

- x Friday - no lecture.
- x Hw 1 (Spectral)



# CS450: Numerical Analysis

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18/10/2023

# Linear Least Square

$$a \cdot x = b \in \mathbb{R}$$

$$a \neq 0 \rightarrow x = \frac{b}{a}$$



- Suppose we want to solve a linear system  $\underbrace{Ax = b}$ , with  $A$  and  $b$  being known, what does this mean?
  - What does  $Ax$  mean?
  - What does  $Ax = b$  mean?
- What happens if  $A$  is not a square matrix?
- Instead of solving  $Ax = b$ , we aim to find  $x$  to minimize  $\|Ax - b\|_2$ 
  - Generally, a perfect fitting may not be possible, and we look for an approximation
  - In data science, this is called Linear Regression

$$[ \vec{a}_1 \vec{a}_2 \dots \vec{a}_n ] \cdot x = b$$

Combination of  $a_1 \dots a_n \rightarrow b$

# Solving the Linear Least Square

- How to find  $\mathbf{x}^* = \operatorname{argmin}_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{b}\|_2$  where  $\mathbf{A} \in R^{m \times n}$ ?
  - The residual error can be written as

$$Err(\mathbf{x}) = (\mathbf{Ax} - \mathbf{b})^T (\mathbf{Ax} - \mathbf{b})$$

- Let  $\frac{\partial Err(\mathbf{x})}{\partial \mathbf{x}} = 2\mathbf{A}^T(\mathbf{Ax} - \mathbf{b}) = \mathbf{0}$ , which is equivalent to  $(\mathbf{A}^T\mathbf{A})\mathbf{x} = \mathbf{A}^T\mathbf{b}$
- If  $\mathbf{A}^T\mathbf{A}$  is nonsingular, we obtain the solution as

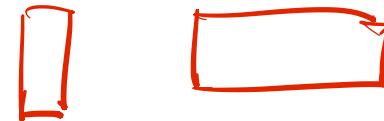
$$\underbrace{\mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}}$$

- This is known as the **normal equation**

*assess the error  
condition #*

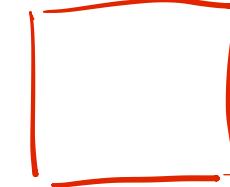


# Recall: Matrix Condition Number



- Given a square matrix  $A$ , the condition number is

$$\kappa(A) = \|A\| \cdot \|A^{-1}\|$$



$$\underbrace{A^T A = A A^{-1} = I}$$

- The usefulness of the condition number is in **assessing the accuracy of solutions to linear systems**
- In other words, it **measures the danger of unacceptable round off error in solving linear systems** (i.e.  $Ax = b$ )
- How can we define condition number for rectangular matrices?

# Conditioning of Rectangular Matrix

$$\underline{A^{-1}A = AA^{-1} = I}$$

$$I \leftarrow \underline{(A^{-1})} A x = A^{-1} b$$

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

- Given an overdetermined system  $\underline{Ax = b}$  where  $A \in R^{m \times n}, m > n$  and

$$\boxed{\text{rank}(A) = n,}$$

$$\checkmark \quad \downarrow x$$

$$\hookrightarrow \underline{(A^T A)x = A^T b}$$

$$\square \tilde{I} = I$$

$$x = \underline{(A^T A)^{-1} A^T b}$$

$$\boxed{A} \rightarrow \|A\|_2 ?$$

- recall that  $\kappa(A) = \underline{\|A\|_2 \cdot \|A^{-1}\|_2}$
- we can calculate  $\|A\|_2$ , but  $A$  is not invertable, therefore, ...
- we define a pseudoinverse of  $A$  by  $\underline{A^+ = (A^T A)^{-1} A^T}$ , note that  $\underline{A^+ A = I}$

