CS 450: Numerical Analysis

Chapter 1 – Scientific Computing

Lecture 1

Numerical analysis introduction, motivation, and applications
Posedness, error, and conditioning

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What is Numerical Analysis?

- **Numerical Problems:**
  
  inputs → problem → solution

  \[ x \rightarrow f \rightarrow f(x) \]

- **Error Analysis:**
  
  quality of approximation

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

  \( \hat{f}(x) \) computed solution
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 require \[5\] DoFs

\[N\]-particle system *configuration* described by \[3N\] DoFs

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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
Sources of Error

- **Representation of Numbers:**
  
  - *Cannot store all digits of π (most finite memory, solution store leading digits)*

- **Propagated Data Error:**
  
  - We are given \( \hat{x} \approx x \), error = \( f(x) - \hat{f}(x) \)

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

  - Error of numerical method (approximation)
  - Error introduced by FLP arithmetic
Error Analysis

- **Forward Error:**
  
  \[
  \text{absolute } f(x) - \hat{f}(x) \approx f(x) - \hat{f}(\hat{x})
  \]

  \[
  \text{relative } \frac{\text{absolute error}}{\text{true solution}}
  \]

- **Backward Error:**

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

  \[
  y = f(x + \text{error}) \] backward stable

  if backward error is bounded by a ‘small enough’ measure
Conditioning

- **Absolute Condition Number:**
  \[ k_{\text{abs}} = \frac{\text{perturbation in output}}{\text{perturbation in input}} \]
  where \( \min_{\text{over inputs}} \max_{\text{perturbation in input}} \).

- **(Relative) Condition Number:**
  \[ 1 \left( \frac{f(x + \delta x) - f(x)}{f(x)} \right) \]
  with \( \delta x \).
Posedness and Conditioning

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

\[ \kappa = \infty \]

Relative condition number

\[ \kappa_{\text{abs}} - \text{absolute cond.} \]
Stability and Accuracy

- **Accuracy:**
  
  how close to solution is the computed answer

- **Stability:**
  
  how sensitive computed solution is to perturbations in input