Computational Physics Homework Assignment #2

Derivative, Integration, Matrix, and Coupled Oscillators

November 25 , 2024; Due December 2, 2024

Reading Assignment

1. Read lecture notes and references;
2. Study sample programs and prepare your own programs with any languages you prefer.

Laboratory Assignments (Total Points 125 = 30 + 30 + 30 + 35)

1. **Derivatives** (30 Points: 15, 15)

   (a) Consider the function $f(x) = xcosh(x)$ at $x = 1$ Calculate its first and second derivatives for $h = 0.50, 0.45, ..., 0.05$, using the forward and central difference formulae. Plot the log error versus $log(h)$. Compare your results with that of Richardson extrapolation.

   (b) Use the two-point, three-point, and five-point formulae to estimate the first five derivatives of $f(x)$ at $x = 0$,

$$f(x) = \frac{e^x}{sin^3(x) + cos^3(x)} \ .$$

   As a check, $f^{(v)}(x = 0) = -164$. You are recommended to change the value of in the fashion of $h = 1/2^n, n = 1, 2, ...$

2. **Integration** (30 Points: 10, 10, 10)
   Using the asymptotic error formulae for the Trapezoid and the Simpson's rules, estimate the number of subdivisions n for the following integrals to the given accuracy ϵ.

$$I_1 = \int_1^3 dx \log(x), \qquad \epsilon = 10^{-8} \ .$$

$$I_2 = \int_{-1}^1 dx e^{-x^2}, \qquad \epsilon = 10^{-10} \ .$$

$$I_1 = \int_{1/2}^{5/2} \frac{dx}{1 + x^2}, \qquad \epsilon = 10^{-12} \ .$$

3. **Hilbert Matrix** (30 Points)

Study the Hilbert Matrix

$$H_n = \begin{pmatrix} \frac{1}{1} & \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{n} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \cdots & \frac{1}{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{1}{n} & \frac{1}{n+1} & \frac{1}{n+2} & \cdots & \frac{1}{2n-1} \end{pmatrix}$$

Diagonalizing H_n and calculate the ratio of the largest eigenvalue to the smallest eigenvalue, $\log(max|\lambda|/min|\lambda|)$, and plot it as a function of n for $n = 2, 3, \cdots, 8$. Discuss your results. Do the problem for both single and double precisions. Indicate which diagonalization routine you are using.

4. **Coupled Oscillators** (35 Points: 10,10,15)
Use program similar to *Oscillators* to solve the dynamics equation of motion for $N = 12$ oscillators with the initial conditions $u_j(t=0) = 0, v_3(t=0) = 1$. Compare numerical results of $u_j(t)$ with the analytic one.

   (a) What is the maximum deviation of $u_j(t)$?

   (b) How well is the total energy conserved as function of Δt?

   (c) How well is the total energy conserved as function of Δt if one uses Runge-Kutta 4th order algorithm?