Computational Physics Final Exam

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Abstract

When you hand in the homework, you should gather all your files into a single tarball file as follows.

- Use an unix command `tar -czf <file name>.tar.gz <file 1> <file 2>` $\cdots$.
- For undergraduate students, put a copy of a tarball <file name>.tar.gz into a directory: `/physics/upload/comp2023/<user-ID>`.
- For graduate students, put a copy of a tarball <file name>.tar.gz into a directory: `/physics/upload/acomp2023/<user-ID>`.
- You must use the GNU `make` command and `Makefile` to compile the code.
- You must make a README file which describes how to run your code. The README file should include your name and student ID.
- You must use `gnuplot` to make a plot into a PDF format.

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I. FINDING ROOTS [15 POINTS]

Let us consider a function $f(x)$ defined as

$$f(x) = \cos[\, g \ \tan(h)] \tag{1}$$
$$g(x) = \frac{3\pi \cdot x^3}{x^6 + 1} \tag{2}$$
$$h(x) = \frac{2\pi \cdot x^2}{x^8 + 1} e^{-x^2} \tag{3}$$

1. Make a plot of $f(x)$ as a function of x in the range of $x \in [0, 10]$.

   `[HINT]` You may use the `gnuplot` program in the linux system.

2. Find all the roots in the range of $x \in [0, +\infty]$, using the Newton method. The values of the roots must have a numerical precision better than 1.0×10^{-10}.

II. QUADRATURE METHOD AND MONTE CARLO METHOD [25 POINTS]

In the homework problems, you learned how to scan your handwriting note into a `PDF` file. Write down an answer to this problem on your note by hand, scan it into a `PDF` file, and submit it to your storage in the Newton computer.

In the class, you learned about the quadrature method to calculate an integral in the d dimensional space.

$$I_d = \int_V f(\mathbf{x}) d^d x \tag{4}$$
$$\mathbf{x} = (x_1, x_2, \ldots, x_d) \tag{5}$$

In this problem, we want to determine in which condition on d the Monte Carlo method gets more efficient than the Bode rule.

1. In the class you learned about the Bode rule in the quadrature method. Let us consider an integral in one-dimensional space.

$$\begin{aligned} I_1 &= \int_a^b f(x)dx \\ &= \int_0^{4h} g(x)dx + \int_{4h}^{8h} g(x)dx + \cdots + \int_{(M-4)h}^{Mh} g(x)dx \end{aligned} \tag{6}$$

where $b > a$ and

$$g(x) = f(a+x) \tag{7}$$

$$h = \frac{b-a}{M} \tag{8}$$

Here, M is the number of the lattice points and h is a lattice spacing. The unit integral in this case is

$$I_u = \int_{-2h}^{+2h} f(x)dx \tag{9}$$

Describe how to calculate I_u using the Bode rule obtain the uncertainty of the Bode rule in terms of h.

2. Let us consider the full integral in one-dimensional space. Please explain how to calculate I_1 using the Bode rule. Describe the uncertainty of the Bode rule in terms of h (the lattice spacing).

3. Now, let us consider the integral I_d in d-dimensional space. Explain how to calculate I_d using the Bode rule. Describe the uncertainty of I_d obtained using the Bode rule in terms of h.

4. Now let us set the total number of the lattice points to N in d-dimensional space. Express h in terms of N. Obtain the uncertainty (σ_B) of I_d obtained using the Bode rule in terms of N.

5. Now obtain the uncertainty (σ_M) of I_d calculated using the Monte Carlo method in terms of N (the total number of the data points).

6. Compare σ_B and σ_M, and obtain the critical dimension d_c under the condition: if $d > d_c$, $\sigma_B > \sigma_M$ for a large sample size $N \ggg 1$.

7. Write down all the answers on your node by hand, and scan them into a `PDF` file. You must submit it to your storage in the Newton computer.