$G_1, G_2 \neq 0$

$$\|A\|_2 = \max_{\|x\|_2=1} \|Ax\|_2$$

$$= \max \{G_1, G_2\} \rightarrow G_{\max}$$

$$A^+ = \underline{(A^T A)^{-1} A^T} \rightarrow 2 \times 3$$

$$A = \begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \\ a_3 & b_3 \end{bmatrix} \xrightarrow[\text{SVD}]{3 \times 2} \begin{bmatrix} U \end{bmatrix} \begin{bmatrix} G_1 & 0 \\ 0 & G_2 \\ 0 & 0 \end{bmatrix} \xrightarrow[2 \times 2]{V^T} \square V^T$$

$$A^+ = \underline{(A^T A)^{-1} A^T}$$

$$A^+ A = \underline{(A^T A)^{-1} A^T A} = I$$

$$\underline{AA^+ = ? I}$$

# Conditioning of Rectangular Matrix

- What does  $A^+$  imply?
- For linear system  $\underbrace{Ax = b}$ , a solution given by  $\boxed{x^+ = A^+b}$  is the **minimum norm** least square solution
- Example: The shortest least squares solution to the following

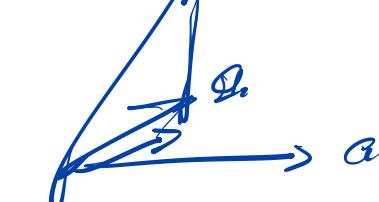
$$\begin{cases} 3 \cdot x_1 + 0 \cdot x_2 = 6 \\ 0 \cdot x_1 + 0 \cdot x_2 = 8 \end{cases}$$

$\rightarrow$

$$\underbrace{\begin{bmatrix} 3 & 0 \\ 0 & 0 \end{bmatrix}}_A \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 8 \end{bmatrix}$$

$\text{col}([2], [0])$

$b = [8]$



is given by

$\|x^+\| \leq \|x\|$

$$\underline{x^+ = A^+b = \begin{bmatrix} 1/3 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 6 \\ 8 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}}$$

$\rightarrow [6] \leftarrow [2]$

$\downarrow A^+$

$A^+A = I$   $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$

$A^+ = \underline{(A^T A)^{-1} A^T}$

# Conditioning of Rectangular Matrix (cont'd)



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$$\boxed{\square} \rightarrow \kappa(A) = \frac{\sigma_{\max}}{\sigma_{\min}}$$

$A \in \mathbb{R}^{m \times n}$

$\text{rank}(A) = n$



- The condition number of a rectangular matrix  $A$  is defined as

$$\kappa(A) = \|A\|_2 \cdot \|A^+\|_2$$

$$\Delta L \xrightarrow{?} G_{\max}$$

$$A = \begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \\ a_3 & b_3 \end{bmatrix}$$

$3 \times 2$ ,  
 $\text{rank}(A) = 2$

- What if  $\text{rank}(A) < n$ ?  $\kappa(A) = \infty$

- We also define  $\kappa(A) = \sigma_{\max}/\sigma_{\min}$ , is it still true here?

SVD:  $A = U \begin{bmatrix} G_1 & 0 \\ 0 & G_2 \\ 0 & 0 \end{bmatrix} V^T$        $U \in \mathbb{R}^{3 \times 3}$        $V \in \mathbb{R}^{2 \times 2}$

$$A^T A = V \begin{bmatrix} G_1^2 & 0 \\ 0 & G_2^2 \end{bmatrix} V^T \downarrow$$

$$(A^T A)^{-1} = V^T \begin{bmatrix} \frac{1}{G_1^2} & 0 \\ 0 & \frac{1}{G_2^2} \end{bmatrix} V$$

$$(A^T A)^{-1} A^T = V^T \begin{bmatrix} \frac{1}{G_1} & 0 \\ 0 & \frac{1}{G_2} \end{bmatrix} U \Rightarrow \|(A^T A)^{-1} A^T\|_2 = \max \left\{ \frac{1}{G_1}, \frac{1}{G_2} \right\}$$

$$\Rightarrow \kappa(A) = \frac{\sigma_{\max}}{\sigma_{\min}}$$

$$= \frac{1}{G_{\min}}$$

# Example (1)

- Calculate the condition number of the following rectangular matrix  $A \in \mathbb{R}^{6 \times 3}$

$$Ax = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \cong \begin{bmatrix} 1237 \\ 1941 \\ 2417 \\ 711 \\ 1177 \\ 475 \end{bmatrix} = b$$

