

Least Square Solution

given $AX=b$ $\rightarrow$ 3 possibilities

- (1) unique solution
- (2) infinitely many solns
- (3) no solution
(inconsistent)

When does $AX=b$ have a solution?
(i.e. the system is consistent)

$$AX = b$$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

$\underbrace{a_{m1}}_{u_1} \quad \underbrace{a_{m2}}_{u_2} \quad \cdots \quad \underbrace{a_{mn}}_{u_n}$

Columns of A $\rightarrow$

$$\begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b \end{bmatrix}$$

$$\Leftrightarrow \vec{x_1} \vec{u_1} + \vec{x_2} \vec{u_2} + \cdots + \vec{x_n} \vec{u_n} = \vec{b}$$

Solving $AX=b \iff$ Write / express b as
a linear combination
of the columns of A

$AX=b$ is solvable

$\iff b$ can be written as a lin comb. of
the columns of A .

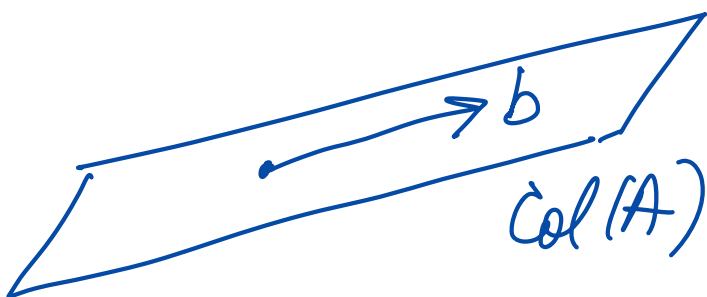
$\iff b \in \text{Span}\{\text{columns of } A\}$

$= \{ \text{all lin comb. of cols of } A \}$

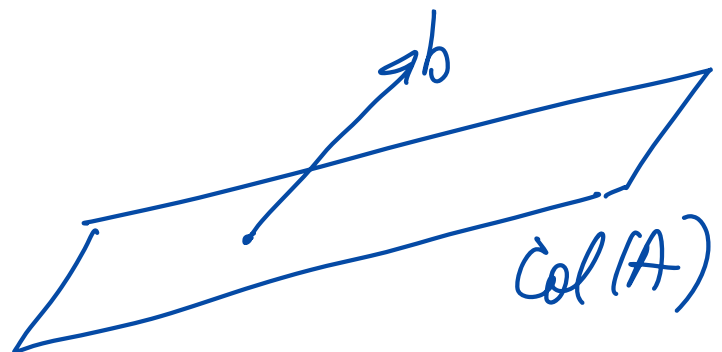
$= \{ c_1 u_1 + \dots + c_n u_n ; c_i \in \mathbb{R} \}$

