Homework 2; due on Tuesday, October 4

PY 502, Computational Physics (Fall 2011)

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1) INTEGRABLE SINGULARITIES

Consider the function

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

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 $\epsilon \approx 0$.

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

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

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

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 $n = 0, 1, \ldots, n_{\max}$, where N_0 and $n_{\max}$ are numbers given by the user.

You can use the time-saving trick, discussed in class, of using the result of step n in the evaluation of step $n + 1$, but you do not have to. Note that in the case of these open-interval formulas the trick is a little bit more complicated because the points x_0 and x_N have to be treated differently than we did for the closed interval.

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;

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

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 γ_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 γ_1=2 and γ_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;

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

What values do you obtain for the first and second order exponents γ_1 and γ_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, e.g., the line fitting program developed in homework assignment 1 (where in this case the data have no relevant error bars and you can set them to an arbitrary non-zero constant, e.g., 1), or any other fitting program you have access to. 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 γ_1 and γ_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 ρ_1 and ρ_2. The material with density ρ_2 is located within a cylinder of radius r_2, as illustrated in Fig. 1, and the material of density ρ_1 fills up the rest of the sphere. Write a program that calculates 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.

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

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

where $r_\perp(x, y, z)$ is the perpendicular distance of the point (x, y, z) from the axis of rotation. Enclose the sphere in a box with side $L = 2r_1$ in order to easily do the calculation using (x, y, z) points. Use the fortran 90 intrinsic random number generator `random_number`, with seeds read from a file `seed.in` (all seed integers written on a single line). The program should read the following input from a file `read.in`:

```
r1,r2,rho1,rho2,eps,
```

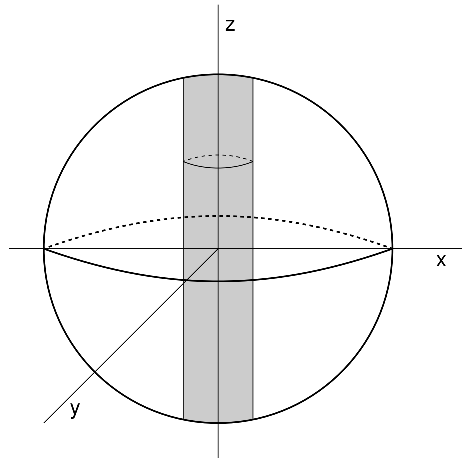

Figure 1: A solid sphere of radius r_1 with an inner solid cylinder of radius r_2. The cylinder consists of a material with density ρ_2; the rest of the sphere consists of a material with density ρ_1.

where `r1,r2` are the two radii (in m), `rho1,rho2` are the densities (in kg/m^3), and `eps` is a desired minimum relative accuracy of the results. Write the program so that the number of points generated per bin is 10^6 and bin avrages $\bar{I}_1\bar{I}_2,\ldots$ (for both the I_z and I_x moments of inertia) are generated until the relative standard deviation (i.e., the standard deviation divided by the average) of the full average $I = \sum \bar{I}_i$ is less than `eps` for both I_1 and I_2. At least 10 bins should be carried out regardless of the accuracy achieved until then. The results, along with the number of bins used, should be written to the screen.

As a specific case, do the calculation for a copper (8930 kg/m^3) sphere of radius 5 cm with an inner gold (19320 kg/m^3) cylinder of radius 1 cm. Use 10^{-4} for the accuracy `eps`. State the result as a comment at the end of the program file (use `!` at the beginning of each comment line so that the program still can be compiled).