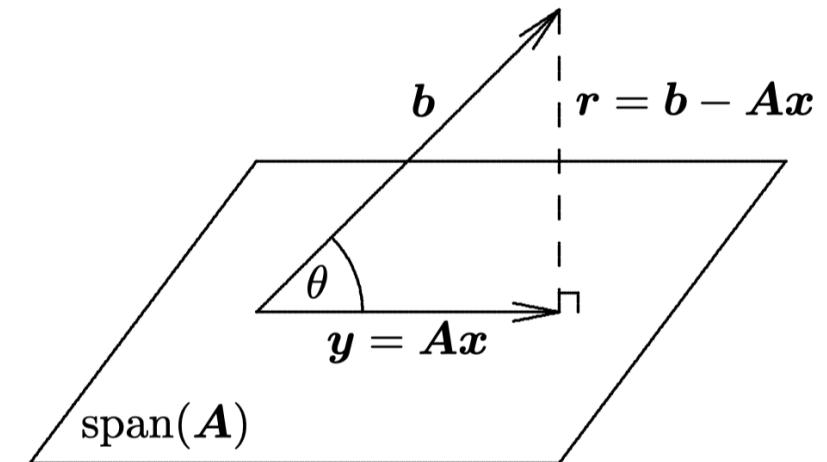
→  $\underbrace{A^+ = (A^T A)^{-1} A^T}_{\text{ }} = \frac{1}{4} \begin{bmatrix} 2 & 1 & 1 & -1 & -1 & 0 \\ 1 & 2 & 1 & 1 & 0 & -1 \\ 1 & 1 & 2 & 0 & 1 & 1 \end{bmatrix}$

- Consequently,  $\|A\|_2 = 2$  and  $\|A^+\|_2 = 1$ , which gives  $\kappa(A) = \|A\|_2 \cdot \|A^+\|_2 = 2$

# Conditioning of Linear Least Square

$$\boxed{Ax = b} \rightarrow A(x + \Delta x) = b + \Delta b$$

- Back to the problem of finding  $x^* = \operatorname{argmin}_x \|Ax - b\|_2$  where  $A \in R^{m \times n}$
- Unlike the conditioning of a linear system  $\underline{Ax = b}$ , which only depends on the condition of the  $A$ ; the conditioning/sensitivity of the solution to an LSQ depends on both  $A$  and  $b$ 
  - It is more stable when  $b$  lies near  $\operatorname{span}(A)$
  - It is sensitive if  $b$  lies near orthogonal to  $\operatorname{span}(A)$



# Conditioning of LSQ (cont'd)



$$a = b \cdot \cos \theta$$

$$\frac{\| \Delta x \|_2}{\| x \|_2} \leq \square \frac{\| \Delta b \|_2}{\| b \|_2} ?$$

$$\begin{aligned} x &= \arg \min \frac{\| Ax - b \|_2}{\text{rank } A = n} \\ Ax &= b \end{aligned}$$

- Recall that solution of the normal equation  $A^T A x = A^T b$  solves the LSQ
- For a perturbation on the RHS, it gives  $A^T A(\underline{x} + \Delta x) = A^T(\underline{b} + \Delta b)$ , i.e.,

$A^T A \Delta x = A^T \Delta b$ . As such,  $\Delta x = (A^T A)^{-1} A^T \Delta b = A^+ \Delta b$ , and this leads to:

$$\left\{ \begin{array}{l} (A^T A)x = A^T b \\ (A^T A)(x + \Delta x) = A^T(b + \Delta b) \end{array} \right.$$

