Assignment for Lecture 2

TAYLOR'S EXPANSION, NUMERICAL CALCULUS AND MONTE CARLO INTEGRATION

Lecture Date: 3/10/2026

"C" denotes for "computational" problems, language suggestion: Python/Julia

please include codes and results with analyses for computational problems

please write in pdf format and submit to `bjcai@fudan.edu.cn` ***before the lecture of 3/17/2026***

1. What is the error for the five-point algorithm for calculating second-order derivative?

2. Prove the approximate algorithm for first-order derivative:

$$f'(x) \approx \frac{1}{45}\mathrm{diff}(h) - \frac{4}{9}\mathrm{diff}\left(\frac{h}{2}\right) + \frac{64}{45}\mathrm{diff}\left(\frac{h}{4}\right) + \mathcal{O}(h^6), \;\; \mathrm{diff}(h) \equiv \frac{f(x+h)-f(x-h)}{2h}. \tag{1-1}$$

3. For the free harmonic oscillator in the absence of damping force, one has $x(t+\delta t) = x(t) + v(t)\delta t$, $v(t+\delta t) = v(t) - \omega_0^2 x(t)\delta t$; however, the energy is not conserved. One algorithm to deal with the energy problems is to use the following update,

$$x(t+\delta t) = x(t) + \left(v(t) - \frac{1}{2}\omega_0^2 x(t)\delta t\right)\delta t, \tag{1-2}$$

$$v(t+\delta t) = v(t) - \left(\omega_0^2 x(t) + \frac{1}{2}\omega_0^2 v(t)\delta t\right)\delta t. \tag{1-3}$$

   It is called the symplectic method. Prove in this scheme:

$$E(t+\delta t) \approx E(t) + \mathcal{O}(\delta t^3), \tag{1-4}$$

   indicating that this algorithm is improved compared with the conventional one.

4. [C] Calculate $\int_0^5 \tanh x \, \mathrm{d}x$ using trapezoidal and rectangular rules, with step $h = 0.1$ or $h = 0.4$.

5. [C] The sample variance of an estimator is defined as

$$\nu = \frac{1}{m-1}\sum_{i=1}^{m}\left(\langle\mathcal{O}\rangle - \widetilde{\mathcal{O}}^{(i)}\right)^2, \tag{1-5}$$

   and if all the $\widetilde{\mathcal{O}}^{(i)}$'s are uncorrelated, the standard error of the mean $\langle\mathcal{O}\rangle$ is obtained as $\sigma_{\langle\mathcal{O}\rangle} = (\nu/m)^{1/2}$. Calculate the sample variance of the estimator for π using the Markov chain random walk as a function of m under different step parameter δ.