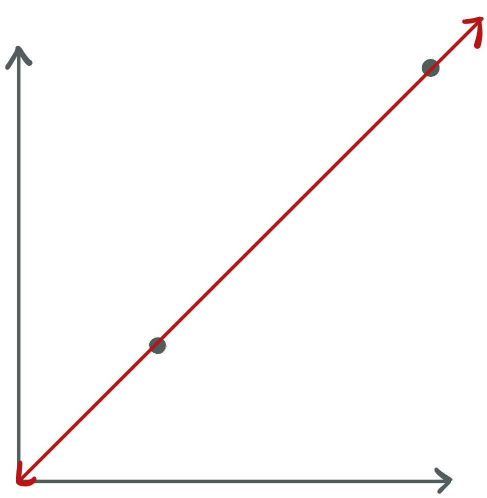
Least Squares.

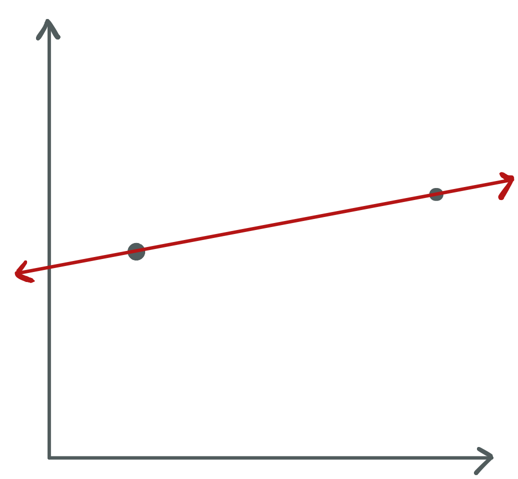
Goal: find a <u>line that best</u> represents some data.

→ line of best fit.

<u>2 pts in $\mathbb{R}^2$</u> → for any $\mathbb{R}^n$.

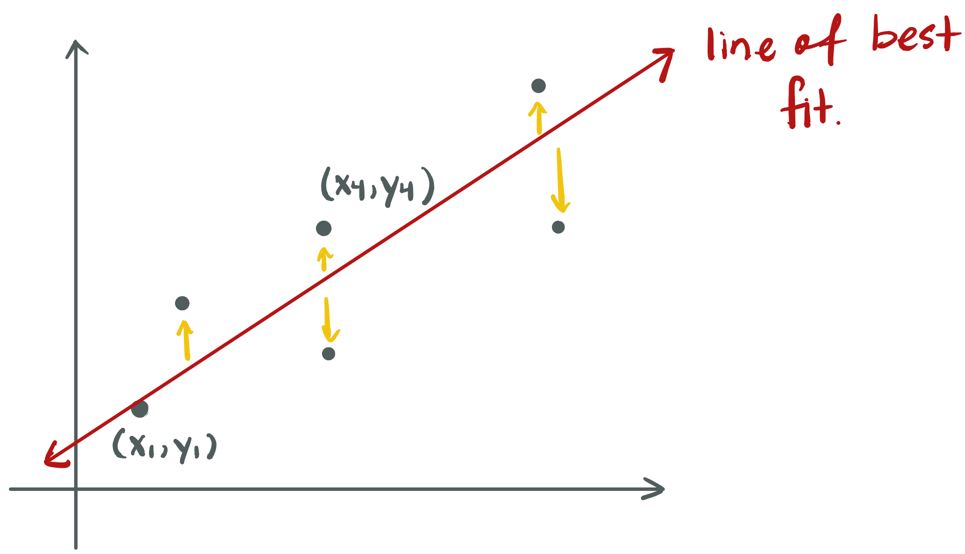
We can always find a straight line through 2 lines.





More than 2 pts in $\mathbb{R}^2$

No longer likely that there is a (straight) line through all the points.



