Numerical Analysis / Scientific Computing

CS450

Andreas Kloeckner, Xiaoyu Wei

Fall 2021

Scientific Computing Area

Outline

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:

- Stock market → predictions 'Simulations'
  - engineering models
  - differential equations (ODE/PDE)
- Marketing/Adv. → ML models
- Protein engineering →
- signal processing

What do we study, and how?

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

- As opposed to discrete
- Putting real numbers in a computer

What's the general approach?

- Pick a representation
- Existence / uniqueness

What makes for *good* numerics?

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

- Real numbers don't exist in computers
- Answers be approximate

- Put upper bound on the error

How fast can we expect the computation to complete?

- What algorithms do we use?
- What's the cost?
- How do we model the cost?

- Are they efficient? (on a machine)

mult: n^2 → $5n^2$ → $O(n^2)$

$A = ab^T$

$= a(b^T x) = (ab^T)x$

Implementation concerns

How do numerical methods *get implemented*?

- interfaces / abstractions (BLAS / numpy)
- What is available?
- Is a method easy to implement?
- How do we build it on existing machinery?
- Does the impl. that influence the error?

Class web page

https://bit.ly/cs450-f21

- 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)
- Virtual Machine Image
- Piazza
- Policies
- Video
- Inclusivity Statement

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

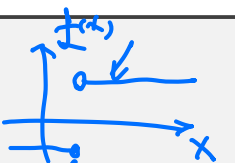
These notes (and the accompanying demos) are open-source!

Bug reports and pull requests welcome:
https://github.com/inducer/numerics-notes

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

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

- Have a solu
- Unique solu
- Output depends cont. on inputs.



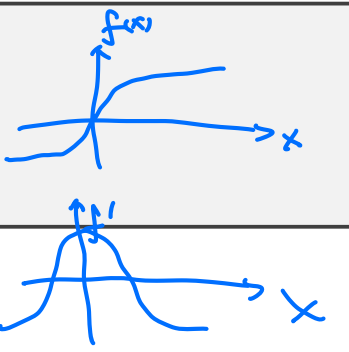
If it satisfies these criteria, the problem is called *well-posed*. Otherwise, *ill-posed*.

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*?

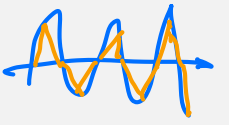
Large error.



Approximation

When does approximation happen?

- rounding error
- over/under flow.
- truncation error



Demo: Truncation vs Rounding

Example: Surface Area of the Earth

Compute the surface area of the earth.
What parts of your computation are approximate?

$A = 4\pi r^2$

Measuring Error

How do we measure error?

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

Abs. error = approx value − true value

rel. error = $\frac{\text{observed}}{|\text{true value}|}$

Estimate

→ proving upper bounds

"a priori"

"a posteriori"

Recap: Norms

What's a norm?

$f : \mathbb{R}^n \to \mathbb{R}_0^+$ "returns a magnitude of the vec

$\|\vec{x}\|$

Define *norm*.