Lecture 09 Accuracy and Stability

Songting Luo

Department of Mathematics lowa State University

MATH 562 Numerical Analysis II

1 Floating Point Arithmetic

2 Accuracy and Stability

1 Floating Point Arithmetic

2 Accuracy and Stability

• Consider $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$, with $\mathbf{A} \in \mathbb{C}^{m \times n}$

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

• If **A** is square and nonsingular, since $\|\mathbf{x}\|/\|\mathbf{A}\mathbf{x}\| \le \|\mathbf{A}^{-1}\|$,

$$\kappa \leqslant \|\mathbf{A}\| \|\mathbf{A}^{-1}\|$$

Question: For what x is equality achieved if 2-norm is used?

• Consider $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$, with $\mathbf{A} \in \mathbb{C}^{m \times n}$

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

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

$$\kappa \leqslant \|\mathbf{A}\| \|\mathbf{A}^{-1}\|$$

- Question: For what **x** is equality achieved if 2-norm is used?
- \bullet Answer: \boldsymbol{x} is equal to right singular vector corresponding to smallest singular value of \boldsymbol{A}

• Consider $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$, with $\mathbf{A} \in \mathbb{C}^{m \times n}$

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

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

$$\kappa \leqslant \|\mathbf{A}\| \|\mathbf{A}^{-1}\|$$

- Question: For what **x** is equality achieved if 2-norm is used?
- \bullet Answer: \boldsymbol{x} is equal to right singular vector corresponding to smallest singular value of \boldsymbol{A}
- Question: What is condition number of Ax if A is singular?

• Consider $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$, with $\mathbf{A} \in \mathbb{C}^{m \times n}$

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

• If **A** is square and nonsingular, since $\|\mathbf{x}\|/\|\mathbf{A}\mathbf{x}\| \le \|\mathbf{A}^{-1}\|$,

$$\kappa \leqslant \|\mathbf{A}\| \|\mathbf{A}^{-1}\|$$

- Question: For what **x** is equality achieved if 2-norm is used?
- \bullet Answer: \boldsymbol{x} is equal to right singular vector corresponding to smallest singular value of \boldsymbol{A}
- Question: What is condition number of Ax if A is singular?
- Answer: $\leq \infty$ (is ∞ if $\mathbf{x} \in null(\mathbf{A})$.
- What is the condition number for $f(b) = A^{-1}b$?

• Consider $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$, with $\mathbf{A} \in \mathbb{C}^{m \times n}$

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

• If **A** is square and nonsingular, since $\|\mathbf{x}\|/\|\mathbf{A}\mathbf{x}\| \le \|\mathbf{A}^{-1}\|$,

$$\kappa \leqslant \|\mathbf{A}\| \|\mathbf{A}^{-1}\|$$

- Question: For what **x** is equality achieved if 2-norm is used?
- \bullet Answer: \boldsymbol{x} is equal to right singular vector corresponding to smallest singular value of \boldsymbol{A}
- Question: What is condition number of Ax if A is singular?
- Answer: $\leq \infty$ (is ∞ if $\mathbf{x} \in null(\mathbf{A})$.
- What is the condition number for $\mathbf{f}(\mathbf{b}) = \mathbf{A}^{-1}\mathbf{b}$?
 - Answer: $\kappa \leq \|\mathbf{A}\| \|\mathbf{A}^{-1}\|$.

Condition Number of Matrix

We define condition number of matrix A as

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

- It is the upper bound of the condition number of f(x) = Ax for any x.
- Another way to interpret $\kappa(\mathbf{A})$ is

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

- For 2-norm, $\kappa(\mathbf{A}) = \sigma_1/\sigma_n$
- 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)
- Note: condition number of a problem is a property of a problem, and is independent of its algorithm

Floating Point Arithmetic

2 Accuracy and Stability

Accuracy

- Roughly speaking, accuracy means that "error" is small in an asymptotic sense, say $O(\epsilon_{machine})$
- Notation $\phi(t)=O(\psi(t))$ means $\exists C$ s.t., $|\phi(t)|\leqslant C|\psi(t)|$ as t approaches 0 (or ∞)
 - Example: $\sin^2 t = O(t^2)$ as $t \to 0$.
- If ϕ depends on s and t, then $\phi(s,t)=O(\psi(t))$ means $\exists C$ s.t., $\phi(s,t)\leqslant C|\psi(t)|$ for any s as t approaches 0 (or ∞)
 - Example: $\sin^2 t \sin^2 s = O(t^2)$ as $t \to 0$.
- When we say $O(\epsilon_{machine})$, we are thinking of a series of idealized machines for which $\epsilon_{machine}$ can be arbitrarily small

More on Accuracy

 \bullet An algorithm $\tilde{\mathbf{f}}$ is accurate if relative error is in the order of machine precision, i.e.,

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

i.e. $\leq C_1 \epsilon_{machine}$ as $\epsilon_{machine} \to 0$, where constant C_1 may depend on the condition number and the algorithm itself

• In most cases, we expect

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

i.e., $\leq C\kappa\epsilon_{machine}$ as $\epsilon_{machine} \to 0$, where constant C should be independent of κ and value of \mathbf{x} (although it may depends on the dimension of \mathbf{x})

- How do we determine whether an algorithm is accurate or not?
 - It turns out to be an extremely subtle question
 - A forward error analysis (operation by operation) is often too difficult and impractical, and cannot capture dependence on condition number
 - An effective solution is backward error analysis

1 Floating Point Arithmetic

2 Accuracy and Stability

- We say an algorithm is stable if it gives "nearly the right answer to nearly the right question"
- More formally, an algorithm $\tilde{\mathbf{f}}$ for problem \mathbf{f} is stable if (for all \mathbf{x})

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

for some $\tilde{\mathbf{x}}$ with $\|\tilde{\mathbf{x}} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\| = O(\epsilon_{machine})$.

