Numerical Methods
Exercise Sheet 4

HS 16
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`http://www.physik.uzh.ch/en/teaching/PHY233/HS2016.html`

Issued: 17.10.2016
Due: 24.10.2016 16:00

Exercise 1: Numerical derivatives (40 Pts.)

In this exercise you will will produce different implementations of numerical derivatives.

Consider the function $d(x) = x \cdot e^{-x^2}$.

a) Implement a forward difference quotient and compute $\partial_x d(x)$ at $x = 1$, for three different increments $h = \{10^{-1}, 10^{-2}, 10^{-3}\}$. (10 points)

b) Implement a central difference quotient and compute $\partial_x d(x)$ at $x = 1$, for three different increments $h = \{10^{-1}, 10^{-2}, 10^{-3}\}$. (10 points)

c) Compare and comment on the results obtained in the two former tasks. (10 points)

d) Optional: Compute $\partial_x d(x)|_{x=1}$ analytically. Then plot, as a function of h, the difference between analytical and numerical derivative for the two different algorithms. (10 points)

Exercise 2: Newton–Raphson method in D=1 (60 Pts.)

In this exercise you will be asked to implement the Newton–Raphson method to find the root of a simple one-dimensional equation: $\cos 3x + \frac{1}{3}\sin x = 0$.

a) Calling $f(x) = \cos 3x + \frac{1}{3}\sin x$, implement the $N = 1$ iterative function $\Phi[f](x) = x - \frac{f(x)}{f'(x)}$. Use the central difference quotient method to implement $f'(x)$. (10 points)

b) Implement the Newton–Raphson method and find a root x_1 of $f(x) = 0$, within an absolute precision $t = 10^{-8}$. Use $x = 0.5$ as starting point. (10 points)

c) We are interested in finding other roots of $f(x) = 0$ in the domain $x \in (0, \pi)$. For this purpose, it would be preferable to get rid of the already-found x_1 root. The function $g(x) \equiv \frac{f(x)}{x - x_1}$ is what we are looking for, since the equation $g(x) = 0$ share all the roots with the former equation $f(x) = 0$, except for x_1.

   Find another root x_2 of $f(x) = 0$, exploiting the function $g(x)$ defined above. Use $x = 0.8$ as starting point of the Newton–Raphson method. Again, the target precision is $t = 10^{-8}$. (15 points)

d) What happens if we use $x = 0.8$ as starting point in task (b)? Comment the result. (5 points)

e) Optional: $f(x)$ has also roots outside our domain of interest, $x \in (0, \pi)$. For example, performing task (c) starting from $x = 0.5$ would lead us to one of such unwanted solutions. Can you think of any solution to this problem? (20 points)

Exercise 3: Theory exercise: order of convergence of the Newton-Raphson method (40 Pts.)

In this exercise you will analyse the local order of convergence of the Newton-Raphson method for a degenerate case: $h(x) = (1-x)^2 e^{-x}$ around 1.

a) Compute analytically $\Phi[h](x) = x - \frac{h(x)}{h'(x)}$. (10 points)

b) Evaluate the local rate of convergence p of $\Phi[h](x)$ around 1, defined as the integer p for which $\exists C > 0 : |\Phi[h](x) - 1| \leq C \cdot |x-1|^n$.

   (Hint: remember that $\Phi[h](1) = 1$, that is $|\Phi[h](x) - 1| = |\Phi[h](x) - \Phi[h](1)|$. The latter can be evaluated through a Taylor expansion). (20 points)

c) Optional: What is the analytical reason for p to have such value? (10 points)

Maximum number of points for mandatory tasks on 24.10 : 100
Maximum possible number of points for tasks on 24.10 : 140