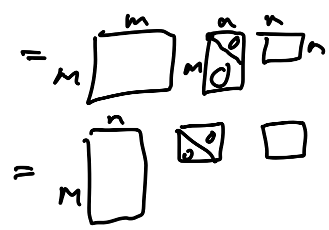
Welcome to Ma 221 !

Finish Norms, SVD, condition number

SVD $\overset{m\times n}{A} = U\Sigma V^T$ $\qquad m \geq n$

$V^{n\times n}, U^{m\times m}$ orthog

$\Sigma = \text{diag}(\sigma_1, \ldots \sigma_n) \qquad \sigma_1 \geq \ldots \geq \sigma_n \geq 0$



"thin svd"

Solve $Ax = b$ square $n \times n$

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

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

cost $= O(n^2)$, LU cheaper

Also solves $x = \underset{x}{\text{argmin}} \|Ax - b\|_2$

$x = \underbrace{V \Sigma^{-1} U^T}_{\text{Moore-Penrose pseudoinverse}} b$ with thin SVD

works for low rank too

QR factorization cheaper for LS

SVD more reliable when
A (near) low rank, error bounds too

Fact 3: A symmetric with
evals $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_n)$
orthonormal evecs $V = [v(1), \dots, v(n)]$

then $A = V \Lambda V^T \quad (AV = V\Lambda)$

$= \text{SVD if } \lambda_i \geq 0$

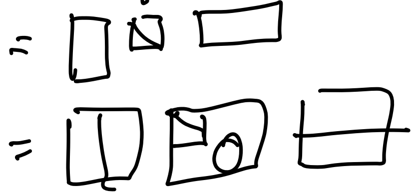
otherwise $= \underbrace{(VD)}_{U} \underbrace{(D\Lambda)}_{\Sigma} V^T$

$D = \mathrm{diag}(\mathrm{sign}(\lambda_i))$

Fact 4: using thin SVD

$$A^T A = (U\Sigma V^T)^T (U\Sigma V^T)$$
$$= V \Sigma^T (U^T U) \Sigma V^T$$
$$= V \Sigma^T \Sigma V^T$$
$$= \text{eigendecomp of } A^T A$$

Fact 5: $AA^T = U \Sigma \Sigma^T U^T$ with thin SVD



Fact 6: $H = \begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix}^{(m+n)\times(m+n)}$

H has evals $\pm\sigma_i$

evecs $\frac{1}{\sqrt{2}} \begin{bmatrix} v(i) \\ \pm u(i) \end{bmatrix}$

$\Rightarrow$ algs for sym eig and SVD closely related

Fact 7: $\|A\|_2 = \sigma_1 \qquad \|A^{-1}\|_2 = \frac{1}{\sigma_n}$

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

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

Fact 8: Let S be a unit sphere in $\mathbb{R}^n$ then $A \cdot S$ is an ellipsoid centered at 0 with principal axes $\sigma_i u_i$

proof: $s = [s_1, \ldots, s_n]$. $\|s\|_2 = 1$

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

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

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

Fact 9: Suppose

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0 = \sigma_{r+1} = \cdots = \sigma_n$$

$\Rightarrow$ rank$(A) = r$

null space = span$(v_{r+1}, \ldots v_n)$

range space = span$(u_1, \ldots, u_r)$

$$Ax = U \Sigma V^T x$$

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

Fact 10: Matrix A_k of rank k closest to A in 2-norm is

$$A_k = \sum_{i=0}^{k} u_i \sigma_i v_i^T = U \Sigma_k V^T$$

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

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

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

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

why is A_k closest such matrix?
Suppose B has rank k, show
$$\|A-B\|_2 \geq \sigma_{k+1}$$

nullspace of B has dimension $n-k$
Space spanned by $\{v_1, \dots, v_{k+1}\}$ has dimension $k+1$

$$\underset{n-k}{\text{nullspace}(B)} \underset{+}{\cap} \underset{k+1}{\text{span}\{v_1, \dots, v_{k+1}\}} \underset{=n+1}{\ni \{h\}}$$