III. MONTE CARLO METHOD AND QUADRATURE METHOD [30 POINTS]

The boson propagator on the 4-dimensional Euclidean lattice is

$$B(k) = \frac{1}{\hat{k}^2} \tag{10}$$

$$\hat{k}^2 = \sum_{\mu=1}^{4} \hat{k}_\mu \cdot \hat{k}_\mu \tag{11}$$

$$\hat{k}_\mu = 2\sin\left(\frac{k_\mu}{2}\right) \tag{12}$$

where k is a 4-dimensional vector: $k = (k_1, k_2, k_3, k_4)$. The tadpole diagram Z_n can be expressed as

$$Z_n \equiv \int_\Omega d\Omega \ \exp(ik.n)B(k) \tag{13}$$

$$\int_\Omega d\Omega = \prod_{\mu=1}^{4} \int_{-\pi}^{+\pi} \frac{dk_\mu}{(2\pi)} \tag{14}$$

where n is a 4-dimensional vector: $n = (n_1, n_2, n_3, n_4)$ with $n_\mu \in Z$. Note that there exists a removable singularity at $k = 0$ in Z_n.

1. Obtain the following integral: Z_{0000}.

   `[HINT]` You may use the Monte Carlo method with weight function $w(k) = 1$.

   `[HINT]` Note that there exists a removable singularity at $|k| = 0$ or $k = (0, 0, 0, 0)$. You may use the subtraction method to take care of this.

   Using the generating functional for the Bessel functions, we can prove the following identity.

   $$Z_n = \int_0^{+\infty} dx \ e^{-8x} \prod_{\mu=1}^{4} I_{n_\mu}(2x) \tag{15}$$

   where $I_{n_\mu}(2x)$ is a modified Bessel function.

2. Using the identity of Eq. (15), it is possible to convert the 4-dimensional intergal into a 1-dimensional integral. Using this identity, calculate the integral Z_{0000} in Problem 1 using the quadrature methods such as Trapezoidal, Simpson, and Bode rules.

   `[HINT]` You may use the numerical recipe subroutines for the Bessel functions which are given to you separately.

3. Compare the results of Problem 1 with those for Problem 2. Which method is more efficient? Explain the reason why it is more efficient.

IV. LEAST χ^2 FITTING [30 POINTS]

Find a data file "`dat.2023-12-15`". This file has the data format of two columns: the first column gives values for the x variable and the second column gives values for the function $y(x)$. Please note that $0 \le x \le 6$. Each line of the data has a x value and the corresponding $y(x)$ value.

1. $\langle$ `File I/O` $\rangle$ Make a code to read in the data of $(x, y(x,i))$ and determine the number of the whole data sets. You must use the `feof()` function to check the end of file.

2. $\langle$ `Statistical Analysis` $\rangle$ Make a code to calculate the average and statistical error of $y(x)$ for each x value. Let us say that $y(x,i)$ represents the data at coordinate x for the ith data set. Then the statistical average ($\langle y(x) \rangle$) and the covariance matrix (C_{ij}) is defined as

$$\langle y(x) \rangle = \frac{1}{N} \sum_i y(x,i) \tag{16}$$

$$C_{ij} = \frac{1}{N(N-1)} \sum_k \Big[y(x_i,k) - \langle y(x_i) \rangle \Big] \Big[y(x_j,k) - \langle y(x_j) \rangle \Big] \tag{17}$$

3. $\langle$ `Print results` $\rangle$ Print results for the average and covariance matrix for $y(x)$ as a function of x into a file named `stat.out`.

4. $\langle$ `Plot results` $\rangle$ Make a plot of the average $\langle y(x) \rangle$ and its statistical uncertainty $\sigma_{y(x)}$ as a function of x. The plot must be made into a PDF format (plot file name: `fig_4.pdf`).

5. $\langle$ `Fitting` $\rangle$ From the statistical analysis on the results for $y(x)$, let us guess that the functional form for the data $y(x)$ is $f(x) = ax^3 + bx^2 \sin(x) + c\sqrt{x} + d$, and then obtain the statistical average of a, b, c, and d using the least χ^2 fitting.

6. $\langle$ `Data analysis` $\rangle$ Obtain the error matrix for a, b, c, and d.

7. $\langle$ `Quality of fitting` $\rangle$ Obtain the χ^2 value from the fitting results. Obtain the confidence level using the quadrature method for the integral.

8. $\langle$ `Hypothesis testing` $\rangle$ Using the confidence level, you can determine whether the quadratic functional form for $f(x)$ is acceptable or should be rejected. Please give your reason for the hypothesis testing.