linalg4 — LEAST SQUARES AND THE NORMAL EQUATIONS

Data $\mathcal{D}_3 = \{(-2,4), (0,2), (4,10)\}$

Basis $\mathcal{B}_2 = \{1, x\}$

fewer basis functions than data points (taken from $y = \frac{1}{2}x^2 + 2$)

"fit a line through three data points"

Vandermonde system

$$\begin{pmatrix} \phi_1(x_1) & \phi_2(x_1) \\ \phi_1(x_2) & \phi_2(x_2) \\ \phi_1(x_3) & \phi_2(x_3) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \Rightarrow \begin{pmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \\ 10 \end{pmatrix}$$

$$V\vec{c} = \vec{y}$$

overdeterminded system

$$y = c_1 + c_2 x$$

$$\begin{pmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \\ 10 \end{pmatrix}$$

cannot solve
(inconsistent system)

$c_1 = 2$
$c_2 = -1$
$c_1 + 4c_2 = -2 \neq 10$

$$\begin{pmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ 5 \end{pmatrix}$$

can solve
(consistent system)

$$\begin{pmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

generally inconsistent

Given up on solving exactly; find $(c_1, c_2)^T$ as close to solution as possible.

Residual vector

$$\begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} = \begin{pmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} - \begin{pmatrix} 4 \\ 2 \\ 10 \end{pmatrix}$$

$$\vec{r} = V\vec{c} - \vec{y}$$

2-norm $\|\vec{r}\| = \sqrt{r_1^2 + r_2^2 + r_3^2}$

Minimize $\|\vec{r}\|^2$ (same as minimizing $\|\vec{r}\|$)

$$\begin{aligned} \|\vec{r}\|^2(c_1, c_2) = {} & (c_1 - 2c_2 - 4)^2 \\ & + (c_1 - 2)^2 \\ & + (c_1 + 4c_2 - 10)^2 \end{aligned}$$

Problem: Choose c_1, c_2 to make following as small as possible

$$\|\vec{r}\|^2(c_1,c_2) = (c_1-2c_2-4)^2+(c_1-2)^2+(c_1+4c_2-10)^2$$

Calculus solution

$$0 = \frac{\partial\|\vec{r}\|^2}{\partial c_1} = 2(c_1-2c_2-4)+2(c_1-2)+2(c_1+4c_2-10)$$
$$= 2(3c_1+2c_2-16)$$

$$0 = \frac{\partial\|\vec{r}\|^2}{\partial c_2} = -4(c_1-2c_2-4)+8(c_1+4c_2-10)$$
$$= 2(2c_1+20c_2-32)$$

$$\boxed{\begin{pmatrix} 3 & 2 \\ 2 & 20 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 16 \\ 32 \end{pmatrix}}$$

Another way to (more quickly) get same equations

$$\begin{pmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \\ 10 \end{pmatrix} \qquad \underline{V\vec{c} = \vec{y}}$$

