Lecture 11
Conditioning of Least Squares Problems; Stability of Least Squares Algorithms

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Outline

1. Conditioning of Least Squares Problems

2. Stability of Least Squares Algorithms

Accuracy of Backward Stable Algorithm

Theorem

If a backward stable algorithm $\tilde{\mathbf{f}}$ *is used to solve a problem* $\mathbf{f}$ *with condition number* κ *using floating-point numbers satisfying the two axioms, then*

$$\|\tilde{\mathbf{f}}(\mathbf{x}) - \mathbf{f}(\mathbf{x})\|/\|\mathbf{f}(\mathbf{x})\| = O(\kappa(\mathbf{x})\epsilon_{machine})$$

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Proof

Backward stability means $\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}})$ for $\tilde{\mathbf{x}}$ such that
$\|\tilde{\mathbf{x}} - \mathbf{x}\| / \|\mathbf{x}\| = O(\epsilon_{machine})$
Definition of condition number gives

$$\|\mathbf{f}(\tilde{\mathbf{x}}) - \mathbf{f}(\mathbf{x})\| / \|\mathbf{f}(\mathbf{x})\| \leqslant (\kappa(\mathbf{x}) + o(1)) \|\tilde{\mathbf{x}} - \mathbf{x}\| / \|\mathbf{x}\|$$

where $o(1) \to 0$ as $\epsilon_{machine} \to 0$.
Combining the two gives desired result.

Outline

Four Conditioning Problems

- Least squares problem: Given $\mathbf{A} \in \mathbb{C}^{m\times n}$ with full rank and $\mathbf{b} \in \mathbb{C}^{m}$,

$$\min_{\mathbf{x}\in\mathbb{C}^n} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|$$

- It is solution is $\mathbf{x} = \mathbf{A}^+\mathbf{b}$. Another quantity is $\mathbf{y} = \mathbf{A}\mathbf{x} = \mathbf{P}\mathbf{b}$, where $\mathbf{P} = \mathbf{A}\mathbf{A}^+ = \mathbf{A}(\mathbf{A}^*\mathbf{A})^{-1}\mathbf{A}^*$ (i.e., orthogonal projection of $\mathbf{b}$ onto range of $\mathbf{A}$) (refer to figure)
- Consider $\mathbf{A}$ and $\mathbf{b}$ as input data, and $\mathbf{x}$ and $\mathbf{y}$ as output. We then have four conditioning problems:

Input \ Output	$\mathbf{y}$	$\mathbf{x}$
$\mathbf{b}$	$\kappa_{\mathbf{b}\to\mathbf{y}}$	$\kappa_{\mathbf{b}\to\mathbf{x}}$
$\mathbf{A}$	$\kappa_{\mathbf{A}\to\mathbf{y}}$	$\kappa_{\mathbf{A}\to\mathbf{x}}$

- These conditioning problems are important and subtle.

Some Prerequisites

- We focus on the second column, namely $\kappa_{\mathbf{b}\to\mathbf{x}}$ and $\kappa_{\mathbf{A}\to\mathbf{x}}$
- However, understanding $\kappa_{\mathbf{b}\to\mathbf{y}}$ and $\kappa_{\mathbf{A}\to\mathbf{y}}$ is prerequisite
- Three quantities: (All in 2-norms)
  - Condition number of $\mathbf{A}$:

$$\kappa(\mathbf{A}) = \|\mathbf{A}\|\|\mathbf{A}^+\| = \sigma_1/\sigma_n$$

  - Angle between $\mathbf{b}$ and $\mathbf{y}$:

$$\theta = \cos^{-1}\frac{\|\mathbf{y}\|}{\|\mathbf{b}\|},\ (0 \leqslant \theta \leqslant \pi/2)$$

  - Orientation of $\mathbf{y}$ with $range(\mathbf{A})$:

$$\eta = \frac{\|\mathbf{A}\|\|\mathbf{x}\|}{\|\mathbf{y}\|},\ (1 \leqslant \eta \leqslant \kappa(\mathbf{A}))$$

Sensitivity of $\mathbf{y}$ to Perturbations in $\mathbf{b}$

- Intuition: The larger θ is, the more sensitive $\mathbf{y}$ is in terms of relative error
- Analysis: $\mathbf{y} = \mathbf{P}\mathbf{b}$, so

$$\kappa_{\mathbf{b}\to\mathbf{y}} = \frac{\|\mathbf{P}\|}{\|\mathbf{y}\|/\|\mathbf{b}\|} = \frac{\|\mathbf{b}\|}{\|\mathbf{y}\|} = \frac{1}{\cos\theta}$$

where $\|\mathbf{P}\| = 1$

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$\mathbf{b}$	$\frac{1}{\cos\theta}$	
$\mathbf{A}$		

