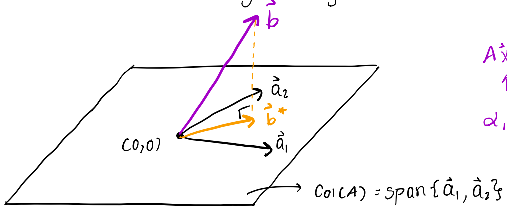
★ LEAST SQUARES

purpose: when an exact solution may not exist, so you want to find the best estimate for the solution

Q: when does an exact solution to $A\vec{x} = \vec{b}$ not exist?
A: $\vec{b}$ is not in the col(A)

Q: what does this look like graphically? → consider the 2D case
A:



$A\vec{x} = \vec{b}$
↑ no solution
$\alpha_1 \vec{a}_1 + \alpha_2 \vec{a}_2 \neq \vec{b}$

→ $A\vec{x} = \vec{b}^*$
↑ exists

practical purpose: when you have α unknowns, you generally need α measurements for the measurements to work they need to be:

1. lin. independent
2. accurate

Q: what happens if measurements are not accurate?
A: we take more than α measurements to find the best estimate for the unknowns

$A = \alpha \times \alpha \Rightarrow \begin{bmatrix} \\ \\ \\ \end{bmatrix}$ α columns
\# rows = # measurements

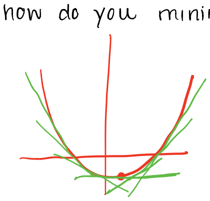
how it works: we want to find an $\vec{x}^*$ such that $A\vec{x}^*$ is as close to $\vec{b}$ as possible since there may not be an $\vec{x}$ where $A\vec{x} = \vec{b}$

∴ we want to find $\vec{x}^*$ that minimizes the distance between $A\vec{x}^*$ and $\vec{b}$

① algebraic $\min_{\vec{x}^*} \|A\vec{x}^* - \vec{b}\|^2$

$\|A\vec{x}^* - \vec{b}\|^2$
$= \|\vec{b} - A\vec{x}^*\|^2$

Q: how do you minimize functions? → consider a function $f(x) = x^2 - 2x - 3$
A:

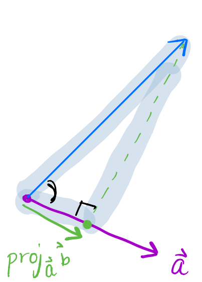


$f'(x) = \frac{d}{dx}(x^2 - 2x - 3)$
$0 = 2x - 2$
$\underline{\underline{x = 1}}$

→ $\vec{x}^* = (A^T A)^{-1} A^T \vec{b}$

② geometric

projections:

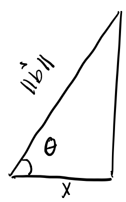


→ $proj_{\vec{a}}\vec{b}$ → project $\vec{b}$ onto $\vec{a}$
: how much of $\vec{b}$ lies in the same direction as $\vec{a}$

$= \frac{\langle \vec{b}, \vec{a} \rangle}{\|\vec{a}\|^2} \cdot \vec{a}$

Q: how can you derive $proj_{\vec{a}}\vec{b}$?

A:



$\cos\theta = \frac{x}{\|\vec{b}\|}$

$\langle \vec{b}, \vec{a} \rangle = \|\vec{a}\| \|\vec{b}\| \cos\theta$

$\langle \vec{b}, \vec{a} \rangle = \|\vec{a}\| \cancel{\|\vec{b}\|} \frac{x}{\cancel{\|\vec{b}\|}}$

$\underbrace{\frac{\langle \vec{b}, \vec{a} \rangle}{\|\vec{a}\|}} = x$

direction: $\frac{\vec{a}}{\|\vec{a}\|}$

$proj_{\vec{a}}\vec{b} = \frac{\langle \vec{b}, \vec{a} \rangle}{\|\vec{a}\|^2} \cdot \vec{a}$

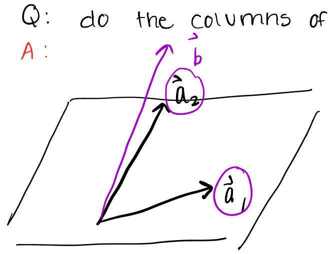
you can think of projections as finding the closest estimate

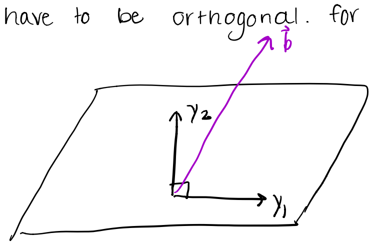
↳ this sounds like least squares!

