CSC338 Midterm Feb 26. 3:10pm – 4 pm.

Bring your:
- pen or pencil
- non-programmable calculator
- single-sided aid sheet (8.5 × 11)
  - ↳ cannot be photocopied: you must produce your own aid sheet

Coverage: Lecture 1–6, up to but excluding QR factorization
Tutorials 1–6
Homework 1–5.

Practise tests are on the course website.

↳ Google doc to share solutions?

↳ Post study material on Piazza and I will pin.

please don't post (except aid sheets)

We will resume lecture at 4:20 pm.

CSC 338 Numerical Methods Lecture 6

Linear Least Squares Setup:

We wish to solve the system $A\underline{x} = \underline{b}$ with $A \in \mathbb{R}^{m \times n}$, $m > n$

So we solve for $\underline{x}$ that minimizes $\|A\underline{x} - \underline{b}\|_2$.

Last class, we showed that $\|A\underline{x} - \underline{b}\|_2$ is minimized when $\underline{x}$ satisfies the normal equation $\underbrace{A^TA}_{n \times n}\underline{x} = \underbrace{A^T\underline{b}}_{n \times 1}$

Normal Equation Method Summary

$$A\underline{x} \approx \underline{b} \xrightarrow{\text{normal equation}} \overbrace{(A^TA)}^{\text{symmetric positive definite}}\underline{x} = A^T\underline{b} \xrightarrow{\text{cholesky factorization}} (LL^T)\underline{x} = A^T\underline{b}$$

Rectangular System — Square System — Triangular System

Today:
1. Geometry of the normal equation
2. Normal equation method conditioning
3. Conditioning of $A\underline{x} = \underline{b}$, $A \in \mathbb{R}^{m \times n}$, $m > n$.
4. QR ~~transform~~ factorization & Householder Transformation

Def Two vectors $\underline{u}, \underline{v} \in \mathbb{R}^m$ are orthogonal (perpendicular, normal) if $\underline{u}^T\underline{v} = 0$.

Recall $\underline{u}^T\underline{v} = \|\underline{u}\|_2\|\underline{v}\|_2 \cos(\theta)$. where θ is the angle between $\underline{u}$ and $\underline{v}$.

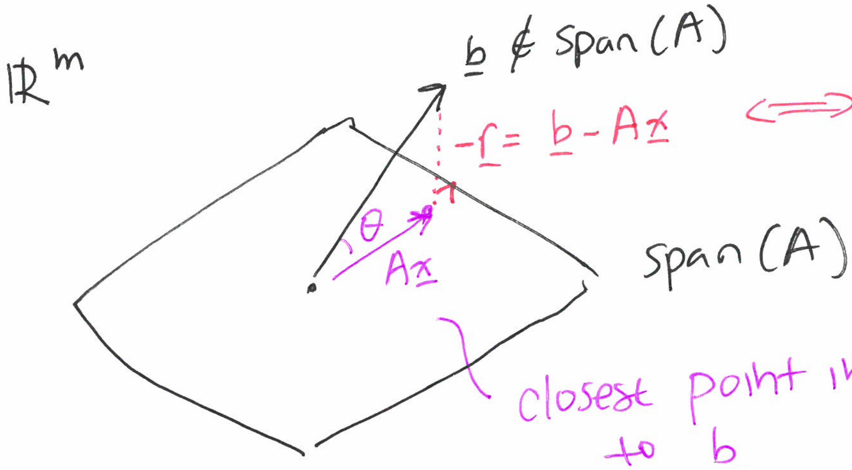
So $\underline{u}^T\underline{v} = 0$ means $\theta = 90°$

$= \frac{\pi}{2}.$

From the normal equation $A^T A \underline{x} = A^T \underline{b}$

$$\Rightarrow \underbrace{A^T}_{n\times m}\underbrace{(A\underline{x}-\underline{b})}_{m\times 1 \text{ vector}} = \underline{0}$$

So each column of A is perpendicular to $\underline{r} = A\underline{x} - \underline{b}$



$\Longleftrightarrow$ to minimize $\|\underline{r}\|_2$, $\underline{r}$ should be perpendicular to span(A)

closest point in span(A) to $\underline{b}$

Conditioning of $A\underline{x} \approx \underline{b}$, $A \in \mathbb{R}^{m\times n}$, $m > n$

Since $A \in \mathbb{R}^{m\times n}$ not square, $\text{cond}(A) = \|A\|\cdot\|A^{-1}\|$ not defined.

