AMS526: Numerical Analysis I (Numerical Linear Algebra)

Lecture 7: Sensitivity of Linear Systems

Xiangmin Jiao

Stony Brook University

Outline

Condition Number of Matrix

- Consider $f(x) = Ax$, with $A \in \mathbb{R}^{m \times n}$

$$\kappa = \frac{\|J\|}{\|f(x)\|/\|x\|} = \frac{\|A\|\|x\|}{\|Ax\|}$$

- If A is square and nonsingular, since $\|x\|/\|Ax\| \leq \|A^{-1}\|$

$$\kappa \leq \|A\|\|A^{-1}\|$$

- We define *condition number of matrix A* as

$$\kappa(A) = \|A\|\|A^{-1}\|$$

- It is the upper bound of the condition number of $f(x) = Ax$ for any x
- For any induced matrix norm, $\kappa(I) = 1$ and $\kappa(A) \geq 1$
- Note about the distinction between the condition number of a *problem* (the map $f(x)$) and the condition number of a *problem instance* (the evaluation of $f(x)$ for specific x)

Geometric Interpretation of Condition Number

- Another way to interpret at $\kappa(A)$ is

$$\kappa(A) = \sup_{\delta x, x} \frac{\|\delta f\| / \|\delta x\|}{\|f(x)\| / \|x\|} = \frac{\sup_{\delta x} \|A \delta x\| / \|\delta x\|}{\inf_{x} \|Ax\| / \|x\|}$$

- Question: For what x and δx is the equality achieved?

Geometric Interpretation of Condition Number

- Another way to interpret at $\kappa(A)$ is

$$\kappa(A) = \sup_{\delta x, x} \frac{\|\delta f\|/\|\delta x\|}{\|f(x)\|/\|x\|} = \frac{\sup_{\delta x} \|A\delta x\|/\|\delta x\|}{\inf_x \|Ax\|/\|x\|}$$

- Question: For what x and δx is the equality achieved?
  Answer: When x is in direction of minimum magnification, and δx is in direction of maximum magnification
- Define *maximum magnification* of A as

$$\text{maxmag}(A) = \max_{\|x\|=1} \|Ax\|$$

  and *minimum magnification* of A as

$$\text{minmag}(A) = \min_{\|x\|=1} \|Ax\|$$

- Then condition number of matrix is $\kappa(A) = \text{maxmag}(A)/\text{minmag}(A)$
- For 2-norm, $\kappa(A) = \sigma_1/\sigma_n$, the ratio of largest and smallest singular values (in later sections)

Example of Ill-Conditioned Matrix

Example

Let $A = \begin{bmatrix} 1000 & 999 \\ 999 & 998 \end{bmatrix}$. It is easy to verify that

$A^{-1} = \begin{bmatrix} -998 & 999 \\ 999 & -1000 \end{bmatrix}$. So

$$\kappa_\infty(A) = \kappa_1(A) = 1999^2 = 3.996 \times 10^6.$$

Example of Ill-Conditioned Matrix

Example

A famous example is Hilbert matrix, defined by $h_{ij} = 1/(i+j-1)$, $1 \leq i,j \leq n$. The matrix is ill-conditioned for even quite small n. For $n \leq 4$, we have

$$H_4 = \begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix},$$

with condition number $\kappa_2(H_4) \approx 1.6 \times 10^4$, and $\kappa_2(H_8) \approx 1.5 \times 10^{10}$.

Outline

Condition Number of Linear System

- What is the condition number for $f(b) = A^{-1}b$?

Condition Number of Linear System

- What is the condition number for $f(b) = A^{-1}b$?
  Answer: $\kappa \leq \kappa(A) \equiv \|A\|\|A^{-1}\|$, as in matrix-vector multiplication

Theorem

Let A be nonsingular, and let x and $\hat{x} = x + \delta x$ be the solutions of $Ax = b$ and $A\hat{x} = b + \delta b$, respectively. Then

$$\frac{\|\delta x\|}{\|x\|} \leq \kappa(A)\frac{\|\delta b\|}{\|b\|},$$

and there exists $\|b\|$ and $\|\delta b\|$ for which the equality holds.

- Question: For what b and δb is the equality achieved?

