CS 450: Numerical Anlaysis

Chapter 1 – Scientific Computing
Lecture 1
Numerical analysis introduction, motivation, and applications
Posedness, error, and conditioning

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January 18, 2018

What is Numerical Analysis?

- **Numerical Problems:**

inputs problem soln

x f $f(x)$

↑ numerical data ←

- **Error Analysis:**

quality of approximation

$$\text{error} = f(x) - \hat{f}(x)$$

↑ computed solution

Example: Mechanics[1]

- Newton's laws provide incomplete particle-centric picture
- Physical systems can be described in terms of *degrees of freedom* (DoFs)
  - A piston moving up and down requires 1 DoFs
  - 1-particle system requires 3 DoFs
  - 2-particle system requires 6 DoFs
  - 2-particles at a fixed distance requires 5 DoFs
- N-particle system *configuration* described by $3N$ DoFs

basis functions

[1] *Variational Principles of Mechanics*, Cornelius Lanczos, Dover Books on Physics, 1949.

Scientific Computing Applications and Context

- **Mathematical Modelling for Computational Science**

physics – mechanics
– quantum (chemistry)

engineering – control systems (described by a configuration)

biology – DNA

- **Linear Algebra and Computation**

Machine learning – numerical optimization
· linear algebra
– model reduction, reduced repr.
low-rank SVD

Efficiency – HPC — matrix multiplication is ubiquitous

Sources of Error

- **Representation of Numbers:**

  cannot store all digits of π (most)

  finite memory, Solution - store leading significant digits

- **Propagated Data Error:**

  true input

  we are given $\hat{x} \approx x$, error $= f(x) - f(\hat{x})$

- **Computational Error** = $\hat{f}(x) - f(x)$ = **Truncation Error + Rounding Error**

  Truncation Error: error of numerical method (approximation)

  Rounding Error: error introduced by F-P arithmetic

Error Analysis

- **Forward Error:**

absolute $f(x) - \hat{f}(x) \sim f(x) - \hat{f}(\hat{x})$

relative $\dfrac{\text{absolute error}}{\text{true solution}}$

- **Backward Error:**

given $y = \hat{f}(x)$

$y = f(x + \text{backward error})$

backward stable if backward error is bounded by a 'small enough' measure

Conditioning

- **Absolute Condition Number:**

$\kappa_{abs} = \max / \min$ over inputs $\dfrac{\text{perturbation in output}}{\text{perturbation in input}}$

$$\frac{|f(x+\delta x) - f(x)|}{\delta x}$$

- **(Relative) Condition Number:**

perturbation in input

$$\frac{|(f(x+\delta x) - f(x))/f(x)|}{\delta x / x} = \frac{|f'(x)\,x|}{|f(x)|}$$

Numerical Problems

input: x

problem: evaluate $f(x)$

input: $x \in [0, 1]$

problem: evaluate $f(x)$

Posedness and Conditioning

- **What is the condition number of an ill-posed problem?**

$\kappa_{rel} = \infty$ ↑ relative condition number

κ_{abs} – absolute cond.

Stability and Accuracy

- **Accuracy**:

  how close to solution is the computed answer

- **Stability**:

  how sensitive computed solution is to perturbations in input