Numerical Analysis   Mar 12, 2020

When solving $A\vec{x} = \vec{b}$, the absolute condition number:

$$\vec{x} = A^{-1}\vec{b}$$

$$\|\vec{x} - \vec{x}'\| \le \|A^{-1}\| \cdot \|\vec{b} - \vec{b}'\|$$

Relative condition number:

$$\frac{\|\vec{x} - \vec{x}'\|}{\|\vec{x}\|} \le \underbrace{\|A\| \cdot \|A^{-1}\|}_{K(A)} \cdot \frac{\|\vec{b} - \vec{b}'\|}{\|\vec{b}\|}$$

The most important case: $\|\cdot\| = \|\cdot\|_2$.

$$\Rightarrow \quad K_2(A) = \sqrt{\frac{\lambda_1}{\lambda_n}}$$

where λ_1 is largest eigenvalue of A^TA

λ_n is the smallest eigenvalue.

Write A in SVD form:

$$A = U \Sigma V^T$$

Σ: diagonal, with entries $\sigma_1 \ge \dots \ge \sigma_n \ge 0$

U, V: are orthogonal matrices

Then

$$A^TA = V \Sigma^T \underbrace{U^T U}_{I} \Sigma V^T$$

$$= V \Sigma^2 V^T$$

V: eigenvectors of A^TA

Σ^2: eigenvalues of $A^TA \Rightarrow \sigma_1^2 \ge \sigma_2^2 \ge \dots \ge \sigma_n^2$

So therefore:

$$K_2(A) = \sqrt{\frac{\lambda_1}{\lambda_n}} = \sqrt{\frac{\sigma_1^2}{\sigma_n^2}} = \frac{\sigma_1}{\sigma_n}$$

Consequences of $K_2(A)$:

$$\frac{\|\vec{x}-\vec{x}'\|}{\|\vec{x}\|} \leq K_2(A) \frac{\|\vec{b}-\vec{b}'\|}{\|\vec{b}\|}$$

True problem is $A\vec{x}=\vec{b}$

Imagine that $\vec{b}'$ is the floating point representation of $\vec{b}$, meaning $\vec{b}' = \text{round}(\vec{b})$.

If machine precision is ϵ, then $\frac{\|\vec{b}-\vec{b}'\|}{\|\vec{b}\|} \sim O(\epsilon)$.

$\epsilon \sim 10^{-16}$

$$\Rightarrow \frac{\|\vec{x}-\vec{x}'\|}{\|\vec{x}\|} \underset{\approx}{\leq} K_2(A)\cdot\epsilon$$

$\Rightarrow$ The number of significant digits lost in solving $A\vec{x}=\vec{b}$ is $\sim -\log_{10}(K_2(A)\cdot\epsilon)$.

Ex: Double precision floating point $\Rightarrow \epsilon \sim 10^{-16}$

Compute $K_2 = 10^{10}$

$$\Rightarrow \frac{\|\vec{x}-\vec{x}'\|}{\|\vec{x}\|} \leq \epsilon\cdot K_2 = 10^{-6}$$

This doesn't mean that $\frac{\|\vec{x}-\vec{x}'\|}{\|\vec{x}\|}$ cannot be smaller, but it puts a bound on how bad it can be.

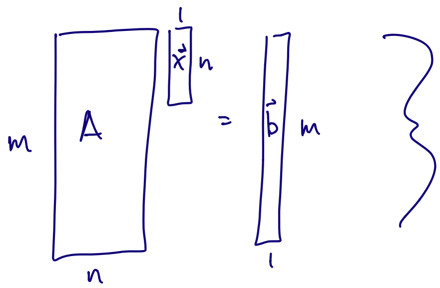
Least Squares

Two canonical problems in linear algebra:

① Solve $A\vec{x} = \vec{b}$ ⟹ A is a square $n \times n$ matrix.

② Find "the best" solution to a system $A\vec{x} = \vec{b}$ where A is an $m \times n$ matrix.

Ex:



In general, not solvable because $m > n$.

