Lecture 6 - Numerical Differential Equations

Class Business

* prayer / spiritual thought
* unit of the day

$$°R = °F + 459.67$$

↑ Rankine ↖ Farenheit

* Rankine is also an absolute temperature scale.

I. Differential Equations

* Differential equations are equations which contain objects with differential operators, e.g.,

$$\frac{d^2x}{dt^2} + 5x = 0$$

* In chemical engineering, we often encounter a class of differential equations we call rate equations.

Rate equations are first-order, ODEs where the derivative is with respect to time,

$$\frac{dy}{dt} = f(y,t)$$

$$y(0) = y_0$$

comments:

- first order: $\frac{dy}{dt}$ is a first derivative.

- ODE: ordinary differential equation
  - ↳ no partial derivatives, Derivatives of one variable only
- derivative w.r.t. time only: $\frac{dy}{dt}$. this is the rate.
- $y(0) = y_0$ is the initial condition

example:

I drive home at 30 mph. Find my position as a function of time.

$$\frac{dy}{dt} = v \qquad v = 30 \text{ mph}$$

$$y(t=0) = y_0$$

solve analytically:

$$\frac{dy}{dt} = v$$

$$dy = v\,dt$$

$$\int dy = \int v\,dt$$ indefinite integral

$$y = vt + c$$ ← use $y(0) = y_0$ to find c

$$y(0) = 0 + c \Rightarrow c = y(0) = y_0$$

$$\boxed{y = vt + y_0}$$

* what if I can't do the integral?
  - Non-linear
  - multiple, coupled rate equations
  - What if it is just messy?

  } Try a numerical approach.

II. Methods for Rate Equations

A. Explicit Euler method.

$$\frac{dy}{dt} = f(y,t) \quad \leftarrow \text{How solve numerically?}$$

$y(0) = y_0$

(i) Pick discrete time points

(ii) Approximate the derivative

(i)

n	0	1	2	3	4	....	
t	0	0.5	1	1.5	2	2.5	...
y	y_0	?					

(ii)

$$\frac{dy}{dt} \approx \frac{\Delta y}{\Delta t} \quad (\text{if } \Delta t \text{ is small})$$

$$= \frac{y_{n+1} - y_n}{t_{n+1} - t_n} \quad \text{e.g.} \quad \frac{y_1 - y_0}{t_1 - t_0}$$

Putting (i) & (ii) together:

use the y & t we know at point n.

$$\frac{y_{n+1} - y_n}{t_{n+1} - t_n} = f(y_n, t_n)$$

normally Δt is a constant value.

solve for y_{n+1}

$$\boxed{y_{n+1} = y_n + \Delta t\, f(y_n, t_n)}$$

Explicit Euler Method

Activity

* Do an example of explicit euler method in Excel
* let students practice
* what happens when Δt is too big? Method is unstable

B. Multiple variables

* what happens when we have more than one, coupled rate equations?

e.g.
$$\frac{dy_1}{dt} = f_1(y_1, y_2, t)$$
$$\frac{dy_2}{dt} = f_2(y_1, y_2, t)$$

* Nothing much changes. We still discretize and approximate the derivative.

$$\frac{y_{1,n+1} - y_{1,n}}{\Delta t} = f_1(y_{1,n}, y_{2,n}, t_n)$$

$$\frac{y_{2,n+1} - y_{2,n}}{\Delta t} = f_2(y_{1,n}, y_{2,n}, t_n)$$

$$y_{1,n+1} = y_{1,n} + \Delta t\, f_1(y_{1,n}, y_{2,n}, t)$$
$$y_{2,n+1} = y_{2,n} + \Delta t\, f_2(y_{1,n}, y_{2,n}, t)$$

* We can generalize this in vector format

$$\boxed{\underline{y}_{n+1} = \underline{y}_n + \Delta t\, \underline{f}(\underline{y}_n, t)}$$

Activity

* Do an example of explicit Euler with multiple variables
* Let students practice.