, Dec. 1

#### GEPP as LU factorization

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

$$P \cdot A = L \cdot U = \left( \begin{array}{c} \\ \\ \end{array} \right) \cdot \left( \begin{array}{c} \\ \\ \end{array} \right).$$

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

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

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

elimination:

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

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

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

pivoting:

$$\operatorname{piv}_1 \stackrel{def}{=} \operatorname{argmax}_{1 \leq j \leq n} |a_{j1}|, \quad \overline{P} = \left\{ \begin{array}{ll} I, & \text{if } \operatorname{piv}_1 = 1, \\ P_{1,\operatorname{piv}_1} & \text{if } \operatorname{piv}_1 \geq 2. \end{array} \right.$$

elimination:

$$\overline{P} \cdot A = \begin{pmatrix} 1 & & \\ 1 & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{0} & \frac{a_{12}}{a_{22}} & \cdots & \frac{a_{1n}}{a_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \begin{pmatrix} \mathbf{I} \stackrel{def}{=} \begin{pmatrix} I_{21} & & \\ \vdots & & \\ I_{n1} & & \end{pmatrix} \end{pmatrix}$$

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elimination:

$$\overline{P} \cdot A = \begin{pmatrix} 1 \\ 1 \\ l \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{0} & \frac{a_{12}}{a_{22}} & \cdots & \frac{a_{1n}}{a_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2} & \cdots & a_{nn} \end{pmatrix}, \quad \begin{pmatrix} \mathbf{I} \stackrel{def}{=} \begin{pmatrix} l_{21} \\ \vdots \\ l_{n1} \end{pmatrix} \end{pmatrix}$$

► Induction hypothesis:

$$\widehat{\mathbf{P}} \cdot \left( \begin{array}{ccc} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{array} \right) = \widehat{\mathbf{L}} \cdot \widehat{\mathbf{U}}.$$

$$= \left(\begin{array}{c|c} 1 & \\ \hline \widehat{P} \cdot I & \widehat{P} \end{array}\right) \cdot \left(\begin{array}{c|c} \frac{a_{11} & \left(\begin{array}{ccc} a_{12} & \cdots & a_{1n} \\ a_{22} & \cdots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n2} & \cdots & a_{nn} \end{array}\right) \right)$$

$$= \left(\begin{array}{c|c} 1 & \\ \hline \widehat{P} \cdot I & I_{n-1} \end{array}\right) \cdot \left(\begin{array}{c|c} \frac{a_{11} & \left(\begin{array}{ccc} a_{12} & \cdots & a_{1n} \\ \end{array}\right)}{\widehat{P} \cdot \left(\begin{array}{ccc} a_{22} & \cdots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n2} & \cdots & a_{nn} \end{array}\right) \end{array}\right)$$

$$= \left(\begin{array}{c|c} 1 & \\ \hline \widehat{P} \cdot I & I_{n-1} \end{array}\right) \cdot \left(\begin{array}{c|c} a_{11} & \left(\begin{array}{ccc} a_{12} & \cdots & a_{1n} \\ \hline \end{array}\right) \\ \hline = \left(\begin{array}{c|c} 1 & \\ \hline \widehat{P} \cdot I & \widehat{L} \end{array}\right) \cdot \left(\begin{array}{c|c} a_{11} & \left(\begin{array}{ccc} a_{12} & \cdots & a_{1n} \\ \hline \end{array}\right) \\ \hline U \\ \end{array}\right)$$

$$def$$

putting it together,

$$\frac{\begin{pmatrix} 1 & \\ & \hat{P} \end{pmatrix} \cdot \overline{P} \cdot A = \begin{pmatrix} 1 & \\ & \hat{P} \end{pmatrix} \cdot \begin{pmatrix} 1 & \\ & 1 & \\ & & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{1} & \frac{a_{12}}{1} & \cdots & \frac{a_{1n}}{1} \\ & \frac{a_{22}}{2} & \cdots & \frac{a_{2n}}{2n} \\ & \vdots & \ddots & \vdots \\ & a_{n2} & \cdots & a_{nn} \end{pmatrix} }{\begin{pmatrix} \frac{a_{11}}{1} & \begin{pmatrix} a_{12} & \cdots & a_{1n} & \\ & a_{22} & \cdots & a_{2n} \\ & \vdots & \ddots & \vdots \\ & a_{n2} & \cdots & a_{nn} \end{pmatrix}} \end{pmatrix} }$$

$$= \begin{pmatrix} \frac{1}{1} & \\ & \hat{P} \cdot I & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{1} & \begin{pmatrix} a_{12} & \cdots & a_{1n} & \\ & \vdots & \ddots & \vdots \\ & a_{n2} & \cdots & a_{nn} \end{pmatrix} \\ = \begin{pmatrix} \frac{1}{1} & \\ & \hat{P} \cdot I & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{1} & \begin{pmatrix} a_{12} & \cdots & a_{1n} & \\ & \hat{I} \cdot \hat{U} & \\ & & \hat{U} \end{pmatrix} \\ = \begin{pmatrix} \frac{1}{1} & \\ & \hat{P} \cdot I & \hat{I} \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{1} & \begin{pmatrix} a_{12} & \cdots & a_{1n} & \\ & \hat{I} \cdot \hat{U} & \\ & \hat{U} \end{pmatrix} \\ \end{pmatrix}$$

$$\frac{def}{=} \begin{pmatrix} \frac{1}{1} & \\ & \frac{1}{1} & \frac{1}{1} \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{1} & \begin{pmatrix} a_{12} & \cdots & a_{1n} & \\ & \hat{I} \cdot \hat{U} & \\ & \hat{U} \end{pmatrix} \\ \end{pmatrix}$$
What if A is singular?