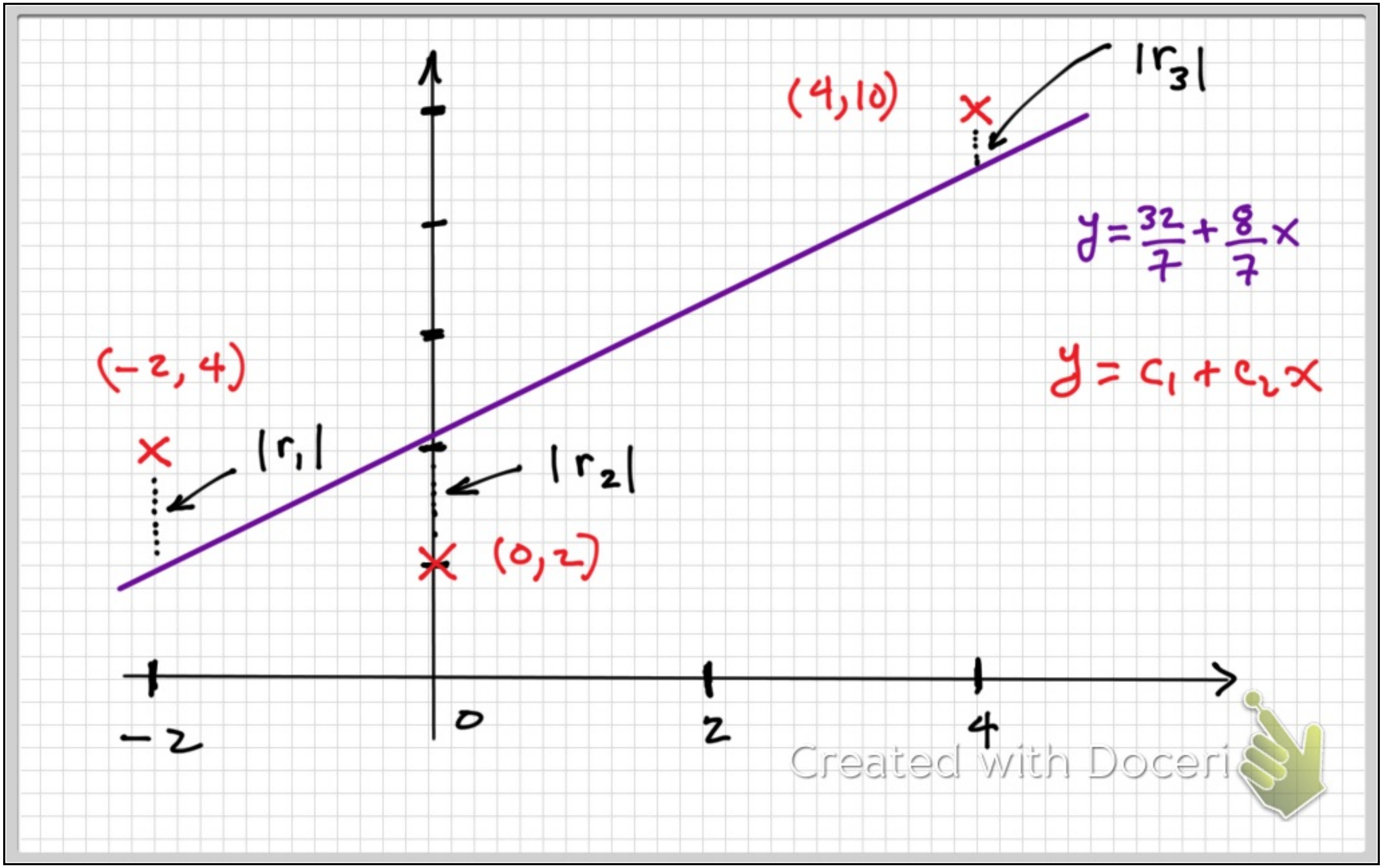
form the "normal equations" $V^T V \vec{c} = V^T \vec{y}$

$$\begin{pmatrix} 1 & 1 & 1 \\ -2 & 0 & 4 \end{pmatrix} \begin{pmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ -2 & 0 & 4 \end{pmatrix} \begin{pmatrix} 4 \\ 2 \\ 10 \end{pmatrix}$$

$$\boxed{\begin{pmatrix} 3 & 2 \\ 2 & 20 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 16 \\ 32 \end{pmatrix}}$$

SAME AS BEFORE

! solution
$(c_1, c_2) = \left(\frac{32}{7}, \frac{8}{7}\right)$


(4,10)
$|r_3|$
$y=\frac{32}{7}+\frac{8}{7}x$
$y=c_1+c_2x$
(-2,4)
$|r_1|$
$|r_2|$
(0,2)
-2
0
2
4
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Ex $\mathcal{D}_4 = \{(-1,1), (0,1), (1,3), (2,11)\}$

taken from $y = \frac{2}{3}x^3 + x^2 + \frac{1}{3}x + 1$

$\mathcal{B}_3 = \{1, x, x^2\}$

$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 3 \\ 11 \end{pmatrix}$$

$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 3 \\ 11 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 0 & 1 & 2 \\ 1 & 0 & 1 & 4 \end{pmatrix}\begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 0 & 1 & 2 \\ 1 & 0 & 1 & 4 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 3 \\ 11 \end{pmatrix}$$

$$\begin{pmatrix} 4 & 2 & 6 \\ 2 & 6 & 8 \\ 6 & 8 & 18 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 16 \\ 24 \\ 48 \end{pmatrix}$$

