

Computational Methods for Engineers

how to waste your time on writing code and have lots of
fun

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Jan 2020

Outline

- ▶ Goals of this course
- ▶ Integrating math/physics/code
- ▶ Python
- ▶ Your commitment

Scientific Computing

aka: Computational Science, Scientific Computation

- ▶ Simulations
- ▶ Data fitting and analysis
- ▶ Optimization
- ▶ Visualization
- ▶ ...

Goal: Gain understanding through analysis of mathematical models implemented on computers.

Steps in Computational Science

- ▶ A story - observation
- ▶ Mathematical model
- ▶ Discretization of the model
- ▶ Solving the model
- ▶ Parameters fitting
- ▶ Visualizing the result

Example I: Newton's apple



- ▶ Observation - Apple is falling
- ▶ Math model

$$\frac{d^2x}{dt^2} = -g$$

(but what is g ?)

- ▶ Discretization

$$\frac{x(t_{i+1}) - 2x(t_i) + x(t_{i-1}))}{\Delta t^2} = -g.$$

- ▶ Solve

$$x(t_{i+1}) = -g\Delta t^2 + 2x(t_i) - x(t_{i-1})$$

- ▶ Measure and find an approximation to g
- ▶ Visualize

Example I: Newton's apple

Data assimilation

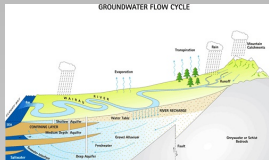
What is g ?

Observations (noisy)

$$t = [0, 1, 2, 3] \quad x = [0, 4.4, 21.0, 54.2]$$

- ▶ Can the mathematical model (reasonably) explain the data?
- ▶ What is the (best) value of g ?

Example II: Ground water flow



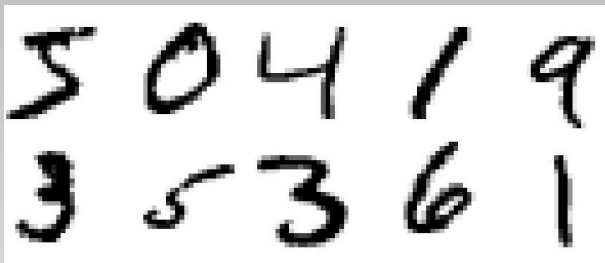
- ▶ Observation - Water flow in the ground
- ▶ Math model

$$\nabla \cdot \sigma \nabla p = q \quad \rho_t + \nabla \cdot (\sigma \nabla p) \rho = 0$$

- ▶ Discretization ... (you will know all about this)
- ▶ Solve ... (you will know all about this)
- ▶ Visualize

Example III: Pattern identification

Simplest example - Character recognition. We have digits ($[0, \dots, 9]$) in an image and we want to get them explicitly.



Mathematical model - ???

Example III: Pattern identification

Machine learning, try the following model known as
Convolution Neural Network

$$\mathbf{y} = \mathbf{w}^{\top} \tanh(\mathbf{K} \star \mathbf{x} + \mathbf{b})$$

No physical basis so we hope it can do the trick ...

Example III: Pattern identification

$$\mathbf{y} = \mathbf{w}^T \tanh(\mathbf{K} \star \mathbf{x} + \mathbf{b})$$

- ▶ \mathbf{y} vector of 10, with probabilities of the digits
Example: $[0, 0.65, 0, 0, 0, 0, 0, 0.35, 0, 0]$ imply 65% the number 1 and 35% the number 7
- ▶ \mathbf{x} the image
- ▶ \mathbf{K} , \mathbf{b} and \mathbf{w} parameters

Example III: Pattern identification

Pattern recognition can be applied for many problems when the math is too complex or unknown

- ▶ Climate prediction
- ▶ Weather
- ▶ Flow in complex systems
- ▶ Much more ...

Goal of this course

- ▶ Describe useful physical models in earth science
 1. Flow in porous media
 2. Pressure system
 3. Heat propagation
- ▶ Learn how to simulate them on the computer
- ▶ Learn how to integrate field data into physical models

Integration of Physics/Math/Computing

This course has a new paradigm. We

- ▶ Describe the physics
- ▶ Develop a mathematical model
- ▶ Write code to simulate this model

We will cover most of the math you need but we will use

- ▶ Vector calculus
- ▶ Differential equations
- ▶ Linear algebra
- ▶ Python programming

Computing

- ▶ The course will involve **lots** of programming and computing
- ▶ Bring your laptop
- ▶ Code will be handled through GitHub
- ▶ Working in groups, encouraged!

Python

- ▶ We will be coding with Python and use Jupyter Notebooks
- ▶ Main packages we use: NumPy and Torch.
- ▶ Tutorials on Python and using NumPy and PyTorch can be found at
<http://cs231n.github.io/python-numpy-tutorial/>
<https://pytorch.org/tutorials/>

Grading

- ▶ Homework and programming assignments 40%
- ▶ Midterms 30%
- ▶ Final 30%

You need a pass in the final and homework to pass the course