DS-288 Numerical Methods
UMC-202 Introduction to Numerical Methods
Due date: October 20, 2025 (11:59 PM)

Homework-3

Total 100 points | Weightage 10%

Read the following instructions carefully.

- Write your NAME and SR. NUMBER on the first page of the report(only one PDF for all questions in order). Start each question on a new page.
- In coding exercises, also give algorithm/background theory in the **report** and discuss attached plots briefly to get full credit for that question.
- Only LaTeX version of the report is **acceptable** (find the attached demo LaTeX file). Use Python/Matlab for coding. Give proper annotations and comments in code wherever required.
- Submit your report as a single PDF named **LastFiveDigitsSRNo_Name.pdf**.(e.g 12345_Ram_charan.pdf)
- For each question, give a separate code file `.ipynb`, i.e., for Question 1 name **LastFiveDigitsSRNo_q1.ipynb**.(e.g 12345_q1.ipynb)
- Upload both the **PDF** and **.ipynb** files to Teams **(without zipping)**.
- Don't use any inbuilt functions for solving problems unless specified; use a proper algorithm to get credits. Marks will be deducted if plagiarism is found in the report or codes. Late submissions won't be accepted.
- Using LLM's for writing the report is strictly prohibited.

---

1. [**Theoretical**] Derive the Simpson's 1/3 rule formula for approximating $\int_a^b f(x)dx$ using a quadratic Lagrange interpolating polynomial through three equally spaced points. Give a reason why Simpson's 1/3 rule gives exact results for polynomials up to degree 3, even though it's derived from a quadratic polynomial. [10 marks]

2. Implement the composite Simpson's 1/3 rule for a function $f(x)$ over $[a, b]$ with n subintervals, where n is even. Test the implementation on

$$I = \int_0^1 \frac{1}{1+x^2}dx = \frac{\pi}{4}$$

by performing convergence analysis for $n = 4, 8, 16, 32, 64, 128$ by plotting the error against h on a log-log scale. [15 marks]

3. For the function $f(x) = e^x \sin x$, compute an approximation of $f'(\pi/4)$ using the three-point forward difference formula, three-point backward difference formula, and five-point central difference formula with step sizes $h = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-7}$.

   - Construct a comparison table displaying the results from all three methods.
   - Generate absolute error plots for each numerical scheme and identify the order of accuracy from the plots (plot absolute error versus step size using log-log scale with reference slope lines).
   - Identify the best step size from the given values of h that produces the smallest error and provide an explanation of the behavior observed in the error plots.

   [25 marks]

4. Write a function **poly_least_squares(x, y, degree)** that computes the polynomial least squares approximation for a given set of data points. The function should take arrays x and y representing the data, along with an integer degree representing the desired degree of the polynomial. It should return the coefficients of the best-fit polynomial in descending order of powers. Use your function to find the coefficients of the best-fit polynomial for the given data sets. Plot the fitted curve and original data points between the minimum and maximum of the given x values. Also, compute and print the Mean Squared Error (MSE) between the actual and predicted values.

   [25 marks]

Table 1: Dataset (a) - Degree 2 polynomial

x	0	1	2	3	4
y	1	2.2	3.9	6.1	8.0

Table 2: Dataset (b) - Degree 4 polynomial

x	-3	-2	-1	0	1	2	3
y	-2.5	-1.0	0.5	0.0	0.6	2.5	1.0

NOTE: Inbuilt functions can be used only to get the solution of linear system of equations.

5. A key integral in probability and statistics is the Gaussian integral, which is the integral of the standard normal distribution's probability density function over the entire real line:

$$I = \int_{-\infty}^{\infty} e^{-x^2}\, dx$$

The exact value of this integral is known to be $\sqrt{\pi} \approx 1.77245385$. Since we cannot compute an integral over an infinite domain directly with simple numerical methods, we must approximate it by integrating over a finite, symmetric interval $[-a, a]$ for a sufficiently large value of a.

Your task is to investigate how the choice of both the interval endpoint a and the number of subintervals n affects the approximation.

(a) Write the formula for **Composite Trapezoidal Rule** along with the error, in your report. Choose the following set of interval endpoints to test, $a = \{0.5, 1, 2, 5\}$.

(b) For **each** chosen value of a, use the **Composite Trapezoidal Rule** to approximate the integral $I_a = \int_{-a}^{a} e^{-x^2}\, dx$. Perform this approximation for $n = 10, 50, 500$, and 3000 subintervals.

(c) For each combination of a and n, calculate the absolute error, defined as $|I_{\text{exact}} - I_{\text{approximate}}|$. Take $I_{\text{exact}} = \sqrt{\pi}$.

(d) Present your results in a single table with columns for a, n, Approximate Value, and Absolute Error.

(e) Create a plot showing how the absolute error changes as a increases for a fixed large value of n (e.g., $n = 3000$). Discuss what this plot tells you about choosing an appropriate interval for approximating an integral over an infinite domain.

[25 marks]