Feb. 24, 2025 (Due: 08:00 Mar. 3, 2025)

1. Write a program to find

$$\inf_{x>0} \frac{x^3 \mathrm{e}^{2x} - 1 - 3\ln x}{x}.$$

What do you observe?

2. Use bisection and *regula falsi*, respectively, over the interval $[0, 1]$ to find the root of $x^{64} - 0.1 = 0$ with absolute accuracy 10^{-12}. Visualize the convergence history of these methods in one figure.

3. When applying Newton's method to solve the equation $f(x) = 0$, we usually require that $f'(x_*) \neq 0$, i.e., the root x_* is a simple one. Without such a condition, Newton's method is still applicable to find x_* while the convergence is no longer quadratic. In the following let us assume that $f(x)$ is sufficiently smooth to avoid complications in theoretical analysis.

(a) Use Newton's method to solve $1 + \cos x = 0$ around $x_0 = 3$ and plot the convergence history.

(b) Let x_* be a root of $f(x)$ with multiplicity higher than one, i.e.,

$$h(x_*) = f'(x_*) = 0.$$

Show that Newton's method converges (locally) linearly around x_*.

(c) Let x_* be a root of $f(x)$ with multiplicity $m > 1$, i.e.,

$$f(x_*) = f'(x_*) = \cdots = f^{(m)}(x_*) = 0 \neq f^{(m+1)}(x_*).$$

We can modify Newton's method as

$$x_{k+1} = x_k - \frac{(m+1)f(x_k)}{f'(x_k)}$$

to achieve local quadratic convergence. Try to explain why such a modification improves the convergence.

4. In this exercise, you will determine the pH of rainwater by measuring the partial pressure of carbon dioxide (CO_2). For simplicity, we suppose that the only chemical reactions in rainwater are

$$\begin{aligned} \mathrm{H_2O} &\rightleftharpoons \mathrm{H^+ + OH^-}, \\ \mathrm{CO_2 + H_2O} &\rightleftharpoons \mathrm{H^+ + HCO_3^-}, \\ \mathrm{HCO_3^-} &\rightleftharpoons \mathrm{H^+ + CO_3^{2-}}. \end{aligned}$$

The following nonlinear system of equations governs the chemistry of rainwater:

$$\begin{aligned} K_{\mathrm{W}} &= [\mathrm{H}^+][\mathrm{OH}^-], \\ K_1 &= 10^6 \frac{[\mathrm{H}^+][\mathrm{HCO}_3^-]}{K_{\mathrm{H}} \cdot p_{\mathrm{CO}_2}}, \\ K_2 &= \frac{[\mathrm{H}^+][\mathrm{CO}_3^{2-}]}{[\mathrm{HCO}_3^-]}, \\ [\mathrm{H}^+] &= [\mathrm{OH}^-] + [\mathrm{HCO}_3^-] + 2[\mathrm{CO}_3^{2-}], \end{aligned}$$

where $K_{\mathrm{H}} = 10^{-1.46}$ is Henry's constant, and $K_1 = 10^{-6.3}$, $K_2 = 10^{-10.3}$ and $K_{\mathrm{W}} = 10^{-14}$ are equilibrium constants.

Let us use $p_{\mathrm{CO}_2} = 375$ (ppm), which was the partial pressure of CO_2 at Mauna Loa (Hawaii) in 2003. Estimate the corresponding pH of rainwater.

Solve this problem using the multivariable version of Newton's method and two variants of Broyden's method.

5. (optional) Visualize the curve $y = (x-2)^9$ around $x = 2$, where the function $f(x) = (x-2)^9$ is evaluated through an expanded form. What is the attainable accuracy if bisection is used to find the root of this function?

6. (optional) Give a local convergence analysis on Steffensen's method.