Exercise sheet 2

Exercise 1 : Simpson's method

1. Recall the error estimate for the *trapezoid method* obtained in the lecture : Let I_1 be the result of a numerical integration obtained with N_1 steps, and I_2 the result obtained with $N_2 = 2\,N_1$ steps, then the error ϵ_2 on I_2 is approximately given by

$$\epsilon_2 \approx \frac{1}{3}(I_2 - I_1)\,.$$

Show that for *Simpson's method*, the same reasoning leads to the error estimate

$$\epsilon_2 \approx \frac{1}{15}(I_2 - I_1)\,.$$

2. Write a function `int_simpson(f, a, b, N)` similar to the function `int_trapez` of the lecture, but which uses Simpson's method.
3. Compute

$$I = \int_0^{\pi} x^2 \sin x \;\mathrm{d}x$$

with the trapezoid method and with Simpson's method for $N = 10, 100, 1000, 2000$, and compare with the exact analytic result $I = \pi^2 - 4$. For $N_1 = 1000$ and $N_2 = 2000$, estimate the errors on I_2 using the above formulas, and compare with the actual errors $I - I_2$.
4. Implement an adaptive version of Simpson's method, similar to the one of the lecture for the trapezoid method.

Hints : Define

$$S_i = \frac{f(a)}{3} + \frac{f(b)}{3} + \frac{2}{3}\sum_{\substack{2\le k\le N_i-2\\ k \text{ even}}} f(a+kh_i)\,, \qquad T_i = \frac{2}{3}\sum_{\substack{1\le k\le N_i-1\\ k \text{ odd}}} f(a+kh_i)$$

and show that $S_i = S_{i-1} + T_{i-1}$ and that $I_i = h_i(S_i + 2T_i)$. This recurrence relation allows to use the result of the previous iteration to efficiently compute the contribution to I_i from even-index points S_i, just as in the adaptive trapezoid method. Only the new points in T_i have to be added explicitly.

Exercise 2 : Gauss-Legendre quadrature

In the Debye model, the heat capacity of a solid is given by

$$C_V = 9\,n\,V\,k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D/T} \frac{x^4\,e^x}{(e^x-1)^2}\,\mathrm{d}x$$

where V is the volume, n is the number density, $k_B = 1.38\cdot 10^{-23}$ JK^{-1} is Boltzmann's constant, T is the temperature, and Θ_D is a material-dependant constant called the Debye temperature.

1. Write a function `CV(T)` which calculates C_V as a function of temperature for an aluminium cube of $10 \times 10 \times 10$ cm^3 ($n = 6.022 \cdot 10^{28}$ m^{-3}, $\Theta_D = 428$ K). Use Gaussian quadrature with $N = 50$ nodes.
2. Plot $C_V(T)$ between $T = 5$ K and $T = 500$ K.

Exercise 3 : The Lennard-Jones potential in the WKB approximation

In quantum mechanics, the Lennard-Jones potential can be used to phenomenologically model the attraction between two atoms or molecules. In one dimension it is given by

$$V(x) = \varepsilon \left(\left(\frac{x_0}{x}\right)^{12} - 2\left(\frac{x_0}{x}\right)^{6} \right)$$

where ε and x_0 are constants. The energy levels E_n of the bound states in this potential are negative numbers, $E_n < 0$. They can be computed numerically using the semi-classical WKB approximation, in which the E_n are implicitly given as the solutions of the equations

$$W(E_n) = \hbar\pi \left(n + \frac{1}{2}\right) , \qquad n \in \mathbb{N} .$$

Here $W(E_n)$ is defined by an integral :

$$W(E_n) = \int_{x_+}^{x_-} \sqrt{2m\,(E_n - V(x'))}\,\mathrm{d}x' , \qquad x_\pm = x_0 \left(1 \pm \sqrt{1 + \frac{E_n}{\varepsilon}}\right)^{-1/6} .$$

Compute the energies E_0, E_1 and E_2 in units where $x_0 = 1$, $m = 1$, $\hbar = 1$ and $\varepsilon = 100$. To do so, numerically find the zeros of the functions $f(E_n) = W(E_n) - \hbar\pi\left(n + \frac{1}{2}\right)$ by one of the root-finding methods of exercise sheet 1, with the integrals $W(E_n)$ computed by Gaussian quadrature. It may be useful to plot these functions first (e.g. for values of E_n between -100 and -1) in order to get an idea about the approximate locations of their zeros.

Exercise 4 : Numerical derivatives

1. Show that

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{1}{12}h^2 f''''(x) + \mathcal{O}(h^3) .$$

2. (a) Write a function `f(x)` which returns $f(x) = \frac{1}{2}(1 + \tanh(x))$ (use the pre-defined function `numpy.tanh`). Plot its graph on the interval $[-3, 3]$.
   (b) Calculate $f'(x)$ analytically.
   (c) On the interval $[-3, 3]$, plot the difference between the exact analytic function $f'(x)$ and the numerical derivative of $f(x)$. To evaluate the latter, use central differencing with $h = 10^{-4}$, $h = 10^{-5}$ et $h = 10^{-6}$. Compare the three graphs and explain what you observe.