Numerical Methods - Lab. 2

Numerical methods for finding roots

1. Use the graphical approach to determine the mass of the bungee jumper who will have a velocity of 36m/s at the 4th second of the free fall. Use a drag coefficient of 0.25 kg/m, and gravitational acceleration $g = 9.81\text{m/s}^2$.

2. Write a function implementing the *Incremental search* to identify brackets within the interval $[3, 6]$ for the function
$$f(x) = \sin(10x) + \cos(3x).$$

3. Use *bisection* to solve problem 1. with an approximate error of at most 0.5% ($\varepsilon_s = 0.5\%$). Plot the true and the approximate errors (in the same figure).

4. Determine the lowest positive root of $f(x) = x^3 - 6x^2 + 11x - 6.1$:

   a Graphically.

   b Using the Newton-Raphson method (three iterations, $x_i = 3.5$).

   c Using the secant method (three iterations, $x_{i-1} = 2.5$ and $x_i = 3.5$.

   d Using the modified secant method (three iterations, $x_i = 3.5$, $\delta = 0.01$)

   e Find all roots with Mathematica (*Roots*).

5. Employ fixed-point iteration to locate the root of $f(x) = \sin\sqrt{x} - x$. Use an initial guess of $x_0 = 0.5$ and iterate until $\varepsilon_a < 0.01\%$. Verify that the process is linearly convergent.

6. Use the Newton-Raphson method to find the root of $f(x) = \mathrm{e}^{-0.5x}(4 - x) - 2$. Employ initial guesses of **(a)** 2, **(b)** 6, and **(c)** 8. Explain your results.

Modeling and bracketing methods

7. It is well documented that the atmospheric levels of several so-called "greenhouse" gases have been increasing over the past 50 years. For example, the figure below shows data for the partial pressure of carbon dioxide (CO_2) collected at Mauna Loa, Hawaii from 1958 through 2008. The trend in these data can be nicely fit with a quadratic polynomial,
$$p_{\text{CO}_2} = 0.012226(t - 1983)^2 + 1.418542(t - 1983) + 342.38309.$$
   These data indicate that levels have increased a little over 22% over the period, from 315 to 386 ppm.

   One question that we can address is how this trend is affecting the pH of rainwater. Outside of urban and industrial areas, it is well documented that carbon dioxide is the primary determinant of the pH of the rain. pH is the measure of the activity of hydrogen ions and, therefore, its acidity or alkalinity. For dilute aqueous solutions, it can be computed as
$$pH = -\log_{10}[H^+],$$
   where $[H^+]$ is the molar concentration of hydrogen ions.

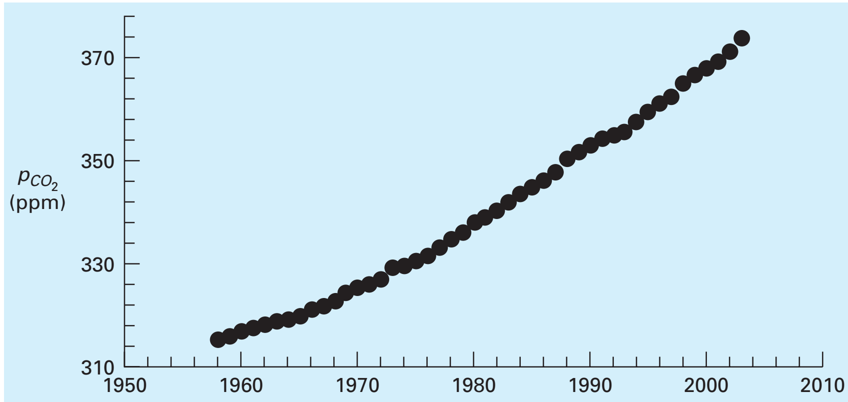

Figure 1: Average annual partial pressures of atmospheric carbon dioxide (ppm) measured at Mauna Loa, Hawaii.

The following five equations govern the chemistry of rainwater:

$$K_1 = 10^6 \frac{[H^+][HCO_3^-]}{K_H p_{\mathrm{CO}_2}} \tag{0.1}$$

$$K_2 = \frac{[H^+][CO_3^{-2}]}{[HCO_3^-]} \tag{0.2}$$

$$K_w = [H^+][OH^-] \tag{0.3}$$

$$c_T = \frac{K_H p_{\mathrm{CO}_2}}{10^6} + [HCO_3^-] + [CO_3^{-2}] \tag{0.4}$$

$$0 = [HCO_3^-] + 2[CO_3^{-2}] + [OH^-] - [H^+] \tag{0.5}$$

where K_H is Henry's constant, and K_1, K_2, and K_w are equilibrium coefficients. The five unknowns are c_T (the total inorganic carbon), $[HCO_3^-]$ (bicarbonate), $[CO_3^{-2}]$ (carbonate), $[H^+]$ (hydrogen ion), and $[OH^-]$ (hydroxyl ion). Notice how the partial pressure of CO_2 shows up in equations (0.1) and (0.4).

Use these equations to compute the pH of rainwater, given that $K_H = 10^{-1.46}$, $K_1 = 10^{-6.3}$, $K_2 = 10^{-10.3}$, and $K_w = 10^{-14}$. Compare the results in 1958 when the p_{CO_2} was 315, and in 2008 when it was 386 ppm. When selecting a numerical method for your computation, consider the following:

- You know with certainty that the pH of rain in pristine areas always falls between 2 and 12.
- You also know that pH can only be measured to two places of decimal precision.