

### Least square solution

- $A\underline{x} \neq \underline{b}$   $\underline{b} - A\underline{x} = \underline{e}$  The length of  $\underline{e}$  or  $\|\underline{e}\|^2$  越小越好

ex: Find the closest line to the points

$$\begin{aligned} b &= C + Dt \\ C + D \cdot 0 &= 6 \\ C + D \cdot 1 &= 0 \Rightarrow A\underline{x} = \underline{b}, A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix}, \underline{x} = \begin{bmatrix} C \\ D \end{bmatrix}, \underline{b} = \begin{bmatrix} 6 \\ 0 \\ 0 \end{bmatrix} \Rightarrow A\underline{x} = \underline{b} \text{ 無解} \end{aligned}$$

The best fit is  $\hat{\underline{x}}$  such that  $\underline{p} = A\hat{\underline{x}}$  is the projection of  $\underline{b}$  onto  $C(A)$ .

$$A^T(\underline{b} - A\hat{\underline{x}}) = \underline{0} \Rightarrow A^TA\hat{\underline{x}} = A^T\underline{b} \Rightarrow \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} \hat{C} \\ \hat{D} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 6 \\ 0 \\ 0 \end{bmatrix} \Rightarrow \begin{bmatrix} 3 & 3 & 3 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} \hat{C} \\ \hat{D} \end{bmatrix} = \begin{bmatrix} 6 \\ 0 \\ 0 \end{bmatrix} \Rightarrow \hat{\underline{x}} = \begin{bmatrix} \hat{C} \\ \hat{D} \end{bmatrix} = \begin{bmatrix} 5 \\ -3 \end{bmatrix}$$

Best line:  $b = 5 - 3t$

- By linear algebra,  $\underline{b} = \underbrace{\underline{p}}_{C(A)} + \underbrace{\underline{e}}_{N(A)}$  We know that  $A\underline{x} = \underline{b} = \underline{p} + \underline{e}$  無解 and  $A\hat{\underline{x}} = \underline{p}$  有解

$$\|A\underline{x} - \underline{b}\|^2 = \|A\underline{x} - \underline{p} - \underline{e}\|^2 = (A\underline{x} - \underline{p} - \underline{e})^T (A\underline{x} - \underline{p} - \underline{e}) = \|A\underline{x} - \underline{p}\|^2 + \|\underline{e}\|^2$$

$\langle (A\underline{x} - \underline{p})^T \underline{e} = 0 \text{ since } A\underline{x} - \underline{p} \in C(A) \text{ and } \underline{e} \in N(A^T) \rangle \Rightarrow \|A\underline{x} - \underline{b}\|^2$  is minimized when  $\underline{x} = \hat{\underline{x}}$  ( $A\hat{\underline{x}} = \underline{p}$ )

i.e.  $\min_{\underline{x}} \|A\underline{x} - \underline{b}\|^2 = \|A\hat{\underline{x}} - \underline{b}\|^2 = \|A\hat{\underline{x}} - \underline{p}\|^2 + \|\underline{e}\|^2 = \|\underline{e}\|^2$  where  $A^T A \hat{\underline{x}} = A^T \underline{b}$  and  $\underline{p} = A \hat{\underline{x}}$

- By calculus,  $E = \|A\underline{x} - \underline{b}\|^2 = (C+D \cdot 0 - 6)^2 + (C+D \cdot 1)^2 + (C+D \cdot 2)^2$

$$\frac{\partial E}{\partial C} = 2(C+D \cdot 0 - 6) + 2(C+D \cdot 1) + 2(C+D \cdot 2) = 0$$

$$\frac{\partial E}{\partial D} = 2(C+D \cdot 1) + 4(C+D \cdot 2) = 0$$

$$\begin{cases} 6C + 6D = 12 \\ 6C + 10D = 0 \end{cases} \Rightarrow D = -3, C = 5 \Rightarrow b = 5 - 3t$$

The partial derivatives of  $\|A\underline{x} - \underline{b}\|^2$  are 0 when  $A^T A \hat{\underline{x}} = A^T \underline{b}$ ,  $\min_{\underline{x}} \|A\underline{x} - \underline{b}\|^2 = \|\underline{e}\|^2$

- When  $A\underline{x} = \underline{b}$  無解, the least square solution  $\hat{\underline{x}}$  satisfies  $A^T A \hat{\underline{x}} = A^T \underline{b}$

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## Curve Fitting

- Fitting a Straight Line : Fit height  $b_i$  at  $t_i$  by  $C+Dt$

solution:  $\begin{cases} C+Dt_1 = b_1 \\ \vdots \\ C+Dt_m = b_m \end{cases} \Rightarrow \begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$  ( $Ax=b$  無解)

best fit:  $A^T A = \begin{bmatrix} 1 & \cdots & 1 \\ t_1 & \cdots & t_m \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} = \begin{bmatrix} m & \sum_i t_i \\ \sum_i t_i & \sum_i t_i^2 \end{bmatrix}$        $A^T b = \begin{bmatrix} 1 & \cdots & 1 \\ t_1 & \cdots & t_m \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} \sum_i b_i \\ \vdots \\ \sum_i t_i b_i \end{bmatrix}$

Solve  $\begin{bmatrix} m & \sum_i t_i \\ \sum_i t_i & \sum_i t_i^2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \sum_i b_i \\ \vdots \\ \sum_i t_i b_i \end{bmatrix}$

The best  $\hat{x} = (C, D)$  minimizes  $\|Ax - b\|^2 = \|A\hat{x}\|^2 = \sum_i (C + Dt_i - b_i)^2$

- Fitting a Parabola : Fit heights  $b_i$  at  $t_i$  by  $C+Dt+Et^2$

solution:  $\begin{cases} C+Dt_1+Et_1^2 = b_1 \\ \vdots \\ C+Dt_m+Et_m^2 = b_m \end{cases} \Rightarrow \begin{bmatrix} 1 & t_1 & t_1^2 \\ \vdots & \vdots & \vdots \\ 1 & t_m & t_m^2 \end{bmatrix} \begin{bmatrix} C \\ D \\ E \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$  ( $Ax=b$  無解)  $\Rightarrow$  Solve  $A^T A \hat{x} = A^T b$  for  $\hat{x}$

## Orthogonal Bases and Gram-Schmidt

Def: The vectors  $q_1, \dots, q_n$  are orthogonal if  $q_i^T q_j = 0$  whenever  $i \neq j$

Claim: If nonzero vector  $q_1, \dots, q_n$  are orthogonal, then they are L.I.

pf: Consider  $x_1 q_1 + \dots + x_n q_n = 0$ , then  $x_1 q_1^T q_1 + \dots + x_n q_n^T q_n = q^T \underline{0} = 0 \Rightarrow x_i \|q_i\|^2 = 0$

$\Rightarrow x_1 = 0$ , similarly,  $x_2 = \dots = x_n = 0 \Rightarrow q_1, \dots, q_n$  are L.I.

Def: The vectors  $q_1, \dots, q_n$  are orthonormal if  $q_i^T q_j = \delta_{ij}$

o A matrix  $Q$  with orthonormal columns satisfies  $Q^T Q = \begin{bmatrix} q_1^T \\ \vdots \\ q_n^T \end{bmatrix} [q_1 \cdots q_n] = I$

When  $Q$  is 方陣,  $Q^T Q = I \Rightarrow Q^T = Q^{-1}$ . In this case,  $Q$  is called an orthogonal matrix.

ex: Rotation:  $Q = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$       Reflection:  $Q = I - 2 \underline{u} \underline{u}^T$ ,  $\underline{u}$ : any unit vector