We can use least-squares to find a good line.

find a,b that make this sum the smallest.

a,b parameters

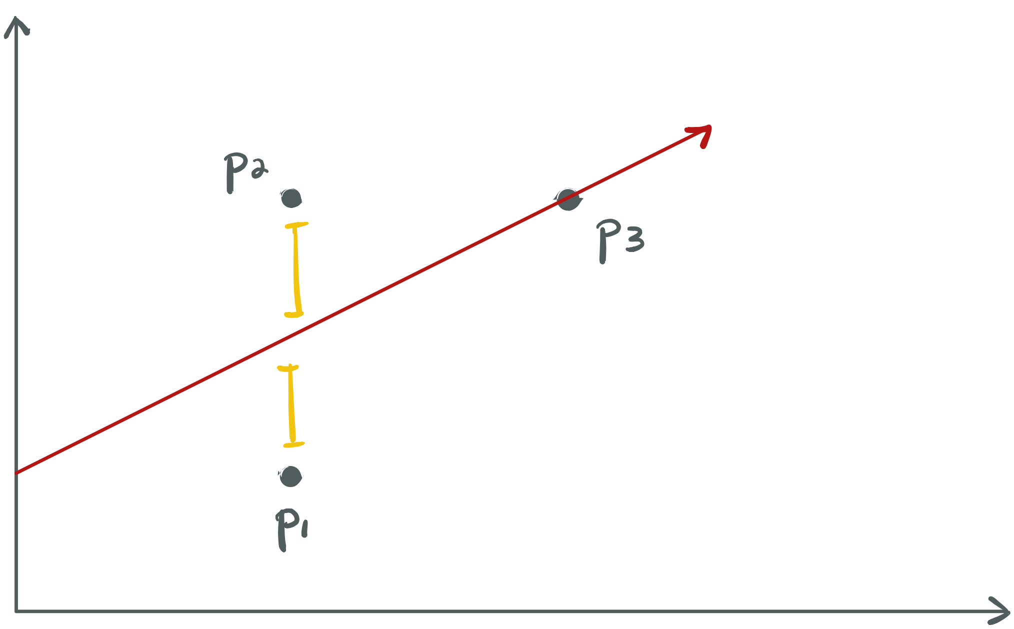
$$f(a,b) := \min_{a,b} \sum_{i=1}^{N} (ax_i + b - y_i)^2$$

$y = ax + b \leftarrow$ best fit line.

Example 1. Find the least-squares regression line for the data,

$$\{ \underset{\substack{\parallel \\ p_1 \\ \parallel \\ (x_1, y_1)}}{(2,1)}, \underset{\substack{\parallel \\ p_2}}{(2,3)}, \underset{\substack{\parallel \\ p_3}}{(4,3)} \}$$

Step 0.5. draw a picture.



Step 1. Write out the matrix problem

$$A = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \end{bmatrix}$$

x-value 1's.

A is $n \times 2$, n = number of points. because pts in $\mathbb{R}^2$

$$\vec{x} = \begin{array}{cl} \begin{bmatrix} a \\ b \end{bmatrix} & \begin{array}{l} \leftarrow \text{slope of line} \\ \leftarrow \text{y-intercept} \end{array} \end{array} \qquad \vec{b} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

y-values

Step 2. Multiply both sides of the equation by A^T. $(A^TA\vec{x} = A^T\vec{b})$

$$\begin{bmatrix} 2 & 2 & 4 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 2 & 1 \\ 4 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 2 & 2 & 4 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \\ 3 \end{bmatrix}$$

$$\begin{bmatrix} 24 & 8 \\ 8 & 3 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 20 \\ 7 \end{bmatrix}$$

Claim: A^TA is invertible and so I can solve for $\vec{x}$.

in almost all cases.

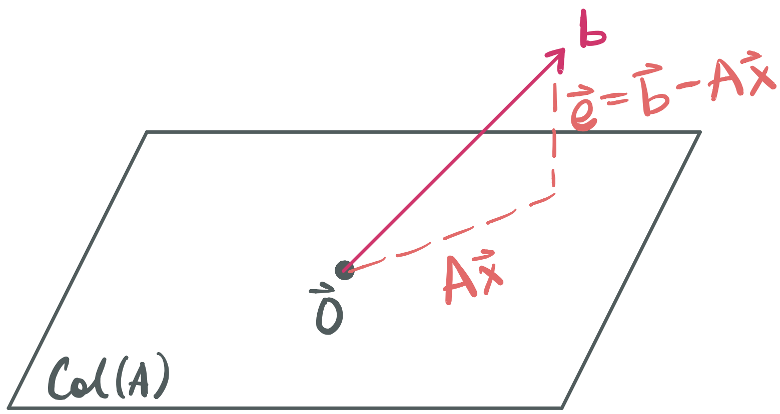
Step 3. Now solve for $\vec{x}$.