<u>Def</u> The pseudoinverse A^+ of an $m\times n$ matrix, $m > n$, $\text{rank}(A) = n$ is

$$\underbrace{A^+}_{n\times m} = \underbrace{(A^T A)^{-1}}_{n\times n}\underbrace{A^T}_{n\times m}$$

Note that $A^+ A = (A^T A)^{-1} A^T A = I$

The least-squares solution to $A\underline{x} \approx \underline{b}$ is given by

$$\underline{x} = A^+ b$$

<u>Def</u> For $A \in \mathbb{R}^{m\times n}$ with $m > n$

$$\text{cond}(A) = \begin{cases} \|A\|\cdot\|A^+\| & \text{if } \text{rank}(A) = n \\ \infty & \text{if } \text{rank}(A) < n \end{cases}$$

Unlike in a square system, the conditioning of $\underline{A\underline{x}} \approx \underline{b}$ depends on both A and $\underline{b}$.

We use θ to represent the angle betwen $\underline{b}$ and $y = A\underline{x}$ (closest point to $\underline{b}$ in span(A)).

Then $\cos(\theta) = \dfrac{\text{adj}}{\text{hyp}} = \dfrac{\|A\underline{x}\|_2}{\|\underline{b}\|_2}$.

If we perturb $\underline{b}$ by $\underline{\Delta b}$ and obtain the perturbed solution $(\underline{x} + \underline{\Delta x})$, $\underline{x}$ is solution to $\min_{\underline{x}} \|A\underline{x} - \underline{b}\|_2$

$$A^TA(\underline{x} + \underline{\Delta x}) = A^T(\underline{b} + \underline{\Delta b})$$ ~ normal equation

$$A^TA\underline{\Delta x} = A^T\underline{\Delta b}$$ ~ Because $A^TA\underline{x} = A^T\underline{b}$

$$\underline{\Delta x} = (A^TA)^{-1}A^T\underline{\Delta b}$$
$$= A^+\underline{\Delta b}$$

$$\frac{\|\underline{\Delta x}\|_2}{\|\underline{x}\|_2} \le \frac{\|A^+\|_2 \|\underline{\Delta b}\|_2}{\|\underline{x}\|_2}$$ ~ property of $\|A\|_2$ matrix norm

$$\frac{\|\underline{\Delta x}\|_2}{\|\underline{x}\|_2} \le \|A^+\|_2 \frac{\|A\|_2}{\|A\|_2} \frac{\|\underline{b}\|_2}{\|\underline{b}\|_2} \frac{\|\underline{\Delta b}\|_2}{\|\underline{x}\|_2}.$$

$$= \text{cond}(A) \frac{\|\underline{b}\|_2}{\|A\|_2\|\underline{x}\|_2} \frac{\|\underline{\Delta b}\|}{\|\underline{b}\|_2}$$

$$\le \text{cond}(A) \frac{\|\underline{b}\|_2}{\|A\underline{x}\|_2} \frac{\|\underline{\Delta b}\|}{\|\underline{b}\|_2}$$ ~ $\|A\underline{x}\|_2 \le \|A\|_2 \|\underline{x}\|_2$

$$\underbrace{\frac{\|\Delta \underline{x}\|_2}{\|\underline{x}\|_2}}_{\text{relative error in computed solution}} \le \underbrace{\mathrm{cond}_2(A)\,\frac{1}{\cos(\theta)}}_{\text{Conditioning of } A\underline{x} \approx \underline{b} \text{ with respect to perturbations in } \underline{b}} \underbrace{\frac{\|\Delta \underline{b}\|_2}{\|\underline{b}\|_2}}_{\text{relative error in } \underline{b} \text{ (relative perturbation)}}.$$

