

CS 450: Numerical Analysis

Chapter 1 – Scientific Computing

Lecture 1

Numerical analysis introduction, motivation, and applications

Posedness, error, and conditioning

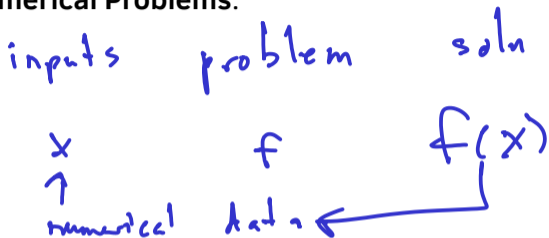
Edgar Solomonik

Department of Computer Science
University of Illinois at Urbana-Champaign

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What is Numerical Analysis?

► Numerical Problems:



► Error Analysis:

quality of approximation

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

$\hat{f}(x)$
↑
computed solution

Example: Mechanics¹

- ▶ 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 n configurations)

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:

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

↓ true input

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

error of numerical method (approximation)

error introduced by F-P arithmetic

Error Analysis

► Forward Error:

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

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

► 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:**

$$\kappa_{abs} = \frac{\text{perturbation in output}}{\text{perturbation in input}}$$

max & min over inputs

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

- ▶ **(Relative) Condition Number:**

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

part. in input

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?

$\kappa_{rel} \propto$



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