PY 502, Computational Physics, Fall 2024

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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 $\epsilon \approx 0$. 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

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

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

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.

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 some software of your choice or a simple program based on the simple formulas we discussed). 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 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.