AMS526: Numerical Analysis I (Numerical Linear Algebra)

Lecture 10: Condition Numbers; Accuracy and Stability

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Outline

Overview of Error Analysis

- Error analysis is important subject of numerical analysis
- Given a problem f and an algorithm $\tilde{f}$ with an input x, the *absolute error* is $\|\tilde{f}(x) - f(x)\|$ and relative error is $\|\tilde{f}(x) - f(x)\| / \|f(x)\|$
- What are possible sources of errors?

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- Given a problem f and an algorithm $\tilde{f}$ with an input x, the *absolute error* is $\|\tilde{f}(x) - f(x)\|$ and relative error is $\|\tilde{f}(x) - f(x)\| / \|f(x)\|$
- What are possible sources of errors?
  - Round-off error (input, computation), truncation (approximation) error
- We would like the solution to be *accurate*, i.e., with small errors
- The error depends on property (*conditioning*) of the problem, property (*stability*) of the algorithm

Absolute Condition Number

- Condition number is a measure of *sensitivity* of a problem
- *Absolute condition number* of a problem $\boldsymbol{f}$ at $\boldsymbol{x}$ is

$$\hat{\kappa} = \lim_{\varepsilon \to 0} \sup_{\|\delta \boldsymbol{x}\| \leq \varepsilon} \frac{\|\delta \boldsymbol{f}\|}{\|\delta \boldsymbol{x}\|}$$

  where $\delta \boldsymbol{f} = \boldsymbol{f}(\boldsymbol{x} + \delta \boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x})$

- Less formally, $\hat{\kappa} = \sup_{\delta \boldsymbol{x}} \frac{\|\delta \boldsymbol{f}\|}{\|\delta \boldsymbol{x}\|}$ for infinitesimally small $\delta \boldsymbol{x}$
- If $\boldsymbol{f}$ is differentiable, then

$$\hat{\kappa} = \|\boldsymbol{J}(\boldsymbol{x})\|$$

  where $\boldsymbol{J}$ is the Jacobian of $\boldsymbol{f}$ at $\boldsymbol{x}$, with $J_{ij} = \partial f_i / \partial x_j$, and the matrix norm is induced by vector norms on $\partial \boldsymbol{f}$ and $\partial \boldsymbol{x}$

- Question: What is absolute condition number of $f(x) = \alpha x$?
- Question: Is absolute condition number scale invariant?

Relative Condition Number

- *Relative condition number* of $\boldsymbol{f}$ at $\boldsymbol{x}$ is

$$\kappa = \lim_{\varepsilon \to 0} \sup_{\|\delta \boldsymbol{x}\| \le \varepsilon} \frac{\|\delta \boldsymbol{f}\| / \|\boldsymbol{f}(\boldsymbol{x})\|}{\|\delta \boldsymbol{x}\| / \|\boldsymbol{x}\|}$$

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- Note: we can use different types of norms to get different condition numbers
- If $\boldsymbol{f}$ is differentiable, then

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

- Question: What is relative condition number of $f(x) = \alpha x$?
- Question: Is relative condition number scale invariant?
- In numerical analysis, we in general use relative condition number
- A problem is *well-conditioned* if κ is small and is *ill-conditioned* if κ is large

Condition Numbers

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    - Note: We are talking about the condition number of the problem for a given x
  - Relative condition number $\kappa = \frac{\|\boldsymbol{J}\|}{\|\boldsymbol{f}(\boldsymbol{x})\|/\|\boldsymbol{x}\|} = \frac{1/(2\sqrt{x})}{\sqrt{x}/x} = 1/2$
- Example: Function $f(\boldsymbol{x}) = x_1 - x_2$, where $\boldsymbol{x} = (x_1, x_2)^T$

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- Example: Function $f(\boldsymbol{x}) = x_1 - x_2$, where $\boldsymbol{x} = (x_1, x_2)^T$
  - Absolute condition number of f at x in ∞-norm is $\hat{\kappa} = \|\boldsymbol{J}\|_\infty = \|(1, -1)\|_\infty = 2$
  - Relative condition number $\kappa = \frac{\|\boldsymbol{J}\|_\infty}{\|\boldsymbol{f}(\boldsymbol{x})\|_\infty/\|\boldsymbol{x}\|_\infty} = \frac{2}{|x_1 - x_2|/\max\{|x_1|,|x_2|\}}$
  - κ is arbitrarily large (f is ill-conditioned) if $x_1 \approx x_2$ (hazard of cancellation error)
- Note: From now on, we will talk about only relative condition number

Condition Number of Matrix-Vector Product

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

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

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

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

  - Question: For what $\boldsymbol{x}$ is equality achieved if 2-norm is used?

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  - Question: For what $\boldsymbol{x}$ is equality achieved if 2-norm is used?
  - Answer: $\boldsymbol{x}$ is equal to right singular vector corresponding to smallest singular value of $\boldsymbol{A}$
  - Question: What is condition number of $\boldsymbol{A}\boldsymbol{x}$ if $\boldsymbol{A}$ is singular?
  - Answer: $\leq \infty$ (is ∞ if $\boldsymbol{x} \in \text{null}(\boldsymbol{A})$).

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

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Condition Number of Matrix

- We define condition number of matrix $\boldsymbol{A}$ as

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

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

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

- For 2-norm, $\kappa(\boldsymbol{A}) = \sigma_1/\sigma_n$
- Note about the distinction between the condition number of a *problem* (the map $\boldsymbol{f}(\boldsymbol{x})$) and the condition number of a *problem instance* (the evaluation of $\boldsymbol{f}(\boldsymbol{x})$ for specific $\boldsymbol{x}$)
- Note: condition number of a problem is a property of a problem, and is independent of its algorithm

Outline

Accuracy

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

More on Accuracy

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

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

  i.e., $\leq C_1 \epsilon_{\text{machine}}$ as $\epsilon_{\text{machine}} \to 0$, where constant C_1 may depend on the condition number and the algorithm itself
- In most cases, we expect

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

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