Scilab for Chemical Engineers

TSEC - Online Certificate Course

SAMPLE PROBLEMS

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Numerical Methods continued...

1 Numerical Integration

Let's consider the following data points:

x	y
0.0	0.0000
0.5	0.4794
1.0	0.8415
1.5	0.9975
2.0	0.9093
2.5	0.5985
3.0	0.1411
3.5	-0.3508
4.0	-0.7568
4.5	-0.9775
5.0	-0.9589
5.5	-0.7055
6.0	-0.2794

Table 1: Discrete data points for numerical integration

1.1 Trapezoidal Method

Compute the integral of the given data points using the trapezoidal method.

$$\int_a^b f(x)\,dx \approx (b-a)\cdot\frac{1}{2}(f(a)+f(b)) \tag{1}$$

1.2 Simpson's 1/3rd Rule

Compute the integral of the given data points using Simpson's 1/3rd rule.

$$\int_a^b f(x)dx \approx \frac{h}{3}[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\ldots+2f(x_{n-2})+4f(x_{n-1})+f(x_n)] \tag{2}$$

1.3 Simpson's 3/8th Rule

Compute the integral of the given data points using Simpson's 3/8th rule.

$$\int_a^b f(x)\,dx \approx \frac{3h}{8}\left(f(x_0)+3f(x_1)+3(x_2)+2(x_3)+3(x_4)+...f(x_n)\right) \tag{3}$$

2 Regression

2.1 Line Fitting (Linear Regression)

Fit a straight line to the following data points and compute the coefficients of the line $y = ax + b$.
Data points:

$$x = [1, 2, 3, 4, 5]$$

$$y = [2, 3, 5, 4, 6]$$

The linear regression formula for the slope a and intercept b is given by:

$$a = \frac{n\sum xy - \sum x \sum y}{n\sum x^2 - (\sum x)^2}$$

$$b = \frac{\sum y - a\sum x}{n}$$

The normal equations for linear regression in the matrix form are:

$$\mathbf{AX} = \mathbf{B}$$

Where:

$$\mathbf{A} = \begin{bmatrix} \sum x^2 & \sum x \\ \sum x & n \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} \sum xy \\ \sum y \end{bmatrix}$$

2.2 Polynomial Fitting (Quadratic Polynomial)

Fit a quadratic polynomial $y = ax^2 + bx + c$ to the following data points and compute the coefficients.
Data points:

$$x = [1, 2, 3, 4, 5]$$

$$y = [2, 3, 5, 4, 6]$$

The normal equations for quadratic polynomial fitting are.

$$\mathbf{A} = \begin{bmatrix} \sum x^4 & \sum x^3 & \sum x^2 \\ \sum x^3 & \sum x^2 & \sum x \\ \sum x^2 & \sum x & n \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} \sum x^2 y \\ \sum xy \\ \sum y \end{bmatrix}$$

Solve $\mathbf{AX} = \mathbf{B}$:

3 Ordinary Differential Equations

3.1 Euler's Method

Solve the first-order ODE $\frac{dy}{dt} = -2y$ with initial condition $y(0) = 1$.
Hint:

$$x_{n+1} = x_n + hf(x_n, y_n) \tag{4}$$

3.2 Runge-Kutta Method

Solve the first-order ODE $\frac{dy}{dt} = y - t^2 + 1$ with initial condition $y(0) = 0.5$.
Hint:

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = hf(x_i, y_i)$$

$$k_2 = hf\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(x_i + \frac{h}{2}, y_i + \frac{k_2}{2}\right)$$

$$k_4 = hf(x_i + h, y_i + k_3)$$

3.3 2nd order differential equation: Runge-Kutta Method

Solve the second-order ODE $\frac{d^2y}{dt^2} + 3\frac{dy}{dt} + 2y = 0$ with initial conditions $y(0) = 0$ and $\frac{dy}{dt}(0) = 1$.
Hint: Convert the second-order ODE into a system of first-order ODEs:

$$\frac{dy_1}{dt} = y_2$$

$$\frac{dy_2}{dt} = -3y_2 - 2y_1$$