$= \text{Col}(A)$

AX is solvable $\iff b \in \text{Col}(A)$



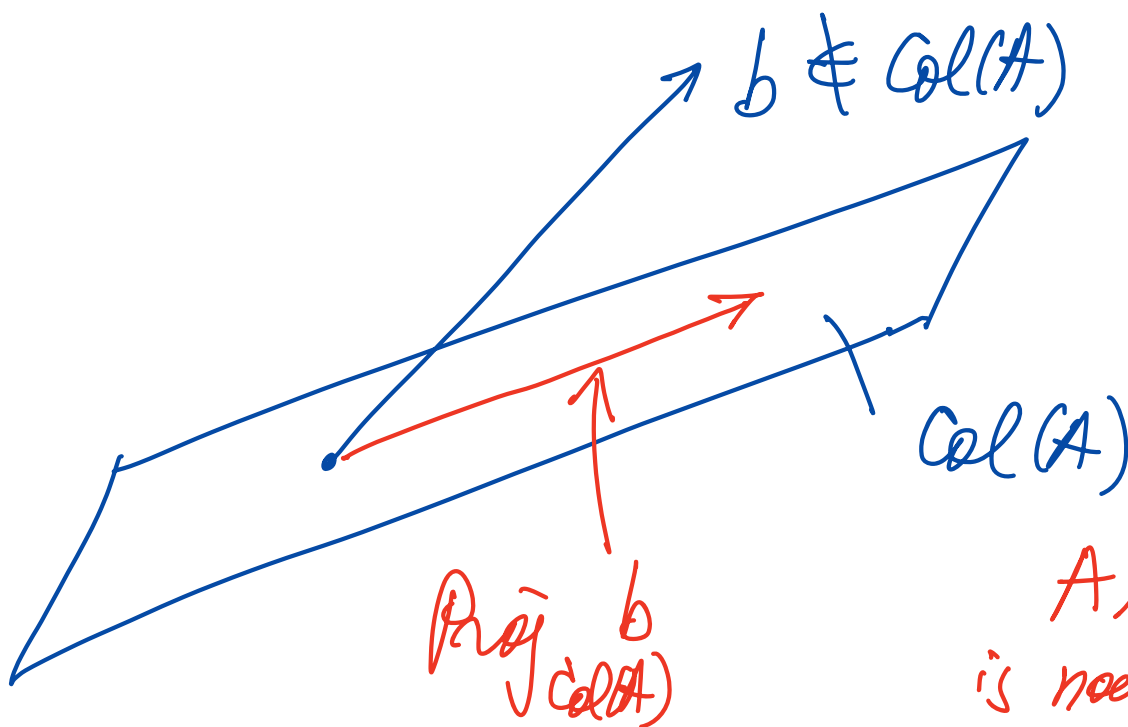
$AX=b$ is solvable



$AX=b$ is not solvable

Suppose $b \notin \text{Col}(A) \Rightarrow AX=b$ is thus not solvable

What is the best way to modify b s.t.
 $AX=b$ is solvable?



$AX=b$
is not solvable

$AX = \text{Proj}_{\text{Col}(A)} b$
is now solvable

$$A\tilde{x} = \text{Proj}_{\text{Col}(A)} b$$

least square solution

e for error

⊥ to all u_i 's

$$b = \underbrace{\text{Proj}_{\text{Col}(A)} b}_{\in \text{Col}(A)} + \underbrace{e}_{\perp \text{Col}(A)}$$

i.e., $\langle e, u_i \rangle = 0$
 $i=1, 2, \dots, n$

$$b = c_1 u_1 + c_2 u_2 + \dots + c_n u_n + e$$

? ? ?

$$\langle b, u_1 \rangle = c_1 \langle u_1, u_1 \rangle + c_2 \langle u_2, u_1 \rangle + \dots + c_n \langle u_n, u_1 \rangle$$

$$\langle b, u_2 \rangle = c_1 \langle u_1, u_2 \rangle + c_2 \langle u_2, u_2 \rangle + \dots + c_n \langle u_n, u_2 \rangle$$

$$\vdots$$

$$\langle b, u_n \rangle = c_1 \langle u_1, u_n \rangle + c_2 \langle u_2, u_n \rangle + \dots + c_n \langle u_n, u_n \rangle$$

(*)

least square solution $\tilde{x}$

$$\begin{bmatrix} \langle b, u_1 \rangle \\ \langle b, u_2 \rangle \\ \vdots \\ \langle b, u_n \rangle \end{bmatrix} = \begin{bmatrix} \langle u_1, u_1 \rangle & \langle u_2, u_1 \rangle & \dots & \langle u_n, u_1 \rangle \\ \langle u_1, u_2 \rangle & \langle u_2, u_2 \rangle & \dots & \langle u_n, u_2 \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle u_1, u_n \rangle & \langle u_2, u_n \rangle & \dots & \langle u_n, u_n \rangle \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}$$

Note: $(*)$ is always solvable!

The solution is called least square solution.

$$\tilde{x} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}$$

Claim

$$(*) \iff$$

$$A^T A x = A^T b$$

(normal equation)

$$A = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix} \quad \text{cols of } A$$

$$A^T = \begin{bmatrix} \text{---} u_1^T \text{---} \\ \text{---} u_2^T \text{---} \\ \vdots \\ \text{---} u_n^T \text{---} \end{bmatrix}$$

