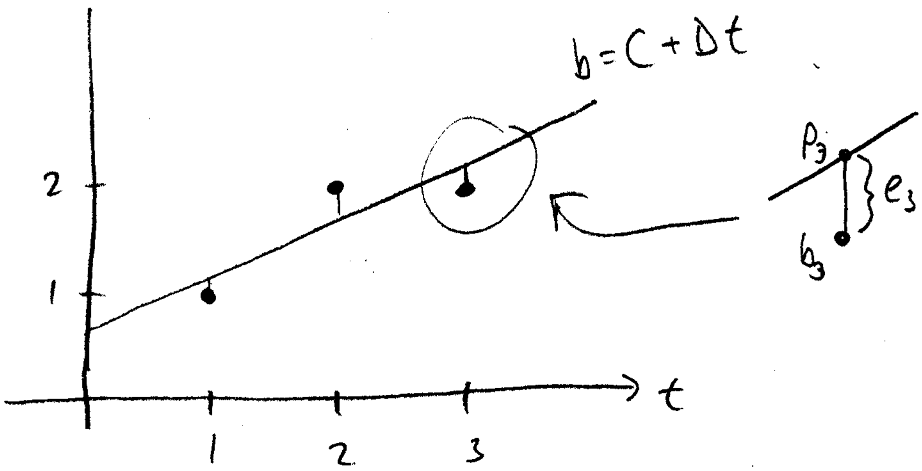
3 Least squares

Goal: Given some data points in $\mathbb{R}^2$, find the "best fit" line.

Ex: Consider 3 points: $(1,1)$, $(2,2)$, $(3,2)$.



e_i = error

p_i = point on the line

Note: $\begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} \in C(A)$

Find the "best" line: $\boxed{b = C + Dt}$

A "perfect sol'n" would solve the following: $\begin{cases} C + D = 1 \\ C + 2D = 2 \\ C + 3D = 2 \end{cases}$

i.e., solve $\underbrace{\begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} C \\ D \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}}_{b}$ (has no sol'n)

Next best thing: Solve $A\hat{x} = \hat{p}$

or $\boxed{A^T A \hat{x} = A^T \hat{p}}$ for $\hat{x} = \begin{bmatrix} \hat{C} \\ \hat{D} \end{bmatrix}$.

Most important eq'n in statistics, estimation.

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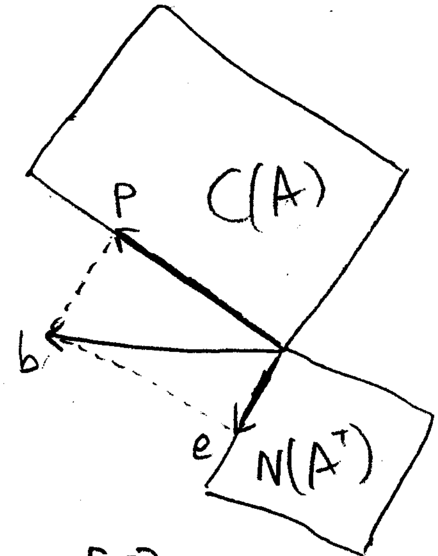
This line minimizes

$$\|Ax-b\|^2 = \|e\|^2 = e_1^2 + e_2^2 + e_3^2$$

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



Solve $A^TA\hat{x} = A^Tb$:

$$A^TA = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 3 & 6 \\ 6 & 14 \end{bmatrix} \qquad A^Tb = \begin{bmatrix} 5 \\ 11 \end{bmatrix}$$

$$\Rightarrow (A^TA)\hat{x} = A^Tb \Rightarrow \left[\begin{array}{cc|c} 3 & 6 & 5 \\ 6 & 14 & 11 \end{array}\right] \Rightarrow \boxed{\begin{array}{l} 3C + 6D = 5 \\ 6C + 14D = 11 \end{array}}$$

"normal eq'ns"

<u>Compare to calculus:</u>

$$\text{Minimize } e_1^2 + e_2^2 + e_3^2 = (C+D-1)^2 + (C+2D-2)^2 + (C+3D-2)^2$$

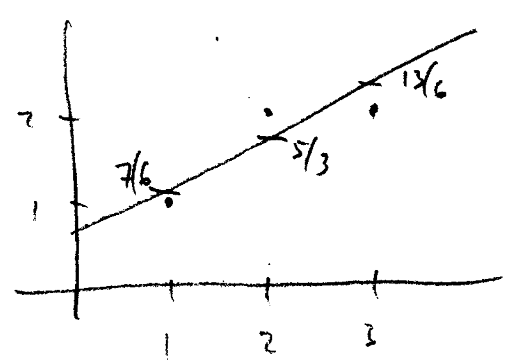
$$\frac{\partial e}{\partial C} = 3C + 6D - 5 = 0, \qquad \frac{\partial e}{\partial D} = 6C + 14D - 11 = 0.$$

Solve normal eq'ns: $\boxed{C = 2/3, \quad D = 1/2}$

Best line: $\boxed{\frac{2}{3} + \frac{1}{2}t}$

$$\begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} = \begin{bmatrix} 7/6 \\ 5/3 \\ 13/6 \end{bmatrix} + \begin{bmatrix} -1/6 \\ 2/6 \\ -1/6 \end{bmatrix}$$

$$b \quad = \quad p \quad + \quad e$$



Remarks:

- $p^T e = -7/36 + 20/36 - 13/36 = 0 \Rightarrow p \perp e$ (as expected)
- $e \perp C(A)$; so $e \perp \begin{bmatrix}1\\1\\1\end{bmatrix}$ and $e \perp \begin{bmatrix}1\\2\\3\end{bmatrix}$.

We've seen that there is no line $b = C + Dt$ through all 3 points.

But what if we try a parabola $b = C + Dt + Et^2$?

We would have to solve
$$\begin{cases} C + D + E = 1 \\ C + 2D + 4E = 2 \\ C + 3D + 9E = 2 \end{cases}$$

We can do this!