## Solving general linear equations with GEPP

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

▶ interchanging components in **b** 

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

solving for b with forward and backward substitution

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

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Cost Analysis

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

# §6.6 Strictly Diagonally Dominant (SDD) Matrices

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

$$|a_{ii}| > \sum_{j=1, i \neq i}^{n} |a_{ij}|$$
 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**.

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

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

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

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

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

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

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

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▶ elimination with  $a_{11} \neq 0$ :

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

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

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ightharpoonup elimination with  $a_{11} \neq 0$ :

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

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

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

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

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

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

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

$$ightharpoonup$$
 for  $i=2,\cdots n$ ,

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

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

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$$\blacktriangleright \text{ for } i=2,\cdots n,$$

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

$$\stackrel{\text{SDD}}{<} \left( |a_{ii}| - |a_{i1}| \right) + \left| \frac{a_{i1}}{a_{11}} \right| \left( |a_{11}| - |a_{1i}| \right) = |a_{ii}| - \left| \frac{a_{i1}}{a_{11}} \right| |a_{1i}|$$

9/3

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

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

### GE on **SDD**: example

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

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

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$$= \begin{pmatrix} 1 \\ \frac{3}{7} & 1 \\ 0 & \frac{35}{29} & 1 \end{pmatrix} \cdot \begin{pmatrix} 7 & 2 & 0 \\ \frac{29}{7} & -1 \\ 0 & \frac{139}{29} \end{pmatrix}$$

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

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

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Example I: matrix

$$\widehat{A} = \begin{pmatrix} \boxed{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = \widehat{A}^T$$

$$\underline{\text{IS NOT SPD:}}$$

$$\left(\begin{array}{c} 1 \\ 0 \\ 0 \end{array}\right)^T \left(\begin{array}{ccc} \boxed{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{array}\right) \left(\begin{array}{c} 1 \\ 0 \\ 0 \end{array}\right) \quad = \quad \mathbf{0}$$

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- $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}^T \begin{pmatrix} \boxed{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \mathbf{0}$  PROOF: Let  $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \neq \mathbf{0},$

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$$\widehat{A} = \begin{pmatrix} \boxed{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = \widehat{A}^T$$
IS NOT SPD:

| Example II: matrix  $A = \begin{pmatrix} \boxed{2} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = A^T$ 

PROOF: Let 
$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \neq \mathbf{0}$$

$$\mathbf{x}^{T} A \mathbf{x} = \begin{pmatrix} x_{1} & x_{2} & x_{3} \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} x_{1} \\ x_{2} \\ x_{3} \end{pmatrix}$$

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- $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}^T \begin{pmatrix} \boxed{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \mathbf{0} \qquad \begin{vmatrix} \frac{2(3-1)^2}{2} \\ \text{PROOF: Let } \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \neq \mathbf{0},$

Example I: matrix
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$$\underline{\text{IS NOT SPD:}}$$
Example II: matrix  $A = \begin{pmatrix} \boxed{2} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = A^T$ 

$$\underline{\text{IS SPD:}}$$

PROOF: Let 
$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \neq \mathbf{0}$$

$$\mathbf{x}^{T} A \mathbf{x} = \begin{pmatrix} x_{1} & x_{2} & x_{3} \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} x_{1} \\ x_{2} \\ x_{3} \end{pmatrix}$$

$$= \begin{pmatrix} x_{1} & x_{2} & x_{3} \end{pmatrix} \begin{pmatrix} 2x_{1} - x_{2} \\ -x_{1} + 2x_{2} - x_{3} \\ -x_{2} + 2x_{3} \end{pmatrix} = 2x_{1}^{2} - 2x_{1}x_{2} + 2x_{2}^{2} - 2x_{2}x_{3} + 2x_{3}^{2}$$

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Example I: matrix
$$\widehat{A} = \begin{pmatrix} \boxed{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = \widehat{A}^T$$
IS NOT SPD:

$$\widehat{A} = \begin{pmatrix} \boxed{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} = \widehat{A}^T$$

$$\underset{\text{IS NOT SPD:}}{\text{IS NOT SPD:}} = \widehat{A}^T$$

$$\underset{\text{IS SPD:}}{\text{IS SPD:}}$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}^{T} \begin{pmatrix} \boxed{0} & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \mathbf{0} \qquad \text{Proof: Let } \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \neq \mathbf{0},$$

$$\mathbf{x}^{T} A \mathbf{x} = \begin{pmatrix} x_{1} & x_{2} & x_{3} \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} x_{1} \\ x_{2} \\ x_{3} \end{pmatrix}$$

$$= \begin{pmatrix} x_{1} & x_{2} & x_{3} \end{pmatrix} \begin{pmatrix} 2x_{1} - x_{2} \\ -x_{1} + 2x_{2} - x_{3} \\ -x_{2} + 2x_{3} \end{pmatrix} = 2x_{1}^{2} - 2x_{1}x_{2} + 2x_{2}^{2} - 2x_{2}x_{3} + 2x_{3}^{2}$$

rearranging 
$$x_1^2 + (x_1^2 - 2x_1 x_2 + x_2^2) + (x_2^2 - 2x_2 x_3 + x_3^2) + x_3^2$$
  