Condition Number of Linear System

- What is the condition number for $f(b) = A^{-1}b$?
  Answer: $\kappa \leq \kappa(A) \equiv \|A\| \|A^{-1}\|$, as in matrix-vector multiplication

Theorem

Let A be nonsingular, and let x and $\hat{x} = x + \delta x$ be the solutions of $Ax = b$ and $A\hat{x} = b + \delta b$, respectively. Then

$$\frac{\|\delta x\|}{\|x\|} \leq \kappa(A) \frac{\|\delta b\|}{\|b\|},$$

and there exists $\|b\|$ and $\|\delta b\|$ for which the equality holds.

- Question: For what b and δb is the equality achieved?
  Answer: When b is in direction of *minimum* magnification of A^{-1}, and δb is in direction of *maximum* magnification of A^{-1}.
  In 2-norm, when b is in direction of *maximum* magnification of A^T, and δb is in direction of *minimum* magnification of A^T.

Singular and Nearly Singular Linear System

- Question: What is condition number of Ax if A is singular?

Singular and Nearly Singular Linear System

- Question: What is condition number of Ax if A is singular?
  Answer: ∞.
- We say a matrix is *nearly singular* if its condition number is very large
- In other words, columns of A are nearly linearly dependent
- If A is nearly singular, for matrix-vector multiplication, Ax, error is large if x is nearly in null space of A
- If A is nearly singular, for linear system $Ax = b$, error is large if b is NOT nearly in null space of A^T
- Therefore, ill-conditioning (near singularity) has a much bigger impact on solving linear system than matrix-vector multiplication!

Ill Conditioning Caused by Poor Scaling

- Some matrices are ill conditioned simply because they are out of scale.

Theorem

Let $A \in \mathbb{R}^{n \times n}$ be any nonsingular matrix, and let a_k, $1 \leq k \leq n$ denote the kth column of A. Then for any i and j with $1 \leq i, j, \leq n$, $\kappa_p(A) \geq \|a_i\|_p / \|a_j\|_p$.

- This theorem indicates that poor scaling inevitably leads to ill conditioning
- A *necessary* condition for a matrix to be well conditioned is that all of its rows and columns are of roughly the same magnitude.

Estimating Condition Number

- We would like to estimate $\kappa_1(A) = \|A\|_1 \|A^{-1}\|_1$ without computing A^{-1}, but allow LU factorization of A
- For any vector $w \in \mathbb{R}^n$ and $\|w\|_1 = 1$, we have lower bound

$$\kappa_1(A) \geq \|A\|_1 \|A^{-1}w\|_1$$

- If w has a significant component in direction near maximum magnification by A^{-1}, then

$$\kappa_1(A) \approx \|A\|_1 \|A^{-1}w\|_1$$

- Note statement on p. 132 of textbook "Actually any w chosen at random is likely to have a significant component in the direction of maximum magnification by A^{-1}" is unjustified for large n in 1-norm
- Good estimators conduct systematic searches for w that approximately maximizes $\|A^{-1}w\|_1$

Outline

Non-singularity of Perturbed Matrix

Theorem

If A is nonsingular and

$$\|\delta A\|/\|A\| < 1/\kappa(A),$$

then $A + \delta A$ is nonsingular.

Non-singularity of Perturbed Matrix

Theorem

If A is nonsingular and

$$\|\delta A\|/\|A\| < 1/\kappa(A),$$

then $A + \delta A$ is nonsingular.

Proof.

$\|\delta A\|/\|A\| < 1/\kappa(A)$ is equivalent to $\|\delta A\|\|A^{-1}\| < 1$. Suppose $A + \delta A$ is singular, then $\exists y \neq 0$ such that $(A + \delta A)y = 0$, and $y = -A^{-1}\delta A y$. Therefore, $\|y\| \leq \|A^{-1}\|\|\delta A\|\|y\|$, or $\|A^{-1}\|\|\delta A\| \geq 1$. □

- If $A + \delta A$ is the singular matrix closest to A, in the sense that $\|\delta A\|_2$ is as small as possible, then $\|\delta A\|_2/\|A\|_2 = 1/\kappa_2(A)$

Linear System with Perturbed Matrix

- Suppose $Ax = b$ and $\hat{A}\hat{x} = b$ where $\hat{A} = A + \delta A$. Let $\delta x = \hat{x} - x$ and $\hat{x} = x + \delta x$.
- We would like to bound $\|\delta x\|/\|x\|$, but first we bound $\|\delta x\|/\|\hat{x}\|$

Theorem

If A is nonsingular, and let $b \neq 0$. Then

$$\frac{\|\delta x\|}{\|\hat{x}\|} \leq \kappa(A)\frac{\|\delta A\|}{\|A\|}.$$

Proof.

