1. This exercise concerns the 2nd derivative of a function $f(x)$. Recall that the forward and backward finite-difference approximations of the 1st derivative are

$$D_+ f(x) = \frac{f(x + h) - f(x)}{h}, \quad D_- f(x) = \frac{f(x) - f(x - h)}{h}.$$ 

a) Show that $D_+ D_- f(x) = D_+(D_- f(x)) = \cdots = \frac{f(x + h) - 2f(x) + f(x - h)}{h^2}$.

b) Show that $D_+ D_- f(x) = f''(x) + ch^2 + \cdots$, where $c$ is a constant independent of $h$. Find the value of $c$ in terms of $f(x)$.

c) Let $f(x) = e^x$, $x = 1$, $h = 0.1, 0.05, 0.025, 0.0125$. Present a table in the following format. Column 1: $h$, column 2: $D_+ D_- f(x)$, column 3: $f''(x) - D_+ D_- f(x)$, column 4: $(f''(x) - D_+ D_- f(x))/h$, column 5: $(f''(x) - D_+ D_- f(x))/h^2$. Present 15 digits past the decimal point (in Matlab, `format long` gives the full 15 digits). What is the limit in each column? Discuss the numerical results in relation to part (b).

2. In class we discussed a problem involving two reversible chemical reactions as an example of a system of nonlinear equations (see page 141 in the textbook or page 6 in the chapter 2 lecture notes). After simplifying, the equations can be written as

$$f(c_1, c_2) = c_1 + c_2 - k_1(a_0 - 2c_1 - c_2)(b_0 - c_1) = 0,$$
$$g(c_1, c_2) = c_1 + c_2 - k_2(a_0 - 2c_1 - c_2)(d_0 - c_2) = 0,$$

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. In order to run the code, you must fill in the two functions and the Jacobian matrix. (Hint: page 256 of the textbook says that $c_1 = 0.10987, c_2 = 0.49001$ after four steps.)

3. page 148 / 7a (warmup exercise on matrices) Find the $\det(D)$ of the matrix $D = \begin{pmatrix} 1 & -1 & 4 \\ 0 & 2 & -2 \\ 0 & 0 & 3 \end{pmatrix}$

4. page 149 / 14 (hint: it is sufficient to show that $AA^{-1} = I$) Let

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

(a) Show that $A$ is nonsingular provided $a_{11}a_{22} - a_{12}a_{21} \neq 0$

(b) If $a_{11}a_{22} - a_{12}a_{21} \neq 0$, show that

$$A^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$$

5. page 157 / 1 (reduce to upper triangular form and solve by back substitution)
\[ 2x_1 - x_2 + x_3 = -1 \]
\[ 4x_1 + 2x_2 + x_3 = 4 \]
\[ 6x_1 - 4x_2 + 2x_3 = -2 \]

6. Which of the following matrices are invertible? Justify your answer. For those that are not invertible, find a nonzero vector \( x \) 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) \( \begin{pmatrix} 1 & 0 & 2 \\ -1 & 3 & 1 \\ 0 & 3 & 3 \end{pmatrix} \)

7. page 159, problem 13 (electric circuit, solve by Gaussian elimination with partial pivoting)
function Newton
    clear; format long;
    c1 = 0.5; c2 = 0.5;
    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)
        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];