Indian Institute of Technology Roorkee

CHN-323
Computer Applications in Chemical Engineering

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Example 1

A first order reaction occurs in a jacketed MFR. The material and energy balance equations are:

$$\frac{dC}{dt} = 0.00005 - C\left[0.005 + \exp\left(\alpha - \frac{11324}{T}\right)\right]$$

$$\frac{dT}{dt} = 1.74 - 0.0057\,T + C\exp\left(\beta - \frac{11324}{T}\right)$$

We have the following experimental "time-series" data. Use the data to estimate the unknown parameters α and β.

t	C	T
0	0.0100	300.00
50	0.0084	303.30
100	0.0068	306.20
150	0.0054	308.62
200	0.0042	310.47
250	0.0034	311.75
300	0.0029	312.55
350	0.0027	313.03
400	0.0025	313.31
450	0.0024	313.48
500	0.0024	313.58

Differential equations

- Ordinary differential equations
  - Initial value problem (IVP)
  - Boundary value problem (BVP)

- Partial differential equations

Initial value problem (IVP)

- Solve

$$\frac{dy}{dt} = 4e^{0.8t} - 0.5y$$

- Initial condition, $y(t = 0) = 2$

Boundary value problem (BVP)

- Diffusion followed by 1st order Rxn in a Slab

$$\frac{d^2y}{dx^2} - y = 0$$

- Boundary conditions

1. $\frac{dy}{dx} = 0$ at $x = 0$
2. $y = 1$ at $x = 1$

Finite-difference approximations

- Finite-difference approximations provide a means to transform derivatives into algebraic form

Forward Difference Formula (1st order accurate)

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

Backward Difference Formula (1st order accurate)

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

Centered Difference Formula (2nd order accurate)

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

Centered Difference Formula for 2nd Derivative (2nd order accurate)

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

Euler's method (IVP)

- Based on forward difference
- Consider the following ODE

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

- Let us take any time t_i, corresponding y is y_i. The ODE should be valid at that point (t_i, y_i)

$$\left.\frac{dy}{dt}\right|_{(t_i, y_i)} = f(t_i, y_i)$$

- *Taking* finite-difference approximation of the derivative at time t_i

$$\frac{y(t_{i+1}) - y(t_i)}{t_{i+1} - t_i} = f(t_i, y_i)$$

- Let $t_{i+1} - t_i = \Delta t$

$$\frac{y(t_{i+1}) - y(t_i)}{\Delta t} = f(t_i, y_i)$$

- Rearranging, we get

$$y(t_{i+1}) = y(t_i) + f(t_i, y_i). \Delta t$$

Example

- Solve

$$\frac{dy}{dt} = 4e^{0.8t} - 0.5y$$

- Initial condition, $y(t = 0) = 2$

Taylor series expansion

- A Taylor series is a series expansion of a function about a point.
- A one-dimensional Taylor series is an expansion of a real function $g(t)$ about a point $t = a$ is given by

$$g(t) = g(a) + g'(a)(t-a) + \frac{g''(a)}{2!}(t-a)^2 + \frac{g^{(3)}(a)}{3!}(t-a)^3 + \cdots + \frac{g^{(n)}(a)}{n!}(t-a)^n + \cdots$$

Derivation of Euler & Runge-Kutta methods

- Consider the following ODE

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

- Let us say that the solution of this ODE is

$$y = g(t)$$

- Taylor series expansion of $g(t)$ about point $t = t_i$

$$g(t) = g(t_i) + g'(t_i)(t - t_i) + \frac{g''(t_i)}{2!}(t - t_i)^2 + \frac{g^{(3)}(t_i)}{3!}(t - t_i)^3 + \cdots + \frac{g^{(n)}(t_i)}{n!}(t - t_i)^n + \cdots$$

- As a numerical solution, we are interested to find y value (or $g(t)$) at time $t = t_{i+1}$.

$$g(t_{i+1}) = g(t_i) + g'(t_i)(t_{i+1} - t_i) + \frac{g''(t_i)}{2!}(t_{i+1} - t_i)^2 + \frac{g^{(3)}(t_i)}{3!}(t_{i+1} - t_i)^3 + \cdots + \frac{g^{(n)}(t_i)}{n!}(t_{i+1} - t_i)^n + \cdots$$

