Computational Physics Lab

(PH49012)

Spring-2021, IIT KGP

Assignment 05

Q1. Create a user-defined function $f(x)$ that returns the value $1 + \frac{1}{2}\tanh 2x$, then use a central difference to calculate the derivative of the function in the range $-2 \le x \le 2$. Calculate an analytic formula for the derivative and make a graph with your numerical result and the analytic answer on the same plot. It may help to plot the exact answer as lines and the numerical one as dots. Use proper legends. In python, you can call tanh function from numpy. (10 points)

Q2. You will find a data set consisted of two columns in the 'Files' section in MS Team. Consider the first column as x values, and the second one as the corresponding functional values. Write a code to perform numerical differentiation on this data set, using Euler's forward (use Euler's backward at the last point), backward (use Euler's forward at the first point) and central difference scheme. Generate two separate plots: (i) The data set (y vs x), (ii) Results obtained after differentiation by three different methods. You can zoom in and see that they do not overlap each other. (10 points)

Q3. (a) Write a program to calculate an approximate value for the integral $\int_0^2 (x^4 - 2x + 1)\mathrm{d}x$ using trapezoidal rule with 10 slices. Take the number of points, N as input.
(b) Run the program and compare your result to the known correct value 4.4. What is the fractional error on your calculation?
(c) Modify the program to use a hundred slices instead, then a thousand. Note the improvement in the result and put your observation as comment within your code. (6+2+2 points)

Q4. Consider the integral

$$E(x) = \int_0^x \mathrm{e}^{-t^2}\mathrm{d}t$$

(a) Write a program to calculate $E(x)$ for values of x from 0 to 3 in steps of 0.1. Use trapezoidal rule to compute the integral.
(b) When you are convinced your program is working, extend it further to make a graph of $E(x)$ as a function of x. (6+4 points)

Q5. Our ability to resolve detail in astronomical observations is limited by the diffraction of light in our telescopes. Light from stars can be treated effectively as coming from a point source at infinity. When such light, with wavelength λ, passes through the circular aperture of a telescope and is focused by the telescope in the focal plane, it produces not a single dot, but a circular diffraction pattern consisting of central spot surrounded by a series of concentric rings. The intensity of the light in this diffraction pattern is given by

$$I(r) = \left(\frac{J_1(kr)}{kr}\right)^2,$$

where r is the distance in the focal plane from the center of the diffraction pattern, $k = 2\pi/\lambda$, and $J_1(x)$ is a Bessel function. The Bessel functions $J_m(x)$ are given by

$$J_m(x) = \frac{1}{\pi}\int_0^\pi \cos(m\theta - x\sin\theta)\mathrm{d}\theta,$$

where m is a nonnegative integer and $x \ge 0$.

Write a python function $J(m, x)$ that calculates the value of $J_m(x)$ using trapezoidal rule with $N = 1000$ points. Use your function in a program to make a plot, on a single graph, of the Bessel functions J_0, J_1 and J_2 as a function of x from $x = 0$ to $x = 20$. (20 points)

(Reference: Q1, Q3, Q4 and Q5 are taken from Computational Physics by Mark Newman)

You may use the following expression for trapezoidal rule:

$$I(a,b) \simeq \frac{1}{2}h\sum_{k=1}^{N}[f(a+(k-1)h) + f(a+kh)] = h\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{N-1} f(a+kh)\right]$$