CS 450: Numerical Analysis

Chapter 1 – Scientific Computing

Lecture 1

Numerical analysis introduction, motivation, and applications

Posedness, error, and conditioning

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Scientific Computing Applications and Context

- **Mathematical modelling for computational science**  
  Typical scientific computing problems are numerical solutions to PDEs
  - Newtonian dynamics: simulating particle systems in time
  - Fluid and air flow models for engineering
  - PDE-constrained numerical optimization: finding optimal configurations (used in engineering of control systems)
  - Quantum chemistry (electronic structure calculations): many-electron Schrödinger equation

- **Linear algebra and computation**
  - Linear algebra and numerical optimization are building blocks for machine learning methods and data analysis
  - Computer architecture, compilers, and parallel computing use numerical algorithms (matrix multiplication, Gaussian elimination) as benchmarks
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

Course Structure

- Complex numerical problems are generally reduced to simpler problems
  
  - eigenvalue problems → linear systems
  - PDEs → algebraic equations
  - optimization → nonlinear solve → linear systems

- The course topics will follow this hierarchical structure
Application

- nonlinear solve
- optimization
- interpolation, differentiation & quadrature
- numerical PDEs

medic's algebra
Numerical Analysis

- **Numerical Problems involving Continuous Phenomena:**
  
  As opposed to discrete

  solve \( f(x) \) for input \( x \), so

  \[ f(\hat{x}) \approx f(x) \quad \text{as} \quad \delta \to 0 \]

  If not \( \text{ill-posed} \)

  \( \text{well-posed} \)

- **Error Analysis:**

  error vs complexity

  Absolute error: approx. soln - exact \( : \frac{f(x) - \hat{f}(x)}{f(x)} \)

  Relative error: absolute error \( : \frac{f(x) - \hat{f}(x)}{f(x)} \)
Vector quantization $v \in \mathbb{R}^n$ error $\frac{\hat{f}(v) - f(v)}{\|v\|}$
Sources of Error

- Representation of Numbers:
  - Scientific notation (significant digits)
    - $3.14 \times 10^0$, $1.011 \times 2$
    - Precision $\rightarrow$ number of represented significant digits
      - $\neq$ accuracy $\rightarrow |error| = f(x) - x$

- Propagated Data Error:
  - Error introduced at/before input
    - E.g. Experimental measurement

- Computational Error $= \hat{f}(x) - f(x) = \text{Truncation Error} + \text{Rounding Error}$
  - Approximation error made by algorithm
Error Analysis

- **Forward Error:**
  
  absolute & relative

  given input $x$, true solution $f(x)$, computed solution $\hat{f}(x)$

  forward error if $f(x) - \hat{f}(x)$

- **Backward Error:**

  $\Delta x = \hat{x} - x$ where $f(x) = \hat{f}(x)$

  min $\Delta x$ such that $

  \hat{x}$

  relative backward error would be $\frac{\hat{x} - x}{x}$
Conditioning

- Absolute Condition Number:

\[
\lim_{\Delta x \to 0} \max_{\text{perturbations}} \max_{\text{inputs} \in \text{range}} \frac{|f(x + \Delta x) - f(x)|}{|\Delta x|} \quad \text{for } f'(x) \neq 0
\]

- (Relative) Condition Number:

conditioning w.r.t. relative error

\[
\varepsilon_{\text{rel}} = \left| \frac{f'(x) \cdot x}{f(x)} \right|
\]

\[
\varepsilon = \max_{x \in [0,1]} |f'(x)| = |f'(x)|
\]

\[
\lim_{h \to 0} \left| \frac{f(x+h) - f(x)}{h} \right|
\]
What is the condition number of an ill-posed problem?

- forward error vs backward error
- given bound on condition $\kappa$
- and we find a backward error bound of $\|E\|$
- We have forward error bound $\kappa \cdot \|E\|$
Stability and Accuracy

- **Accuracy:**
  how far away we are from desired soln.

- **Stability:**
  sensitivity of algorithm to perturbation/