The condition number of the problem $A\underline{x} \approx \underline{b}$ with respect to perturbations in $\underline{b}$ is $\dfrac{\mathrm{cond}(A)}{\cos(\theta)}$,

which is small when cond(A) is small, and $\cos(\theta) \approx 1$ so the angle θ is small.

Similarly, for a perturbation ΔA on A, we have

$$\frac{\|\Delta \underline{x}\|_2}{\|\underline{x}\|_2} \le \left(\mathrm{cond}(A)^2 \underbrace{\tan(\theta)}_{\text{also depends on } \theta,} + \mathrm{cond}(A)\right) \frac{\|\Delta A\|_2}{\|A\|_2}$$

also small when θ is small

The problem with the normal equation is that its condition number is $\mathrm{cond}(A^T A) = \mathrm{cond}(A)^2$

So the sensitivity of the normal equation is <u>worse</u> than the original equation.

eg// Information can be lost in the cross-product matrix A^TA.

$$A = \begin{bmatrix} 1 & 1 \\ \epsilon & 0 \\ 0 & \epsilon \end{bmatrix} \quad \text{where } 0 < \epsilon < \sqrt{\epsilon_{mach}}$$

in floating-point arithmetic

$$A^TA = \begin{bmatrix} 1+\epsilon^2 & 1 \\ 1 & 1+\epsilon^2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

midterm coverage up to here

So what do we actually do to solve $A\underline{x} \approx \underline{b}$?

Inspiration: to solve $A\underline{x} = \underline{b}$, $A \in \mathbb{R}^{n\times n}$, we found a transformation $MA\underline{x} = M\underline{b}$, $M \in \mathbb{R}^{n\times n}$, M invertible, and (MA) is triangular.

Idea behind QR Factorization

Use a similar idea to G.E. to reduce the system $A\underline{x} \approx \underline{b}$ to another system

$$\begin{array}{r} n\times n \\ (m-n)\times n \end{array}\left\{\begin{bmatrix} R \\ \underline{0} \end{bmatrix}\right. \underbrace{\underline{x}}_{n\times 1} \approx \begin{bmatrix} \underline{c}_1 \\ \underline{c}_2 \end{bmatrix} \begin{array}{l} \} \ n\times 1 \\ \} \ (m-n)\times 1. \end{array}$$

with $A = Q\begin{bmatrix} R \\ 0 \end{bmatrix}$, matrix of zeros, R triangular, where the new system has the same solution to $\min_{\underline{x}} \left\| \begin{bmatrix} R \\ 0 \end{bmatrix}\underline{x} - \begin{bmatrix} \underline{c}_1 \\ \underline{c}_2 \end{bmatrix} \right\|_2$

$$\begin{array}{r} n\times n \\ (m-n)\times n \end{array} \begin{bmatrix} R \\ 0 \end{bmatrix} \underbrace{\underline{x}}_{n\times 1} = \begin{bmatrix} \boxed{\underline{c}_1} \\ \boxed{\underline{c}_2} \end{bmatrix} \begin{array}{l} \} \ n\times 1 \\ \} \ (m-n)\times 1 \end{array}$$

If we have such a system $R\underline{x} = \underline{c}_1$ can be solved exactly

$0\underline{x} = \underline{c}_2$ cannot be solved

So to minimize $\|A\underline{x}-\underline{b}\|_2^2 = \|R\underline{x}-\underline{c}_1\|_2^2 + \|0\underline{x}-\underline{c}_2\|_2^2$.

set $\underline{x}$ to be the solution to $R\underline{x} = \underline{c}_1$,

and $\min \|A\underline{x}-\underline{b}\|_2 = \|\underline{c}_2\|_2$

Q : Can we use G.E. to factorize $A = Q\begin{bmatrix} R \\ 0 \end{bmatrix}$?

