

Numerical methods in chemistry. Exercises 4

Problem 1

Solve the following ordinary differential equation by using the Laplace transform:

$$\begin{aligned}\frac{d^2y}{dt^2} + y &= 3\sin(2t), \\ y(0) &= 3, \\ y'(0) &= 1.\end{aligned}$$

Problem 2

Determine the Fourier series for $f(x) = h(x)$, the Heaviside unit step function, in the range $-\pi \leq x < \pi$ and periodic with period 2π : $f(x) = f(x + 2\pi)$ for all $x \in \mathbb{R}$. Hence find the sum of the series

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{2n-1} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \frac{1}{9} - \cdots.$$

Problem 3

Determine the Fourier series for the function $f(x)$ such that

$$\begin{aligned}f(x) &= 1 - x^2, & -\pi \leq x \leq \pi, \\ f(x) &= f(x + 2\pi), & x \in \mathbb{R}.\end{aligned}$$

Problem 4

Find the Fourier series expansion of the function $f(t)$ where

$$f(t) = \begin{cases} \pi^2 & -\pi < t < 0 \\ (t - \pi)^2 & 0 \leq t < \pi \end{cases},$$

and $f(t) = f(t + 2\pi)$ for all $t \in \mathbb{R}$. Hence determine the sums of the series

$$\sum_{n=1}^{\infty} \frac{1}{n^2} \quad \text{and} \quad \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2}.$$