

Problem Sheet 9a

CH2013: Computational Programming and Simulations Lab

July-Nov 2023

Problem Sheet #9a

11 October 2023

- 1) Write a general purpose program to integrate a function between two limits. The inputs should be lower limit and upper limit and the number of grid points in the interval of integration. Integrate the function x^2 , $\sin(x)$ and $\exp(x)$ in the limits from 0 to 1. Do this for 10 grids and 100 grids and compare the results with analytical solution. Comment on the results.
- 2) Consider the function $\exp(-x)$ and x^2 in the interval 0 to 1. Generate discrete data for this function at N equispaced grid points. Find the first order derivative using the following difference schemes at the mid point 0.5 . Choose N = 11 and 21
 - a) central difference of first order accuracy
 - b) Central different second order accuracy
 - c) Forward difference second order accuracy
 - d) Backward difference second order accuracy
- 3) The first order reaction in a reactor is described by $dC/dt = -kC$. Its solution is given by $C = C_0 \exp(-kt)$.Take $k = 0.1$ Assume you are doing a perfect experiment. Generate data from $t = 0$ to 10 in steps of 0.1. Add a 10 percent error to the data randomly. Use this as the data you got from an experiment. Now find the slope of the data using finite difference method. Plot the derivative Vs C at a point. The slope of this curve is k. Compare the k you obtain with 0.1.