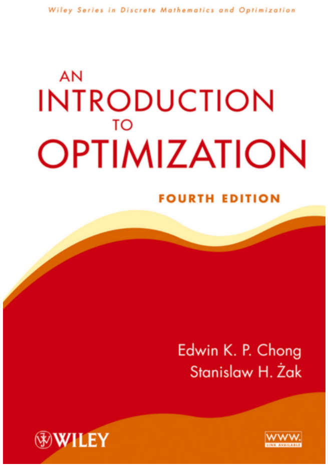

Introduction to Optimization

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Data Science

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Recall

Suppose that we are given m equations in n unknowns of the form

$$\begin{aligned} a_{11}x_1 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + \cdots + a_{2n}x_n &= b_2 \\ &\vdots \\ a_{m1}x_1 + \cdots + a_{mn}x_n &= b_m \end{aligned}$$

In matrix form,

$$Ax = b.$$

◦ The system $Ax = b$ has a solution iff rank A = rank $[A,\ b]$.

Tall matrices

≈ more rows than columns

Consider a system of linear equations

$$Ax = b$$

where $A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m, m \geq n$, and rank $A = n$.

$$\begin{bmatrix} 0 & 8 & 44 \\ 1 & 13 & 33 \\ 1 & 21 & 77 \\ 2 & 34 & 10 \\ 3 & 55 & 87 \\ 5 & 89 & 97 \end{bmatrix}$$

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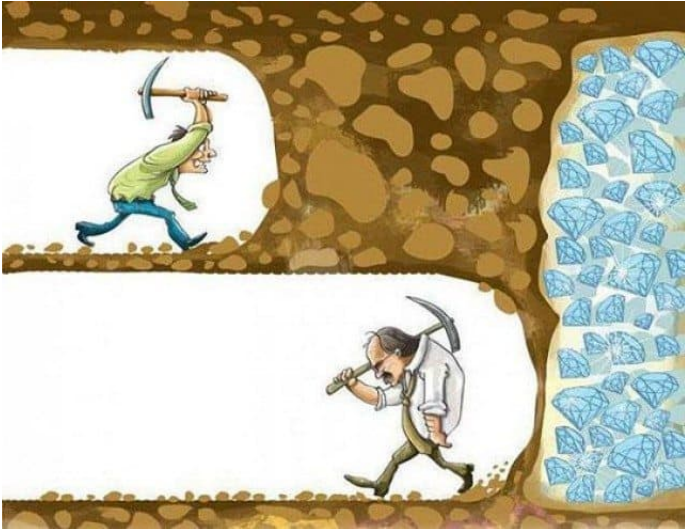
- $\mathrm{Col}(A) \neq \mathbb{R}^m$
- What if $b \notin \mathrm{Col}(A)$?

No solution?



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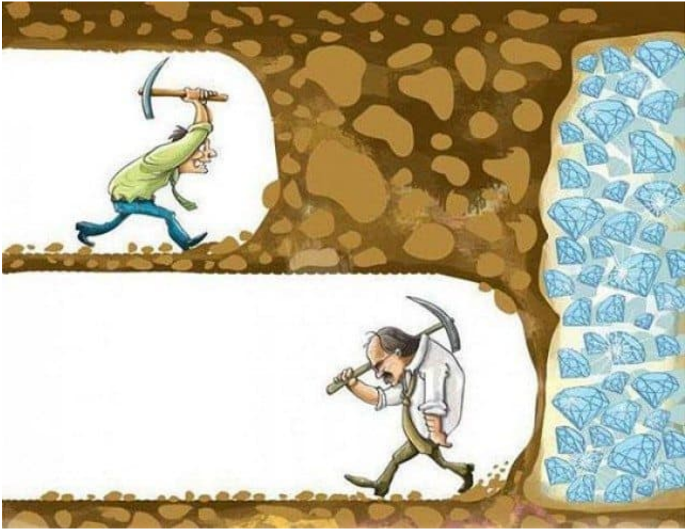

~~No solution~~ Least squares solution

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Find the vector x that minimizes $\|Ax - b\|^2$

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$\equiv$ Find x^* such that for all $x \in \mathbb{R}^n$,

$$\|Ax - b\|^2 \geq \|Ax^* - b\|^2$$

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x^* is the least squares solution to $Ax = b$.

Helper lemma

for finding the least squares solution

Lemma – Let $A \in \mathbb{R}^{m \times n}, m \geq n$. Then,

$$\text{rank } A = n \iff \text{rank } A^\top A = n$$

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Proof sketch –

($\Longrightarrow$) Suppose rank $A = n$. Show that $\mathcal{N}(A^\top A) = \{\mathbf{0}\}$.

Let $x \in \mathcal{N}(A^\top A)$. Then,

$$\|Ax\|^2 = x^\top A^\top Ax$$

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Theorem – The unique vector x^* that minimizes $\|Ax - b\|^2$ is given by the solution to the equation

$$A^\top A x = A^\top b.$$

That is,

$$x^* = (A^\top A)^{-1} A^\top b.$$

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$$\begin{aligned} \|Ax - b\|^2 &= \|Ax - Ax^* + Ax^* - b\|^2 \\ &= \cdots \\ &= \|A(x - x^*)\|^2 + \|Ax^* - b\|^2. \end{aligned}$$

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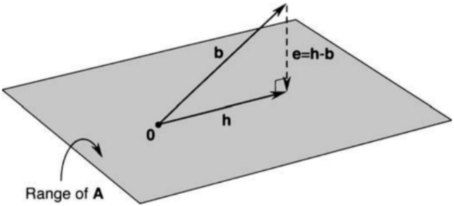
If $x \neq x^*$, then $\|A(x - x^*)\|^2 > 0$ since rank $A = n$.

