Computational Physics — SuSe 2023
0. Exercise Sheet

Handing out: 17.04.2023 — Prof. H. Jelger Risselada
Submission: 21.04.2023 8 pm

Exercise 0: Comprehension Questions — 0 Points

1) What integration routine in 2) and 3) has the best accuracy? Which one is the best to use?
2) To what polynomial degree does Simpson's rule give exact results when approximating integrals of polynomials?

Exercise 1: Numerical differentiation — 8 Points

Numerical differentiation is a fundamental tool of any physicists repertoire in modern times. The goal of this exercise is to practice this method and to create an understanding of the occurring errors.

Calculate the derivatives of the functions

$$f_1(x) = \sin(x) \tag{1}$$

$$f_2(x) = \begin{cases} 2 \cdot \left\lfloor \frac{x}{\pi} \right\rfloor - \cos\left(x \bmod \pi\right)) + 1 & \text{for} \quad x \geq 0 \\ 2 \cdot \left\lfloor \frac{x}{\pi} \right\rfloor + \cos\left(x \bmod \pi\right)) + 1 & \text{for} \quad x < 0 \end{cases} \tag{2}$$

analytically and numerically. The expression $\lfloor\ \rfloor$ is the *floor* function.
Implement the two-point method

$$f'_{\text{two-point}}(x, h) = \frac{f(x+h) - f(x-h)}{2h} \tag{3}$$

and the four-point method

$$f'_{\text{four-point}}(x, h) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}. \tag{4}$$

Use single precision (32-bit) floating point variables in your implementation so that numerical errors are more pronounced.
To analyse the numerical errors of the implemented methods, perform the following steps:

a) Calculate the first derivative of $f_1(x)$ using the two-point method at a suitable point. Plot the value of the derivative as a function of the step size h and make a suitable choice for h. Plot the error $\Delta f'_{1,\text{two-point}}(x)$ of the analytical result on the interval $[-\pi, +\pi]$.

b) Calculate the second derivative $f''_{1,\text{two-point}}(x)$ and, as before, plot the error and compare with the results of the first derivative. Determine a suitable h in an analogous way to a).

c) Now calculate the derivative $f'_{1,\text{four-point}}(x)$ using the four-point method and compare the error with $\Delta f'_{1,\text{two-point}}(x)$.

d) Continue comparing the two-point rule and the four-point rule in the same way using the first derivative of $f_2(x)$.

Exercise 2: Integration routines **6 Points**

Numerical integration is just as important as numerical differentiation in computational physics. Therefore this exercise's goal is to implement three basic integration routines as generally applicable functions.

Implement integration routines for

a) trapezoid rule,

b) Riemann sum,

c) Simpson's rule

with the following four arguments

1. integrand $f(x)$,
2. lower integration limit a,
3. upper integration limit b,
4. interval width h or number of integration intervals N (for Simpson's rule N should be even).

Exercise 3: One-dimensional integrals **6 Points**

Now that we have implemented three different integrations routines, we can apply them to numerically more complex one-dimensional integrals. This exercise, therefore, focuses on the numerical effort needed to attain high accuracy.

Calculate the integrals

a)

$$I_1 = \int_1^{100} \frac{\exp(-x)}{x} \mathrm{d}x \tag{5}$$

(Result: $I_1 \simeq 0.219\,384$)

b)

$$I_2 = \int_0^1 x \sin\left(\frac{1}{x}\right) \mathrm{d}x \tag{6}$$

(Result: $I_2 \simeq 0.378\,530$)

numerically with

1. trapezoid rule,
2. Riemann sum,
3. Simpson's rule.

Halve the interval width h until the relative change of the result becomes smaller than 10^{-4}.