CS 450: Numerical Anlaysis[1]

Introduction to Scientific Computing

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[1] *These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book "Scientific Computing: An Introductory Survey" by Michael T. Heath (slides).*

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*

Example: Mechanics[2]

- 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 ____________ DoFs
  - 1-particle system requires ____________ DoFs
  - 2-particle system requires ____________ DoFs
  - 2-particles at a fixed distance require ____________ DoFs
- N-particle system *configuration* described by $3N$ DoFs

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

Course Structure

- **Complex numerical problems are generally reduced to simpler problems**

- **The course topics will follow this hierarchical structure**

Numerical Analysis

- **Numerical Problems involving Continuous Phenomena**:

- **Error Analysis**:

Sources of Error

***Demo:** Floating Point vs Program Logic*

- **Representation of Numbers**:

- **Propagated Data Error**:

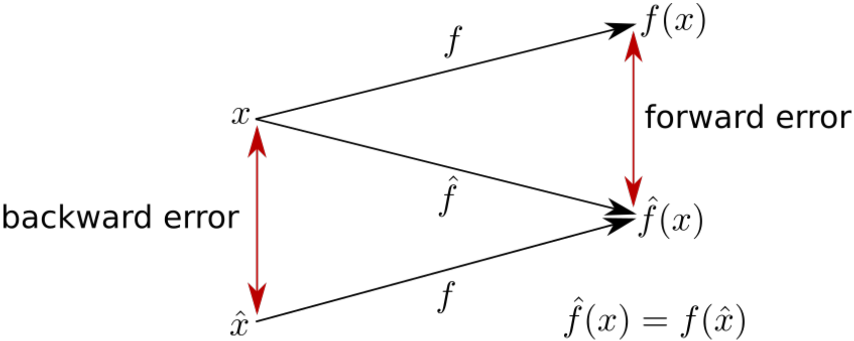
- **Computational Error** = $\hat{f}(x) - f(x)$ = **Truncation Error + Rounding Error**

Error Analysis

- **Forward Error**:

- **Backward Error**:

Visualization of Forward and Backward Error



Conditioning

- **Absolute Condition Number**:

- **(Relative) Condition Number**:

Posedness and Conditioning

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

Stability and Accuracy

- **Accuracy**:

- **Stability**:

Demo: *Truncation vs Rounding*

Error and Conditioning

- Two major sources of error: *roundoff* and *truncation* error.
  - roundoff error concerns floating point error due to finite precision
  - truncation error concerns error incurred due to algorithmic approximation, e.g. the representation of a function by a finite Taylor series

- To study the propagation of roundoff error in arithmetic we can use the notion of conditioning.

Floating Point Numbers

***Demo:** Picking apart a floating point number*
***Demo:** Density of Floating Point Numbers*

- **Scientific Notation**

- **Significand (Mantissa) and Exponent** Given x with s leading bits $x_0, \ldots, x_{s-1}$

Rounding Error

***Demo:** Floating point and the Harmonic Series*
***Demo:** Floating Point and the Series for the Exponential Function*

- **Maximum Relative Representation Error (Machine Epsilon)**

Rounding Error in Operations (I)

Demo: *Catastrophic Cancellation*
Activity: *Cancellation in Standard Deviation Computation*

- **Addition and Subtraction**

Rounding Error in Operations (II)

- **Multiplication and Division**

Exceptional and Subnormal Numbers

- **Exceptional Numbers**

- **Subnormal (Denormal) Number Range**

- **Gradual Underflow: Avoiding underflow in addition**

Floating Point Number Line