Problem set 4

This problem set involves plotting functions. Please refer to `01_PythonIntro/part_3/python_intro_pt3.ipynb` and `01_PythonIntro/part_3/python_intro_pt3.py` for help on how to create plots in Python.

Function derivative approximation

1. Use the formulae

$$\frac{df(x)}{dx} \approx \frac{f(x+h) - f(x-h)}{h},$$

   and

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

   with $h = 0.1$ to find approximate values for df/dx and d^2f/dx^2 at each of the **interior points** (i.e. $x \neq 0$ and $x \neq 0.5$) in the following table

$$\begin{aligned} x &= 0.0, 0.1, 0.2, 0.3, 0.4, 0.5 \\ f(x) &= 1.00000, 1.10517, 1.22140, 1.34986, 1.49182, 1.64872 \end{aligned}$$

2. Use the formulae above (Q1) with $h = 0.2$ to calculate tbe approximate values of df/dx and d^2f/dx^2 at $x = 0.2$ and $x = 0.3$.

   - The function $f(x)$ being approximated is in fact $f(x) = e^x$. Compute the true error of the approximated first and second derivatives obtained using both methods and with $h = 0.1$ and $h = 0.2$ at $x = 0.2$ and $x = 0.3$. Comment on how the errors change as a function of h. Are the errors observed consistent with the known truncation error?
   - Describe how you could compute a second order accurate dertivative estimate at the **end points** $x = 0$ and $x = 0.5$

3. Given a function $f(x)$, the complex step approximation to the derivative at x is given by

$$\frac{df(x)}{dx} = \frac{\mathrm{Im}(f(x+ih))}{h} + O(h^2).$$

We can think of this as a *forward difference* approximation since it involves a Taylor series expansion of f at the point $x + ih$.

- Derive the *backward difference* complex step derivative approximation by considering the Taylor series expansion of f at the point $x - ih$.
- State the order of accuracy of the *backward difference* complex step derivative approximation you derived.

4. We wish to compare the accuracy of the derivative approximation obtained using (i) the forward difference, (ii) the central difference and (iii) the complex step differentiation formulae. We will consider the function

$$f(x) = \frac{\exp(x)}{(\cos(x))^3 + (\sin(x))^3},$$

and we seek a derivative approximation at $x = \pi/4$. Python code to evaluate the exact function and its exact derivative is provided in `func.py`.

- Using values of $h = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, \ldots, 10^{-14}$ compute and store the approximate derivative at $x = \pi/4$ using each method (e.g. (i), (ii), (iii)) for each value of h.
- For each set of approximate derivatives, compute the true error using the provided function (`evaluate_derivative_f`). On a log-log plot, plot the errors (y-axis) vs h (x-axis) you obtained with each of the three methods used to approximate the derivative. Save the plot to a PDF file.
- Comment on what you observe as h decreases.
- You can create a log-log plot using `ax = plt.loglog(xvalues, yvalues)`