

## Homework 2; due on Tuesday, October 3

### PY 502, Computational Physics, Fall 2023

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#### 1) INTEGRABLE SINGULARITIES

Consider the function

$$f(x) = \frac{1}{(\epsilon + x)^\alpha}, \quad (1)$$

with  $\epsilon \geq 0$  and  $0 < \alpha < 1$ . For  $\epsilon = 0$  this function has an integrable singularity at  $x = 0$ . In this assignment you will investigate the convergence of two simple numerical integration schemes for  $\epsilon = 1$ ,  $\epsilon = 0$ , and  $\epsilon \approx 0$ . In the process, you will learn about the concept of “cross-over” behavior (in part C), which is very common in physics.

Write a program implementing the first and second order open-interval integration formulas

$$\int_{x_0}^{x_N} f(x) dx = h \left( \frac{3}{2} f_1 + f_2 + \dots + f_{N-2} + \frac{3}{2} f_{N-1} \right) + O(h^2), \quad (2)$$

$$\int_{x_0}^{x_N} f(x) dx = h \left( \frac{23}{12} f_1 + \frac{7}{12} f_2 + f_3 + \dots + f_{N-3} + \frac{7}{12} f_{N-2} + \frac{23}{12} f_{N-1} \right) + O(h^3). \quad (3)$$

The integration range should be from  $x_0 = 0$  to an upper bound  $x_N$  given by the user. Write the program so that it carries out a series of integrations for different number of intervals  $N$  of the form  $N = N_0 \times 2^n$  with  $n = 0, 1, \dots, n_{\max}$ , where  $N_0$  and  $n_{\max}$  are numbers given by the user.

With the above definitions, the discretization step is  $h(N) = (x_N - x_0)/N$ . You will study the rate of convergence of the first-order and second-order approximants  $I_1(N)$  and  $I_2(N)$  to the exact value  $I$  of the integral by analyzing the error  $\Delta_k(N) = |I_k(N) - I|$ . If the error has a power-law form;

$$\Delta_k(N) = |I_k(N) - I| \propto h^{\gamma_k} \propto N^{-\gamma_k}, \quad k = 1, 2, \quad (4)$$

then data points  $[\ln(h), \ln(\Delta_k(N))]$  calculated for different values of  $N$  (i.e.,  $h$ ) should fall on a straight line with slope  $\gamma_k$ .

#### A) Convergence for a non-singular integrand

Confirm the leading-order error scaling  $\sim h^2$  and  $\sim h^3$  of the integration formulas (2) and (3), respectively, for a non-singular integrand. Use the parameters  $\epsilon = 1$  and  $\alpha = 1/2$  in Eq. (1), upper integration limit  $x_N = 1$ , and initial number of points  $N_0 = 10$ . Produce a graph showing results for  $[\ln(h), \ln(\Delta_k(N))]$  and lines corresponding to the expected exponents  $\gamma_1=2$  and  $\gamma_2=3$ .

#### B) Convergence when the integrand is singular

Investigate the rate of convergence of the approximants  $I_1(N)$  and  $I_2(N)$  to the exact value of the integral when  $\epsilon = 0$  and the upper integration limit  $x_N = 1$ . Use  $N_0 = 10$ . You should again find that the error behaves as a power-law;

$$\Delta_k(N) = |I_k(N) - I| \propto h^{\gamma_k}, \quad k = 1, 2. \quad (5)$$

What values do you obtain for the first and second order exponents  $\gamma_1$  and  $\gamma_2$  in the cases  $\alpha = 1/2$  and  $\alpha = 3/4$ ? You can find the exponent by fitting a straight line to the points  $[\ln(h), \ln(\Delta_k(N))]$  (using some software of your choice or writing a simple program based on the formulas covered at the discussion meeting 9/29). In this case the data have no relevant error bars and, depending on how you do the fitting, you will either not need error bars or you can set them to an arbitrary non-zero constant, e.g., 1. Produce graphs showing the data and line fits. How can you explain the power-laws with the exponents obtained?