=  $x_1^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + x_3^2 > 0$ 

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

$$\begin{array}{lll} \boldsymbol{A}^T & = & \boldsymbol{A}, & \text{therefore} & \boldsymbol{a}_{jk} = \boldsymbol{a}_{kj} & \text{for all } 1 \leq j, \, k \leq n \\ \\ \boldsymbol{a}_{11} & = & \left( \begin{array}{c} 1 \\ 0 \\ \vdots \\ 0 \end{array} \right)^T \cdot \boldsymbol{A} \cdot \left( \begin{array}{c} 1 \\ 0 \\ \vdots \\ 0 \end{array} \right) > 0 \end{array}$$

Let  $A = (a_{ii}) \in \mathbb{R}^{n \times n}$  be SPD, then

$$A^T = A, \quad \text{therefore} \quad a_{jk} = a_{kj} \quad \text{for all } 1 \leq j, k \leq n$$
 
$$a_{11} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}^T \cdot A \cdot \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} > 0$$

elimination without pivoting

$$A = \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ \vdots & & \ddots & & \\ l_{n1} & & & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{0} & \frac{a_{12}}{a_{22}} & \cdots & \frac{a_{1n}}{a_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} & & & \\ for j \ge k = 2, \cdots, n \\ & & & \\ l_{j1} & = \frac{a_{j1}}{a_{11}} \\ & & & \\ a_{j,k} & -= l_{j1} a_{1k} \end{pmatrix}$$

Let  $A = (a_{ii}) \in \mathbb{R}^{n \times n}$  be SPD, then

$$\begin{array}{lcl} \boldsymbol{A}^T & = & \boldsymbol{A}, & \text{therefore} & a_{jk} = a_{kj} & \text{for all } 1 \leq j, k \leq n \\ a_{11} & = & \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}^T \cdot \boldsymbol{A} \cdot \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} > 0 \end{array}$$

elimination without pivoting

$$A = \begin{pmatrix} 1 \\ l_{21} & 1 \\ \vdots & \ddots & \vdots \\ l_{n1} & & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{0} & \frac{a_{12}}{0} & \cdots & \frac{a_{1n}}{0} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} l_{j1} & = \frac{a_{j1}}{a_{11}} \\ a_{j,k} & -= l_{j1} a_{1k} \end{pmatrix}$$

$$Define \ \mathbf{I}_1 \stackrel{def}{=} \begin{pmatrix} l_{21} \\ \vdots \\ l_{n1} \end{pmatrix}, \ \widehat{\mathbf{A}} \stackrel{def}{=} \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ a_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} = \widehat{\mathbf{A}}^T, \text{ then}$$

$$A = \begin{pmatrix} 1 \\ \mathbf{I}_1 & I \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{11} \mathbf{I}_1^T \\ \widehat{\mathbf{A}} \end{pmatrix} \iff \text{Gaussian elimination}$$

Let  $A = (a_{ii}) \in \mathbb{R}^{n \times n}$  be SPD, then

$$\begin{array}{lcl} \boldsymbol{A}^T & = & \boldsymbol{A}, & \text{therefore} & a_{jk} = a_{kj} & \text{for all } 1 \leq j, k \leq n \\ a_{11} & = & \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}^T \cdot \boldsymbol{A} \cdot \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} > 0 \end{array}$$

elimination without pivoting

$$A = \begin{pmatrix} 1 \\ l_{21} & 1 \\ \vdots & \ddots & \vdots \\ l_{n1} & & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{0} & \frac{a_{12}}{0} & \cdots & \frac{a_{1n}}{0} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} l_{j1} & = \frac{a_{j1}}{a_{11}} \\ a_{j,k} & -= l_{j1} a_{1k} \end{pmatrix}$$

$$Define \ \mathbf{l}_1 \stackrel{def}{=} \begin{pmatrix} l_{21} \\ \vdots \\ l_{n1} \end{pmatrix}, \ \widehat{\mathbf{A}} \stackrel{def}{=} \begin{pmatrix} a_{22} & \cdots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n2} & \cdots & a_{nn} \end{pmatrix} = \widehat{\mathbf{A}}^T, \text{ then}$$

$$A = \begin{pmatrix} 1 \\ \mathbf{l}_1 & I \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{11}\mathbf{l}_1^T \\ \widehat{\mathbf{A}} \end{pmatrix} \iff \text{Gaussian elimination}$$

$$= \begin{pmatrix} 1 \\ \mathbf{l}_1 & I \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{11}\mathbf{l}_1^T \\ \widehat{\mathbf{A}} \end{pmatrix} \begin{pmatrix} 1 & \mathbf{l}_1^T \\ I \end{pmatrix} \iff \text{due to symmetry of } A$$

Let  $A = (a_{ii}) \in \mathbb{R}^{n \times n}$  be SPD, then

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

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

elimination without pivoting

**next step**: show  $\widehat{\mathbf{A}}$  remains **SPD** 

$$A = \begin{pmatrix} 1 & & \\ I_1 & I \end{pmatrix} \cdot \begin{pmatrix} a_{11} & & \\ & \widehat{\mathbf{A}} \end{pmatrix} \begin{pmatrix} 1 & & \\ I_1 & I \end{pmatrix}^T$$