LEAST SQUARES: projecting $\vec{b}$ onto Col(A)

Q: do the columns of A have to be orthogonal for least squares to work?

A:





$\underset{2\times 1}{\vec{x}} = (A^TA)^{-1}A^T\vec{b}$

$\vec{x} = \begin{bmatrix} \| proj_{\vec{y}_1}\vec{b} \| \\ \| proj_{\vec{y}_2}\vec{b} \| \end{bmatrix}$

Q: what happens if an exact solution to $A\vec{x} = \vec{b}$ exists, but we accidentally apply least squares?

A:

$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \vec{x} = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$

$\vec{x} = \underbrace{(A^TA)^{-1}} A^T b = A^{-1}\vec{b}$

☆ PROBLEMS

① Your prof. gives you a black box and wants you to predict its behavior for any given input. He has tested it before and has given you the output he measured in the table on the left. He proposes that the black box follows one of the following models:

x	y
x_0	y_0
x_1	y_1
x_2	y_2
x_3	y_3
x_4	y_4

→ • a line through the origin $y = ax$
→ • ~~a polynomial of degree 5~~ $y = a_1 x^5 + a_2 x^4 + \dots + a_5 x + a_6$
→ • a sine wave $y = a\sin(x) + b$
→ • an exponential function $y = ae^{bx}$

How can you determine which model best represents the behavior of the black box?

① $y = ax$

$y_0 = ax_0$
$y_1 = ax_1$
$\vdots$
$y_4 = ax_4$

$$\underbrace{\begin{bmatrix} x_0 \\ \vdots \\ x_4 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} a \end{bmatrix}}_{\vec{x}} = \underbrace{\begin{bmatrix} y_0 \\ \vdots \\ y_4 \end{bmatrix}}_{\vec{b}}$$

$\underset{1\times1}{\vec{x}} = (A^TA)^{-1}A^T\vec{b}$

② $y = a\sin(x) + b$

$$\underbrace{\begin{bmatrix} \sin(x_0) & 1 \\ \sin(x_1) & 1 \\ \vdots & \vdots \\ \sin(x_4) & 1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} a \\ b \end{bmatrix}}_{\vec{x}} = \underbrace{\begin{bmatrix} y_0 \\ \vdots \\ y_4 \end{bmatrix}}_{\vec{b}}$$

$\underset{2\times1}{\vec{x}} = (A^TA)^{-1}A^T\vec{b}$

③ $(y = ae^{bx}) \rightarrow \ln(y) = \ln(ae^{bx})$

$\underbrace{\ln(y)}_{} = \underbrace{\ln(a)}_{} + \underbrace{bx}_{=\uparrow}$

$y_0 = ae^{bx_0}$
$y_1 = ae^{bx_1}$
$\vdots$
$y_4 = ae^{bx_4}$

$$\begin{bmatrix} 1 & x_0 \\ 1 & \vdots \\ \vdots & \vdots \\ 1 & x_4 \end{bmatrix} \begin{bmatrix} \ln(a) \\ b \end{bmatrix} = \begin{bmatrix} \ln(y_0) \\ \vdots \\ \ln(y_4) \end{bmatrix}$$

$\rightarrow y = ae^{bx}$ ↑

$\vec{x} = (A^TA)^{-1}A^T\vec{b} = \begin{bmatrix} \ln(a) \\ b \end{bmatrix}$ ③ $e^{\ln(a)} = \underline{\underline{a}}$

	model 1 pred.	model 2 pred.	model 3 pred.	actual output
x_0	α_0	β_0	γ_0	y_0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
x_4	α_4	β_4	γ_4	y_4
error	$\sum_{i=0}^{4}(y_i - \alpha_i)^2$	$\sum_{i=0}^{4}(y_i - \beta_i)^2$	$\sum_{i=0}^{4}(y_i - \gamma_i)^2$	

pick model w/ smallest error

② Consider $A = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 3 & 0 & 3 & 0 \\ 4 & 0 & 4 & 0 \\ 2 & 3 & 5 & 6 \\ 8 & 0 & 8 & 0 \\ 13 & 0 & 13 & 0 \end{bmatrix}$ and $\vec{b} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

TRUE or FALSE: least squares can be applied to this problem.