LHS of $(*)$



$$A^T b = \begin{bmatrix} \text{---} u_1^T \text{---} \\ \text{---} u_2^T \text{---} \\ \vdots \\ \text{---} u_n^T \text{---} \end{bmatrix} \begin{bmatrix} b \end{bmatrix} = \begin{bmatrix} \langle u_1, b \rangle \\ \langle u_2, b \rangle \\ \vdots \\ \langle u_n, b \rangle \end{bmatrix}$$

$$A^T A = \begin{bmatrix} - & u_1^T & - \\ - & u_2^T & - \\ & \vdots & \\ - & u_n^T & - \end{bmatrix} \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \dots & u_n \\ | & | & & | \end{bmatrix}$$

$$= \begin{bmatrix} \langle u_1, u_1 \rangle & \langle u_1, u_2 \rangle & \dots & \langle u_1, u_n \rangle \\ \langle u_2, u_1 \rangle & \langle u_2, u_2 \rangle & \dots & \langle u_2, u_n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle u_n, u_1 \rangle & \langle u_n, u_2 \rangle & \dots & \langle u_n, u_n \rangle \end{bmatrix}$$

Matrix on the RHS of (*)

Conclusion:

least square solution

normal equation

$$AX = b \quad \Longrightarrow \quad A^T A \tilde{X} = A^T b$$

(might not be solvable) (always solvable)

Note: $A^{m \times n}$, $(A^T)^{n \times m}$, $(A^T A)^{n \times n}$
↖ square matrix

If $(A^T A)^{-1}$ exists, then $\tilde{X} = (A^T A)^{-1} A^T b$

$(A^T A)^{-1}$ exists $\iff$ Columns of A are lin ind.

Example Solve $\begin{bmatrix} 1 & 2 \\ -1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$

not solvable

Normal equation

$$\begin{bmatrix} 1 & -1 & 1 \\ 2 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ -1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 \\ 2 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 3 & 3 \\ 3 & 6 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

$$y = \frac{2}{3}$$

$$x = -\frac{1}{3}$$

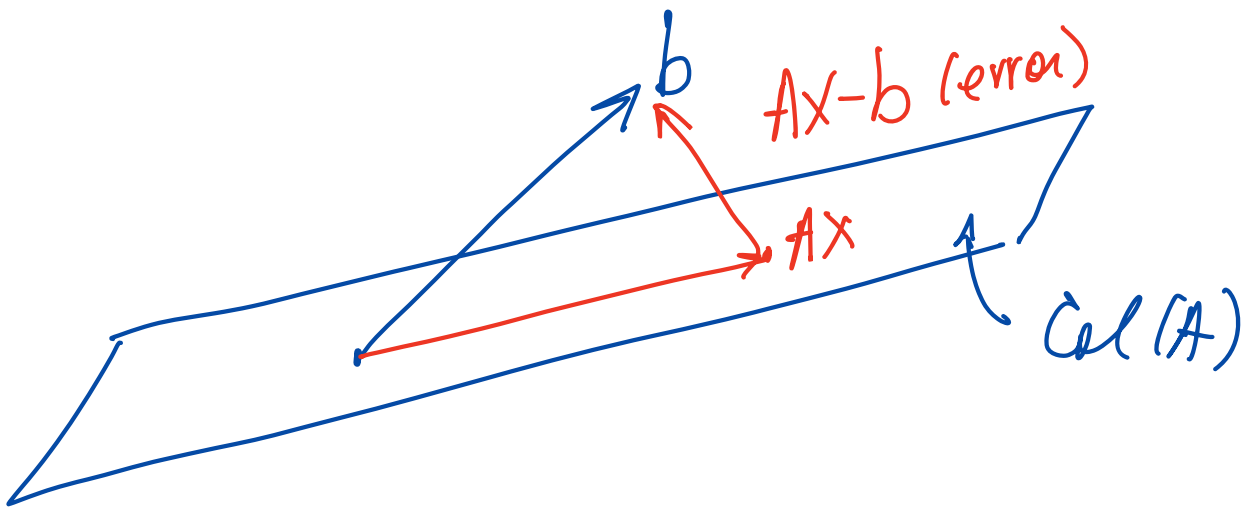
$$\begin{bmatrix} 3 & 3 \\ 3 & 6 \end{bmatrix} \begin{bmatrix} -\frac{1}{3} \\ \frac{2}{3} \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

least square solution

Why called least square solution?