- As $y = g(t)$ and $\frac{dy}{dt} = f(t, y)$, we can write

$$g'(t_i) = f(t_i, y_i),\ g''(t_i) = f'(t_i, y_i)$$

$$g(t_{i+1}) = y_{i+1},\quad g(t_i) = y_i$$

- Let us define $t_{i+1} - t_i = h$

- Incorporating the above, we can write

$$y_{i+1} = y_i + f(t_i, y_i)h + \frac{f'(t_i, y_i)}{2!}h^2 + \frac{f''(t_i, y_i)}{3!}h^3 + \cdots + \frac{f^{(n)}(t_i, y_i)}{n!}h^n + \cdots$$

Euler's method

- If we consider the first two terms only

$$y_{i+1} = y_i + f(t_i, y_i)h$$

- This is Euler's method; it is referred to as Runge-Kutta 1st order method.

- The true error in the approximation is given by

$$\frac{f'(t_i, y_i)}{2!}h^2 + \frac{f''(t_i, y_i)}{3!}h^3 + \cdots + \frac{f^{(n)}(t_i, y_i)}{n!}h^n + \cdots$$

Runge-Kutta 2nd order method

- If we consider the first three terms

$$y_{i+1} = y_i + f(t_i, y_i)h + \frac{f'(t_i, y_i)}{2!}h^2$$

- Example: $\frac{dy}{dt} = e^{-2t} - 3y, \; y(0) = 5$

$$f'(t, y) = \frac{df(t, y)}{dt} = \frac{\partial f(t, y)}{\partial t} + \frac{\partial f(t, y)}{\partial y}\frac{dy}{dt}$$

*Need to find the derivative of $f(t_i, y_i)$ symbolically

*Calculation of $f'(t_i, y_i)$ can be challenging sometimes

Runge-Kutta 2nd order method

Runge-Kutta proposed that

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h$$

where

$$k_1 = f(t_i, y_i)$$

$$k_2 = f(t_i + p_1 h, y_i + q_{11} k_1 h)$$

- This form allows one to take advantage of the 2nd order method without having to calculate $f'(t_i, y_i)$
- However, there are 4 unknown constants, i.e., a_1, a_2, p_1, q_{11}

- Going back to the Taylor series expansion with three terms

$$y_{i+1} = y_i + f(t_i, y_i)h + \frac{f'(t_i, y_i)}{2!}h^2$$

- We know that $f'(t,y) = \frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}\frac{dy}{dt}$, thus

$$y_{i+1} = y_i + f(t_i, y_i)h + \frac{1}{2!}h^2\left[\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}\frac{dy}{dt}\right]_{(t_i, y_i)}$$

- As $\frac{dy}{dt} = f(t,y)$, we can write

$$y_{i+1} = y_i + f(t_i, y_i)h + \frac{1}{2!}h^2\left.\frac{\partial f}{\partial t}\right|_{(t_i, y_i)} + \frac{1}{2!}h^2\left.\frac{\partial f}{\partial y}\right|_{(t_i, y_i)} f(t_i, y_i)$$

- We have written $k_2 = f(t_i + p_1 h, y_i + q_{11} k_1 h)$

- Let us revise Taylor series expansion of $f(x)$ around the point $x = a$ (for a single variable)

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)(x-a)^2}{2!} + \cdots$$

- Similarly, Taylor series expansion of $f(t, y)$ around the point (t_i, y_i) (for two variables)

$$f(t,y) = f(t_i, y_i) + \left.\frac{\partial f}{\partial t}\right|_{(t_i, y_i)} (t - t_i) + \left.\frac{\partial f}{\partial y}\right|_{(t_i, y_i)} (y - y_i) + \cdots$$

- Taking $t = t_i + p_1 h$ and $y = y_i + q_{11} k_1 h$, we can write

$$k_2 = f(t_i + p_1 h, y_i + q_{11} k_1 h) = f(t_i, y_i) + \left.\frac{\partial f}{\partial t}\right|_{(t_i, y_i)} p_1 h + \left.\frac{\partial f}{\partial y}\right|_{(t_i, y_i)} q_{11} k_1 h + \cdots$$

