

Numerical Analysis / Scientific Computing

CS450 / MATH 410 / ECE 481 /

CSE 401

Andreas Kloeckner

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Outline

Introduction to Scientific Computing

Notes

Notes (unfilled, with empty boxes)

Notes (source code on Github)

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:

- ▷ Engineering sim.
- ▷ Machine Learning

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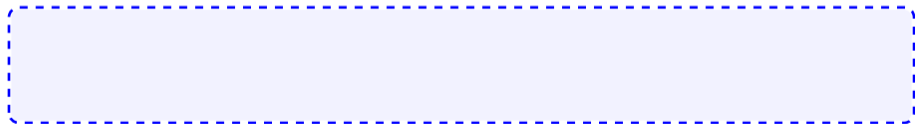
- ▶ Engineering simulation
 - ▶ E.g. Drag from flow over airplane wings, behavior of photonic devices, radar scattering, ...
 - ▶ → Differential equations (ordinary and partial)
- ▶ Machine learning
 - ▶ Statistical models, with unknown parameters
 - ▶ → Optimization
- ▶ Image and Audio processing
 - ▶ Enlargement/Filtering
 - ▶ → Interpolation
- ▶ Lots more.

What do we study, and how?

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



What's the general approach?



What do we study, and how?

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

- ▶ As opposed to *discrete* problems.
- ▶ Including: How can we put a real number into a computer?
(and with what restrictions?)

What's the general approach?

- ▶ Pick a *representation* (e.g.: a polynomial)
- ▶ Existence/uniqueness?

What makes for *good* numerics?

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



How fast can we expect the computation to complete?



What makes for *good* numerics?

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

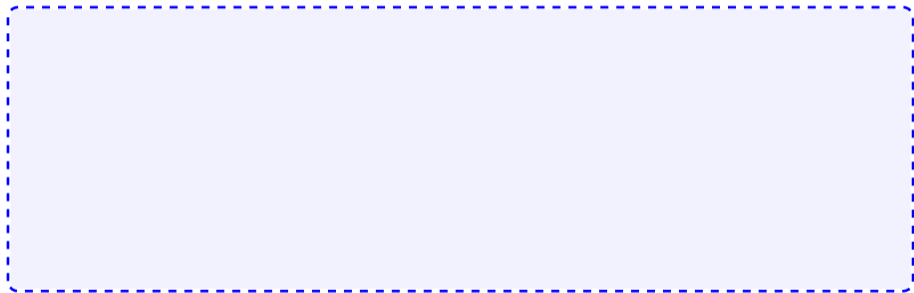
- ▶ Can't even represent numbers exactly.
- ▶ Answers will always be *approximate*.
- ▶ So, it's natural to ask *how far off the mark* we really are.

How fast can we expect the computation to complete?

- ▶ A.k.a. what algorithms do we use?
- ▶ What is the cost of those algorithms?
- ▶ Are they efficient?
(I.e. do they make good use of available machine time?)

Implementation concerns

How do numerical methods *get implemented*?



Implementation concerns

How do numerical methods *get implemented*?

- ▶ Like anything in computing: A layer cake of *abstractions* (“careful lies”)
- ▶ What tools/languages are available?
- ▶ Are the methods easy to implement?
- ▶ If not, how do we make use of existing tools?
- ▶ How robust is our implementation? (e.g. for error cases)

Class web page

<https://bit.ly/cs450-f24>

- ▶ Assignments
 - ▶ HW1 (soon!)
 - ▶ 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. . .



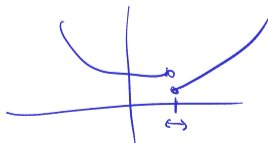
If it satisfies these criteria, the problem is called *well-posed*. Otherwise, *ill-posed*.