$$AX = b \quad (\text{suppose not solvable})$$

$\Rightarrow$ Find X s.t. AX is closest to b
i.e. minimize error $AX - b$



Optimization

$$\min_X f(X) \quad \text{where } f(X) = \|AX - b\|^2$$

Solution X^* satisfies $A^T A X^* = A^T b$

Pf (Coordinate version) $A^{m \times n}$

$$\begin{aligned} f(X) &= \|AX - b\|^2 \\ &= \sum_{i=1}^m ((AX)_i - b_i)^2 \end{aligned}$$

$$= \sum_{i=1}^m \left(\sum_{j=1}^n A_{ij} x_j - b_i \right)^2$$

$$\partial_{x_k} f(x) = \partial_{x_k} \left[\sum_i \left(\sum_j A_{ij} x_j - b_i \right)^2 \right]$$

$$= 2 \sum_i \left(\sum_j A_{ij} x_j - b_i \right) A_{ik}$$

$$= 2 \left[\sum_i \sum_j A_{ij} x_j A_{ik} - \sum_i b_i A_{ik} \right]$$

$$= 2 \left[\sum_j \sum_i A_{ik} A_{ij} x_j - \sum_i A_{ik} b_i \right]$$

$$= 2 \left[\sum_j \left(\sum_i A_{ik} A_{ij} \right) x_j - \sum_i A_{ik} b_i \right]$$

$$= 2 \left[\sum_j \underbrace{\left(\sum_i (A^T)_{ki} A_{ij} \right)}_{(A^T A)_{kj}} x_j - \sum_i (A^T)_{ki} b_i \right]$$

$$= 2 \left[\sum_j (A^T A)_{kj} x_j - (A^T b)_k \right]$$

$$= 2 \left[((A^T A)X)_k - (A^T b)_k \right]$$

$$2x_k f(x) = 0 \iff ((A^T A)X)_k = (A^T b)_k$$

Hence $\nabla f(x) = 0 \iff (A^T A)X = A^T b$

Pf (Matrix Version)

