CHEN 2450
HOMEWORK 8
NONLINEAR EQUATIONS

Submit all your homework using Jupyter notebooks. You are expected to include proper text and discussion for each and every problem including appropriate headings and formatting. You will lose points if your reports are not readable or just include code with a few print out statements. No exceptions.

Problem 1 (25 pts)

Assume that we want to solve the nonlinear equation

$$f(x) = \sin(x)\exp\left(-\frac{x-5}{3}\right) \tag{1}$$

for $f(x) = 2$. (be sure to show all of your work):

1. (5 pts) Write the equation in residual form $r(x) = 0$

   First, we rewrite the problem as $r(x) = 2 - f(x)$ and solve $r(x) = 0$ for x. Therefore,

   $$r(x) = 2 - \sin(x)\exp\left(-\frac{x-5}{3}\right). \tag{2}$$

2. (5 pts) Show the ***first two*** iterations of the Bisection method. Use initial guesses of $a = 1$ and $b = 5$.

   First, we rewrite the problem as $r(x) = 2 - f(x)$ and solve $r(x) = 0$ for x. Therefore,

   $$r(x) = 2 - \sin(x)\exp\left(-\frac{x-5}{3}\right). \tag{3}$$

   For the first iteration, we have $a = 1$, $b = 5$ so that $c = {}^{(5+1)}/_{2} = 3$ and $r(a)r(c) = -2.0568$. Therefore, we choose $[a,c] = [1,3]$ as the new interval.

   The second iteration begins with $a = 1$, $b = 3$ and $c = 2$ so that $f(a)f(c) = 0.562$ and we choose $[b,c] = [3,2]$ as the new interval.

3. (5 pts) Show the ***first two*** iterations of the Regula-Falsi method. Use initial guesses of $a = 1$ and $b = 5$.

   For the first iteration, we have $c = 2.149$, $f(a)f(c) = 0.1985$. Therefore, we choose $[b,c] = [5,2.149]$ as the new interval.

The second iteration begins with $a = 2.149$, $b = 5$ and $c = 2.301$ so that $f(a)f(c) = -0.0279$ and we choose $[a,c] = [2.149, 2.301]$ as the new interval.

4. (5 pts) Show the ***first two*** iterations of the Secant method using an initial guess of $a = 4$ and $b = 5$.

   For the first iteration, we have $a = 4$, $b = 5$ so that $f(a) = 3.1$, $f(b) = 3.0$, $c = 35.42$ and $f(c) = 2.0$.

   The second iteration begins with $a = 5$, $b = 35.42$ so that $f(a) = 0.0281$, $f(b) = 2.0$, $c = 98.86$, and $f(c) = 2.0$.

5. (5 pts) Show the ***first two*** iterations of Newton's method using an initial guess of $x = 1$ and using an *analytic* derivative.We need $r'(x)$ which we obtain from (3) as

$$r'(x) = -\exp\left(\frac{5-x}{3}\right)\left(\cos(x) - \frac{1}{3}\sin(x)\right) \tag{4}$$

   For a guess of $x = 1$ we have $r(x) = -1.1923$ and $r'(1) = -0.9856$. Newton's update is:

$$x^{k+1} = x^k - \frac{r(x^k)}{r'(x^k)} = 1 - \frac{-1.1923}{-0.9856} = -0.2096.$$

   For the second iteration, we have $r(-0.2096) = 3.1815$ and $r'(x) = -5.947$ so that the update provides:

$$x^{k+1} = x^k - \frac{r(x^k)}{r'(x^k)} = -0.2096 - \frac{3.1815}{-5.947} = 0.3253.$$

Problem 2 (35 pts)

When water vapor is heated to sufficiently high temperatures, a significant portion of the water dissociates - that is, splits apart - from oxygen and hydrogen. We assume that this is the only reaction involved in this process. The mole fraction, x, of water that dissociates is given by

$$K = \frac{x}{1-x}\sqrt{\frac{2p_t}{2+x}} \tag{5}$$

where K is the reaction equilibrium constant and p_t is the total pressure of the mixture.

1. (5 pts) Assuming you want to solve for x, this equation in residual form $r(x)$.

2. (30 pts) Write a code that uses Newton's method to determine the mole fraction of water for a mixture with a total pressure of 3.5 atm and a reaction equilibrium constant of 0.04. Use an analytical derivative along with an absolute tolerance of 10^{-3}.

Write your own Newton solver code. You may compare your results to Python's root finding routines. HINT: plot this function first to get an idea of where the root is located and then choose an initial guess accordingly.

Problem 3 (40 pts)

Pipe flow theory in fluid dynamics predicts that the pressure drop in a pipe is given by

$$\Delta p = f\frac{L\rho V^2}{2D} \tag{6}$$

where Δp is the pressure drop (Pa), f is called the friction factor, L is the pipe length in meters, ρ is the fluid density (kg/m^3), V is the mean fluid velocity (m/s), and D is the pipe diameter (m). For turbulent flows, the Colebrook equation allows us to calculate the friction factor f. This formula is given by

$$\frac{1}{\sqrt{f}} = -2\log\left(\frac{\varepsilon}{3.7D} + \frac{2.51}{\mathrm{Re}\sqrt{f}}\right) \tag{7}$$

where ε is the pipe roughness (m), and Re is the Reynolds number given by

$$\mathrm{Re} = \frac{\rho V D}{\mu} \tag{8}$$

with μ denoting the viscosity of the fluid.

1. (20 pts) Determine the pressure drop for air flow for a 0.2-m-long stretch of smooth PVC tubing with diameter $D = 0.005$ m and roughness 0.0015 mm. The air density is 1.23 kg/m^3, $\mu = 1.79 \times 10^{-5}$ N.s/m^2. The air is flowing @ 40 m/s. Use Newton's method to determine the friction factor and then calculate the pressure drop and use an anlytical derivative. A good initial guess can be obtained from: $f = 0.316/\mathrm{Re}^{0.25}$.

2. (20 pts) Repeat the compuation for a commercial steel pipe where $\varepsilon = 0.045$ mm.

Reuse the Newton solver that you wrote for Problem 2. You may compare your results to Python's root finding routines.