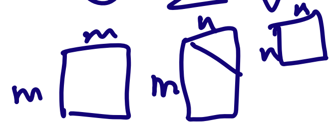
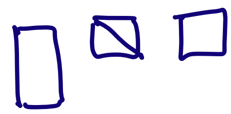
Welcome to Ma221! Lec 5, Fa2024

SVD $A^{m \times n} = U \Sigma V^T$ $\quad$ U, V orthog

$m \geq n$





"thin SVD" if $m > n$

Fact 1: If $A^{n \times n}$, nonsingular can solve $Ax = b$ in $O(n^2)$ more flops

$$x = A^{-1} b = (U \Sigma V^T)^{-1} b = (V \Sigma^{-1} U^T) b$$

$$= V(\Sigma^{-1}(U^T b)) \quad \text{cost } O(n^2)$$

Gauss Elim cheaper

SVD gives error bound

Fact 2: $m > n$ solve $\arg\min_x \|Ax - b\|_2$

$A = U^{m \times n} \Sigma^{n \times n} V^{T\, n \times n}$ $\quad$ thin SVD

$x = V \Sigma^{-1} U^T b$, same as above

proof: $A = \hat{U} \hat{\Sigma} V^T$

$$\hat{U} = m\begin{array}{c} \begin{array}{cc} n & m-n \end{array} \\ \left[U, U' \right] \end{array}, \quad \hat{\Sigma} = \begin{array}{c} n \\ m-n \end{array} \left[\begin{array}{c} \Sigma \\ 0 \end{array} \right]$$

$$\|Ax-b\|_2^2 = \|\hat{U}\hat{\Sigma}V^T x - b\|_2^2$$

$$= \|\hat{U}^T(\quad " \quad)\|_2^2$$

$$= \|\hat{\Sigma}V^T x - \hat{U}^T b\|_2^2$$

$$= \left\| \begin{bmatrix} \Sigma V^T x \\ 0 \end{bmatrix} - \begin{bmatrix} U^T b \\ U^T b \end{bmatrix} \right\|_2^2$$

$$= \|\underbrace{\Sigma V^T x - U^T b}_{\text{make } =0 \text{ to minimize}}\|_2^2 + \|U^T b\|_2^2$$

Solve $\Sigma V^T x = U^T b$

$x = V\Sigma^{-1}U^T b$ same as above

Def $A = U\Sigma V^T$ $m \times n$ $m \geq n$
full rank

$A^+ = V\Sigma^{-1}U^T$

called Moore-Penrose Pseudoinverse

pinv(A) in Matlab

natural generalization A^{-1} to rectangular case

Extends to rank deficient case

underdetermined LS

see Q 3.13 for more properties

QR faster for LS, but SVD

gives us error bounds for LS

Fact 3 $A = A^T$ with evals $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$

evecs $v_1, \dots, v_n$

which are orthonormal

$$V = [v_1, \dots, v_n], \quad \Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

$$A = V \Lambda V^T$$

$= \text{SVD}$ if all $\lambda_i \ge 0$

otherwise $(VD)(\underbrace{D\Lambda}_{\text{all nonnegative entries}})V^T$

$$D_{ii} = \operatorname{sign}(\lambda_i)$$

= SVD except $D\Lambda$ may not be sorted

to reorder, to sort, use permutation matrix P

$$= (\underbrace{VDP}_{\text{orthog}})(P^T D \Lambda P)(\underbrace{P^T V^T}_{\text{orthog}})$$

Fact 4: Using thin SVD of $A = U \Sigma V^T$

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

$$= (V \Sigma^T \underbrace{U^T)(U}_{I} \Sigma V^T)$$

$$= V \underbrace{(\Sigma^T \Sigma)}_{\text{diagonal}} V^T$$

Fact 5: $AA^T = (U \Sigma V^T)(U \Sigma V^T)^T$

$$= (U \Sigma \underbrace{V^T) V}_{I} \Sigma^T U^T$$

$$= U \Sigma \Sigma^T U^T$$

$= U \ \Sigma \ \Sigma^T \ U^T$

$$= \begin{bmatrix} U \end{bmatrix} \left[\begin{array}{c|c} \Sigma^2 & 0 \\ \hline 0 & 0 \end{array}\right] \boxed{U^T}$$

$$= \left[\begin{array}{c|c} U & \tilde{U} \end{array}\right] \left[\begin{array}{c|c} \Sigma^2 & 0 \\ \hline 0 & 0 \end{array}\right] \left[\begin{array}{c|c} U & \hat{U} \end{array}\right]^T$$

