AMS526: Numerical Analysis I (Numerical Linear Algebra for Computational and Data Sciences)

Lecture 12: Conditioning of Least Squares Problems; Stability of Householder Triangularization

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Outline

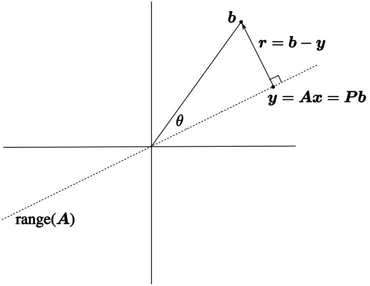
1. Conditioning of Least Squares Problems (NLA§18)
2. Stability of Householder Triangularization (NLA§16,19)

Four Conditioning Problems

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

$$\min_{x \in \mathbb{R}^n} \|b - Ax\|$$

- Its solution is $x = A^+ b$. Another quantity is $y = Ax = Pb$, where $P = AA^+$



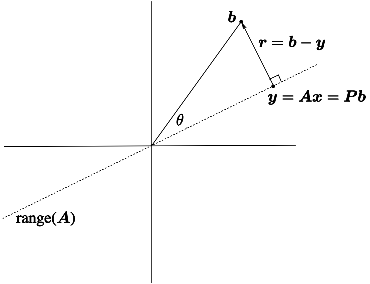
- Consider A and b as input data, and x and y as output. We then have four conditioning problems:

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

- These conditioning problems are important and subtle.

Some Prerequisites

- We focus on the second column, namely $\kappa_{b \to x}$ and $\kappa_{A \to x}$
- However, understanding $\kappa_{b \to y}$ and $\kappa_{A \to y}$ is prerequisite
- Three quantities: (All in 2-norms)
  - Condition number of A: $\kappa(A) = \|A\| \|A^+\| = \sigma_1 / \sigma_n$
  - Angle between b and y: $\theta = \arccos \frac{\|y\|}{\|b\|}$. $(0 \le \theta \le \pi/2)$
  - Orientation of y with range(A): $\eta = \frac{\|A\| \|x\|}{\|y\|}$. $(1 \le \eta \le \kappa(A))$



Sensitivity of y to Perturbations in b

- Intuition: The larger θ is, the more sensitive y is in terms of relative error
- Analysis: $y = Pb$, so

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

where $\|P\| = 1$

Input \ Output	y	x
b	$\frac{1}{\cos\theta}$	
A		

- Question: When is the maximum attained for perturbation δb?

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A		

- Question: When is the maximum attained for perturbation δb?
- Answer: When is δb in range(A)

Sensitivity of x to Perturbations in b

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

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

where $\eta = \|A\| \|x\| / \|y\|$

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

Sensitivity of x to Perturbations in b

- Assume $\cos\theta = O(1)$, $\kappa_{b \to x} = \frac{\kappa(A)}{\eta \cos\theta}$ can lie anywhere between 1 and $O(\kappa(A))$!
- Question: When is the maximum attained for perturbation δb?

Sensitivity of x to Perturbations in b

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

Sensitivity of x to Perturbations in b

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

Sensitivity of y and x to Perturbations in A

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

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

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

Condition Numbers of Linear Systems

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

Input \ Output	y	x
b	1	$\kappa(A)/\eta$
A	$\leq \kappa(A)$	$\leq \kappa(A)$

Outline

Solution of Least Squares Problems

- An efficient and robust approach is to use QR factorization $A = \hat{Q}\hat{R}$
  - b can be projected onto range(A) by $P = \hat{Q}\hat{Q}^T$, and therefore $\hat{Q}\hat{R}x = \hat{Q}\hat{Q}^T b$
  - Left-multiply by $\hat{Q}^T$ and we get $\hat{R}x = \hat{Q}^T b$ (note $A^+ = \hat{R}^{-1}\hat{Q}^T$)

Least squares via QR Factorization
Compute reduced QR factorization $A = \hat{Q}\hat{R}$
Compute vector $c = \hat{Q}^T b$
Solve upper-triangular system $\hat{R}x = c$ for x

- Computation is dominated by QR factorization ($2mn^2 - \frac{2}{3}n^3$)
- What about stability?