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

$$A = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} a_{11} & a_{11} & a_{11} \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}^T$$

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

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

$$\begin{pmatrix} 0 \\ \hat{\mathbf{x}} \end{pmatrix} = \begin{pmatrix} 1 \\ \mathbf{I}_1 \end{pmatrix}^T \cdot \begin{pmatrix} -\mathbf{I}_1^T \hat{\mathbf{x}} \\ \hat{\mathbf{x}} \end{pmatrix}$$

consequently,

$$\widehat{\mathbf{x}}^{T} \cdot \widehat{\mathbf{A}} \cdot \widehat{\mathbf{x}} = \begin{pmatrix} 0 \\ \widehat{\mathbf{x}} \end{pmatrix}^{T} \cdot \begin{pmatrix} a_{11} \\ \widehat{\mathbf{a}} \end{pmatrix} \cdot \begin{pmatrix} 0 \\ \widehat{\mathbf{x}} \end{pmatrix} \\
= \begin{pmatrix} -\mathbf{I}_{1}^{T} \widehat{\mathbf{x}} \\ \widehat{\mathbf{x}} \end{pmatrix}^{T} \cdot \begin{pmatrix} 1 \\ \mathbf{I}_{1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} \\ \widehat{\mathbf{a}} \end{pmatrix} \begin{pmatrix} 1 \\ \mathbf{I}_{1} \end{pmatrix}^{T} \cdot \begin{pmatrix} -\mathbf{I}_{1}^{T} \widehat{\mathbf{x}} \\ \widehat{\mathbf{x}} \end{pmatrix} \\
= \mathbf{x}^{T} \cdot \mathbf{A} \cdot \mathbf{x} > 0$$

## Major Cholesky, 1875 - 1918



- ► Invented Cholesky factorization for geodesic work
- ► Fell for his country (France) in WWI

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

▶ Cholesky for n = 2:

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

Cholesky for  $n \ge 3$ :

$$A = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{21} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \quad [A \text{ is symmetric}]$$

$$= \begin{pmatrix} 1 \\ \mathbf{I} & I_{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_{11} \\ \vdots & \ddots & \vdots \\ a_{n2} & \cdots & a_{nn} \end{pmatrix} \cdot \begin{pmatrix} 1 \\ \mathbf{I} & I_{n-1} \end{pmatrix}^{T},$$
where 
$$\mathbf{I} \stackrel{def}{=} \begin{pmatrix} I_{21} \\ \vdots \\ I_{n-1} \end{pmatrix}.$$

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

induction hypothesis

$$\begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} = \widehat{\mathbf{L}}\widehat{\mathbf{D}}\widehat{\mathbf{L}}^T = \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \\ \mathbf{c} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{c} \\ \mathbf{c} \\ \mathbf{c} \\ \mathbf{c} \end{pmatrix}$$

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

induction hypothesis

$$\left(\begin{array}{c} a_{11} \\ \end{array}\right)$$

 $A = \begin{pmatrix} 1 \\ \mathbf{I} & I \end{pmatrix} \cdot \begin{pmatrix} \mathbf{a}_{11} \\ & \begin{pmatrix} \mathbf{a}_{22} & \cdots & \mathbf{a}_{2n} \\ \vdots & \ddots & \vdots \\ \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nn} \end{pmatrix} \cdot \begin{pmatrix} 1 \\ \mathbf{I} & I \end{pmatrix}^{T},$ 

 $= \begin{pmatrix} 1 \\ \mathbf{I} & I \end{pmatrix} \cdot \begin{pmatrix} a_{11} \\ & \widehat{\mathbf{L}} \widehat{\mathbf{D}} \widehat{\mathbf{L}}^T \end{pmatrix} \cdot \begin{pmatrix} 1 \\ \mathbf{I} & I \end{pmatrix}^I,$ 

$$\int a_{11}$$







$$= \begin{pmatrix} \mathbf{I} & I \end{pmatrix} \cdot \begin{pmatrix} \mathbf{I} & \widehat{\mathbf{L}} \widehat{\mathbf{D}} \widehat{\mathbf{L}}^T \end{pmatrix} \cdot \begin{pmatrix} \mathbf{I} & I \end{pmatrix} ,$$

$$= \begin{pmatrix} \mathbf{I} & 1 \\ \mathbf{I} & \widehat{\mathbf{L}} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{a}_{11} & 1 \\ \mathbf{D} & 1 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{I} & 1 \\ \mathbf{I} & \widehat{\mathbf{L}} \end{pmatrix}^T = \begin{pmatrix} \mathbf{L} \\ \mathbf{L} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{L} \\ \mathbf{L} \end{pmatrix}^T .$$

$$)^T$$

## Cholesky factorization $A = LDL^T$ : example

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

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

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

$$\cdot \begin{pmatrix} 1 \\ -\frac{1}{4} & 1 \\ \frac{1}{4} & 1 \end{pmatrix}^{T}$$