Fact 6: $H = \begin{array}{c} \\ n \\ m \end{array} \begin{array}{c} \begin{array}{cc} n & m \end{array} \\ \left[\begin{array}{c|c} 0 & A^T \\ \hline A & 0 \end{array}\right] \end{array} = H^T$

H has evals $\pm \sigma_i$'s of A + 0s if $m \neq n$

$A = U \Sigma V^T$ evecs $\frac{1}{\sqrt{2}} \begin{bmatrix} v(i) \\ \pm u(i) \end{bmatrix}$

$\Rightarrow$ algs for sym eigenproblem and algs for SVD closely related (proof Q3.14)

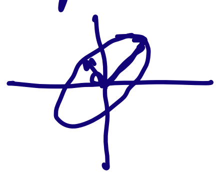
Fact 7: $A^{n \times n} \Rightarrow \|A\|_2 = \sigma_1$, $\|A^{-1}\|_2 = \frac{1}{\sigma_n}$

$\sigma_1 \geq \cdots \geq \sigma_n > 0$

Def: $K(A) = \frac{\sigma_1}{\sigma_n}$ = condition number of A

Fact 8: Let S be unit sphere in $\mathbb{R}^n$

Then $A \cdot S$ is an ellipsoid centered at 0 with principal axes



$\sigma_i u_i$

proof: $s = [s_1, \dots, s_n] \in S$, $\|s\|_2 = 1$

$$As = U\Sigma \underbrace{V^T s}_{\text{unit vector}} = U\Sigma \hat{s} = \sum_i u_i(\sigma_i \hat{s}_i)$$

$$\hat{s} \in S$$

$$u_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, u_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad As = \begin{bmatrix} \sigma_1 \hat{s}_1 \\ \sigma_2 \hat{s}_2 \end{bmatrix} = \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\left(\frac{x}{\sigma_1}\right)^2 + \left(\frac{y}{\sigma_2}\right)^2 = \hat{s}_1^2 + \hat{s}_2^2 = 1$$

Fact 9: Suppose: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0 = \sigma_{r+1} = \dots = \sigma_n$

$r = \text{rank}(A)$

nullspace $= \text{span}\{v_{r+1}, v_{r+2}, \dots, v_n\}$

rangespace $= \text{span}(u_1, u_2, \dots, u_r\}$

$$Ax = U\Sigma(V^T x) = \sum_i u_i \sigma_i (V^T x)_i$$

$$= \sum_{i=1}^{r} u_i \sigma_i (V^T x)_i$$

Fact 10: Matrix A_k of rank k closest to A in $\|\cdot\|_2$ is

$$A_k = \sum_{i=\phi}^{k} u_i \sigma_i v_i^T = U\Sigma_k V^T$$

$$\Sigma_k = \text{diag}(\sigma_1, \dots \sigma_k, 0 \dots 0)$$

In particular closest non-full rank matrix to A is at distance $\sigma_n = \sigma_{min}$

proof: A_k has rank k, and has right distance to A: $A - A_k = \sum_{i=k+1}^{n} u_i \sigma_i v_i^T$

$$\|A - A_k\|_2 = \sigma_{k+1}$$

Why is A_k closest such matrix?

Suppose B has rank k, need to show

$$\|A - B\|_2 \geq \sigma_{k+1}$$

nullspace of B has dimension $n-k$

Space spanned by $\{v_1, \ldots, v_{k+1}\}$ has dimension $k+1$

$$\underset{n-k}{\text{nullspace}(B)} \;\underset{+}{\cap}\; \underset{k+1}{\text{span}\{v_1, \ldots, v_{k+1}\}} \;\underset{= n+1}{\supset} \{h\},\ h \neq 0$$

these two spaces intersect in unit vector h

$$\|A - B\|_2 \geq \|(A-B)h\|_2 = \|Ah\|_2$$

$$= \|U \Sigma \underbrace{V^T h}_{x}\|_2 \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{k+1} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$= \|\Sigma x\|_2 = \left\| \begin{bmatrix} \sigma_1 x_1 \\ \sigma_2 x_2 \\ \vdots \\ \sigma_{k+1} x_{k+1} \end{bmatrix} \right\|_2 \geq \sigma_{k+1} \|x\|_2 = \sigma_{k+1}$$

Start using SVD, norms to analyze condition number for A^{-1} and solving $Ax = b$: if A (and b) change a "little" how much can A^{-1} (and x) change?