Rewrite $(A + \delta A)\hat{x} = b$ as $Ax + A\delta x + \delta A\hat{x} = b$, where $Ax = b$. Therefore,

$$\|\delta x\| \leq \|A^{-1}\|\|\delta A\|\|\hat{x}\|.$$

Therefore,

$$\frac{\|\delta x\|}{\|\hat{x}\|} \leq \|A^{-1}\|\|\delta A\| = \kappa(A)\frac{\|\delta A\|}{\|A\|}.$$

Linear System with Perturbed Matrix Continued

- $Ax = b$ and $\hat{A}\hat{x} = b$ where $\hat{A} = A + \delta A$. Let $\delta x = \hat{x} - x$ and $\hat{x} = x + \delta x$.

Theorem

If A is nonsingular and $\|\delta A\|/\|A\| < 1/\kappa(A)$, and let $b \neq 0$. Then

$$\frac{\|\delta x\|}{\|x\|} \leq \frac{\kappa(A)\|\delta A\|/\|A\|}{1 - \kappa(A)\|\delta A\|/\|A\|}.$$

Proof.

$\|\delta x\| \leq \|A^{-1}\|\|\delta A\|\|\hat{x}\| \leq \|A^{-1}\|\|\delta A\|(\|x\| + \|\delta x\|)$. Therefore,

$$\left(1 - \|A^{-1}\|\|\delta A\|\right) \delta x \leq \|A^{-1}\|\|\delta A\|\|x\|,$$

where $\|A^{-1}\|\|\delta A\| = \kappa(A)\|\delta A\|/\|A\|$. $\square$

We typically expect $\kappa(A)\|\delta A\| \ll \|A\|$, so the denominator is close to 1.

Outline

Perturbed RHS and Matrix

- Suppose $Ax = b$ and $(A + \delta A)(x + \delta x) = (b + \delta b)$, where $\hat{A} = A + \delta A$, $b = b + \delta b$ and $\hat{x} = x + \delta x$.

Theorem

Let A be nonsingular, and suppose $\hat{x} \neq 0$ and $\hat{b} \neq 0$. Then

$$\frac{\|\delta x\|}{\|\hat{x}\|} \leq \kappa(A) \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|\hat{b}\|} + \frac{\|\delta A\|}{\|A\|} \frac{\|\delta b\|}{\|\hat{b}\|} \right) \approx \kappa(A) \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|\hat{b}\|} \right).$$

Theorem

If A is nonsingular and $\|\delta A\|/\|A\| < 1/\kappa(A)$, and let $b \neq 0$, then

$$\frac{\|\delta x\|}{\|x\|} \lesssim \frac{\kappa(A)(\|\delta A\|/\|A\| + \|\delta b\|/\|b\|)}{1 - \kappa(A)\|\delta A\|/\|A\|}.$$

Roughly speaking, $\kappa(A)$ determines loss of digits of accuracy in x in addition to loss of digits of accuracy in perturbations in A and b

A Posteriori Error Analysis Using Residual

- Suppose $\hat{x}$ is a computed solution of $Ax = b$, and residual $\hat{r} = b - A\hat{x}$. How to bound error in $x - \hat{x}$?

Theorem

Let A be nonsingular, let $b \neq 0$. Then

$$\frac{\|\delta x\|}{\|x\|} \leq \kappa(A)\frac{\|\hat{r}\|}{\|b\|}.$$

- If the residual is tiny and A is well conditioned, then $\hat{x}$ is an accurate approximation to x.
- For *a posteriori* error bound, one needs to estimate $\|\hat{r}\|$ and $\kappa(A)$