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.

<table>
<thead>
<tr>
<th>column 1</th>
<th>step index</th>
</tr>
</thead>
<tbody>
<tr>
<td>column 2</td>
<td>$c_1$</td>
</tr>
<tr>
<td>column 3</td>
<td>$c_2$</td>
</tr>
<tr>
<td>column 4</td>
<td>$f(c_1, c_2)$</td>
</tr>
<tr>
<td>column 5</td>
<td>$g(c_1, c_2)$</td>
</tr>
</tbody>
</table>

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 $A^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$.

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) $\begin{pmatrix} 1 & 0 & 2 \\ -1 & 3 & 1 \\ 0 & 3 & 3 \end{pmatrix}$
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];