Welcome to Ma 221!

Norms, SVD, condition number for $Ax=b$

Summary of how we understand accuracy despite roundoff or uncertainty in input:

Show algorithms are backward stable:

Scalar case for $f(x)$

$$\mathrm{alg}(x) = f(x+\delta) \approx f(x) + f'(x)\cdot\delta$$

where δ small compared to x

Error Bound:

$$\underbrace{\left|\frac{\mathrm{alg}(x)-f(x)}{f(x)}\right|}_{\substack{\text{relative}\\ \text{error in}\\ \text{output}}} \lessapprox \left|\frac{f'(x)\cdot\delta}{f(x)}\right| = \underbrace{\left|\frac{f'(x)\cdot x}{f(x)}\right|}_{\substack{\text{condition}\\ \text{number}}} \cdot \underbrace{\left|\frac{\delta}{x}\right|}_{\substack{\text{relative}\\ \text{error in}\\ \text{input}}}$$

Same approach for $Ax=b$, $Ax=\lambda x$, ..

Get $(A+\Delta)\hat{x} = b$ where

Δ "small" compared to A

What is small

Need vector and matrix norms

$x = f(A)$ get $\mathrm{alg}(A) = \hat{x} = f(A+\Delta)$

error $= \hat{x} - x = f(A+\Delta) - f(A)$

If Δ small enough for Taylor exp.

error $\sim J_f(A) \cdot \Delta$ J = Jacobian

want to bound $|\text{error}| \lessapprox |J_f(A)| \cdot |\Delta|$

what does $|\cdot|$ mean?

Matrix and Vector Norms

Def: Let B be linear space $\mathbb{R}^n$ (or $\mathbb{C}^n$)

It is "normed" if there is

$\|\cdot\| : B \to \mathbb{R}$ s.t.

(1) $\|x\| \geq 0$ and $\|x\| = 0$ iff $x = 0$
"positive definite"

(2) $\|c \cdot x\| = |c| \cdot \|x\|$ "homogeneous"

(3) $\|x+y\| \leq \|x\| + \|y\|$ "triangle inequality"

Examples: p-norm $\|x\|_p = \left(\sum_i |x_i|^p\right)^{\frac{1}{p}}$, $p \geq 1$

Euclidean norm = 2-norm $= \|x\|_2$

x real $\Rightarrow \|x\|_2^2 = \sum_i x_i^2 = x^T x$

∞-norm $\|x\|_\infty = \max_i |x_i|$

C- norm $= \|Cx\|$ where
C has full column rank (HWQ1.5)

Lemma (1.4) All norms are equivalent
given any $\|\cdot\|_a$ and $\|\cdot\|_b$
there are positive constants α, β
$\alpha \cdot \|x\|_a \leq \|x\|_b \leq \beta \|x\|_a \quad \forall x$
(proof: compactness)

Lemma is an excuse to use easiest
norm in any proof (HW Q1.14)

Def: Matrix norm: vector norm on m·n vectors
(1) $\|A\| \geq 0$ and $\|A\| = 0$ iff $A = 0$
(2) $\|c \cdot A\| = |c| \cdot \|A\|$
(3) $\|A+B\| \leq \|A\| + \|B\|$

Ex: max norm $= \max_{ij} |A_{ij}|$

Frobenius norm $= \|A\|_F = \left(\sum_{ij} |A_{ij}|^2\right)^{\frac{1}{2}}$

Def Operator norm: given any vector norm

$$\|A\| = \max_{x \neq 0} \frac{\|Ax\|}{\|x\|}$$

Lemma (1.6) An operator norm is a matrix norm

pf: HW Q. 1.15

Lemma (1.7) if $\|A\|$ is an operator norm then $\exists$ x such that $\|x\|=1$ and $\|Ax\|=\|A\|$

proof: $\|A\| = \max_{x\neq 0} \|Ax\| / \|x\|$

$= \max_{x \neq 0} \|A(x/\|x\|)\|$

$= \max_{\text{unit vectors } y} \|Ay\|$

y attaining maximum exists since $\|Ay\|$ continuous on closed bounded set = unit ball

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Orthogonal + Unitary Matrices (needed for SVD)

Notation: $Q^* = (\overline{Q^T})$

Sometimes Q^H

H stands for Hermitian

(if $A=A^H$ called Hermitian)

Def: orthogonal: Q square, real
$Q^{-1} = Q^T$

unitary: Q square, complex
$Q^{-1} = Q^*$

for simplicity, use real case,
all extends to complex case

Fact: Q orthog $\Leftrightarrow Q^T Q = I$

$\Leftrightarrow (i,j)^{th}$ entry of $Q^T Q$

= dot product of columns i and j of Q

$\Leftrightarrow$ all columns of Q are
pairwise orthogonal and unit
vectors

$QQ^T = I$ implies same for rows

Fact: $\|Qx\|_2 = \|x\|_2$
(aka Pythagorean Thm)

