Math 371 Winter 2013 Homework 3 due: Thursday February 7

1. In class we discussed the equation of state of chlorine gas as an example of root-finding. The example uses Newton's method to compute the gas volume, given the pressure and temperature, determined by the van der Waals equation of state, where the initial guess V_0 is given by the ideal gas law. We computed V_0, V_1, V_2 in class and inferred that V_0 has 2 correct digits and V_1 has 5 correct digits. Now compute V_3. How many correct digits does V_2 have? Explain your answer.

2. In class we discussed a problem involving two reversible chemical reactions as an example of a system of nonlinear equations. After simplifying, the equations can be written as

$$f(c_1, c_2) = c_1 + c_2 - k_1(a_0 - 2c_1 - c_2)^2(b_0 - c_1) = 0,$$

$$g(c_1, c_2) = c_1 + c_2 - k_2(a_0 - 2c_1 - c_2)(d_0 - c_2) = 0,$$

where c_1, c_2 are the equilibrium product concentrations arising from the two reactions, k_1, k_2 are the equilibrium reaction constants, and a_0, b_0, d_0 are the initial concentrations of the reactants. Let $a_0 = 20$ mole/liter, $b_0 = d_0 = 10$ mole/liter, $k_1 = 1.63 \times 10^{-4}$, $k_2 = 3.27 \times 10^{-3}$. The Matlab code on the back of this sheet applies Newton's method to solve for c_1, c_2. The code takes six steps starting from initial guess $c_1 = c_2 = 0.5$ mole/liter and it prints the results in a table with the following format.

column 1: n (step index)
column 2: c_1
column 3: c_2
column 4: $f(c_1, c_2)$
column 5: $g(c_1, c_2)$

Your assignment is to run the code and present the table of results in your writeup. Put the code into an m-file (all the functions should go into the same m-file). To run the code, you must fill in the two functions $f(c_1, c_2), g(c_1, c_2)$ and the Jacobian matrix. To check your code, note that the last value in column 2 should be 0.109867175948009. Which reaction produced more product, reaction #1 or reaction #2?

In the following problems, you should find the answer by hand, but you may check your answer using Matlab. On an exam you may be asked to solve such problems by hand.

3. Let $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$. Show that $A^{-1} = \dfrac{1}{ad - bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$.

4. Which of the following matrices are invertible? Justify your answer. For those matrices that are not invertible, find a vector $x \neq 0$ such that $Ax = 0$.

a) $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ b) $\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ c) $\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ d) $\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$ e) $\begin{pmatrix} 1 & 0 & 2 \\ -1 & 3 & 1 \\ 0 & 3 & 3 \end{pmatrix}$

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%
% Math 371, exercise on Newton's method for solving a nonlinear system
%
function Newton
clear; format long;
c1 = 0.5; c2 = 0.5; % initial guess
for n = 1:6
    result(n,1) = n-1;
    result(n,2) = c1;
    result(n,3) = c2;
    result(n,4) = f(c1,c2);
    result(n,5) = g(c1,c2);
    answer = [c1; c2] - jacobian(c1,c2)\[f(c1,c2); g(c1,c2)];
    c1 = answer(1); c2 = answer(2);
end
result
%
function ffun = f(c1,c2)
a0 = 20; b0 = 10; d0 = 10; k1 = 1.63e-4; k2 = 3.27e-3;
ffun = % fill in 1st function
%
function gfun = g(c1,c2)
a0 = 20; b0 = 10; d0 = 10; k1 = 1.63e-4; k2 = 3.27e-3;
gfun = % fill in 2nd function
%
function j = jacobian(c1,c2)
a0 = 20; b0 = 10; d0 = 10; k1 = 1.63e-4; k2 = 3.27e-3;
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];
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