$c_1 = \frac{2}{5}$

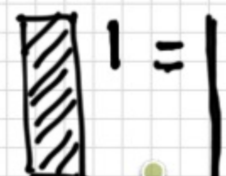
$c_2 = \frac{6}{5}$

$c_3 = 2$

Two theoretical results. Consider $A \in \mathbb{R}^{m \times n}$, where $m > n$ (more rows than columns).

$$\underbrace{\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}}_{\vec{x}} = \underbrace{\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}}_{\vec{b}}$$

structure

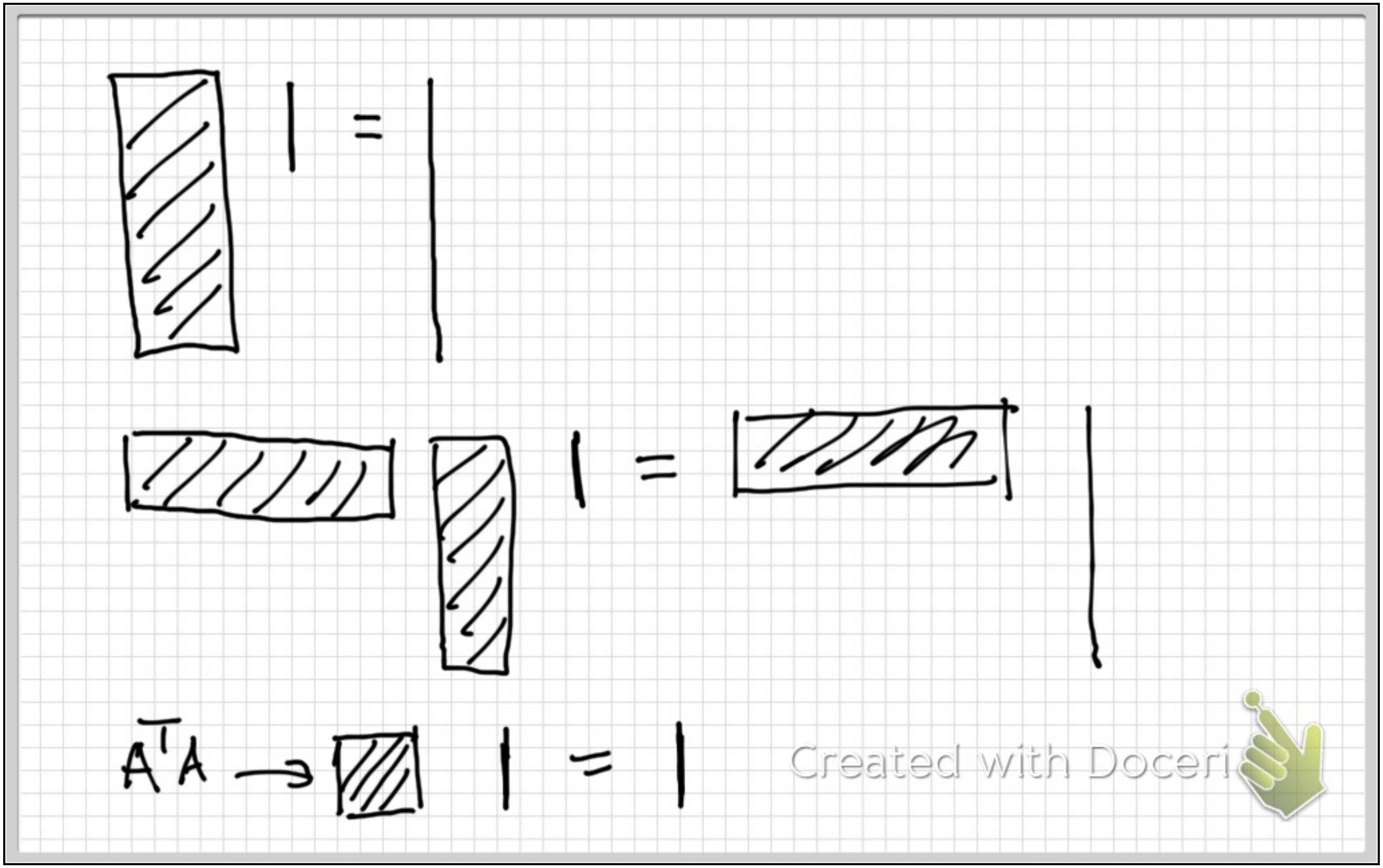


$\boxed{\text{Assume } A \text{ has full rank: columns of } A \text{ are linearly independent.}}$