# Cholesky factorization $A = LDL^T$ : example

Cholesky factorization 
$$A = LDL^T$$
: example
$$A = \begin{pmatrix} 4 & -1 & 1 \\ -1 & 4.25 & 2.75 \\ 1 & 2.75 & 3.5 \end{pmatrix} = A^T.$$

$$\begin{pmatrix} \frac{1}{4} & 1 \end{pmatrix} \begin{pmatrix} 3 \\ -\frac{1}{4} & 1 \\ \end{pmatrix} \cdot \begin{pmatrix} 4 \\ & \end{pmatrix}$$

 $= \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & \frac{3}{4} & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & & \\ & 4 & \\ & & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & \frac{3}{4} & 1 \end{pmatrix} .$ 

$$=\begin{pmatrix}1\\-\frac{1}{4}&1\\\frac{1}{4}&1\end{pmatrix}\cdot\begin{pmatrix}4\\&\begin{pmatrix}1\\\frac{3}{4}&1\end{pmatrix}\cdot\begin{pmatrix}4\\&1\end{pmatrix}\cdot\begin{pmatrix}1\\\frac{3}{4}&1\end{pmatrix}^{T}\\\begin{pmatrix}\frac{1}{4}&1\\\frac{1}{2}&1\end{pmatrix}^{T}$$

 $A = \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{4} & & 1 \end{pmatrix} \cdot \begin{pmatrix} 4 & & \\ & 4 & 3 \\ & 3 & \frac{13}{2} \end{pmatrix} \cdot \begin{pmatrix} 1 & & \\ -\frac{1}{4} & 1 & \\ \frac{1}{2} & & 1 \end{pmatrix}'$ 

### Cholesky factorization is a special LU factorization

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

## Cholesky factorization is a special LU factorization

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"But Cholesky factorization should not have a  $D \cdots$ "

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- only L need to be computed, saving half of the work in factorization.
- ▶ total cost: about  $\frac{1}{3}n^3$  operations.

"But Cholesky factorization should not have a  $D \cdots$ "

$$D = \begin{pmatrix} d_1 & & \\ & \ddots & \\ & & d_n \end{pmatrix} = \left(D^{\frac{1}{2}}\right)^2, \quad \text{for } D^{\frac{1}{2}} \stackrel{\text{def}}{=} \begin{pmatrix} d_1^{\frac{1}{2}} & & \\ & \ddots & \\ & & d_n^{\frac{1}{2}} \end{pmatrix}$$

$$A = L\left(D^{\frac{1}{2}}\right)^{2}L^{T} = \left(LD^{\frac{1}{2}}\right)\left(LD^{\frac{1}{2}}\right)^{T} = \left(\square\right) \cdot \left(\square\right)^{T}$$

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

$$= \begin{pmatrix} \frac{2}{1} & 2 & \\ \frac{1}{2} & \frac{3}{2} & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{2}{1} & 2 & \\ \frac{1}{2} & \frac{3}{2} & 1 \end{pmatrix}^{T}$$

### Review: Natural Splines equations in matrix form

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

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

where

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

A is SDD, SPD, and tri-diagonal

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

$$A \ = \ \left( \begin{smallmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{smallmatrix} \right)$$

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

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

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A is SDD, SPD, and tri-diagonal

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

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

LU should GREATLY simplify since A has so many zero entries

#### **Tri-diagonal** LU factorization with $a_{ii} \neq 0$

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

#### **Tri-diagonal** LU factorization with $a_{ii} \neq 0$

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} & a_{23} \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & a_{n,n-1} & a_{n,n} \end{pmatrix} \left( \text{set } l_{21} = \frac{a_{21}}{a_{11}} \text{ and } a_{22} = a_{22} - l_{21} a_{12} \right)$$

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

#### **Tri-diagonal** LU factorization with $a_{jj} \neq 0$

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} & a_{23} \\ & \ddots & & \ddots & & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & a_{n,n-1} & a_{n,n} \end{pmatrix} \left( \text{set } l_{21} = \frac{a_{21}}{a_{11}} \text{ and } a_{22} = a_{22} - l_{21} a_{12} \right)$$

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

 $\triangleright$  elimination = computing  $l_{21}$  and  $\mathbf{a}_{22}$  (3 operations)

### **Tri-diagonal** LU factorization with $a_{ii} \neq 0$

Recursively on all trailing matrices,

Recursively on all training matrices,
$$\begin{pmatrix} 1 & & & \\ & & & \\ & & & \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & & \\ & & & \\ & & & \\ \end{pmatrix}$$

 $A = \begin{pmatrix} 1 & & & & & \\ l_{21} & 1 & & & & \\ & \ddots & \ddots & & & \\ & & l_{n-1,n-2} & 1 & & \\ & & & l_{n,n-1} & 1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & & & \\ & a_{22} & a_{23} & & & \\ & & \ddots & & \ddots & \\ & & & a_{n-1,n-1} & a_{n-1,n} \\ & & & & a_{n,n} \end{pmatrix} \qquad b \text{ for } j = 1, \dots, n-1$ 

grand total: 3n operations, if  $\mathbf{a}_{ii} \neq 0$  for all  $j \mid$ 

▶ Assume  $|a_{11}| \ge |a_{21}|$ . Let  $l_{21} = \frac{a_{21}}{a_{11}}$  and  $\overline{a}_{22} = a_{22} - l_{21} a_{12}$ , then

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

elimination only means computing  $\emph{I}_{21}$  and  $\overline{\mathbf{a}}_{22}$ 