(explain on board)

Geometric picture of the least squares solution



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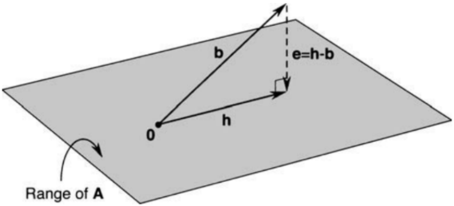

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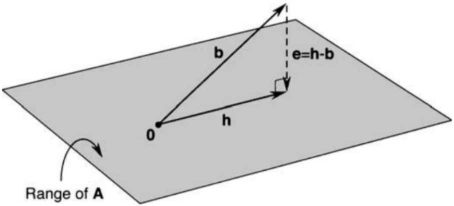

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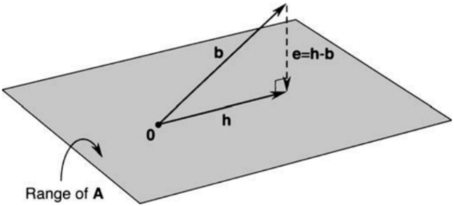

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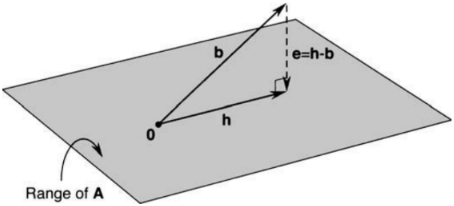

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- Since $h \in \mathrm{Col}(A)$, we can write

  $$h = Ax^* \qquad \text{for some } x^*.$$

(continue on board)

A 2D example

(show on board)

Let

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

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Line fitting

We model test scores based on hours studied:

#hours studied	Test score
1	50
2	60
3	65
4	70

(plot on board)

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Assuming $Ax = b$, this gives us:

$$A = \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \\ 4 & 1 \end{bmatrix}, \quad b = \begin{bmatrix} 50 \\ 60 \\ 65 \\ 70 \end{bmatrix} \qquad \text{with } x = \begin{bmatrix} m \\ c \end{bmatrix}$$

Least squares solution

We solve using the least squares formula:

$$x^* = (A^\top A)^{-1} A^\top b$$

Step-by-step:

$$A^\top A = \begin{bmatrix} 30 & 10 \\ 10 & 4 \end{bmatrix}, \quad A^\top b = \begin{bmatrix} 645 \\ 245 \end{bmatrix}$$

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Inverse of $A^\top A$:

$$(A^\top A)^{-1} = \frac{1}{20} \begin{bmatrix} 4 & -10 \\ -10 & 30 \end{bmatrix}$$

Solving for $x = \begin{bmatrix} m \\ c \end{bmatrix}$

Now compute:

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So, the best fit line is:

$$\boxed{y = 6.5t + 45}$$

Interpretation

predict test scores for "any" number of study hours

- $m = 6.5$: every hour of study $\Longrightarrow$ score of 6.5 points.
- $c = 45$: a student who doesn't study would score 45.

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- Suppose I get one more measurement:

#hours studied	Test score
1	50
2	60
3	65
4	70
5	92

Do the whole calculation from scratch?

Recursive least squares

Update the least squares solution x^* to accommodate new data point(s).

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– The solution to the least squares problem with A_0 and $b^{(0)}$ is given by

$$x^{(0)} = {G_0}^{-1} A_0^\top b^{(0)} \qquad ; \qquad G_0 = A_0^\top A_0$$

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– Suppose we are given more data: A_1 and $b^{(1)}$.

Recursive least squares

General form

We seek to minimize

$$\left\| \begin{bmatrix} A_0 \\ A_1 \end{bmatrix} x - \begin{bmatrix} b^{(0)} \\ b^{(1)} \end{bmatrix} \right\|^2 .$$

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$$x^{(1)} = G_1^{-1} \begin{bmatrix} A_0 \\ A_1 \end{bmatrix}^\top \begin{bmatrix} b^{(0)} \\ b^{(1)} \end{bmatrix}$$

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We want to write $x^{(1)}$ in terms of **old estimate**: $x^{(0)}$ and **new data**: $A_1, b^{(1)}$;
(possibly use G_0 also)

Recursive least squares

Update equations

$$x^{(1)} = G_1^{-1} \begin{bmatrix} A_0 \\ A_1 \end{bmatrix}^\top \begin{bmatrix} b^{(0)} \\ b^{(1)} \end{bmatrix} \qquad ; \qquad G_1 = \begin{bmatrix} A_0 \\ A_1 \end{bmatrix}^\top \begin{bmatrix} A_0 \\ A_1 \end{bmatrix}$$

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$$= A_0^\top b^{(0)} + A_1^\top b^{(1)}.$$

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\end{aligned}$$

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$$x^{(1)} = G_1^{-1}\left[G_1 x^{(0)} - A_1^\top A_1 x^{(0)} + A_1^\top b^{(1)}\right] \qquad ; \qquad G_1 = G_0 + A_1^\top A_1$$

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&= G_1 x^{(0)} - A_1^\top A_1 x^{(0)}.
\end{aligned}$$

Recursive least squares

Update equations

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