Backward Stability of Householder Triangularization

- For a QR factorization $A = QR$ computed by Householder triangularization, the factors $\tilde{Q}$ and $\tilde{R}$ satisfy

$$\tilde{Q}\tilde{R} = A + \delta A, \quad \|\delta A\|/\|A\| = O(\epsilon_{\text{machine}}),$$

  i.e., exact QR factorization of a slightly perturbed A
- $\tilde{R}$ is R computed by algorithm using floating points
- However, $\tilde{Q}$ is product of *exactly orthogonal* reflectors

$$\tilde{Q} = \tilde{Q}_1 \tilde{Q}_2 \dots \tilde{Q}_n$$

  where $\tilde{Q}_k$ is given by computed $\tilde{v}_k$, since Q is not formed explicitly

Backward Stability of Solving $Ax = b$ with QR

Algorithm: Solving $Ax = b$ by QR Factorization Compute $A = QR$ using Householder, represent Q by reflectors Compute vector $y = Q^T b$ implicitly using reflectors Solve upper-triangular system $Rx = y$ for x

- All three steps are backward stable
- Overall, we can show that

$$(A + \Delta A)\tilde{x} = b, \quad \|\Delta A\|/\|A\| = O(\epsilon_{\text{machine}})$$

as we prove next

Backward Stability of Solving $Ax = b$ with Householder Triangularization

Proof: Step 2 gives

$$(\tilde{Q} + \delta Q)\tilde{y} = b, \quad \|\delta Q\| = O(\epsilon_{\text{machine}})$$

Step 3 gives

$$(\tilde{R} + \delta R)\tilde{x} = \tilde{y}, \quad \|\delta R\|/\|\tilde{R}\| = O(\epsilon_{\text{machine}})$$

Therefore,

$$b = (\tilde{Q} + \delta Q)(\tilde{R} + \delta R)\tilde{x} = \left[\tilde{Q}\tilde{R} + (\delta Q)\tilde{R} + \tilde{Q}(\delta R) + (\delta Q)(\delta R)\right]\tilde{x}$$

Step 1 gives

$$b = \left[A + \underbrace{\delta A + (\delta Q)\tilde{R} + \tilde{Q}(\delta R) + (\delta Q)(\delta R)}_{\Delta A}\right]\tilde{x}$$

where $\tilde{Q}\tilde{R} = A + \delta A$

Proof of Backward Stability Cont'd

$\tilde{Q}\tilde{R} = A + \delta A$ where $\|\delta A\|/\|A\| = O(\epsilon_{\text{machine}})$, and therefore

$$\frac{\|\tilde{R}\|}{\|A\|} \leq \|\tilde{Q}^T\| \frac{\|A + \delta A\|}{\|A\|} = O(1)$$

Now show that each term in ΔA is small

$$\frac{\|(\delta Q)\tilde{R}\|}{\|A\|} \leq \|(\delta Q)\| \frac{\|\tilde{R}\|}{\|A\|} = O(\epsilon_{\text{machine}})$$

$$\frac{\|\tilde{Q}(\delta R)\|}{\|A\|} \leq \|\tilde{Q}\| \frac{\|\delta R\|}{\|\tilde{R}\|} \frac{\|\tilde{R}\|}{\|A\|} = O(\epsilon_{\text{machine}})$$

$$\frac{\|(\delta Q)(\delta R)\|}{\|A\|} \leq \|\delta Q\| \frac{\|\delta R\|}{\|A\|} = O(\epsilon^2_{\text{machine}})$$

Overall,

$$\frac{\|\Delta A\|}{\|A\|} \leq \frac{\|\delta A\|}{\|A\|} + \frac{\|(\delta Q)\tilde{R}\|}{\|A\|} + \frac{\|\tilde{Q}(\delta R)\|}{\|A\|} + \frac{\|(\delta Q)(\delta R)\|}{\|A\|} = O(\epsilon_{\text{machine}})$$

Since the algorithm is backward stable, it is also accurate.

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 $\tilde{x}$ has the property

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

for some $\delta A \in \mathbb{R}^{m \times n}$.

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