$\downarrow$

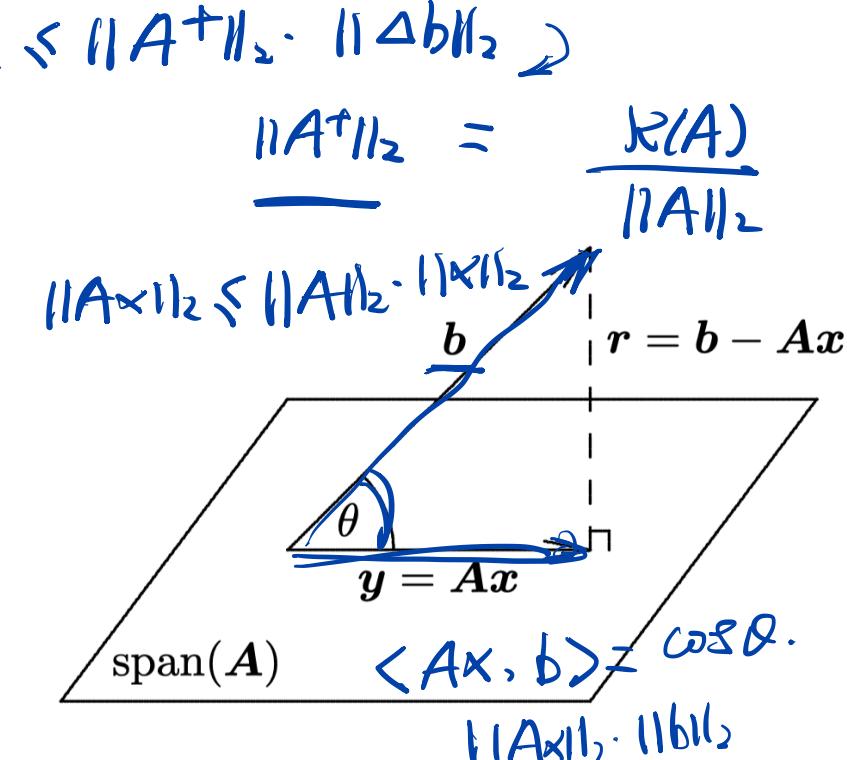
$$(A^T A) \cdot \Delta x = A^T \Delta b$$

$$\begin{aligned} \Delta x &= (A^T A)^{-1} A^T \Delta b \\ &= A^+ \Delta b \end{aligned}$$

What determines  $\theta$ ?

What values of  $\theta$  are bad?

$$\begin{aligned} \frac{\| \Delta x \|_2}{\| x \|_2} &\leq \| A^+ \|_2 \frac{\| \Delta b \|_2}{\| x \|_2} \quad (\| \Delta x \|_2 \leq \| A^+ \|_2 \cdot \| \Delta b \|_2) \\ &= \underbrace{\text{cond}(A)}_{\frac{\| A \|_2}{\| A^+ \|_2}} \frac{\| b \|_2}{\| A \|_2 \cdot \| x \|_2} \frac{\| \Delta b \|_2}{\| b \|_2} \\ &\leq \underbrace{\text{cond}(A)}_{\frac{1}{\cos(\theta)}} \frac{\| b \|_2}{\| A x \|_2} \frac{\| \Delta b \|_2}{\| b \|_2} \end{aligned}$$



# Solving Linear Systems



- For a square matrix  $A$ , how to (systematically) solve for  $Ax = b$ ?
    - Transform it into one whose solution is the same but easier to compute
  - Example: solve for  $x_1, x_2, x_3, x_4$  for the following

$$\begin{array}{l} E_2 - 2 \times E_1 \\ \downarrow \\ E_3 - 3 \times E_1 \\ \rightarrow \\ E_9 + E_1 \rightarrow \end{array}$$

$$\begin{aligned}
 E_1 : \quad & \cancel{x_1} + x_2 + 3x_4 = 4, \\
 \underline{E_2} : \quad & \cancel{2x_1} + -x_2 - x_3 \cancel{+ 5x_4} = -1, \\
 E_3 : \quad & 3x_1 - x_2 - x_3 + 2x_4 = -3, \\
 E_4 : \quad & -x_1 + 2x_2 + 3x_3 - x_4 = 4,
 \end{aligned}$$

$$\begin{array}{l}
 \text{nxn} \\
 \downarrow \\
 A\mathbf{x} = \mathbf{b} \quad \downarrow \\
 \left[ \begin{array}{cccc|c}
 a_{11} & a_{12} & \cdots & a_{1n} & \\
 0 & & & & \\
 0 & & & & \\
 \vdots & & & & \\
 0 & & & & \\
 \end{array} \right] \quad \mathbf{x} \neq \mathbf{0} \Rightarrow \mathbf{b}' \\
 \xrightarrow{\quad \leftarrow \quad} \quad A_{n-1} \cdot x_{n-1} = b_{n-1} \\
 n-1 < n-1
 \end{array}$$