$$f(x) = \|AX - b\|^2 = \langle AX - b, AX - b \rangle$$

$$= (AX - b)^T (AX - b)$$

$$= (x^T A^T - b^T)(AX - b)$$

$$= x^T A^T A X - x^T A^T b - b^T A X - b^T b$$

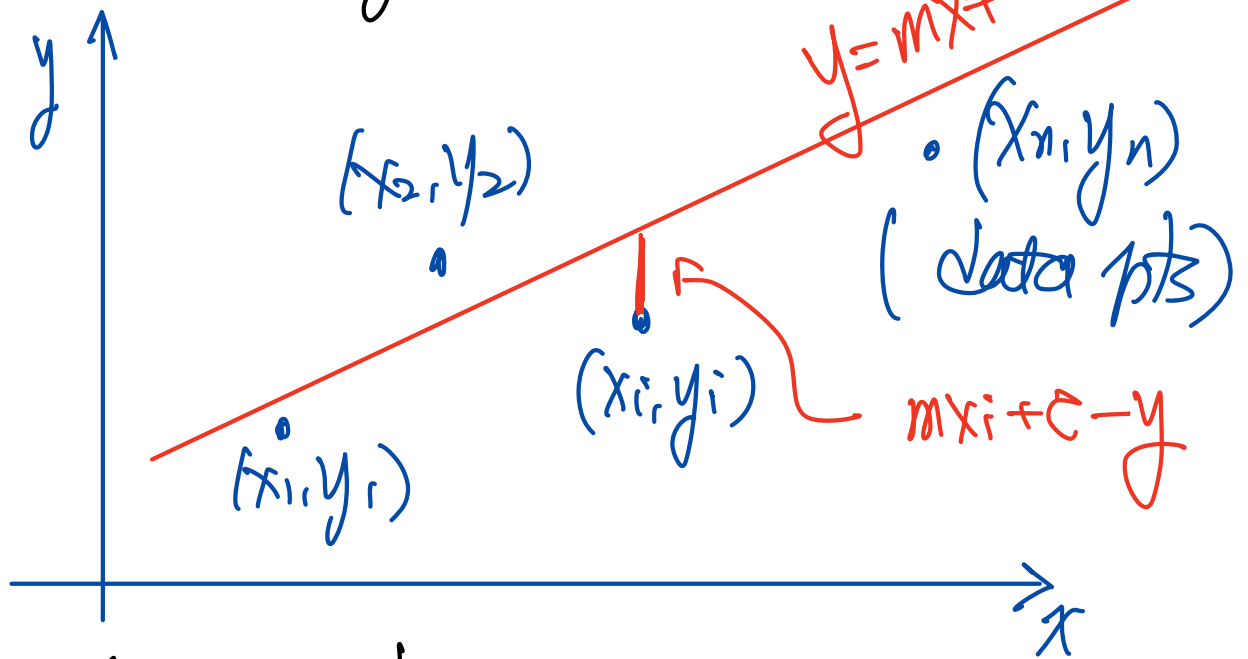
the same as both are numbers

$$= x^T A^T A X - 2 x^T A^T b - b^T b$$

$$\nabla f(x) = 2 A^T A X - 2 A^T b = 0$$

$$\iff A^T A X = A^T b$$

Best Fit Straight Line



Find m, c s.t

$$\begin{cases} mx_1 + c = y_1 \\ mx_2 + c = y_2 \\ \vdots \\ mx_n + c = y_n \end{cases}$$

$$\Leftrightarrow \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

normal equation

$$\begin{bmatrix} x_1 & x_2 & \cdots & x_n \\ 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \\ 1 \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} x_1 & \cdots & x_n \\ 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

$$\begin{bmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & n \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} \sum x_i y_i \\ \sum y_i \end{bmatrix}$$

(Alternative Derivation)

$$e(m, c) = \sum_{i=1}^n (m x_i + c - y_i)^2 \quad \text{mean square error}$$

$$\begin{aligned} \frac{\partial e}{\partial m} &= 2 \sum_{i=1}^n (m x_i + c - y_i) x_i \\ &= 2 \left[m \left(\sum_{i=1}^n x_i^2 \right) + c \left(\sum_{i=1}^n x_i \right) - \left(\sum_{i=1}^n x_i y_i \right) \right] \end{aligned}$$

$$\begin{aligned} \frac{\partial e}{\partial c} &= 2 \sum_{i=1}^n (m x_i + c - y_i) \\ &= 2 \left[m \left(\sum_{i=1}^n x_i \right) + n c - \sum_{i=1}^n y_i \right] \end{aligned}$$

$$\left(\frac{\partial e}{\partial m} = 0, \frac{\partial e}{\partial c} = 0 \right) \Rightarrow$$

$$m \left(\sum_{i=1}^n x_i^2 \right) + c \left(\sum_{i=1}^n x_i \right) = \left(\sum_{i=1}^n x_i y_i \right)$$

$$m \left(\sum_{i=1}^n x_i \right) + n c = \left(\sum_{i=1}^n y_i \right)$$

$$\begin{bmatrix} \sum_i x_i^2 & \sum_i x_i \\ \sum_i x_i & n \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} \sum_i x_i y_i \\ \sum y_i \end{bmatrix}$$

i.e.

$$\begin{bmatrix} \|x\|^2 & \bar{x} \\ \bar{x} & n \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} \langle x, y \rangle \\ \bar{y} \end{bmatrix}$$

$$\begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} \|x\|^2 & \bar{x} \\ \bar{x} & n \end{bmatrix}^{-1} \begin{bmatrix} \langle x, y \rangle \\ \bar{y} \end{bmatrix}$$

$$= \frac{\begin{bmatrix} n & -\bar{x} \\ -\bar{x} & \|x\|^2 \end{bmatrix}}{n\|x\|^2 - (\bar{x})^2} \begin{bmatrix} \langle x, y \rangle \\ \bar{y} \end{bmatrix}$$

$$m = \frac{n\langle x, y \rangle - \bar{x} \bar{y}}{n\|x\|^2 - (\bar{x})^2},$$

$$c = \frac{\|x\|^2 \bar{y} - \bar{x} \langle x, y \rangle}{n\|x\|^2 - (\bar{x})^2}$$