

Numerical Analysis / Scientific Computing

CS450 / CSE 401 / ECE 491
/ MATH 450

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Outline

Introduction to Scientific Computing

Notes

Notes (unfilled, with empty boxes)

About the Class

Errors, Conditioning, Accuracy, Stability

Floating Point

Systems of Linear Equations

Linear Least Squares

Eigenvalue Problems

Nonlinear Equations

Optimization

Interpolation

Numerical Integration and Differentiation

Initial Value Problems for ODEs

Boundary Value Problems for ODEs

Partial Differential Equations and Sparse Linear Algebra

Fast Fourier Transform

Additional Topics

What's the point of this class?

'*Scientific Computing*' describes a family of approaches to obtain approximate solutions to problems *once they've been stated mathematically*.

Name some applications:

- Numerical simulation (e.g. engineering)
 - ↳ differential equations
- machine learning/stats
 - statistical models
 - optimization
- Image and audio processing

What do we study, and how?

Problems with real numbers (i.e. continuous problems)

\mathbb{T} \leadsto how \mathbb{R} go into a computer

What's the general approach?

- how to represent the solution
- existence / uniqueness

What makes for *good* numerics?

How good of an answer can we expect to our problem?

- how to even measure sol. quality
- given that we can't even represent numbers (!!)

How fast can we expect the computation to complete?

- math. statement (discrete)
 - method
 - algorithm
- cost $\left\{ \begin{array}{l} \text{asymptotic } O(n^3) \\ \text{efficiency} \end{array} \right.$
- efficient?

Implementation concerns

How do numerical methods *get implemented*?

- like anything in computing: lies
- tools/languages : "tower of abstractions"
 - ↳ methods
 - ↳ robustness / guarantees

Class web page

<https://bit.ly/cs450-f22>

- ▶ Assignments
 - ▶ HW1!
 - ▶ Pre-lecture quizzes
 - ▶ In-lecture interactive content (bring computer or phone if possible)
- ▶ Textbook
- ▶ Exams
- ▶ Class outline (with links to notes/demos/activities/quizzes)
- ▶ Discussion forum
- ▶ Policies
- ▶ Video

Programming Language: Python/numpy

- ▶ Reasonably readable
- ▶ Reasonably beginner-friendly
- ▶ Mainstream (top 5 in 'TIOBE Index')
- ▶ Free, open-source
- ▶ Great tools and libraries (not just) for scientific computing
- ▶ Python 2/3? 3!
- ▶ `numpy`: Provides an array datatype
Will use this and `matplotlib` all the time.
- ▶ See class web page for learning materials

Demo: Sum the squares of the integers from 0 to 100. First without `numpy`, then with `numpy`.

Supplementary Material

- ▶ [Numpy \(from the SciPy Lectures\)](#)
- ▶ [100 Numpy Exercises](#)
- ▶ [Dive into Python3](#)

Sources for these Notes

- ▶ M.T. Heath, *Scientific Computing: An Introductory Survey*, Revised Second Edition. Society for Industrial and Applied Mathematics, Philadelphia, PA. 2018.
- ▶ [CS 450 Notes by Edgar Solomonik](#)
- ▶ Various bits of prior material by Luke Olson

Open Source <3

These notes (and the accompanying demos) are open-source!

Bug reports and pull requests welcome:

<https://github.com/inducer/numerics-notes>

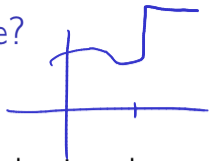
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What problems *can* we study in the first place?



To be able to compute a solution (through a process that introduces errors), the problem...

- existence
- uniqueness
- depend continuously on the inputs

If it satisfies these criteria, the problem is called **well-posed**. Otherwise, *ill-posed*.

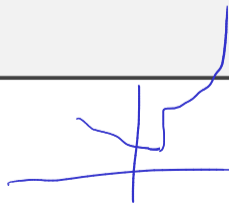
→ otherwise trouble
if inputs are perturbed
(say by rounding error)

Dependency on Inputs

We excluded discontinuous problems—because we don't stand much chance for those.

... what if the problem's input dependency is just *close to discontinuous*?

- sensitive output to input
- absence of error amplification



Approximation

$$f(x+h) \approx \sum_{i=0}^n \frac{f^{(i)}(x)}{i!} h^i$$

When does approximation happen?

Before computation:

- modeling
- measurement

During computation:

- rounding
- truncation / discretization

Demo: Truncation vs Rounding [cleared]

Example: Surface Area of the Earth

Compute the surface area of the earth.

What parts of your computation are approximate?

$$4\pi r^2$$

Measuring Error

How do we measure error?

Idea: Consider all error as being *added onto* the result.

$$\text{Relative error} = \frac{\text{abs. error}}{\text{mag. of true value}} = \frac{|x - \tilde{x}|}{|x|}$$

$$\text{abs. error} = \text{mag. of true answer} - \text{approx. answer} = |x - \tilde{x}|$$

Recap: Norms

$$\begin{pmatrix} 1 \\ 3 \\ 5 \end{pmatrix}$$

↑ vector

What's a norm?

$$f: \mathbb{R}^n \rightarrow \mathbb{R}_0^+$$

$$\|\vec{x}\|$$

Define *norm*.

$\|\cdot\|: \mathbb{R}^n \rightarrow \mathbb{R}_0^+$ is called a norm iff

$$\|\vec{x}\| > 0 \Leftrightarrow \vec{x} \neq \vec{0}$$

$$\|\gamma \vec{x}\| = |\gamma| \|\vec{x}\|$$

$$\|\vec{x} + \vec{y}\| \leq \|\vec{x}\| + \|\vec{y}\|$$

Norms: Examples

Examples of norms?

$$\left\| \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \right\|_2 = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$$

Demo: Vector Norms [cleared]

Norms: Which one?

Does the choice of norm really matter much?