# Solving Linear Systems (cont'd)

$$Ax = b \Rightarrow MAx = Mb$$

- Example: solve for  $x_1, x_2, x_3, x_4$  for the following

$$\left[ \begin{array}{cccc} 1 & 0 & 0 & 1 \\ -2 & 1 & 0 & 0 \\ -3 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{array} \right] = M$$

$$E_1 : x_1 + x_2 + 3x_4 = 4,$$

$$E_2 : 2x_1 + x_2 - x_3 + x_4 = 1,$$

$$E_3 : 3x_1 - x_2 - x_3 + 2x_4 = -3,$$

$$E_4 : -x_1 + 2x_2 + 3x_3 - x_4 = 4,$$

$$x = (MA)^{-1}Mb$$

$$= A^{-1}M^{-1}Mb$$

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

- Step #1: use  $E_1$  to eliminate the unknown  $x_1$  from  $E_2, E_3$ , and  $E_4$



$$E_1 : x_1 + x_2 + 3x_4 = 4,$$

$$E_2 : -x_2 - x_3 - 5x_4 = -7,$$

$$E_3 : -4x_2 - x_3 - 7x_4 = -15,$$

$$E_4 : 3x_2 + 3x_3 + 2x_4 = 8.$$

- Q: why the solutions remained the same after this process?

# Solving Linear Systems

- Given a square matrix  $A$ , if we want to solve for  $Ax = b$ , then premultiply both sides with any non-singular matrix  $M$  would not affect the solution
- Why?: solution to  $MAx = Mb$  is given by

$$x = (MA)^{-1}Mb = A^{-1}M^{-1}Mb = A^{-1}b$$

# Solving Linear Systems (cont'd)

- Step #1: use  $E_1$  to eliminate the unknown  $x_1$  from  $E_2, E_3$ , and  $E_4$

$$\begin{aligned}
 E_1 : & \quad x_1 + x_2 + 3x_4 = 4, \\
 E_2 : & \quad -x_2 - x_3 - 5x_4 = -7, \\
 E_3 : & \quad -4x_2 - x_3 - 7x_4 = -15, \\
 E_4 : & \quad 3x_2 + 3x_3 + 2x_4 = 8.
 \end{aligned}$$

- Continue the process, and finally reduce to the following

$$\begin{aligned}
 E_1 : & \quad x_1 + x_2 + 3x_4 = 4, \\
 E_2 : & \quad -x_2 - x_3 - 5x_4 = -7, \\
 E_3 : & \quad 3x_3 + 13x_4 = 13, \\
 E_4 : & \quad -13x_4 = -13. \quad \rightarrow \quad x_4 = \frac{-13}{-13} = 1
 \end{aligned}$$

- The matrix is in triangular form, can be solved via backward-substitution

# Triangular Linear Systems

- What type of linear system is easy to solve?
  - If one equation in the system involves only one component of solution, then that component can be computed by division
  - If another equation in system involves only one additional solution component, then by substituting one known component into it, we can solve for other component
  - If this pattern continues, all components of solution can be computed in succession
  - System with this property is called **triangular**

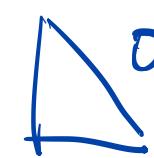
$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = a_{1,n+1}$$

$$a_{22}x_2 + \cdots + a_{2n}x_n = a_{2,n+1}$$

$$\vdots \quad \vdots$$

$$a_{nn}x_n = a_{n,n+1}$$

# Triangular Matrices



$$Ax = b \Rightarrow Lx = b'$$

$$Ux = \bar{b}$$

- Two specific triangular forms are of particular interest
  - Lower triangular: all entries above main diagonal are zero,  $a_{ij} = 0$  for  $i < j$
  - Upper triangular: all entries below main diagonal are zero,  $a_{ij} = 0$  for  $i > j$
- Successive substitution process described earlier is especially easy to formulate for lower or upper triangular systems
- Any triangular matrix can be permuted into upper or lower triangular form by suitable row permutation