Answer: unfortunately no, because Q needs to preserve the norm of the residual, and elementary elimination matrices do not.

e.g. $A = \begin{bmatrix} 1 & 2 \\ -1 & 1 \end{bmatrix}$ $\quad \underline{b} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$.

If we have $\underline{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ then $\|A\underline{x}-\underline{b}\|_2$
$= \left\| \begin{bmatrix} 3 \\ 0 \end{bmatrix} - \begin{bmatrix} 2 \\ 0 \end{bmatrix} \right\| = 1$.

not equal

Eliminate below first diagonal:

$A' = \begin{bmatrix} 1 & 2 \\ 0 & 3 \end{bmatrix}$ $\quad \underline{b}' = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$

So $\|M(A\underline{x}-\underline{b})\|_2 = \|A'\underline{x}-\underline{b}'\|_2 = \left\| \begin{bmatrix} 3 \\ 3 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \end{bmatrix} \right\|_2 = \sqrt{2}$

We need another set of transformations that are norm preserving.

Def : A square matrix Q is orthogonal if its columns are orthonormal, i.e. $Q^TQ = I$.

1. Orthogonal matrices are norm preserving

$$\|Q\underline{v}\|_2^2 = (Q\underline{v})^T(Q\underline{v}) = \underline{v}^T\underbrace{Q^TQ}_{I}\underline{v} = \underline{v}^T\underline{v} = \|\underline{v}\|_2^2$$

2. A product of orthogonal matrices is orthogonal

$$(Q_1Q_2)^T(Q_1Q_2) = Q_2^T \underbrace{Q_1^TQ_1}_{I} Q_2 = Q_2^TQ_2 = I.$$

<u>Idea</u>: we will use orthogonal transformations to factor

$$A = Q\begin{bmatrix} R \\ 0 \end{bmatrix}.$$

Just like in G.E., we will annihilate values in A below the diagonals, one column at a time.

$$A = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix}$$

we will find Q_1 such that

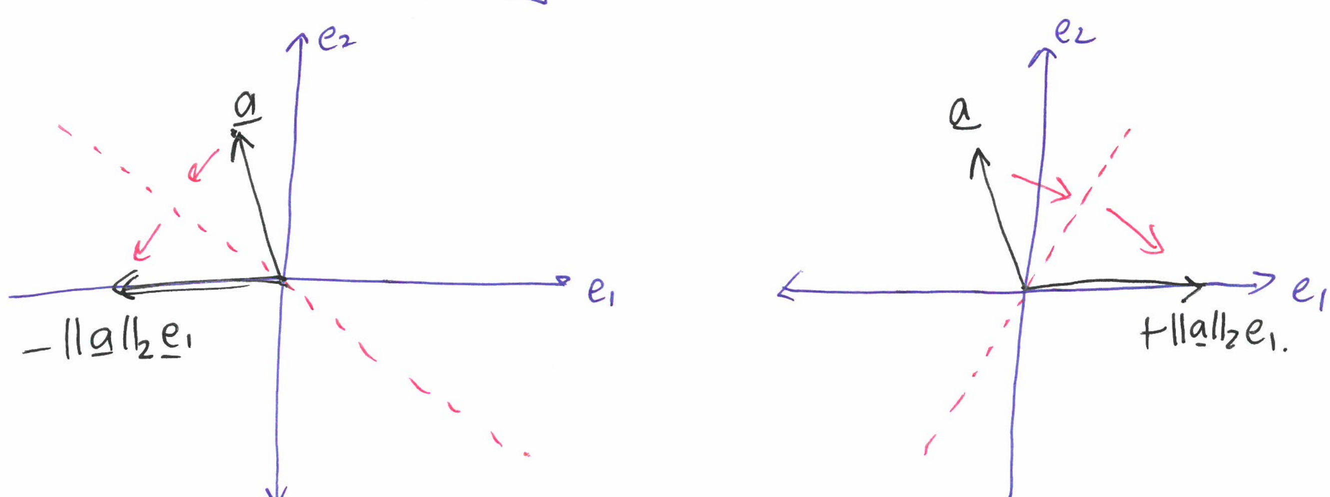
$$Q_1\underline{a}_1 = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

then repeat for other columns.