▶ Assume  $|a_{11}| \ge |a_{21}|$ . Let  $l_{21} = \frac{a_{21}}{a_{11}}$  and  $\overline{a}_{22} = a_{22} - l_{21} a_{12}$ , then

• Assume  $|a_{11}| \ge |a_{21}|$ . Let  $l_{21} = \frac{a_{21}}{a_{11}}$  and  $\overline{a}_{22} = a_{22} - l_{21} a_{12}$ , then

$$A \quad = \quad \begin{pmatrix} \frac{1}{b_1} & 1 & & & \\ & \ddots & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & 1 & \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{\bar{a}_{12}} & \frac{a_{12}}{\bar{a}_{22}} & a_{23} & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & a_{n,n-1} & a_{n,n} \end{pmatrix}$$

elimination only means computing  $\emph{I}_{21}$  and  $\overline{\mathbf{a}}_{22}$ 

Trailing matrix 
$$\begin{pmatrix} \overline{a}_{22} & a_{23} & & & & \\ & \ddots & & \ddots & & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \end{pmatrix} \quad \textbf{tri-diagonal}$$

• Otherwise  $|a_{21}| > |a_{11}|$ . Let  $l_{21} = \frac{a_{11}}{a_{21}}$  and  $(\bar{a}_{22}, \bar{a}_{23}) = (a_{12} - l_{21} a_{22}, -l_{21} a_{23})$ 

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

elimination only means computing  $\emph{I}_{21},~\overline{a}_{22}$  and  $\overline{a}_{23}.$  Trailing matrix tri-diagonal

• Assume  $|a_{11}| \ge |a_{21}|$ . Let  $l_{21} = \frac{a_{21}}{a_{11}}$  and  $\overline{a}_{22} = a_{22} - l_{21} a_{12}$ , then

$$A \quad = \quad \begin{pmatrix} \frac{1}{b_1} & 1 & & & \\ & \ddots & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & 1 & \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{\bar{a}_{12}} & \frac{a_{12}}{\bar{a}_{22}} & a_{23} & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & a_{n,n-1} & a_{n,n} \end{pmatrix}$$

elimination only means computing  $\emph{I}_{21}$  and  $\overline{\textbf{a}}_{22}$ 

Trailing matrix 
$$\begin{pmatrix} \overline{a}_{22} & a_{23} & & & & \\ & \ddots & & \ddots & & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \end{pmatrix} \quad \textbf{tri-diagonal}$$

• Otherwise  $|a_{21}| > |a_{11}|$ . Let  $l_{21} = \frac{a_{11}}{a_{21}}$  and  $(\bar{a}_{22}, \bar{a}_{23}) = (a_{12} - l_{21} a_{22}, -l_{21} a_{23})$ 

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

elimination only means computing  $l_{21}$ ,  $\overline{a}_{22}$  and  $\overline{a}_{23}$ . Trailing matrix **tri-diagonal** 

## tri-diagonal LU factorization with partial pivoting (II)

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

## tri-diagonal LU factorization with partial pivoting (II)

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

$$\mathbf{P}_1 \cdot A = \begin{pmatrix} \frac{1}{l_{21}} & 1 & & \\ & & \ddots & & \\ & & & 1 & \\ & & & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{a_{11}}{l_{21}} & \frac{a_{12}}{l_{22}} & \frac{a_{13}}{a_{23}} & & \\ & \ddots & \ddots & & \ddots & \\ & & a_{n-1,n-2} & a_{n,n-1} & a_{n-1,n} \\ & & & & a_{n,n-1} & a_{n,n} \end{pmatrix}$$

cost: at most 4 operations per elimination step, with or without pivoting

$$\text{Recursively:} \quad \widehat{\textbf{P}} \cdot \begin{pmatrix} ^{a_{22}} & ^{a_{23}} & & \\ & \ddots & & \\ & ^{a_{n-1,n-2}} & ^{a_{n-1,n-1}} & ^{a_{n-1,n}} \\ & & ^{a_{n-1,n-2}} & ^{a_{n-1,n-1}} & ^{a_{n-1,n}} \end{pmatrix} = \widehat{\textbf{L}} \cdot \widehat{\textbf{U}}$$

- ▶ Û: upper triangular with bandwidth at most 3.
- L: unit lower triangular with one non-zero in each column below diagonal.

## tri-diagonal LU factorization with partial pivoting (III)

$$\text{Together: } \mathbf{P}_1 \cdot A = \begin{pmatrix} \frac{1}{l_{21}} & & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{\mathbf{a}_{11}}{l_{21}} & & & & \\ & \frac{\mathbf{a}_{22}}{l_{23}} & & & & \\ & \ddots & \ddots & & \\ & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & a_{n,n-1} & a_{n,n} \end{pmatrix} \end{pmatrix}$$

$$\underbrace{\left(\left(\begin{array}{ccc|c} 1 & \\ & \widehat{\mathbf{P}} \end{array}\right) \cdot \mathbf{P}_{1}\right)}_{P} \cdot A = \left(\frac{1}{|\mathbf{I}_{1}|} \right) \cdot \left(\frac{\mathbf{a}_{11} \mid (\mathbf{a}_{12} \mid \mathbf{a}_{13} \mid)}{|\widehat{\mathbf{L}} \cdot \widehat{\mathbf{U}}|}\right), \quad \left(\mathbf{I}_{1} = \widehat{\mathbf{P}} \left(\begin{array}{ccc|c} I_{21} \\ \hline \end{array}\right)\right)$$

