Problem Set 1

due date: 2023/4/14, PM 12:00

Pls send an attached email to jqian@ecust.edu.cn inlcuding both your `.ipynb` file and the corresponding `.html` or `.pdf` file. The homework topics below doesn't need to be inlcuded.

1. In the class, you have been told the second forward-difference approximitions given by

$$f'(x) = \frac{4f(x+\frac{h}{2}) - f(x+h) - 3f(x)}{h} + \frac{h^2}{12}f'''(x) + \cdots.$$

   Show it by combining the Taylor series for $f(x+h)$ and $f(x+h/2)$.

2. The second central-difference approximation can be wriiten as

$$f'(x) = \frac{27f(x+\frac{h}{2}) + f(x-\frac{3h}{2}) - 27f(x-\frac{h}{2}) - f(x+\frac{3h}{2})}{24h} + \frac{3}{640}h^4 f^{(5)}(x) + \cdots.$$

   Show it by substracting two pairs of Taylor series: $f(x+h/2)$ and $f(x-h/2)$, on the one hand,$f(x+3h/2)$ and $f(x-3h/2)$ on the other.

3. This problem deals with the error assessment of the first central-difference approximation of the second derivative $f''(x)$.
   (a) Start with the error analysis, including both approximation and roundoff error. Derive expressions for the optimal h_{opt} and $\mathcal{E}_{opt}$.
   (b) Then, produce numerical estimates for h_{opt} and $\mathcal{E}_{opt}$.

4. You will find a file named `velocities.txt` which contains two columns of numbers, the first representing the time t in seconds and the second the velocities in meters per second of a particle. Write a program to do the following
   (a) Load the data from the file and use the trapzoidal to calculate the distance $x(t)$. Hint: use `np.loadtxt` to read the data.
   (b) Plot the distance $x(t)$ and $v(t)$ as a function of t on the same figure.

5. Create a user-defined function $f(x)$ that return the value $1 + 0.5\tanh(2x)$, then use the central difference to calculate the derivative $f'(x)$ in the range $-2 \leq x \leq 2$. Plot a graph your numerical results and the analytic solution on the same figure. Hint: It may be good to plot the exact answer as lines and the numerical one as dots.

6. Produce a table of x_i and $e^{sin(2x_i)}$ values, where x_i goes from 0 to 1.6 in steps of 0.08.
   (a) Plot the forward-difference and central-difference results (for the first derivative) given these values. (Hint: if you cannot produce a result for a specific x, don't.) Then, introduce a curve for the analytical derivative.
   (b) Use Richardson extrapolation for the forward difference for points on a grid and add an extra set of points to the plot. You can use the following expression

$$R_{fd} = 2D_{fd}(h) - D_{fd}(2h) + \mathcal{O}(h^2).$$

7. Consider the integral

$$E(x) = \int_0^x e^{-t^2} dt.$$

   (a) Write a program to calculte $E(x)$ for values of $x \in [0, 3]$ in steps of 0.1. Choose for youself which method you will use for performing the integral and a suitable number of slices.

(b) When you are convinced your program is working, extend it further to make a graph of $E(x)$ as a function of x.

8. The Gamma function is defined by the integral $\Gamma(a) = \int_0^\infty x^{a-1} e^{-x}$.
(a) Write a program to make a graph of the value of the integrand as a function of $x \in [0, 5]$, with three separate curves for $a = 2, 3, 4$, respectively.
(b) Show analytically that the maximum falls at $x = a - 1$.
(c) Most of the area under the integrand curve falls near the maximum. It indicates that, to calculate the Gamma function accurately, we need to do a good job of this part of the integral. One can change the variable to change the range of the integral from $[0, \infty]$ to a finite range.

9. Use a build-in random number generator to perform the 10-dimension Monte Carlo integral

$$I = \int_0^1 dx_1 \int_0^1 dx_2 \cdots \int_0^1 dx_{10} (x_1 + x_2 + \cdots x_{10})^2$$

(a) Conduct 16 trials and take the average as your answer, and then check against the exact answer, 155/6.
(b) Try sample sizes of $N = 10, 20, \cdots, 10000$. Plot the relative error vs. $1/\sqrt{N}$ and see if linear behavior occurs.
(c) Show that for a dimension $D \simeq 3 - 4$, the error of the multidimensional Monte-Carlo integral is approximately equal to that of conventional methods, and for larger D, the Monte-Carlo method is more accurate.