- The solution has been proposed as

$$y_{i+1} = y_i + (a_1k_1 + a_2k_2)h$$

- Substituting for k_1 and k_2

$$k_1 = f(t_i, y_i)$$

$$y_{i+1} = y_i + \left[a_1 f(t_i, y_i) + a_2\left\{f(t_i, y_i) + \left.\frac{\partial f}{\partial t}\right|_{(t_i, y_i)} p_1 h + \left.\frac{\partial f}{\partial y}\right|_{(t_i, y_i)} q_{11} k_1 h\right\}\right] h$$

$$y_{i+1} = y_i + (a_1 + a_2) f(t_i, y_i)h + a_2 p_1 \left.\frac{\partial f}{\partial t}\right|_{(t_i, y_i)} h^2 + a_2 q_{11} \left.\frac{\partial f}{\partial y}\right|_{(t_i, y_i)} f(t_i, y_i) h^2$$

- Comparing

$$y_{i+1} = y_i + (a_1 + a_2)f(t_i, y_i)h + a_2 p_1 \left.\frac{\partial f}{\partial t}\right|_{(t_i,y_i)} h^2 + a_2 q_{11} \left.\frac{\partial f}{\partial y}\right|_{(t_i,y_i)} f(t_i, y_i)h^2$$

$$y_{i+1} = y_i + f(t_i, y_i)h + \frac{1}{2!}h^2 \left.\frac{\partial f}{\partial t}\right|_{(t_i,y_i)} + \frac{1}{2!}h^2 \left.\frac{\partial f}{\partial y}\right|_{(t_i,y_i)} f(t_i, y_i)$$

- We can get values the following equations

$$a_1 + a_2 = 1$$
$$a_2 p_1 = 1/2$$
$$a_2 q_{11} = 1/2$$

3 equations, 4 unknowns -> infinite choices of a_1, a_2, p_1, q_{11}

One of the solutions is
$a_1 = a_2 = 1/2,\ p_1 = q_{11} = 1$

Substituting the suggested values of constants, we can define 2nd order Runge-Kutta formulae as

$$y_{i+1} = y_i + \frac{h}{2}(k_1 + k_2)$$

where

$$k_1 = f(t_i, y_i)$$

$$k_2 = f(t_i + h, y_i + k_1 h)$$

Runge-Kutta 4th order method

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

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h\left[\frac{\boldsymbol{k}_1}{6} + \frac{\boldsymbol{k}_2}{3} + \frac{\boldsymbol{k}_3}{3} + \frac{\boldsymbol{k}_4}{6}\right]$$

$$\begin{aligned}
\boldsymbol{k}_1 &= \boldsymbol{f}(t_n, \boldsymbol{y}_n) \\
\boldsymbol{k}_2 &= \boldsymbol{f}\left(t_n + \frac{h}{2}, \boldsymbol{y}_n + \frac{h}{2}\boldsymbol{k}_1\right) \\
\boldsymbol{k}_3 &= \boldsymbol{f}\left(t_n + \frac{h}{2}, \boldsymbol{y}_n + \frac{h}{2}\boldsymbol{k}_2\right) \\
\boldsymbol{k}_4 &= \boldsymbol{f}\left(t_n + h, \boldsymbol{y}_n + h\boldsymbol{k}_3\right).
\end{aligned}$$

Example

- Solve

$$\frac{dy}{dt} = 4e^{0.8t} - 0.5y$$

- Initial condition, $y(t = 0) = 2$

- Solve this problem by Euler method, RK-2, and RK-4 and compare the solutions.

Example

Let us consider a simple isothermal reaction $A \rightarrow B$ taking place in a MFR with constant holdup V. The kinetics of the reaction is given by second order reaction. The material balance for the reactor is written as

$$V \frac{dC_A}{dt} = F\left(C_{AF} - C_A\right) - k\, C_A^2\, V$$

where C_{AF} is the concentration of A in the reactor inlet stream (mol/m^3), C_A is the instantaneous concentration of A in the reactor (the exit stream composition is equal to the reactor composition for an ideal MFR), F is the inlet flow rate (also the effluent flow rate) in m^3/min, k is the reaction rate constant in m^3/(mol*min) and V is the reactor holdup in m^3. The nominal values are: F = 9 m^3/min, C_{AF} = 5 mol/m3, k = 2 m^3/(mol*min) and V = 1 m^3. If the feed concentration changes from 5 mol/m^3 to 6 mol/m^3, how does the concentration of A in the reactor evolve with time?

Example continued…

- Due to some constraints, it is required to reduce the effluent concentration of species A below 1 mol/m^3. The operation team suggests the use of a train of MFRs of similar size (same holdup). How many reactors will be needed to achieve the desired operation?
- For the above train of MFRs, Determine how the concentration of reactant A changes in the Nth reactor when the feed concentration to the first reactor changes from 5 to 6 mol/m^3.