$$= \left(\frac{1}{|\mathbf{I}_{1}|} \right) \cdot \left(\frac{\mathbf{a}_{11} \mid (\mathbf{a}_{12} \mid \mathbf{a}_{13} \mid)}{|\widehat{\mathbf{U}}|}\right) \stackrel{def}{=} L \cdot U$$

total cost: at most 4 n operations and n comparisons

### And that is it.



- ► Covers every section in Chapters 1-6, excluding
  - ► FALSE POSITION METHOD IN SECTION 2.3,
  - ► SECTION 5.8,
  - ► SCALED PARTIAL OR COMPLETE PIVOTING IN SECTION 6.2.

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- ► OH: MW 1:30-3:00PM in 861 Evans or by appointment.

Let 
$$f(x) = x^2 - a$$
 for  $a > 0$ 

Apply Secant method to solve the equation f(x) = 0 with initial guesses  $x_0 > x_1 > \sqrt{a}$ :

$$x_{k+1} = x_k - \frac{f(x_k) (x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}, \text{ for } k = 1, 2, \cdots.$$

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$$x_{k+1} = x_k - \frac{f(x_k) \ \left(x_k - x_{k-1}\right)}{f(x_k) - f(x_{k-1})}, \quad \textit{for} \quad k = 1, 2, \cdots. \quad \textit{Show that the iteration always converges}$$

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SOLUTION: Since  $x_0 > x_1 > \sqrt{a} > 0$ , the denominator for k = 1

$$f(x_k) - f(x_{k-1}) = x_k^2 - x_{k-1}^2 = (x_k - x_{k-1})(x_k + x_{k-1}) \neq 0$$

thus  $x_2$  is defined. In general, for  $k \ge 1$ ,

$$x_{k+1} = x_k - \frac{\left(x_k^2 - a\right)\left(x_k - x_{k-1}\right)}{\left(x_k - x_{k-1}\right)\left(x_k + x_{k-1}\right)} = x_k - \frac{\left(x_k^2 - a\right)}{x_k + x_{k-1}} = \frac{x_k x_{k-1} + a}{x_k + x_{k-1}}$$

It follows that 
$$x_{k+1} - \sqrt{a} = \frac{x_k x_{k-1} + a - \sqrt{a} \left( x_k + x_{k-1} \right)}{x_k + x_{k-1}} = \frac{\left( x_k - \sqrt{a} \right) \left( x_{k-1} - \sqrt{a} \right)}{x_k + x_{k-1}} > 0$$
 (1)

To show Secant iteration is defined, we must show  $x_{k+1} \neq x_k$  for all k. However, if  $x_{k+1} = x_k$  for some k, then

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From (1),  $x_k > \sqrt{a}$  for all k, and therefore (1) implies for all k,  $0 < x_{k+1} - \sqrt{a} < x_k - \sqrt{a}$ 

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SOLUTION: Since  $x_0 > x_1 > \sqrt{a} > 0$ , the denominator for k = 1

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It follows that 
$$x_{k+1} - \sqrt{s} = \frac{x_k x_{k-1} + s - \sqrt{s} \left( x_k + x_{k-1} \right)}{x_k + x_{k-1}} = \frac{\left( x_k - \sqrt{s} \right) \left( x_{k-1} - \sqrt{s} \right)}{x_k + x_{k-1}} > 0$$
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To show Secant iteration is defined, we must show  $x_{k+1} \neq x_k$  for all k. However, if  $x_{k+1} = x_k$  for some k, then

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From (1),  $x_k > \sqrt{a}$  for all k, and therefore (1) implies for all k,  $0 < x_{k+1} - \sqrt{a} < x_k - \sqrt{a}$ 

Therefore the sequence  $\{x_k\}_{k=0}^{\infty}$  monotonically decreases with a lower bound. It must converge.

Let polynomial

$$P_n(x) \quad \stackrel{def}{=} \quad a_0 + a_1(x-x_0) + a_2(x-x_0)^2 + \cdots + a_{n+1}(x-x_0)^2 \left(x-x_1\right) \cdots \left(x-x_{n-1}\right) \quad (1)$$

interpolate function f(x) at distinct points  $x_0, x_1, \dots, x_n$  such that

$$P_n(x_j)=f(x_j), \quad j=0,1,\cdots,n \quad \text{and that } P_n'(x_0)=f'(x_0). \qquad \text{Show that} \quad a_2=f[x_0,x_0,x_1].$$

Let polynomial

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Solution: Let  $x = x_0$  in equation (1) to reach  $a_0 = P_n(x_0) = f(x_0)$ . Additionally,

$$\frac{P_n(x) - f(x_0)}{x - x_0} = a_1 + a_2(x - x_0) + \dots + a_{n+1}(x - x_0)(x - x_1) \cdots (x - x_{n-1})$$

Let  $x \longrightarrow x_0$  gives  $a_1 = P'_n(x_0) = f'(x_0)$ . Now let  $x = x_1$ , we get

$$f[x_0, x_1] = f[x_0, x_0] + a_2(x_1 - x_0)$$

which implies

$$a_2 = f[x_0, x_0, x_1].$$

Let  $0 < \alpha_1 < \alpha_2 < 1$ , and let N(h) be an approximation to a value M for every h > 0 such that

$$M = N(h) + k_1 h + k_2 h^2 + k_3 h^3 + \cdots$$

Find  $\mu_1$  and  $\mu_2$  such that the expression  $\frac{N(h)+\mu_1}{1+\mu_1+\mu_2}\frac{N(\alpha_2 h)}{N(\alpha_2 h)}$  is an  $O(h^3)$  approximation to M.

