Problem Set 2 (9/11, 13, 16)
Due on Fri, Sep 27

1) Consider $f(x) = x^2 - 5$. Since $f(2) = -1 < 0$ and $f(3) = 4 > 0$, it follows that $f(x)$ has a root r in the interval $[2, 3]$. Compute an approximation to r and fill the following table. Take 10 steps in each case. Do the results agree with the theory discussed in class?

   (a) Use bisection method with starting interval $[a, b] = [2, 3]$.

   (b) Use fixed-point iteration with $g_1(x) = 5/x$, $g_2(x) = x - (x^2 - 5)$, $g_3(x) = x - \frac{1}{3}(x^2 - 5)$, $x_0 = 2.5$.

   (c) Use Newton's method with $x_0 = 2.5$.

n	x_n	$\|r - x_n\|$
1	*	*
2	*	*
$\vdots$	$\vdots$	$\vdots$

2) Let us consider the equation of state of chlorine gas. The ideal gas law is given by

$$PV = nRT,$$

where P is pressure, V is volume, T is temperature, n is the number of moles, and R is the gas constant ($R = 0.08206\,\text{atm} \cdot \text{liter}/(\text{mole} \cdot \text{K})$). We get van der Waals equation by improving the left-hand side as

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT,$$

where $a = 6.29\,\text{atm} \cdot \text{liter}^2/\text{mole}^2$ (accounts for intermolecular attractive forces), and $b = 0.0562\,\text{liter}/\text{mole}$ (accounts for size of gas molecules). Let us find V by Newton's method when $n = 1\,\text{mole}$, $P = 2\,\text{atm}$, and $T = 313\,\text{K}$. We give the starting guess V_0 by the ideal gas law. We introduce $f(V)$ as

$$f(V) = \left(P + \frac{n^2 a}{V^2}\right)(V - nb) - nRT.$$

   (a) Find $f'(V)$.

   (b) Find V_0.

   (c) Find V_1, V_2.

   (d) We infer that V_0 has 2 correct digits and V_1 has 5 correct digits. Compute V_3. How many correct digits does V_2 have? Explain your answer.

3) Consider the following system of nonlinear equations.

$$\begin{cases} f(x, y) = (x - 1)^2 + y^2 - 4 = 0, \\ g(x, y) = xy - 1 = 0. \end{cases} \tag{1}$$

This corresponds to finding the intersection of a circle and a hyperbola. Find an approximate solution using Newton's method for systems. Take two steps starting from $(x_0, y_0) = (3, 0)$. Present the iterates (x_i, y_i) and residual values $f(x_i, y_i)$, $g(x_i, y_i)$ for $i = 0, 1, 2$. Present also intermediate calculations.

4) Let us solve the system (1) by Matlab. By using the Matlab code below as a template, write your own code and find a solution. The solution must have at least 4 significant digits. For $i = 1, 2$, do (x_i, y_i), $f(x_i, y_i)$, $g(x_i, y_i)$ agree with the values found in 2)? If so, it seems that the Matlab code is working correctly.

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%
% Template for Problem 4)
%
function Newton
clear; format long;
x = 3.0; y = 0.0; % initial guess
nmax = 2; % number of iterations (Choose a suitable number)
for n = 1:nmax
     result(n,1) = n-1;
     result(n,2) = x;
     result(n,3) = y;
     result(n,4) = f(x,y);
     result(n,5) = g(x,y);
     answer = [x; y] - jacobian(x,y)\[f(x,y); g(x,y)];
     x = answer(1); y = answer(2);
end
result
%
function ffun = f(x,y)
ffun = % fill in 1st function
%
function gfun = g(x,y)
gfun = % fill in 2nd function
%
function j = jacobian(x,y)
j11 = % fill in 11 element
j12 = % fill in 12 element
j21 = % fill in 21 element
j22 = % fill in 22 element
j = [j11 j12; j21 j22];
```