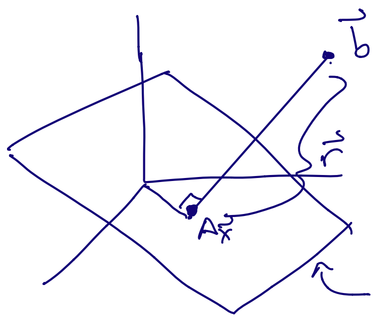
One version of "the best" solution is the least squares solution:

Least squares: For $A \in \mathbb{R}^{m \times n}$, with $m > n$, find $\vec{x}$ such that $\|A\vec{x} - \vec{b}\|_2$ is as small as possible.

↳ The fact that this is the 2-norm is important

Ex: $A \in \mathbb{R}^{3 \times 2}$

Geometrically



$$\min \|A\vec{x} - \vec{b}\|_2$$

minimize the distance between $\vec{b}$ and $A\vec{x}$.

column space of A
col(A)

We also have that

$$\|A\vec{x} - \vec{b}\|_2^2 = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} a_{ij} x_j - b_i \right)^2 = f(\vec{x})$$

If all you knew was calculus, then you could solve this by find the solution to

$$\left.\begin{aligned} \frac{\partial f}{\partial x_1} &= 0 \\ &\vdots \\ \frac{\partial f}{\partial x_n} &= 0 \end{aligned}\right\}$$

Finding a zero of f'

⟹ minimization or maximization

Let $\vec{r} = \vec{b} - A\vec{x}$ = residual vector.

$\Rightarrow \|\vec{r}\|$ = distance from $\mathrm{col}(A)$ to $\vec{b}$.

perpendicular.

If $\vec{x}$ is the least squares solution, then $\vec{r} \perp \mathrm{col}\, A$,

in particular, $A^T\vec{r} = \vec{0}$.

$$\Rightarrow A^T\vec{r} = \vec{0} = A^T(\vec{b} - A\vec{x})$$
$$= A^T\vec{b} - A^TA\vec{x}$$

$\Rightarrow$ The least squares solution $\vec{x}$ solves $\underbrace{A^TA\vec{x} = A^T\vec{b}}_{\text{"normal equations"}}$.

These equations have at least one solution.

From a numerical point of view, how best to find $\vec{x}$ to $\min \|A\vec{x} - \vec{b}\|_2$?

Options: (1) Solve the normal equations:

$$A^TA\vec{x} = A^T\vec{b}$$

$m \times n$

Drawback: Solving $A^TA\vec{x} = A^T\vec{b}$ has a condition number that is the square of $A\vec{x} = \vec{b}$.

Ex: If A is $m \times n$ with rank n, then

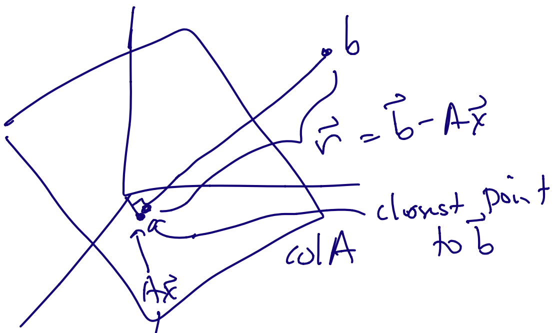
$$A = U_{m\times n} S_{n\times n} V^T_{n\times n} \Rightarrow \mathrm{cond}(A) = \frac{\sigma_1}{\sigma_n}$$

$$A^TA = V S^2 V^T \Rightarrow \mathrm{cond}(A^TA) = \frac{\sigma_1^2}{\sigma_n^2}$$

So if $\mathrm{cond}(A) = 10^4$, then $\mathrm{cond}(A^TA) = 10^8$.

Option (2) Use calculus to $\min \|A\vec{x} - \vec{b}\|$

Goal: $\min \|A\vec{x} - \vec{b}\|$ <u>without</u> solving the normal equations.



<u>Idea</u>: Construct a linear system that is consistent (i.e. has a solution), without computing A^TA.