$\Rightarrow$ these two spaces intersect in some unit vector h

$$\|A-B\|_2 \geq \|(A-B)h\|_2 = \|Ah\|_2$$
$$= \|U\Sigma \underbrace{V^T h}_{x}\|_2 \qquad x = \begin{bmatrix} x_1 \\ \vdots \\ x_k \\ x_{k+1} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$
$$= \|\Sigma x\|_2 = \left\| \begin{bmatrix} \sigma_1 x_1 \\ \vdots \\ \sigma_{k+1} x_{k+1} \\ 0 \\ \vdots \end{bmatrix} \right\|_2 \geq \sigma_{k+1} \|x\|_2$$
$$= \sigma_{k+1}$$

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

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

Generalizes to matrices:

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

then $I-X$ nonsingular

$$(I-X)^{-1} = \sum_{i=0}^{\infty} X^i, \quad \|(I-X)^{-1}\| \le \frac{1}{1-\|X\|}$$

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

$\|X^i\| \le \|X\|^i \to 0$ as $i \to \infty$

$\Rightarrow$ each entry of $I + X + X^2 + \cdots$ bounded by a convergent geometric series $\Rightarrow$ converges

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

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

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

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

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

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

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

Later: generalize for matrix functions $f(X)$, eg $e^X = \sum_{i=0}^{\infty} \frac{X^i}{i!}$

Lemma: Suppose A invertible

Then $A - E$ invertible if $\|E\| < \frac{1}{\|A^{-1}\|}$, in which case

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

$$\|(A-E)^{-1}\| \leq \frac{\|A^{-1}\|}{1 - \underbrace{\|E\| \cdot \|A^{-1}\|}_{<1}}$$

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

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

if $\|X\| < 1$ $\quad \|EA^{-1}\| \leq \|E\| \cdot \|A^{-1}\| < 1$

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

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

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

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

$$\underbrace{\frac{\|(A-E)^{-1}-A^{-1}\|}{\|A^{-1}\|}}_{\text{relative error in output}} \le \underbrace{\frac{\|A^{-1}\|\cdot\|A\|}{1-\|E\|\cdot\|A^{-1}\|}} \underbrace{\frac{\|E\|}{\|A\|}}_{\text{rel error in input}}$$

condition number of A : $\kappa(A) = \|A\|\cdot\|A^{-1}\|$

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 from A to nearest singular matrix

$= 1/\kappa(A)$

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

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

relative dist to singularity =

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

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

$$= \|\Sigma^{-1}\|_2 = \frac{1}{\sigma_{min}}$$

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

Extend analysis to solving

$Ax=b$ vs $(A-E)\hat{x} = b+f$

$\hat{x} = x+\delta$ goal: bound $\|\delta\|$

Subtract: $A\cdot\delta x - E\cdot x - E\cdot\delta x = f$

$$(A-E)\delta x = f + Ex$$

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

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

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

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

$$\underbrace{\frac{\|\delta x\|}{\|x\|}}_{\text{relative change in } x} \le \frac{\|A^{-1}\|\cdot\|A\|}{1-\|E\|\cdot\|A^{-1}\|}\left(\frac{\|f\|}{\|x\|\cdot\|A\|}+\frac{\|E\|}{\|A\|}\right)$$

$$\le \underbrace{\frac{\|A^{-1}\|\cdot\|A\|}{1-\|E\|\cdot\|A^{-1}\|}}_{\text{condition number}}\left(\underbrace{\frac{\|f\|}{\|b\|}}_{\text{rel change in } f}+\underbrace{\frac{\|E\|}{\|A\|}}_{\text{rel change in } A}\right)$$

All our algorithms will try to guarantee $\frac{\|f\|}{\|b\|}$ and $\frac{\|E\|}{\|A\|}$ are small ("backward stable") hopefully O(macheps)

Practical Question:
given $\hat{x}$ what is backward error?

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

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

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

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

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

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

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

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

small residual $\Rightarrow$ small backward error

If want better accuracy, can use iterative refinement (Newton)

Practical error bounds

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

computing A^{-1} costs $O(n^3)$ extra, we want just $O(n^2)$

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

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

use gradient ascent
"go uphill" pick next x to
increase $\|A^{-1}x\|$
each step costs $O(n^2)$
$O(5)$ steps in practice

Thm (D., Diament, Malajovich, 2000)
to estimate $\|A^{-1}\|$ with any
constant factor guaranteed,
costs as much as matrix
multiply