Recall if $|x|<1$ $\quad \frac{1}{1-x} = 1+x+x^2+\cdots$

Generalize to matrices

Lemma: If operator norm $\|X\|<1$

then $I-X$ nonsingular,

$$(I-X)^{-1} = I + X + X^2 + \cdots = \sum_{i=0}^{\infty} X^i$$

$$\|(I-X)^{-1}\| \leq \frac{1}{1-\|X\|}$$

proof: claim $I+X+X^2\cdots$ converges

$$\|X^i\| \leq \|X\|^i \to 0 \quad \|X\|<1$$

each entry of $I+X+X^2+\cdots$

bounded by a convergent geometric sum

$\Rightarrow$ converges

$$(I-X)\underbrace{(I+X+X^2+\cdots+X^i)}_{\text{converges to } (I-X)^{-1}}$$

$$= I - X^{i+1} \to I \quad \text{as } i\to\infty$$

$$\|I+X+X^2+\cdots\|$$

$$\leq \|I\| + \|X\| + \|X^2\| + \cdots$$

$$\leq \|I\| + \|X\| + \|X\|^2 + \cdots$$

$$= 1 + \|X\| + \|X\|^2 + \cdots$$

$$= \frac{1}{1-\|X\|}$$

Later: generalize for matrix functions

e.g. $$e^x = \sum_{i=0}^{\infty} \frac{1}{i!} x^i$$

Lemma: Suppose A invertible

Then $A-E$ invertible if $\|E\| < \frac{1}{\|A^{-1}\|}$

in which case

$$(A-E)^{-1} = A^{-1} + A^{-1}(EA^{-1}) + A^{-1}(EA^{-1})^2 + \cdots$$

$$\|(A-E)^{-1}\| \le \frac{\|A^{-1}\|}{1 - \|E\|\cdot\|A^{-1}\|} \quad \text{when } \|E\| < \frac{1}{\|A^{-1}\|}$$

proof: $$(A-E)^{-1} = ((I - EA^{-1})A)^{-1}$$

$$= A^{-1}(I - \underbrace{EA^{-1}}_{X})^{-1}$$

$$= A^{-1}(I + X + X^2 + \cdots)$$

$$= A^{-1}(I + (EA^{-1}) + (EA^{-1})^2 + \cdots)$$

$$\|(A-E)^{-1}\| \le \|A^{-1}\| \frac{1}{1 - \|EA^{-1}\|} \le \frac{\|A^{-1}\|}{1 - \|E\|\cdot\|A^{-1}\|}$$

if $\|E\|\cdot\|A^{-1}\| < 1$

Finally: how much can A^{-1} and $(A-E)^{-1}$ differ?

Lemma: Suppose A invertible and $\|E\| < \frac{1}{\|A^{-1}\|}$

$$\|(A-E)^{-1} - A^{-1}\| \le \frac{\|A^{-1}\|^2 \cdot \|E\|}{1 - \|E\|\cdot\|A^{-1}\|}$$

proof: $$(A-E)^{-1} - A^{-1} = A^{-1}(EA^{-1}) + A^{-1}(EA^{-1})^2 + \cdots$$

$$= (A^{-1}EA^{-1})(I + EA^{-1} + (EA^{-1})^2 + \cdots)$$

take norms

$$\|(A-E)^{-1}-A^{-1}\| \le \|A^{-1}EA^{-1}\| \frac{1}{1-\|EA^{-1}\|}$$

$$\|(A-E)^{-1}-A^{-1}\| \le \frac{\|A^{-1}\|^2\|E\|}{1-\|E\|\cdot\|A^{-1}\|}$$

$$\underbrace{\frac{\|(A-E)^{-1}-A^{-1}\|}{\|A^{-1}\|}}_{\substack{\text{relative error}\\ \text{in output}}} \le \underbrace{\frac{\|A^{-1}\|\cdot\|A\|}{1-\|E\|\cdot\|A^{-1}\|}}_{\substack{\text{condition}\\ \text{number}\\ \kappa(A)=\|A^{-1}\|\cdot\|A\|}} \cdot \underbrace{\frac{\|E\|}{\|A\|}}_{\substack{\text{relative error}\\ \text{in input}}}$$

