Computational Methods for Geological Engineers

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Learning Outcomes

At the end of the course, participants will be able to:

- Code mathematical and physical models in pytorch
- Solve some ODE's
- Find parameters within the simulation

Approximate schedule

Week	Technical Programming	Analytical Skills
Week 1	intro to python	Intro to O/PDEs
Week 2	loops and vectorization	Separable ODEs
Week 3	functions and classes, Finite difference	Integrating factors
Week 4-5	Solving IVP's particle propagation	Integrating factors
Week 6-7	Nonlinear equations	Second order equations
Week 8	Implicit methods	Systems
Week 9-10	The discrete Laplacian	BVPs
Week 11-12	Parameter estimation	
Week 13	Catch-up	

- **Programming Quiz:** Jan 24
- **Midterm** Feb 28

Motivation

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

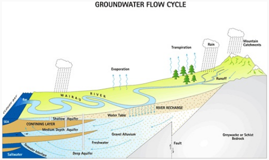
What is g?

Observations (noisy)

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

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

Example II: Ground water flow



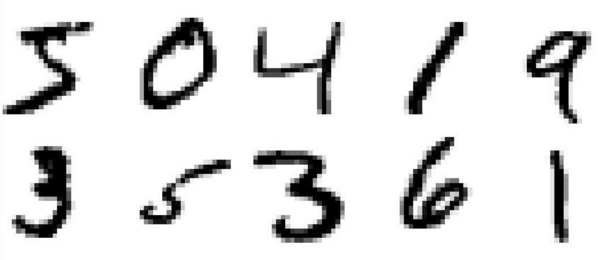
- Observation - Water flow in the ground
- Math model

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

- 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,...,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

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

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

Example III: Pattern identification

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

- 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
- x the image
- K, b and 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
- 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 with pytorch

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 VS code (primarily) and 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/

Python

We will be using two types of Python environments

- A Python Integrated development environment (IDE)
  - VS code
  - Spyder
  - PyCharm
  - Choose your own (your own support)
- Jupyter notebook `https://jupyter.org/`

Grading

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

Ordinary Differential Equations

ODE's - Ordinary differential equations

$$\frac{d\mathbf{y}}{dt} = f(t, \mathbf{y}; p)$$

or more specifically

$$\frac{d}{dt}\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} f_1(y_1, \ldots, y_n; p) \\ \vdots \\ f_n(y_1, \ldots, y_n; p) \end{pmatrix}$$

Appear in many applications

- Particle flow
- Disease propagation
- Fake news detection
- Geochemistry
- ...

ODE's - Classification

- Linear first order
- Linear higher order
- Nonlinear first order
- Nonlinear higher order
- System, linear
- System, nonlinear

Separation of variables

We have a special case

$$\frac{dy}{dx} = f(x, y) = \frac{g(x)}{w(y)}$$

Then

$$w(y)dy = g(x)dx$$

$$\int^{y} w(y)dy = \int^{x} g(x)dx + C$$

Integrate and solve for $y(x)$

Examples

Exponential model

$$\frac{dy}{dx} = \lambda y$$

Examples

Logistic model

$$\frac{dy}{dx} = \lambda y \left(1 - \frac{y}{a}\right)$$

Hint -

$$\frac{1}{y(1-y/a)} = \frac{1}{y} + \frac{1}{a+y}$$