Sensitivity of $\mathbf{y}$ to Perturbations in $\mathbf{b}$

- Intuition: The larger θ is, the more sensitive $\mathbf{y}$ is in terms of relative error
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- Question: When the maximum is attained for perturbation $\delta\mathbf{b}$?
- Answer: when $\delta\mathbf{b} \in range(\mathbf{A})$

Sensitivity of $\mathbf{x}$ to Perturbations in $\mathbf{b}$

- Intuition: It depends on how sensitive $\mathbf{y}$ is to $\mathbf{b}$, and how $\mathbf{y}$ lies within $range(\mathbf{A})$
- Analysis: $\mathbf{x} = \mathbf{A}^+\mathbf{b}$, so

$$\kappa_{\mathbf{b}\to\mathbf{x}} = \frac{\|\mathbf{A}^+\|}{\|\mathbf{x}\|/\|\mathbf{b}\|} = \|\mathbf{A}^+\|\frac{\|\mathbf{b}\|}{\|\mathbf{y}\|}\frac{\|\mathbf{y}\|}{\|\mathbf{x}\|} = \|\mathbf{A}^+\|\frac{1}{\cos\theta}\frac{\|\mathbf{A}\|}{\eta} = \frac{\kappa(\mathbf{A})}{\eta\cos\theta}$$

where $\eta = \|\mathbf{A}\|\|\mathbf{x}\|/\|\mathbf{y}\|$

Input \ Output	$\mathbf{y}$	$\mathbf{x}$
$\mathbf{b}$	$\frac{1}{\cos\theta}$	$\frac{\kappa(\mathbf{A})}{\eta\cos\theta}$
$\mathbf{A}$		

Sensitivity of $\mathbf{x}$ to Perturbations in $\mathbf{b}$

- Assume $\cos\theta = O(1)$, $\kappa_{\mathbf{b}\to\mathbf{x}} = \frac{\kappa(\mathbf{A})}{\eta\cos\theta}$ can lie anywhere between 1 and $O(\kappa(\mathbf{A}))$!

Sensitivity of $\mathbf{x}$ to Perturbations in $\mathbf{b}$

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- Question: When the maximum is attained for perturbation $\delta\mathbf{b}$?
- Answer: When $\delta\mathbf{b}$ is in subspace spanned by left singular vectors corresponding to smallest singular values

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- Question: When the maximum is attained for perturbation $\delta\mathbf{b}$?
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- Question: What if $\mathbf{A}$ is a nonsingular matrix?

Sensitivity of $\mathbf{x}$ to Perturbations in $\mathbf{b}$

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- Question: When the maximum is attained for perturbation $\delta\mathbf{b}$?
- Answer: When $\delta\mathbf{b}$ is in subspace spanned by left singular vectors corresponding to smallest singular values
- Question: What if $\mathbf{A}$ is a nonsingular matrix?
- Answer: $\kappa_{\mathbf{b}\to\mathbf{x}} = \frac{\kappa(\mathbf{A})}{\eta\cos\theta}$ can lie anywhere between 1 and $O(\kappa(\mathbf{A}))$

Sensitivity of $\mathbf{x}, \mathbf{y}$ to Perturbations in $\mathbf{A}$

- The relationship are nonlinear, because $range(\mathbf{A})$ changes due to $\delta\mathbf{A}$
- Intuitions:
  - The larger θ is, the more sensitive $\mathbf{y}$ is in terms of relative error.
  - Tilting of $range(\mathbf{A})$ depends on $\kappa(\mathbf{A})$.
  - For $\mathbf{x}$, it depends where $\mathbf{y}$ lies within $range(\mathbf{A})$

Input \ Output	$\mathbf{y}$	$\mathbf{x}$
$\mathbf{b}$	$\frac{1}{\cos\theta}$	$\frac{\kappa(\mathbf{A})}{\eta\cos\theta}$
$\mathbf{A}$	$\leqslant \frac{\kappa(\mathbf{A})}{\cos\theta}$	$\kappa(\mathbf{A}) + \frac{\kappa(\mathbf{A})^2\tan\theta}{\eta}$

- For second row, bounds are not necessarily tight
- Assume $\cos\theta = O(1)$, $\kappa_{\mathbf{A}\to\mathbf{x}}$ can lie anywhere between $\kappa(\mathbf{A})$ and $O(\kappa(\mathbf{A})^2)$