Instead of solving $A\vec{x} = \vec{b}$, (which has no solution),

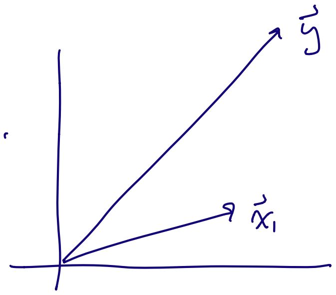
solve $A\vec{x} = \vec{b}' \leftarrow \vec{b}' =$ orthogonal projection of $\vec{b}$ onto the column space of A.

$$\boxed{A\vec{x} = \text{proj}_{\text{col}A}\vec{b}} = \vec{b}'$$

How do we compute $\text{proj}_{\text{col}A}\vec{b}$?

How do we compute a projection of one vector onto another?

In 2D.

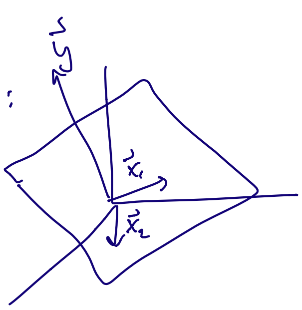


The orthogonal projection of $\vec{y}$ onto $\vec{x}_1$ is the component of $\vec{y}$ pointing in the $\vec{x}_1$ direction.

$$\text{proj}_{\vec{x}_1}\vec{y} = \underbrace{\left(\vec{y}, \frac{\vec{x}_1}{\|\vec{x}_1\|}\right)}_{\text{inner product}} \frac{\vec{x}_1}{\|\vec{x}_1\|}$$

$\frac{\vec{x}_1}{\|\vec{x}_1\|} \longrightarrow$ unit vector pointing in the direction of $\vec{x}_1$.

<u>In 3D</u>:



$\text{proj}_X \vec{y}$ = the component of $\vec{y}$ in the $\vec{x}_1$-$\vec{x}_2$ plane.

$$= (\vec{y}, \hat{x}_1)\,\hat{x}_1 + \left(\underbrace{\vec{y} - (\vec{y}, \hat{x}_1)\,\hat{x}_1}_{\substack{\text{the remaining part of} \\ \vec{y} \text{ after projecting onto } \hat{x}_1}}, \hat{x}_2\right)\hat{x}_2$$

$\hat{x}_1 = \frac{\vec{x}_1}{\|\vec{x}_1\|}$

If $(\hat{x}_1, \hat{x}_2) = 0$, (orthogonal), then
$\text{proj}_X \vec{y} = (\vec{y}, \hat{x}_1)\,\hat{x}_1 + (\vec{y}, \hat{x}_2)\,\hat{x}_2$ | Gram Schmidt process.

So this suggests that we want to find an orthonormal basis for col(A), $U = \text{span}\{\hat{u}_1, \ldots, u_n\}$ and then project $\vec{b}$ onto U, forming $\vec{b}'$.

$$\vec{b}' = (\vec{b}, \hat{u}_1)\hat{u}_1 + (\vec{b}, \hat{u}_2)\hat{u}_2 + \ldots + (\vec{b}, \hat{u}_n)\hat{u}_n$$

$$= \begin{pmatrix} \hat{u}_1 & \hat{u}_2 & \cdots & \hat{u}_n \end{pmatrix} \begin{pmatrix} (\vec{b}, \hat{u}_1) \\ (\vec{b}, \hat{u}_2) \\ \vdots \\ (\vec{b}, \hat{u}_n) \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} \hat{u}_1 & \hat{u}_2 & \cdots & \hat{u}_n \end{pmatrix}} \begin{pmatrix} \hat{u}_1^T \\ \hat{u}_2^T \\ \vdots \\ \hat{u}_n^T \end{pmatrix} \vec{b}$$

$$= \underbrace{U U^T \vec{b}}$$

orthogonal projection of $\vec{b}$ onto the columnspace of A

$\Rightarrow$ The linear system $A\vec{x} = UU^T\vec{b}$ is consistent.