Fact $\kappa(A) \ge 1$

proof: $1 = \|I\| = \|A\cdot A^{-1}\| \le \|A\|\cdot\|A^{-1}\| = \kappa(A)$

Thm: $\min\left\{\frac{\|E\|}{\|A\|} : A-E \text{ singular}\right\}$

$=$ relative distance to nearest singular matrix

$= 1/\kappa(A)$

proof for $\|\cdot\|_2$ using SVD

$\min\{\|E\|_2 : A-E \text{ singular}\} = \sigma_{min}$

relative dist to singularity $=$

$$\frac{\sigma_{min}(A)}{\|A\|_2} = \frac{\sigma_{min}}{\sigma_{max}}$$

$$\|A^{-1}\|_2 = \|(U\Sigma V^T)^{-1}\|_2 = \|V\Sigma^{-1}U^T\|_2 = \|\Sigma^{-1}\|_2$$
$$= \frac{1}{\sigma_{min}}$$

$$\frac{\sigma_{min}}{\sigma_{max}} = \frac{1}{\sigma_{max}/\sigma_{min}} = \frac{1}{\|A\|_2 \cdot \|A^{-1}\|_2} = \frac{1}{\kappa(A)}$$

Extend analysis to solving $Ax=b$
vs $(A-E)\hat{x} = b+f$
$\hat{x} = x+\delta$, want to bound $\|\delta\|$

Subtract: $A\cdot\delta - E\cdot x - E\cdot\delta = f$
$$(A-E)\delta = f + E\cdot x$$
$$\delta = (A-E)^{-1}(f+Ex)$$

$$\|\delta\| = \|(A-E)^{-1}(f+Ex)\|$$
$$\le \|(A-E)^{-1}\| \cdot \|f+Ex\|$$
$$\le \frac{\|A^{-1}\|}{1-\|E\|\cdot\|A^{-1}\|} \cdot (\|f\| + \|E\|\cdot\|x\|)$$

$$\frac{\|\delta\|}{\|x\|} \le \frac{\|A^{-1}\|\cdot\|A\|}{1-\|E\|\cdot\|A^{-1}\|}\left(\frac{\|f\|}{\|A\|\cdot\|x\|} + \frac{\|E\|}{\|A\|}\right)$$

$$\le \frac{\|A^{-1}\|\cdot\|A\|}{1-\|E\|\cdot\|A^{-1}\|}\left(\frac{\|f\|}{\|b\|} + \frac{\|E\|}{\|A\|}\right)$$

rel change in x — condition number — rel change in f — rel change in A

backward stability $\Rightarrow$ $\frac{\|f\|}{\|b\|} = O(\text{macheps})$
$\|E\|/\|A\| = O(\text{macheps})$

Practical question: Given $\hat{x}$, what is its backward error?

Compute residual $r = A\hat{x} - b$

$$r = A\hat{x} - Ax = A(\hat{x} - x) = A \cdot \text{error}$$

$$\text{error} = A^{-1} \cdot r \qquad \|\text{error}\| \le \|A^{-1}\| \cdot \|r\|$$

Thm Smallest E in norm such that $(A+E)\hat{x} = b$ has norm $\|E\| = \dfrac{\|r\|}{\|\hat{x}\|}$

proof: $r = A\hat{x} - b = -E\hat{x}$

$$\|r\| = \|E\hat{x}\| \le \|E\| \cdot \|\hat{x}\|$$

$$\frac{\|r\|}{\|\hat{x}\|} \le \|E\|$$

attainable! in 2-norm: $E = \dfrac{-r \cdot \hat{x}^T}{\|\hat{x}\|_2^2}$

$$\|E\|_2 = \frac{\|r\|_2 \cdot \|\hat{x}\|_2}{\|\hat{x}\|_2^2} = \frac{\|r\|_2}{\|\hat{x}\|_2}$$

Small residual $\Rightarrow$ small backward error

if not small enough, can use iterative refinement (Newton)

Practical error bounds

how to bound $\|A^{-1}\|$ cheaply?

computing A^{-1} costs $O(n^3)$

more than Gauss Elim

Goal: estimate for $O(n^2)$ cost

$$\|A^{-1}\| = \max_{\|x\|=1} \|A^{-1}x\|$$

$$= \max_{\|x\|\le 1} \|A^{-1}x\|$$

use gradient ascent "go uphill"

pick next x to increase

$\|A^{-1}x\|$, each step costs $O(n^2)$

in practice, 5 steps work

Thm (D., Diament, Malojovich, 2000)

to estimate $\|A^{-1}\|$ with any

constant factor guarantee

costs as much as matrix multiply