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/Syster
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 -

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

END LECTURE 2

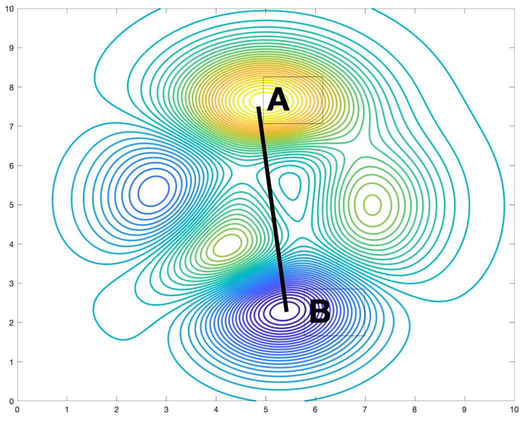
Finite Difference

Goal: Approximate the derivative

Why

- To solve ODE's on the computer (to come)
- To understand data
- For design

Example: Path design



What is the slope of the proposed path from A to B?

Is it too steep?

Finite Difference

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \ldots$$

"Solve" for $f'(x)$

$$\frac{f(x+h) - f(x)}{h} = f'(x) + \frac{1}{2}f''(x)h + \frac{1}{6}f'''(x)h^2 + \ldots$$

Think small h, the leading error behaves like h

$$\frac{f(x+h) - f(x)}{h} = f'(x) + \mathcal{O}(h)$$

Similarly (to be derived at home)

$$\frac{f(x) - f(x-h)}{h} = f'(x) + \mathcal{O}(h)$$

Higher Order Finite Difference

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \ldots$$

$$\begin{aligned}
\frac{f(x+h) - f(x)}{h} &= f'(x) + \frac{1}{2}f''(x)h + \frac{1}{6}f'''(x)h^2 + \ldots \\
\frac{f(x) - f(x-h)}{h} &= f'(x) - \frac{1}{2}f''(x)h + \frac{1}{6}f'''(x)h^2 + \ldots
\end{aligned}$$

Add them together to obtain

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{1}{6}f'''(x)h^2 + \ldots$$

Or equivalent

$$\frac{f(x+h) - f(x)}{h} = f'(x + h/2) + \mathcal{O}(h^2)$$

Finite Difference on a mesh

Components

- A mesh $\mathbf{x} = [x_1, x_2, \ldots, x_n]^\top$
- The functions on the mesh $\mathbf{f} = [f(x_1), \ldots, f(x_n)]^\top$
- Approximate the derivative at x_j

$$f'(x_j) + \mathcal{O}(h) = \frac{f(x_j + h) - f(x_j)}{h} = \frac{f(x_{j+1}) - f(x_j)}{h}$$

- Approximate the derivative at $x_{j+\frac{1}{2}}$

$$f'(x_{j+\frac{1}{2}}) + \mathcal{O}(h^2) = \frac{f(x_j + h) - f(x_j)}{h} = \frac{f(x_{j+1}) - f(x_j)}{h}$$

The forward Euler Method

Numerically solve the ODE

$$y' = f(t, y)$$

Use forward difference to obtain

$$\frac{y(t+h) - y(t)}{h} = f(t, y)$$

or

$$y(t+h) = y(t) + hf(t, y)$$

Indexing

$$\mathbf{y} = [y(t=0), y(t=h), y(t=2h), ..., y(t=Nh)] = [\mathbf{y}_0, \ldots, \mathbf{y}_N]$$

we write

$$\mathbf{y}_{j+1} = \mathbf{y}_j + hf(t_j, \mathbf{y}_j)$$

The forward Euler Method

How to pick h?

- Solve the problem on two (nested) grids and compare the results
- Mesh size H

$$\mathbf{y}_{coarse} = [y(0), y(H), y(2H), ..., y(NH)]$$

- Do it again for $h = H/2$ and obtain

$$\mathbf{y}_{fine} = [y(0), y(h), y(2h), ..., y(2Nh)]$$

- Compare

$$\mathbf{r} = [y_{coarse}(H) - y_{fine}(2h), y_{coarse}(2H) - y_{fine}(4h) ...., y_{coarse}(NH) - y_{fine}(2Nh)]$$

- If error small enough stop.

END LECTURE 3