Condition Numbers of Linear Systems

- Linear systems $\mathbf{Ax} = \mathbf{b}$ for nonsingular $\mathbf{A} \in \mathbb{C}^{m \times m}$ is a special case of least squares problems, where $\mathbf{y} = \mathbf{b}$
- If $m = n$, then $\theta = 0$, so $\cos\theta = 1$ and $\tan\theta = 0$

Input \ Output	$\mathbf{y}$	$\mathbf{x}$
$\mathbf{b}$	1	$\frac{\kappa(\mathbf{A})}{\eta}$
$\mathbf{A}$	$\leqslant \kappa(\mathbf{A})$	$\kappa(\mathbf{A})$

Outline

1. Conditioning of Least Squares Problems

2. Stability of Least Squares Algorithms

Algorithms for Solving Least Squares Problems

- There are many variants of algorithms for solving least squares problems
  - Householder **QR** (with/without pivoting, explicit or implicit **Q**): Backward stable
  - Classical Gram-Schmidt: Unstable
  - Modified Gram-Schmidt with explicit **Q**: Unstable
  - Modified Gram-Schmidt with augmented system of equations with implicit **Q**: Backward stable
  - Normal equations (solve $\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}$): Very unstable
  - Singular value decomposition: Stable and most accurate
- Note that in general, only SVD is robust for solving rank deficient least squares problems

Backward Stability of Householder Triangularization

Theorem

Let the full-rank least squares problem be solved using Householder triangularization on a computer satisfying the two axioms of floating point numbers. The algorithm is backward stable in the sense that the computed solution $\tilde{\mathbf{x}}$ *has the property*

$$\|(\mathbf{A} + \delta\mathbf{A})\tilde{\mathbf{x}} - \mathbf{b}\| = \min, \quad \frac{\|\delta\mathbf{A}\|}{\|\mathbf{A}\|} = O(\epsilon_{machine})$$

for some $\delta\mathbf{A} \in \mathbb{C}^{m\times n}$

- Backward stability of the algorithm is true whether $\hat{\mathbf{Q}}^*\mathbf{b}$ is computed via explicit formation of $\hat{\mathbf{Q}}$ or computed implicitly
- Backward stability also holds for Householder triangularization with arbitrary column pivoting $\mathbf{AP} = \hat{\mathbf{Q}}\hat{\mathbf{R}}$

Gram-Schmidt Orthogonalization

- Note that Gram-Schmidt orthogonalization in general is unstable, due to loss of orthogonality
- However, Gram-Schmidt can be stabilized using an augmented system of equations:
  - Compute QR of augmented matrix: $[\mathbf{Q}, \mathbf{R}_1] = mgs([\mathbf{A}, \mathbf{b}])$
  - Extract $\mathbf{R}$ and $\hat{\mathbf{Q}}^*\mathbf{b}$ for $\mathbf{R}_1$: $\mathbf{R} = \mathbf{R}_1(1:n, 1:n); \mathbf{Qb} = \mathbf{R}_1(1:n, n+1)$
  - Back solve: $\mathbf{x} = \mathbf{R}\backslash\mathbf{Qb}$

Theorem

The solution of the full-rank least squares problem by Gram-Schmidt orthogonality is backward stable in the sense that the computed solution $\tilde{\mathbf{x}}$ has the property

$$\|(\mathbf{A} + \delta\mathbf{A})\tilde{\mathbf{x}} - \mathbf{b}\| = \min, \quad \frac{\|\delta\mathbf{A}\|}{\|\mathbf{A}\|} = O(\epsilon_{machine})$$

for some $\delta\mathbf{A} \in \mathbb{C}^{m\times n}$, provided that $\hat{\mathbf{Q}}^*\mathbf{b}$ is formed implicitly.

Other Methods

- The method of normal equation solves $\mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}$

Theorem

The solution of the full-rank least squares problem via normal equation is unstable. Stability can be achieved, however, by restriction to a class of problems in which $\kappa(\mathbf{A})$ is uniformly bounded above or $\tan\theta/\eta$ is uniformly bounded below.

- Solution using SVD: $\mathbf{A} = \hat{\mathbf{U}}\hat{\Sigma}\mathbf{V}^*, \mathbf{x} = \mathbf{V}\hat{\Sigma}^{-1}\hat{\mathbf{U}}^*\mathbf{b}$

Theorem

The solution of the full-rank least squares problem by the SVD is backward stable.