Numerisches Praktikum – Numerical Practical Training

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Root finding

Return by 9:15 a.m. tomorrow

Free Training

- Write a program code to calculate the root $x_\star$ (i.e., with $f(x_\star) = 0$) of some given function f(x) using the four methods presented in the lecture:
  1. Bisection method
  2. Regula falsi (Interpolation)
  3. Newton-Raphson
  4. Secant method
- Solve the quadratic equation $x^2 + x - 1 = 0$ using these four methods. Plot the graph first to find proper starting values for the iteration.

Assignment for the Afternoon / Homework

- **Exercise 1, 8 points**: Convergence (I).
  Solve the equation $f(x) = \cos(x) - \frac{1}{4}$ with your program using $x_a = 0$ and $x_b = \pi/2$ (for methods 1, 2 and 4) and $x_a = \pi/2$ (for Newton-Raphson) as initial values. Calculate and write out both the absolute true error ($|e_n| = |x_n - x_*|$) and the absolute true relative error $|f_n| = |x_n - x_*|/|x_*|$ for the first 20 iterations.
- **Exercise 2, 6 points**: Convergence (II).
  Plot $|e_n/e_0|$, where e_0 is the error for $n = 0$, versus the iteration step n from the data in Ex. 1 in a logarithmic plot. Compare your results to the expected convergence behaviour of these methods.
- **Exercise 3, 6 points**: Double-well potential
  $f(x) = 0.1\,x^4 - 4\,x^2 - 10$. Double-well potentials play an important role in quantum mechanics and molecular dynamics to describe the motion of a particle in the force field of two others. Determine the root of $f(x)$ with the four root-finding methods. Start the iteration with the initial values $x_a = 2.5$ and $x_b = 7.0$ (use $x_a = 2.5$ for the Newton-Raphson algorithm). Discuss the results of the four methods in terms of their convergence behaviour. Give an example in which the bisection method cannot be applied or would give a wrong result (i.e., not converge to a root of $f(x)$).