Department of molecular science and nanosystems 2023/24
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Exercise Sheet 5

Exercise 1: Prepare a script that computes the roots of the problem $f(x) = 0$ with the following methods

a) Bisection method

b) Chord's method

c) Secant Method

d) Newton's Method

INPUT:

- a, b the boundary of the domain,
- f the function
- x_0 the initial condition
- ε the stopping criteria

OUTPUT:

- number of iterations k to converge
- the plot of the sequence $\{x_k\}$ for $k = 0, 1, \ldots, k_{max}$
- order of convergence p_k for each iteration of the method.

You might then test your code for the following functions

a) $f(x) = x^2 - x - 2$

b) $f(x) = \sqrt{x+2} - x$

c) $f(x) = 1 + \frac{2}{x} - x$

d) $f(x) = x + 2(\log(x) - 1)$

e) $f(x) = e^x - x^2$

f) $f(x) = \frac{1}{x} - e^{\sqrt{x}}$

g) $f(x) = x - e^{-x^2}$

h) $f(x) = x^3 - \sin(x)$

Exercise 2 Prepare a script that computes the roots of $F : \mathbb{R}^2 \to \mathbb{R}^2$ using

- Newton's method
- Approximation of the Jacobian

Test your code for the following examples:

- $F(x, y) = (x + 2y - 3, 2x^2 + y^2 - 5)$ where $J_F(x, y) = \begin{pmatrix} 1 & 2 \\ 4x & 2y \end{pmatrix}$. One solution can be found in $[1, 2] \times [0.5, 1.5]$ and it is $(x, y) \approx (1.488, 0.756)$. Are there other roots?
- $F(x, y) = (x^2 + y^2 - 1, \sin \frac{\pi}{2} x + y^3)$ where $J_F(x, y) = \begin{pmatrix} 2x & 2y \\ \frac{\pi}{2} \cos \frac{\pi}{2} x & 3y^2 \end{pmatrix}$. One solution can be approximated by $(x, y) \approx (0.4761, -0.8794)$. Are there other roots?

Compare the CPU times for the two methods, the order of convergence and the number of iterations needed to achieve the desired tolerance.