

Assignment 1: Computational

Due Date: 06/02/2022(Sunday)

Problem 1: **Numerical Differentiation:** Consider the function $f(x) = x^2$ and,

1. Plot the function $f(x)$
2. Find the derivative numerically and plot the result(df/dx) alongside the analytical solution. (*While numpy is allowed, Do not use special packages to do the numerical derivative*)

Problem 2: **Numerical integration:** Given $I = \int_0^\pi \sin(x)dx$, Define a function to calculate the integral by Simpsons's 1/3 Rule and compare with the analytical result.

Problem 3: **Boundary Value Problem:** Solve the following boundary value problem(BVP).(Hint: shooting method).

$$y'' = -y + \frac{2(y')^2}{y}, \quad -1 < x < 1$$

Problem 4:**Infinite Square Well:** Solve the Schrödinger equation for Infinite Square Well and plot the ground state and two excited states of energy. Also compare the numerical result with the analytical result.

$$V(x) = \begin{cases} \infty, & x < 0 \\ 0, & 0 \leq x \leq a \\ \infty, & x > a \end{cases}$$

Problem 5: **Quantum Harmonic Oscillator:** Solve the Schrödinger equation for Quantum Harmonic Oscillator in 1D and plot the eigenfunctions for $n = 0, 1, 2$. Also compare the numerical result with the analytical result.

$$V(x) = \frac{1}{2}m\omega^2 x^2$$