Then $A\vec{x} = \vec{0} \implies \vec{x} = \vec{0}$

$$x_1\vec{a}_1 + x_2\vec{a}_2 + \cdots + x_n\vec{a}_n = \vec{0}$$

<u>Fact</u>: $A \in \mathbb{R}^{m\times n}$, $m > n$, of full rank. Then $A^TA \in \mathbb{R}^{n\times n}$ is <u>nonsingular</u>.


A^TA →
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Lemma ①. Suppose $A \in \mathbb{R}^{m \times n}$, $m > n$, has full rank. Then unique solution $\vec{x}_{LS}$ to normal equations $A^T A \vec{x}_{LS} = A^T \vec{b}$ minimizes $\|\vec{r}(\vec{x})\| = \|A\vec{x} - \vec{b}\|$ over all $\vec{x} \in \mathbb{R}^n$.

<u>Proof</u>: Any $\vec{x}$ can be expressed as

$$\vec{x} = \vec{x}_{LS} + \underbrace{(\vec{x} - \vec{x}_{LS})}_{\vec{e}} = \vec{x}_{LS} + \vec{e}$$

$$\|A\vec{x}-\vec{b}\|^2 = (A\vec{x}-\vec{b})^T(A\vec{x}-\vec{b})$$

$$= (A\vec{x}_{LS}+A\vec{e}-\vec{b})^T(A\vec{x}_{LS}+A\vec{e}-\vec{b})$$

$$= (A\vec{x}_{LS}-\vec{b})^T(A\vec{x}_{LS}-\vec{b})$$

combine these terms

$$\left\{\begin{array}{l} + (A\vec{x}_{LS}-\vec{b})^T A\vec{e} \\ + (A\vec{e})^T(A\vec{x}_{LS}-\vec{b}) \end{array}\right.$$

$$+ (A\vec{e})^T(A\vec{e})$$

$$\|A\vec{x}-\vec{b}\|^2 = (A\vec{x}_{LS}-\vec{b})^T(A\vec{x}_{LS}-\vec{b})$$

$$+ 2(A\vec{e})^T(A\vec{x}_{LS}-\vec{b})$$

$$+ (A\vec{e})^T A\vec{e}$$

$$= \|A\vec{x}_{LS}-\vec{b}\|^2 + \|A\vec{e}\|^2$$

$$+ 2\vec{e}^{\,T}\underbrace{(A^TA\vec{x}_{LS} - A^T\vec{b})}_{0}$$

$$= \|A\vec{x}_{LS}-\vec{b}\|^2 + \|A\vec{e}\|^2$$

Shows $\|A\vec{x}-\vec{b}\| \geq \|A\vec{x}_{LS}-\vec{b}\|$ with $=$ only for $\vec{x}=\vec{x}_{LS}$

Lemma (2). $A \in \mathbb{R}^{m \times n}$, $m > n$, with full rank. $\vec{x}_{LS}$ is unique solution to $A^T A \vec{x}_{LS} = A^T \vec{b}$.

Then
$$\left(\vec{\nabla} \|A\vec{x} - \vec{b}\|^2\right)\Big|_{\vec{x} = \vec{x}_{LS}} = \vec{0}$$

<u>Proof</u> See PDF notes. Relies on

$$\frac{\partial x_k}{\partial x_j} = \delta_{kj} \quad \text{(Kronecker delta)}$$

compare w/ $\frac{\partial x}{\partial x} = 1$ but $\frac{\partial y}{\partial x} = 0 = \frac{\partial z}{\partial x}$