- We say an algorithm is backward stable if it gives "exactly the right answer to nearly the right question"
- More formally, an algorithm $\hat{\mathbf{f}}$ for problem \mathbf{f} is stable if (for all \mathbf{x})

$$\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}})$$

for some $\tilde{\mathbf{x}}$ with $\|\tilde{\mathbf{x}} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\| = O(\epsilon_{machine})$.

Is stability or backward stability stronger?

- We say an algorithm is stable if it gives "nearly the right answer to nearly the right question"
- More formally, an algorithm $\tilde{\mathbf{f}}$ for problem \mathbf{f} is stable if (for all \mathbf{x})

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

for some $\tilde{\mathbf{x}}$ with $\|\tilde{\mathbf{x}} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\| = O(\epsilon_{machine})$.

- We say an algorithm is backward stable if it gives "exactly the right answer to nearly the right question"
- More formally, an algorithm $\hat{\mathbf{f}}$ for problem \mathbf{f} is stable if (for all \mathbf{x})

$$\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}})$$

for some $\tilde{\mathbf{x}}$ with $\|\tilde{\mathbf{x}} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\| = O(\epsilon_{machine})$.

- Is stability or backward stability stronger?
 - Backward stability is stronger.

- We say an algorithm is stable if it gives "nearly the right answer to nearly the right question"
- More formally, an algorithm $\tilde{\mathbf{f}}$ for problem \mathbf{f} is stable if (for all \mathbf{x})

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

for some $\tilde{\mathbf{x}}$ with $\|\tilde{\mathbf{x}} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\| = O(\epsilon_{machine})$.

- We say an algorithm is backward stable if it gives "exactly the right answer to nearly the right question"
- More formally, an algorithm $\hat{\mathbf{f}}$ for problem \mathbf{f} is stable if (for all \mathbf{x})

$$\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}})$$

for some $\tilde{\mathbf{x}}$ with $\|\tilde{\mathbf{x}} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\| = O(\epsilon_{machine})$.

- Is stability or backward stability stronger?
 - Backward stability is stronger.
- Does (backward) stability depend on condition number of f(x)?

- We say an algorithm is stable if it gives "nearly the right answer to nearly the right question"
- More formally, an algorithm $\tilde{\mathbf{f}}$ for problem \mathbf{f} is stable if (for all \mathbf{x})

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

for some $\tilde{\mathbf{x}}$ with $\|\tilde{\mathbf{x}} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\| = O(\epsilon_{machine})$.

- We say an algorithm is backward stable if it gives "exactly the right answer to nearly the right question"
- More formally, an algorithm f for problem f is stable if (for all x)

$$\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}})$$

for some $\tilde{\mathbf{x}}$ with $\|\tilde{\mathbf{x}} - \tilde{\mathbf{x}}\|/\|\mathbf{x}\| = O(\epsilon_{machine})$.

- Is stability or backward stability stronger?
 - Backward stability is stronger.
- Does (backward) stability depend on condition number of f(x)?
 - No.



Stability of Floating Point Arithmetic

- Backward stability of floating point operations is implied by these two floating point axioms:
 - $\forall x \in \mathbb{R}, \exists \epsilon, |\epsilon| \leq \epsilon_{machine}, \text{ s.t., } fl(x) = x(1+\epsilon)$
 - For floating-point numbers $x, y, \exists \epsilon, |\epsilon| \leq \epsilon_{machine}$ s.t. $x \circledast y = (x * y)(1 + \epsilon)$
- Example: Subtraction $f(x_1,x_2)=x_1-x_2$ with floating-point operation

$$\widetilde{f}(x_1, x_2) = fl(x_1) \ominus fl(x_2)$$

- Axiom 1 implies $fl(x_1)=x_1(1+\epsilon_1), fl(x_2)=x_2(1+\epsilon_2)$, for some $|\epsilon_1|, |\epsilon_2| \leqslant \epsilon_{machine}$
- Axiom 2 implies $fl(x_1) \ominus fl(x_2) = (fl(x_1) fl(x_2))(1 + \epsilon_3)$ for some $|\epsilon_3| \leqslant \epsilon_{machine}$

$$fl(x_1) \ominus fl(x_2) = (x_1(1+\epsilon_1) - x_2(1+\epsilon_2))(1+\epsilon_3)$$

= $x_1(1+\epsilon_1)(1+\epsilon_3) - x_2(1+\epsilon_2)(1+\epsilon_3)$
= $x_1(1+\epsilon_4) - x_2(1+\epsilon_5)$

where $|\epsilon_4|, |\epsilon_5| \leq 2\epsilon_{machine} + O(\epsilon_{machine}^2)$

Stability of Floating Point Arithmetic Cont'd

- Example: Inner product $f(\mathbf{x}, \mathbf{y}) = \mathbf{x}^* \mathbf{y}$ using floating-point operations \otimes and \oplus is backward stable
- Example: outer product $f(\mathbf{x},\mathbf{y})=\mathbf{x}\mathbf{y}^*$ using floating-point operations \otimes and \oplus is not backward stable
- Example: f(x) = x + 1 is computed as $\tilde{f}(x) = fl(x) \oplus 1$ is not backward stable
- Example: f(x,y) = x + y computed as $\tilde{f}(x,y) = fl(x) \oplus fl(y)$ is backward stable

Accuracy of Backward Stable Algorithm

Theorem

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

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

Proof

Backward stability means $\mathbf{f}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}})$ 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.

◆ロ > ◆母 > ◆ き > ◆き > き の < の </p>