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**Computational Physics**
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Blatt 1 vom 16.10.2018
Abgabe bis 12:30 Uhr am 23.10.2018

**<u>Problem 1.1</u>: Numerical Integration**

The error function is defined by the integral

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, \mathrm{d}t\,. \tag{1}$$

a) Write a computer programme that computes the numerical approximation of the integral using:

   i) The trapezoidal rule with $N$ nodes

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{h}{2}\sum_{i=0}^{N-1}\left[f(x_i)+f(x_{i+1})\right] \tag{2}$$

   ii) The Simpson rule with $N$ nodes (with $N$ a even integer number).

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{h}{3}\left[f(x_0) + 2\sum_{i=1}^{N/2-1} f(x_{2i}) + 4\sum_{i=1}^{N/2} f(x_{2i-1}) + f(x_N)\right] \tag{3}$$

   with $h = (b-a)/N$.

b) Use the programs to estimate erf(0.4). And compare both the trapezoidal and Simpson rules for $N = 4$ with the exact value $\mathrm{erf}(0.4) = 0.428392$.

**<u>Problem 1.2</u>: Newton-Raphson Method**

By the Newton-Raphson method, one can estimate the root of a function $f(x)$ as

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}. \tag{4}$$

The goal of this exercise is to understand (i) the importance of the initial value, and (ii) obtain the rate of the convergence of the method numerically to find the roots of following function

$$f(x) = 3x^4 + 4x^3 - x^2 - 2x$$

a) Calculate the roots of $f(x)$ analytically?

b) Now use a combination of bisection and the Newton-Raphson method to determine the roots of $f(x)$. (you do not need a code!)

c) Now use $x_0 \in \{-4 \cdots 4\}$ as the initial value to calculate the roots numerically. What do you observe?

d) In practice, usually the derivative is not known analytically and one should approximate it. Now approximate the derivative in Eq. (4) by

$$f'(x_n) = \frac{f(x_n + h) - f(x_n)}{h} \quad \text{with} \quad h = 0.01.$$

and find the roots with this approximation. Is the convergence still quadratic?