

Lecture 6 - Numerical Differential Equations

Class Business

* prayer / spiritual thought

* unit of the day

$$^{\circ}R = ^{\circ}F + 459.67$$

$\uparrow$ $\nwarrow$
 Rankine Fahrenheit

* Rankine is also an absolute temperature scale.

I. Differential Equations

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

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

* 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.

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

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

solve analytically:

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

$$dy = v dt$$

$$\int dy = \int v dt \quad \text{indefinite integral}$$

$$y = vt + c \quad \leftarrow \text{use } y(0) = y_0 \text{ to find } c$$

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

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

* 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

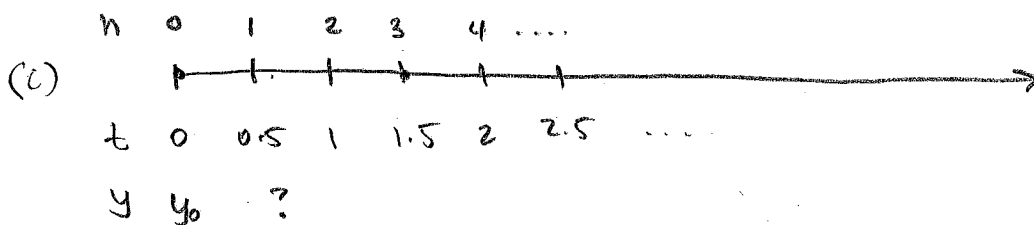
A. Explicit Euler method.

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

$$y(0) = y_0$$

(i) Pick discrete time points

(ii) Approximate the derivative



(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:

normally
 Δt is a
constant
value.

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

use the y & t we know at point n .

↓ solve for y_{n+1}

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

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

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

Activity

* Do an example of explicit Euler with multiple variables

* let students practice.