March 7, 2022 (Due: 08:00 March 14, 2022)

1. 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

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

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

$$\begin{aligned} K_W &= [H^+][OH^-], \\ K_1 &= 10^6 \frac{[H^+][HCO_3^-]}{K_H \cdot p_{CO_2}}, \\ K_2 &= \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]}, \\ [H^+] &= [OH^-] + [HCO_3^-] + 2[CO_3^{2-}], \end{aligned}$$

where $K_H = 10^{-1.46}$ is Henry's constant, and $K_1 = 10^{-6.3}$, $K_2 = 10^{-10.3}$ and $K_W = 10^{-14}$ are equilibrium constants.

Let us use $p_{CO_2} = 375$ 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 multivariable methods, such as Newton's method or Broyden's method.

2. Polynomial interpolation provides one way to approximate a given function. For instance, let $0 = x_1 < x_2 < \cdots < x_n = 2\pi$ be equally spaced interpolation nodes. The interpolation polynomial passing through all $(x_i, \sin x_i)$'s can be used to approximate the sine function $f(x) = \sin x$. Try to visualize the difference between the interpolation polynomial and the sine function for a few different choices of n.

What happens if the same technique is applied to approximate the rational function $f(x) = (1 + 25x^2)^{-1}$ over $[-1, 1]$ (using equally spaced interpolation nodes)?

3. Polynomial interpolation are useful not only in modeling, but also in pure mathematics. For instance, the Chinese Remainder Theorem can be derived from Lagrange's approach. This exercise is another example.

Let $f(x)$ be a real polynomial of degree n. Suppose that there exists $i \in \mathbb{Z}$ such that $f(i)$, $f(i+1)$, …, $f(i+n)$ are all integers. Show that $f(k) \in \mathbb{Z}$ for any $k \in \mathbb{Z}$. Is it also true that $f(x) \in \mathbb{Z}[x]$, i.e., $f(x)$ has integer coefficients?