Let  $0<\alpha_1<\alpha_2<1$ , and let N(h) be an approximation to a value M for every h>0 such that

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SOLUTION: We write

$$M = N(h) + k_1 h + k_2 h^2 + k_3 h^3 + \cdots$$

$$M = N(\alpha_1 h) + k_1 (\alpha_1 h) + k_2 (\alpha_1 h)^2 + k_3 (\alpha_1 h)^3 + \cdots$$

$$M = N(\alpha_2 h) + k_1 (\alpha_2 h) + k_2 (\alpha_2 h)^2 + k_3 (\alpha_2 h)^3 + \cdots$$

It follows that 
$$M = \frac{N(h) + \mu_1 \, N(\alpha_1 \, h) + \mu_2 \, N(\alpha_2 \, h)}{1 + \mu_1 + \mu_2} + \frac{1 + \mu_1 \, \alpha_1 + \mu_2 \, \alpha_2}{1 + \mu_1 + \mu_2} \, k_1 h + \frac{1 + \mu_1 \, \alpha_1^2 + \mu_2 \, \alpha_2^2}{1 + \mu_1 + \mu_2} \, k_2 h^2 + O(h^3)$$

Thus, we must choose  $\mu_1$  and  $\mu_2$  such that

$$1+\mu_1~\alpha_1+\mu_2~\alpha_2=0, \qquad 1+\mu_1~\alpha_1^2+\mu_2~\alpha_2^2=0$$
 which leads to  $\left(\begin{array}{c} \mu_1\\ \mu_2 \end{array}\right)=-\left(\begin{array}{cc} \alpha_1&\alpha_2\\ \alpha_1^2&\alpha_2^2 \end{array}\right)^{-1}\left(\begin{array}{cc} 1\\ 1 \end{array}\right)$ 

Consider an initial value ODE

$$y' = f(t, y), \quad y(t_0) = Y_0, \quad (1)$$

and a method for solving (1)

$$w_{j+1} = w_j + h\left(\alpha f(t_{j+1}, w_{j+1}) + \beta f(t_j, w_j) + \gamma f(t_{j-1}, w_{j-1})\right), \quad (2)$$

for  $j = 0, 1, 2, \cdots$ .

Find relations on coefficients  $\alpha$ ,  $\beta$ ,  $\gamma$  so that (2) is a second-order method for solving (1).

Consider an initial value ODE

$$y' = f(t, y), \quad y(t_0) = Y_0, \quad (1)$$

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for  $i = 0, 1, 2, \cdots$ .

Find relations on coefficients  $\alpha$ ,  $\beta$ ,  $\gamma$  so that (2) is a second-order method for solving (1).

Solution: By definition, 
$$y'(t_j) = f(t_j, y(t_j)), \ y''(t_j) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} \ f$$

LTE 
$$= \frac{y(t_{j+1}) - y(t_j)}{h} - \left(\alpha f(t_{j+1}, y(t_{j+1})) + \beta f(t_j, y(t_j)) + \gamma f(t_{j-1}, y(t_{j-1}))\right)$$
$$= y'(t_j) + \frac{h}{2}y''(t_j) - (\alpha + \beta + \gamma) f(t_j, y(t_j)) - \left(\alpha h \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} f\right) - \gamma h \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} f\right)\right) + O(h^2)$$

Thus the relations are

$$\alpha + \beta + \gamma = 1,$$
  $\alpha - \gamma = \frac{1}{2}$ 

Let  $h_i > 0$  for  $j = 0, 1, \dots, n$ , and let

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

Show that A is symmetric positive definite.

Let  $h_i > 0$  for  $j = 0, 1, \dots, n$ , and let

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Show that A is symmetric positive definite.

SOLUTION: *A* is symmetric. Let  $\mathbf{x} = \begin{pmatrix} \mathbf{x} \\ \vdots \\ \mathbf{x}_n \end{pmatrix}$  non-zero. Then

$$\begin{split} \mathbf{x}^T \, A \mathbf{x} &= 2 \left( \sum_{j=1}^n x_j^2 (h_j + h_{j-1}) \right) + 2 \left( \sum_{j=2}^n x_j x_{j-1} h_{j-1} \right) \\ &= 2 \left( \sum_{j=1}^n x_j^2 (h_j + h_{j-1}) \right) + \left( \sum_{j=2}^n \left( (x_j + x_{j-1})^2 - x_j^2 - x_{j-1}^2 \right) h_{j-1} \right) \\ &= \left( \sum_{j=1}^n x_j^2 (h_j + h_{j-1}) \right) + x_n^2 \, h_n + x_1^2 \, h_0 + \left( \sum_{j=2}^n \left( x_j + x_{j-1} \right)^2 h_{j-1} \right) \\ &> 0 \end{split}$$