Householder Transformation

We seek an orthogonal transform that annihilates all but the first component of a vector.

eg// in 2D, $\underline{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \xrightarrow{Q\underline{a}} \begin{bmatrix} \alpha \\ 0 \end{bmatrix}$ with $\|Q\underline{a}\|_2 = \|\underline{a}\|_2$



Householder transform ⇒ reflection about dotted line.

<u>Def</u> A Householder transform or elementary reflector is a matrix of the form $H = I - 2\frac{\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}}$ where $\underline{v} \neq 0$.

we can show that H is orthogonal (exercise)

So given a vector $\underline{a}$, we need to choose a vector $\underline{v}$ such that $H\underline{a} = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \cdot \underline{e}_1$

We need
$$\alpha \underline{e}_1 = H\underline{a}$$
$$= \left(I - 2\frac{\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}}\right)\underline{a}$$
$$= \underline{a} - 2\underline{v}\frac{\underline{v}^T\underline{a}}{\underline{v}^T\underline{v}}$$
Scalar.
$$\Rightarrow \underline{v} = (\underline{a} - \alpha\underline{e}_1)\frac{\underline{v}^T\underline{v}}{\underline{v}^T\underline{a}}$$

Since $\|\underline{v}\|_2$ divides out in the formula for H, we can take $\underline{v} = \underline{a} - \alpha\,\underline{e}_1$.

To preserve norm, we need $\|\alpha\underline{e}_1\|_2 = \|\underline{a}\|_2$

so $\alpha = \pm\|\underline{a}\|_2$

Choose the sign to avoid cancellation in $\underline{v} = \underline{a} - \alpha\underline{e}_1$ based on the first component of $\underline{a}$.

eg// $\underline{a} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix}$ we want an orthogonal transform that transforms $\underline{a}$ to $\begin{bmatrix} \alpha \\ 0 \\ 0 \end{bmatrix}$

Choose $\underline{v} = \underline{a} - \alpha \underline{e}_1$

$$= \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \alpha \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$\|a\|_2 = \sqrt{4+1+4} = 3$

$$= \begin{bmatrix} 2-\alpha \\ 1 \\ 2 \end{bmatrix}$$

choose $\alpha = -3$

$$= \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$$

verify $H\underline{a} = \underline{a} - 2 \dfrac{\underline{v}^T\underline{a}}{\underline{v}^T\underline{v}} \cdot v$

$$= \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - 2 \frac{\overset{15}{2\cdot5 + 1\cdot1 + 2\cdot2}}{\underset{30}{5\cdot5 + 1\cdot1 + 2\cdot2}} \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$$

$$= \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$$

$$= \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \\ 0 \end{bmatrix} \text{ as expected.}$$

~~Scratch~~

SCRATCH NOTES

$$Q = \begin{bmatrix} | & | & | & | \\ q_1 & q_2 & q_3 & q_4 \\ | & | & | & | \end{bmatrix}$$

$\cos(\theta)\|q_4\|\|q_1\|$

$\|q_1\|_2$

$$Q^TQ = \begin{bmatrix} q_1^Tq_1 & q_2^Tq_1 & q_3^Tq_1 & q_4^Tq_1 \\ q_1^Tq_2 & q_2^Tq_2 & \cdots & \\ \vdots & & & \end{bmatrix} = I$$

$\|q_2\|_2$.