# Solving Linear Systems (cont'd)

- Example: Solve the following triangular system

$$\begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

- Using back-substitution for this upper triangular system, last equation,  $4x_3 = 8$  , is solved directly to obtain  $x_3 = 2$
- Next,  $x_3$  is substituted into second equation to obtain  $x_2 = 2$
- Finally, both  $x_3$  and  $x_2$  are substituted into first equation to obtain  $x_1 = -1$

# Elimination

- To transform general linear system into triangular form, we need to replace selected nonzero entries of matrix by zeros
- This can be accomplished by taking linear combinations of rows
- Consider a two-dimensional vector  $\mathbf{a} = [a_1 \ a_2]$
- If  $a_1 \neq 0$ , then

$$\begin{bmatrix} 1 & 0 \\ -a_2/a_1 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} a_1 \\ 0 \end{bmatrix}$$

# Elementary Elimination Matrices

- More generally, we can annihilate all entries below  $k$ -th in a  $n$ -dimensional vector  $\mathbf{a}$  by transformation

$$\mathbf{M}_k \mathbf{a} = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -m_{k+1} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -m_n & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ a_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where  $m_i = \frac{a_i}{a_k}$ ,  $i = k + 1, \dots, n$

- Divisor  $a_k$ , called pivot, must be nonzero

# Elementary Elimination Matrices (cont'd)

Example: For a vector  $\mathbf{a} = [2, 4, -2]^T$ , the elementary elimination matrices  $\mathbf{M}_1$  and  $\mathbf{M}_2$  are (recall:  $m_i = \frac{a_i}{a_k}$ ,  $i = k + 1, \dots, n$ )

$$\mathbf{M}_1 \mathbf{a} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$$

$$\mathbf{M}_2 \mathbf{a} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 0 \end{bmatrix}$$

# Elementary Elimination Matrices (cont'd)



- Matrix  $\mathbf{M}_k$ , called elementary elimination matrix, adds multiple of row  $k$  to each subsequent row, with multipliers  $m_i$  chosen so that result is zero
- $\mathbf{M}_k$  is unit lower triangular and nonsingular
- $\mathbf{M}_k = \mathbf{I} - \mathbf{m}_k \mathbf{e}_k^T$ , where  $\mathbf{m}_k = [0, \dots, 0, m_{k+1}, \dots, m_n]^T$  and  $\mathbf{e}_k$  is the  $k$ -th column of identity matrix
- $\mathbf{M}_k^{-1} = \mathbf{I} + \mathbf{m}_k \mathbf{e}_k^T$ , which means  $\mathbf{M}_k^{-1} = \mathbf{L}_k$  is the same as  $\mathbf{M}_k$  except signs of multipliers are reversed

# Elementary Elimination Matrices (cont'd)

- If  $\mathbf{M}_j$ ,  $j > k$ , is another elementary elimination matrix, with vectors of multipliers  $\mathbf{m}_j$ , then

$$\begin{aligned}\mathbf{M}_k \mathbf{M}_j &= (\mathbf{I} - \mathbf{m}_k \mathbf{e}_k^T)(\mathbf{I} - \mathbf{m}_j \mathbf{e}_j^T) \\ &= \mathbf{I} - \mathbf{m}_k \mathbf{e}_k^T - \mathbf{m}_j \mathbf{e}_j^T + \mathbf{m}_k \mathbf{e}_k^T \mathbf{m}_j \mathbf{e}_j^T \\ &= \mathbf{I} - \mathbf{m}_k \mathbf{e}_k^T - \mathbf{m}_j \mathbf{e}_j^T\end{aligned}$$

where means product is essentially “union”, and similarly for product of inverses,  $\mathbf{L}_k \mathbf{L}_j$