

Assignment 8 (Optional)

Problem 1

The second derivative of a function can be approximated using the central finite difference formula:

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

- (a) Write a Python function that returns the numerical approximation of the second derivative of a function using the central finite difference formula. The function for the derivative should take as inputs the function `f`, a point `x`, and the step size `h`. `h` should be a keyword parameter with the default step size $h = 10^{-3}$.
- (b) Use your function to compute the second derivative of

$$f(x) = e^{2x}$$

at $x = 1$. Compute also the analytical value of $f''(1) = 4e^2$. How does the numerical derivative compare to the analytical solution?

- (c) Investigate how the numerical error depends on the step size. For $f(x) = e^{2x}$ at $x = 1$, run your calculation using

$$h = 10^{-n}, \quad n \in [0.5, 7]$$

choosing at least 10 values of n in this interval. For each h , compute the absolute error with respect to the analytical value. Make a plot of the logarithm of the absolute error versus the logarithm of h .

- (d) Comment on the trends you observe from the previous question. Why do you think the error starts rising for very small h ? Based on your plot, estimate a value of h that gives the smallest error.

Problem 2

- (a) Create a Python class that represents a typical organic molecule composed solely of C, H, and O atoms. When initializing the class, it should take as input the number of C, H, and O atoms in the molecule. Set the default value for the number of O atoms to zero, so that the class can be created by only specifying the number of C and H atoms.
- (b) Create a method inside the class that prints the chemical formula of the molecule. If the number of O atoms is zero, the printed formula should omit oxygen.
- (c) Create a method inside the class that returns the molecular weight of the molecule.
- (d) Create a class object for benzene and formaldehyde, and print both the chemical formula and the molecular weight of each.