Numerical Methods
Bachelor in Physics

# Practicum 5: Numerical differentiation and integration

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1. Richardson extrapolation. In many problems, such as numerical differentiation and integration, we calculate an approximated value for the quantity of interest, using a certain step size. We actually want to know the value for an infinitesimally small step size. However, it is impossible to choose an arbitrarily small step size, since this will lead to large 'rounding errors'. Luckily, we can estimate the result for a step size going to zero, by making an extrapolation of the results obtained with different step sizes.

   Call $F(h)$ the value obtained with step size $h$. Assume that

   $$F(h) = a_0 + a_1 h^p + O(h^r)$$

   with $p$ as the lowest order of the error estimation. We will assume that the order $p$ and $r$ are known and $r > p$, in contrast to the values $a_0$ and $a_1$ which are unknown. After all, $F(0) = a_0$ is the quantity of interest. We calculate $F$ for two different step sizes, e.g. $h$ and $h/q$ where $q$ is an integer. It holds true that

   $$F(h/q) = a_0 + a_1(h/q)^p + O(h^r).$$

   From these two equations, we can easily determine $a_0$:

   $$a_0 = \frac{q^p F(h/q) - F(h)}{q^p - 1} + O(h^r) \tag{1}$$

   $$= F(h) + \frac{F(h) - F(h/q)}{q^{-p} - 1} + O(h^r). \tag{2}$$

   The accuracy of the approximation is now of the order $O(h^r)$ instead of $O(h^p)$. Apply this technique to the central difference approximation of the first derivative:

   $$F(h) = \frac{f(x+h) - f(x-h)}{2h} \tag{3}$$

   $$f'(x) = F(h) + O(h^2) \tag{4}$$

   Calculate, in this way, the derivative of $\sin(x)$ in $x = 1$. Use step sizes $h = 0.5$ and $h/2 = 0.25$.

2. **For this exercise, you can use the scripts trap.m and trapsimp.m** Richardson extrapolation can also be applied when performing numerical integrations. Calculate the integral

$$\int_0^{\pi/2} \sin(x)dx$$

with the (composite) trapezoidal rule. First, use a step size $h = \pi/2$, and then $h/2 = \pi/4$. Use these results to calculate Richardson's interpolation.

Define $T_{k,0}$ for every integer $k \geq 0$ as an approximation of the integral $\int_a^b f(x)dx$ using the composite trapezoidal rule with grid size $h_k = (b - a)/2^k$. Now we can write down the extrapolated values recursively for $j = 1, \ldots, k$:

$$T_{k,j} = \frac{4^j T_{k,j-1} - T_{k-1,j-1}}{4^j - 1}.$$

Convince yourselves that this is equivalent with the Romberg integration formula. We can write this down as

$$\begin{array}{lllll} T_{0,0} & & & & \\ T_{1,0} & T_{1,1} & & & \\ T_{2,0} & T_{2,1} & T_{2,2} & & . \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{array}$$

You have already calculated $T_{0,0}$, $T_{1,0}$, and the extrapolated value $T_{1,1}$.

Show (numerically and annalytically) that the second column is equivalent to the composite Simpson rule.

3. Write a function which calculates the integral of numerical data (use a spline interpolation).

4. Calculate the integral

$$\int_{-1}^{3} f(x)dx = \int_{-1}^{3} (x^3 - x + 5)dx$$

exactly and with Simpson's method. What do you notice? Plot the quadratic interpolant $P_2$ which is used to calculate $S_2$ together with the integrand $x^3 - x + 5$. Make use of the function of the previous exercise, to calculate the difference

$$\int [f(x) - P_2]\, dx$$

in the first and second half of the interval $[-1, 3]$.

5. What should we do when an integrandom diverges in a single point? Since, we can split the original integral, we can reduce the problem to the integral $\int_a^b f(x)dx$ with a singularity in one of the end points, let's say in $a$. First, we have to be sure that the integral exists. For a singularity of the form $f(x) \sim c(x-a)^\gamma$ with $x \to a$, the integral exists if $\gamma > -1$.

   For singularities of the form $f(x) \sim c(x-a)^\gamma$, we can eliminate the singularity by using another variable of integration: $x = a + t^\beta$. The integral becomes

$$\int_a^b f(x)dx = \int_0^{(b-a)^{1/\beta}} f(a+t^\beta)\beta t^{\beta-1}dt = \int_0^{(b-a)^{1/\beta}} G(t)dt.$$

   The new integrand $G(t) \sim ct^{\beta\gamma}\beta t^{\beta-1}$ does not have a singularity if $\beta(\gamma+1)-1 \geq 0$.

   Apply this method to the integral

$$\int_0^1 \frac{e^x}{\sqrt[3]{x}}dx.$$

   This integral has a singularity in $x = 0$. In order to check the behaviour of the singularity, you can use the following the Taylor expansion:

$$\frac{e^x}{\sqrt[3]{x}} = \frac{1 + x + x^2/2 + \cdots}{\sqrt[3]{x}} = \frac{1}{\sqrt[3]{x}} + x^{2/3} + \cdots .$$

   Thus $f(x) \sim x^{-1/3}$ and $\gamma = -1/3$. The integral exists because $\gamma > -1$. Choose $\beta$ in such a way that there is no longer a singularity. Next, calculate the integral. (solution: 2.343591093328065)

6. Apply the same method to the integral

$$\int_0^1 \frac{x^{7/4}e^x}{\sinh^2(x)}dx.$$

   (Solution: 1.913146675663268)