### C) Convergence when the integrand is almost singular

Now consider  $\epsilon = 10^{-5}$  and  $\alpha = 1/2$ . Using the same values as in B) for the other parameters, investigate the convergence rate in the same way as above. You should now see a different behavior for small and large  $n$  (the maximum  $n$  will in principle be dictated by the double-precision floating-point numerical accuracy, but in practice by the time you are willing to run the calculation;  $n \approx 20$  will be sufficient).

What are the exponents  $\gamma_1$  and  $\gamma_2$  for small and large  $n$ ? How can you explain the results? How do you explain the location of the “cross-over” region where the behavior (exponent) changes?

Produce graphs showing the data points  $[\ln(h), \ln(\Delta_k(n))]$  and the lines you have fit to the data.

## 2) MONTE CARLO INTEGRATION

A sphere of radius  $r_1$  consists of two different materials, with densities  $\rho_1$  and  $\rho_2$ . The material with density  $\rho_2$  is located within a cylinder of radius  $r_2$ , as illustrated in Fig. 1, and the material of density  $\rho_1$  fills up the rest of the sphere. Write a program using Monte Carlo integration to calculate the two moments of inertia of this sphere corresponding to rotation about the  $z$  and  $x$  axis. The inner cylinder is centered around the  $z$ -axis, as also shown in the figure.

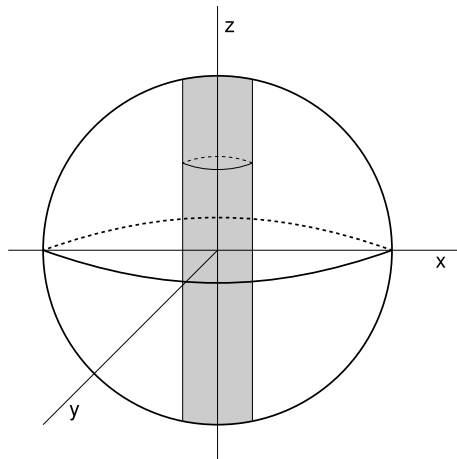


Figure 1: A solid sphere of radius  $r_1$  with an inner solid cylinder of radius  $r_2$ . The cylinder consists of a material with density  $\rho_2$ ; the rest of the sphere consists of a material with density  $\rho_1$ .

Carry out the calculation using Monte Carlo sampling of the moment of inertia integral

$$I = \int dx \int dy \int dz \rho(x, y, z) r_{\perp}^2(x, y, z), \quad (6)$$

where  $r_{\perp}(x, y, z)$  is the perpendicular distance of the point  $(x, y, z)$  from the axis of rotation (here the  $x$  or  $z$  axis, giving  $I_x$  and  $I_z$ ). Enclose the sphere in a box with side  $L = 2r_1$  in order to easily do the calculation using  $(x, y, z)$  points. You can use the Julia default random-number generator.

The program should read the following input from a file `read.in`:

```
r1
r2
rho1
rho2
npt
nbi
```

where `r1,r2` are the two radii (in m), `rho1,rho2` are the densities (in  $\text{kg/m}^3$ ), `npt` is the number of random points generated per “bin” (for which bin averages are computed) and `nbi` is the number of bins (on the basis of which the final average and statistical error are computed).

Bin averages should be computed for both the  $I_z$  and  $I_x$  moments of inertia and these should be written to a file `bin.dat` containing `nbi` lines, each with the bin number followed by the  $I_z$  and  $I_x$  values (write these averages to the file after each bin is completed; it is not necessary to store the data in the program). The final average and error bar (standard deviation of the mean) computed using the bin averages should be written to a file `res.dat`.

As a specific case, do the calculation for a copper ( $8930 \text{ kg/m}^3$ ) sphere of radius 5 cm with an inner gold ( $19320 \text{ kg/m}^3$ ) cylinder of radius 1 cm. Use  $10^6$  points per bin (`npt`) and do the calculation for `nbi=50,500,5000`. For the final case, construct histograms of the bin averages of the two moments of inertia (with the width of the histogram bins chosen in a reasonable way to get of the order tens of histogram bins with significant weight). The report on this problem needs to contain only the final numerical results (averages and standard deviations) for the three runs and the histograms for the last run.