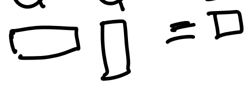
proof: $\|Qx\|_2^2 = (Qx)^T(Qx) = x^T \underbrace{Q^T Q}_{I} x$
$= x^T x = \|x\|_2^2$

Fact: Q, Z orthogonal $\Rightarrow Q \cdot Z$ orthogonal

proof: $(QZ)^T(QZ) = Z^T \underbrace{Q Q^T}_{I} Z = Z^T Z = I$

Fact: if Q $m \times n$, $n < m$ and

$Q^T Q = I_n$ then add $m-n$



more columns to Q, get $m\,[\overset{n}{Q}, \overset{m-n}{\hat{Q}}]$

orthogonal (infinitely many ways to do this, proof later, useful now

Lemma (most proofs in HW Q 1.16)

(1) $\|Ax\| \le \|A\| \cdot \|x\|$ for a vector norm and its operator norm

(2) $\|A \cdot B\| \le \|A\| \cdot \|B\|$ for same operator norm

(3) $\|QAZ\|_2 = \|A\|_2$ if Q, Z orthog.

(4) $\|Q\|_2 = 1$ if Q orthog

(5) $\|A\|_2 = \sqrt{\lambda_{max}(A^T A)}$

(6) $\|A^T\|_2 = \|A\|_2$

proof of (5)

$$\|A\|_2 = \max_{x \ne 0} \frac{\|Ax\|_2}{\|x\|_2}$$

$$= \max_{x \ne 0} \frac{\sqrt{(Ax)^T (Ax)}}{\sqrt{x^T x}}$$

$$= \max_{x \neq 0} \frac{\sqrt{x^T A^T A x}}{\sqrt{x^T x}}$$

$A^T A$ symmetric $\Rightarrow$ has eigendecomposition

(*) $A^T A q_i = \lambda_i q_i$ where λ_i real

q_i all unit orthogonal vectors

$$Q = [q_1, \dots q_n] \qquad \Lambda = \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix}$$

(*) $A^T A Q = Q \Lambda \Rightarrow A^T A = Q \Lambda Q^T$

$$\|A\|_2 = \sqrt{\max_{x \neq 0} \frac{x^T A^T A x}{x^T x}}$$

$$= \sqrt{\max_{x \neq 0} \frac{x^T Q \Lambda Q^T x}{x^T Q \underbrace{Q^T x}_{y}}}$$

$$= \sqrt{\max_{y \neq 0} \frac{y^T \Lambda y}{y^T y}}$$

$$= \sqrt{\max_{y \neq 0} \frac{\sum_i \lambda_i y_i^2}{\sum y_i^2}}$$

$$\leq \sqrt{\max_{y \neq 0} \frac{\sum_i \lambda_{max} y_i^2}{\sum_i y_i^2}} = \sqrt{\lambda_{max}}$$

attainable by $y = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ if $\lambda_{max} = \lambda_1$

SVD = Singular Value Decomposition

Given SVD
- solve $Ax=b$
- solve over or underdetermined LS problems, full rank A or not
- compute evals/evecs of AA^T, A^TA
- compute " " of $A = A^T$
- + error bounds for all these

SVD = Swiss Army Knife of NLA

SVD more expensive than specialized algs, so may not be first resort

History: 1936: first complete version by Eckart + Young

1965: first Backward Stable alg: Golub, Kahan

Faster alg since then: (Chap 5) Ming Gu's currently most popular

Fastest so far: 2010 thesis by Paul Willems – still some hard cases not solved, not in LAPACK (very hard class project!)

Thm: Suppose A $m \times m$. Then $\exists$

orthogonal $U = [u(1), \dots, u(m)]$

diagonal $\Sigma = \mathrm{diag}(\sigma_1, \dots, \sigma_m)$

$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_m \geq 0$

orthogonal $V = [v(1), \dots, v(m)]$

$A = U \Sigma V^T$

$v(i)$ right singular vectors

σ_i singular values

$u(i)$ left sing. vecs.