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

- ▶ Needs to *have* a solution
- ▶ That solution should be *unique*
- ▶ And *depend continuously* on the inputs

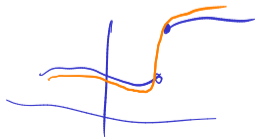
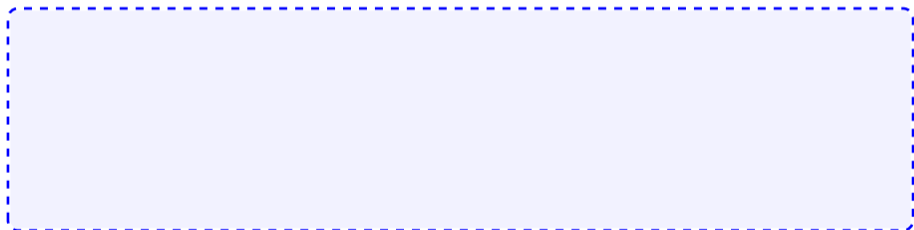
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Dependency on Inputs

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*?



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*?

- ▶ We call those problems *sensitive* to their input data. Such problems are obviously trickier to deal with than non-sensitive ones.
- ▶ Ideally, the computational method will not *amplify* the sensitivity

Approximation

When does approximation happen?

▷ `round`

▷ `trunc`

Demo: Truncation vs Rounding [cleared]

Approximation

When does approximation happen?

- ▶ Before computation
 - ▶ modeling
 - ▶ measurements of input data
 - ▶ computation of input data
- ▶ During computation
 - ▶ truncation / discretization
 - ▶ rounding

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?

$$4\pi r^2$$

Example: Surface Area of the Earth

Compute the surface area of the earth.

What parts of your computation are approximate?

All of them.

$$A = 4\pi r^2$$

- ▶ Earth isn't really a sphere
- ▶ What does radius mean if the earth isn't a sphere?
- ▶ How do you compute with π ? (By rounding/truncating.)

Measuring Error

How do we measure error?

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

$$\begin{aligned} \text{error} &:= \text{true} - \text{approximate} \\ \text{abs. error} &:= |\text{true} - \text{approximate}| \\ \text{rel. error} &:= \frac{\text{abs. error}}{|\text{true}|} \end{aligned}$$

Recap: Norms

What's a norm?

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

"how far away from $\vec{0}$ "

Define *norm*.

$$\|\vec{x}\|: \mathbb{R}^n \rightarrow \mathbb{R}_0^+$$

- $\|\vec{x}\| = 0 \Leftrightarrow \vec{x} = \vec{0}$ ("definiteness")

- $\|\alpha \vec{x}\| = |\alpha| \|\vec{x}\|$

- $\|\vec{x} + \vec{y}\| \leq \|\vec{x}\| + \|\vec{y}\|$ ("triangle inequality")

Norms: Examples

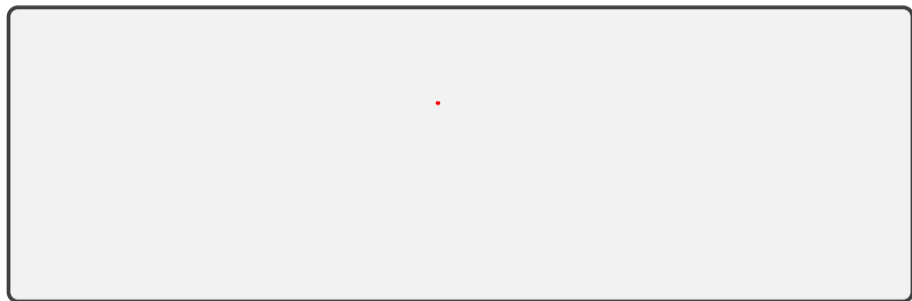
Examples of norms?

$$\|x\|_p = \sqrt[p]{\sum_{i=1}^n |x_i|^p} \quad (p > 1)$$

Demo: Vector Norms [cleared]

Norms: Which one?

Does the choice of norm really matter much?



In these notes: If we write $\|\cdot\|$ without any specifics, then the statement is true for any norm. If a specific norm is needed, the notation will indicate that.