$$\begin{bmatrix} 24 & 8 \\ 8 & 3 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 20 \\ 7 \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \frac{3}{8} & -1 \\ -1 & 3 \end{bmatrix}\begin{bmatrix} 20 \\ 7 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ 1 \end{bmatrix}$$

Least-squares line: $y = \frac{1}{2}x + 1$

WHY THE HECK DOES THIS WORK?



Note:

- $A\vec{x} \in Col(A)$
- $\vec{e} = b - A\vec{x}$ is orthogonal to any vector $v \in Col(A)$.
- $\vec{e} \perp a_1$ and $\vec{e} \perp a_2$ 2nd column of A

$\Rightarrow (a_1)^T \vec{e} = 0$ & $(a_2)^T \vec{e} = 0$.

$$A^T \vec{e} = A^T(\vec{b} - A\vec{x}) = 0.$$

Show $A^T A$ is invertible for A given by (most) least squares problems.

Step 1. Show columns of A are (usually) linearly independent.

The col's of A are LD $\Leftrightarrow x_1 = \cdots = x_n$.

In all other cases, the columns of A are linearly independent.

Step 2. Show $N(A^TA) = N(A)$.

1\. Show $v \in Nul(A) \Rightarrow v \in Nul(A^TA)$

$$v \in Nul(A) \Rightarrow Av = \vec{0}$$
$$\Rightarrow A^TAv = A^T\vec{0} = \vec{0}$$
$$\Rightarrow v \in Nul(A^TA).$$

2\. $v \in Nul(A^TA) \Rightarrow v \in Nul(A)$

$$v \in Nul(A^TA) \Rightarrow A^TAv = \vec{0}$$

$\Rightarrow$ $\underline{\text{i. } Av = \vec{0}}$ or ii. $Av \neq 0$ but $Av \in Nul(A^T)$.

✗ CANT HAPPEN.

ii. $Av \in Nul(A^T)$ & $Av \in Range(A)$

BUT. $Nul(A^T) \perp Range(A)$

Step 3. Conclusion.

1. Col's A are LI (mostly)

   $\Rightarrow \mathrm{Nul}(A) = \{\vec{0}\}$

2. $\mathrm{Nul}(A^TA) = \mathrm{Nul}(A) = \{\vec{0}\}$

3. A^TA is square and $\mathrm{Nul}(A^TA) = \{0\}$

   $\Rightarrow A^TA$ is invertible.

Example 2. Find the best line to fit the set of data,

$$\{(1,1), (2,2), (3,2)\}$$

① $\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$

② $\begin{bmatrix} 1 & 2 & 3 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$

$$\begin{bmatrix} 14 & 6 \\ 6 & 3 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 11 \\ 5 \end{bmatrix}$$

③ $\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & -1 \\ -1 & \frac{7}{3} \end{bmatrix} \begin{bmatrix} 11 \\ 5 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ \frac{2}{3} \end{bmatrix}$

$$y = \frac{1}{2}x + \frac{2}{3}.$$

Example 3. Compute the line that best fits the data,

$$\{(1,3),\ (2,1),\ (1,1),\ (4,3)\}$$

① $$\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 1 & 1 \\ 4 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 1 \\ 3 \end{bmatrix}$$

② $$\begin{bmatrix} 22 & 8 \\ 8 & 4 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 18 \\ 8 \end{bmatrix}$$

③ $$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \frac{1}{6} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{11}{12} \end{bmatrix} \begin{bmatrix} 18 \\ 8 \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \frac{1}{3} \\ 4/3 \end{bmatrix} \Rightarrow y = \frac{1}{3}x + \frac{4}{3}.$$

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

$$\begin{bmatrix} ax_1 + b \\ ax_2 + b \\ ax_3 + b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

if p_1, p_2, p_3 on same line can find $\vec{x}$

looks like eq of a line