More Generally A $m \times n$, $m > n$

U $m \times m$, orthog

V $n \times n$, orthog

Σ $m \times n$, same diag

$$\begin{array}{cc} & n \\ m & \begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ & & \sigma_n \\ & 0 & \end{bmatrix} \end{array}$$

Sometimes write as "thin SVD"

$A = [u(1), \ldots, u(n)] \cdot \mathrm{diag}(\sigma_1, \ldots, \sigma_n) \cdot V^T$

$= \; m \overset{n}{[\;\;]} \; n \overset{n}{[\diagdown]} \; n \overset{n}{[\;\;]}$

Same idea if A $m \times n$, $m < n$

Geometric Interpretation

$A^{m \times n}$: linear map from $\mathbb{R}^n \to \mathbb{R}^m$

with right orthogonal bases for $\mathbb{R}^n$ and $\mathbb{R}^m$, A diagonal (Σ)

"all matrices diagonal"

proof that SVD exists: induction on n $\quad m \geq n$

2 base cases

$A^{m \times n} = 0$: $U = I_m$ $\quad \Sigma = 0$ $\quad V = I_n$

$n = 1$ (one column)

Let U's first column $= \frac{A}{\|A\|_2}$

other columns can be chosen in any way so U orthog

$$\sigma_1 = \|A\|_2 , \quad V = 1$$

$$\Sigma = \begin{bmatrix} \sigma_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Induction step (if $A \neq 0$)

$$\|A\|_2 = \max_{x \neq 0} \|Ax\|_2 / \|x\|_2$$

$$= \max_{\|x\|_2 = 1} \|Ax\|_2$$

Let $v(1)$ be x attaining max

$$\sigma_1 = \|A\|_2 = \|A\,v(1)\|_2$$

$$u(1) = Av(1) / \|A\,v(1)\|_2 = Av(1)/\sigma_1$$

$$\left.\begin{array}{l} V = [v(1), \hat{V}] \\ U = [u(1), \hat{U}] \end{array}\right\} \text{square, orthog}$$

$$\hat{A} = U^T A V = \begin{bmatrix} u(1)^T \\ \hat{U}^T \end{bmatrix} A \begin{bmatrix} v(1), \hat{V} \end{bmatrix}$$

$$= \begin{array}{c c} & \begin{array}{c c} 1 & n-1 \end{array} \\ \begin{array}{c} 1 \\ m-1 \end{array} & \left[\begin{array}{c|c} u(1)^T A v(1) & u^T(1) A \hat{V} \\ \hline \hat{U}^T A\, v(1) & \hat{U}^T A \hat{V} \end{array}\right] \end{array} = \left[\begin{array}{c|c} \sigma_1 & \overbrace{A_{12}}^{=0} \\ \hline \underbrace{A_{21}}_{=0} & A_{22} \end{array}\right]$$

$A_{21} = 0$ by def of $\hat{U}$

$A_{12} = 0$ by def of $\sigma_1 = \|A\|_2$

if $\|A_{12}\| \neq 0$ then

$$\|A\|_2 = \|A^T\|_2 = \|\hat{A}^T\|_2 \geq \|\hat{A}^T \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}\|_2 = \|\begin{bmatrix} \sigma_1 \\ A_{12}^T \end{bmatrix}\|_2$$

$$= \sqrt{\sigma_1^2 + A_{12} A_{12}^T} > \sigma_1 \text{ if } A_{12} \neq 0$$

contradiction

Induction: $A_{22} = U_2 \cdot \Sigma_2 \cdot V_2^T$

$$A = U \hat{A} V^T = U \left[\begin{array}{c|c} \sigma_1 & 0 \\ \hline 0 & U_2 \Sigma_2 V_2^T \end{array}\right] V^T$$

$$= \underbrace{U \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & U_2 \end{array}\right]}_{\text{orthog}} \cdot \underbrace{\left[\begin{array}{c|c} \sigma_1 & 0 \\ \hline 0 & \Sigma_2 \end{array}\right]}_{\text{nonneg diag}} \underbrace{\left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & V_2^T \end{array}\right] V^T}_{\text{orthog}}$$

= SVD as desired

Some (of many) useful properties of SVD

$A^{m \times n}$ $m \geq n$

Fact 1: A $n \times n$, nonsingular

can solve $Ax = b$ in $O(n^2)$ more ops

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

Gaussian elimination cheaper

SVD gives error bound

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

use thin SVD - $A = U\Sigma V^T$ $\quad U$ $m\times n$

Σ, V, $n\times n$

$x = V \cdot \Sigma^{-1} U^T b$ same formula

as square case

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

$$\hat{U} = [U, U']^{m\times m} \text{ square + orthog}$$

$$\hat{\Sigma} = \begin{bmatrix} \Sigma \\ 0 \end{bmatrix}^{m\times n}$$

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

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

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

$$= \left\| \begin{bmatrix} \Sigma V^T x \\ 0 \end{bmatrix} - \begin{bmatrix} U^T b \\ U'^T b \end{bmatrix} \right\|_2^2$$

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

$$+ \|U'^T b\|_2$$

minimize by making first term 0

$$\Sigma V^T x - U^T b = 0 \Rightarrow x = V\Sigma^{-1}U^T b$$

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 of A^{-1}
to rectangular case

Extends to rank deficient case
used for underdetermined
Least Squares Problems too

Q 3.13 has more properties