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	Motivation, why
Week 2	intro to python	Separable ODEs
Week 3	Finite difference	Finite difference
Week 4	Finite difference	Integrating factors
Week 5	Solving IVP's particle propagation	Second order equations/Syste
Week 6	Nonlinear equations	Systems
Week 7	Implicit methods	Boundary Value Problems
Week 8	Matrix methods for BVP	Boundary Value Problems
Week 9-10	Optimization	Optimization
Week 11-12	Parameter estimation	Optimization
Week 13	Catch-up	Catch up

- **Programming Quiz:** Jan 23
- **Midterm I** Feb 27
- **Midterm II** March 27

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
- Initial value problems, Boundary value problems

Types of ODE's

Linear ODE's

$$\dot{y} = f(y)$$

$f(y) = Ay + b$, that is f is linear.

Nonlinear ODE's

$$\dot{y} = f(y)$$

e.g. $f(y) = \cos(y)$, that is f is nonlinear.

Types of ODE's

First order ODE's

$$\dot{y} = f(y)$$

Higher order ODE's

$$y''' = f(y)$$

Types of ODE's

Initial value problems (IVP)

$$y'' = f(y) \quad y'(0) = y_0, \quad y''(0) = y_0''$$

Boundary value problems

$$y''' = f(y) \quad y(0) = y_0, \quad y(1) = y_1$$

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 -

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