Exam III
Administered: Thursday, November 14, 2013
28 points

For each problem part: 0 points if not attempted or no work shown,
1 point for partial credit, if work is shown,
2 points for correct numerical value of solution

Problem 1. (14 points)

Consider the matrix and vector:

$$\underline{\underline{A}} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & 0 \\ 1 & 0 & -2 & 1 \\ 0 & 1 & 1 & -2 \end{bmatrix} \qquad \underline{b} = \begin{bmatrix} 10 \\ 8 \\ -1 \\ -3 \end{bmatrix}$$

Report the following information.
(a) the determinant of $\underline{\underline{A}}$
(b) the rank of $\underline{\underline{A}}$
(c) the rank of the augmented $\underline{\underline{Ab}}$ matrix
(d) the number of solutions to $\underline{\underline{A}}\underline{x} = \underline{b}$
(e) the inverse of $\underline{\underline{A}}$ if it exists
(f) a solution to $\underline{\underline{A}}\underline{x} = \underline{b}$, if it exists
(g) the eigenvalues of $\underline{\underline{A}}$

Solution

I put together this little MatLab script in xm3p01.m

```
clear all;
A = [1 1 1 1; 1 2 1 0; 1 0 -2 1; 0 1 1 -2]
b = [10; 8; -1; -3]
detA = det(A)
rankA = rank(A)
rrefa = rref(A)
Ab = [A,b]
rrefAb = rref(Ab)
rankAb = rank(Ab)
[w,lambda] = eig(A)
invA = inv(A)
x = invA*b
bcheck = A*x
```

This is the output from the script:

```
A =
```

```
     1     1     1     1
     1     2     1     0
     1     0    -2     1
     0     1     1    -2

b =
    10
     8
    -1
    -3
```

(a) the determinant of $\underline{\underline{A}}$

```
detA =     4
```

(b) the rank of $\underline{\underline{A}}$

```
rankA =     4

rrefa =
     1     0     0     0
     0     1     0     0
     0     0     1     0
     0     0     0     1

Ab =
     1     1     1     1    10
     1     2     1     0     8
     1     0    -2     1    -1
     0     1     1    -2    -3

rrefAb =
     1     0     0     0     1
     0     1     0     0     2
     0     0     1     0     3
     0     0     0     1     4
```

(c) the rank of the augmented $\underline{\underline{Ab}}$ matrix

```
rankAb =     4
```

(d) the number of solutions to $\underline{\underline{A}}\underline{x} = \underline{b}$

Since the determinant is not zero, there is one unique solution.

(g) the eigenvalues of $\underline{\underline{A}}$

```
w =

   -0.5781   -0.7435    0.0216   -0.4996
   -0.7785    0.6003   -0.1549    0.0214
   -0.1552   -0.2549    0.7331    0.4268
   -0.1889    0.1478   -0.6619    0.7535

lambda =
```

```
    2.9420         0         0         0
         0    0.3367         0         0
         0         0   -2.8735         0
         0         0         0   -1.4052
```

(e) the inverse of $\underline{\underline{A}}$ if it exists

```
invA =
    1.7500   -1.5000    0.7500    1.2500
   -1.2500    1.5000   -0.2500   -0.7500
    0.7500   -0.5000   -0.2500    0.2500
   -0.2500    0.5000   -0.2500   -0.7500
```

(f) a solution to $\underline{\underline{A}}\underline{x} = \underline{b}$, if it exists

```
x =
     1
     2
     3
     4

bcheck =

    10
     8
    -1
    -3
```

Problem 2. (6 points)

Use the Newton-Raphson method with numerical approximations to the derivative to find the molar volume(s) of ammonia from the the van der Waals equation of state at $T = 500$ K and p = 1013250 bar.
The van der Waals equation of state is given by

$$P = \frac{RT}{V-b} - \frac{a}{V^2}$$

where, $R = 8.314$ J/mol/K. The van der Waals constants for ammonia are $a = 0.4253$ m^6/mol^2, $b = 3.737x10^{-5}$ m^3/mol. The critical temperature of ammonia is $T_c = 430.6$ K.

Solution:

I used the nrnd1.m code.

The input function was

```
function f = funkeval(x)
V = x;
T = 500; % K
p = 1013250; % Pa
R = 8.314; % J/mol/K
b = 3.737e-5; % m^3/mol
a = 0.4253; % m^6/mol^2
f = R*T/(V-b) - a/(V^2) - p;
```

Since the temperature is above the critical temperature, there is only one root.
I used the ideal gas to give me an initial guess for the volume.

```
>> T = 500; % K
p = 1013250; % Pa
R = 8.314; % J/mol/K
>> V = R*T/p
V =    0.0041
```

From the command line I executed the code

```
>> [x0,err] = nrnd1(0.0041)
```

This provided the following output

```
icount = 1 xold = 4.100000e-03 f = -1.532162e+04 df = -2.395452e+08 xnew = 4.036039e-03  err = 1.000000e+02
icount = 2 xold = 4.036039e-03 f = 2.373354e+02 df = -2.470717e+08 xnew = 4.036999e-03  err = 2.379474e-04
icount = 3 xold = 4.036999e-03 f = 7.850452e-02 df = -2.469560e+08 xnew = 4.037000e-03  err = 7.874379e-08

x0 =   0.004036999606166

err =     7.874379241627386e-08
```

This program converged to a solution. The root is 0.00403 m^3/mol.

Problem 3. (8 points)

Use the multivariate Newton-Raphson method with numerical approximations to the derivative to find the solution near [1,1,1] to this set of non-linear algebraic equations

$$f_1 = x_1 + 2x_2 + 3x_3 - 7$$
$$f_2 = x_1^3 - 4x_2^3 + 10x_3^3 - 10$$
$$f_3 = x_2 - \exp(x_3)$$

Solution:

I used the nrndn.m code.

My input function was

```
function f = funkeval(x)
%
%  these two lines force a column vector of length n
%
n = max(size(x));
f = zeros(n,1);
%
%  enter the functions here
%
f(1) = x(1) + 2*x(2) + 3*x(3) - 7;
f(2) = x(1)^3 - 4*x(2)^3 + 10*x(3)^3 - 10;
f(3) = x(2) - exp(x(3));
```

From the command line I executed the code

```
>> [x,err,f] = nrndn([1,1,1],1.0e-6,1)
```

This provided the following output

```
iter =    1, err =  4.11e+00 f =  2.08e+00
 iter =    2, err =  1.65e+00 f =  2.80e+02
 iter =    3, err =  9.50e-01 f =  7.98e+01
 iter =    4, err =  4.54e-01 f =  2.03e+01
 iter =    5, err =  9.82e-02 f =  3.10e+00
 iter =    6, err =  4.02e-03 f =  1.18e-01
 iter =    7, err =  6.37e-06 f =  1.87e-04
 iter =    8, err =  5.78e-11 f =  1.62e-09

x =   2.826498171685380   1.489295813936914   0.398303400146931

err =     5.781682122659449e-11

f =     1.617535538214254e-09
```

This program converged to a solution. The root is $\underline{x} = \begin{bmatrix} 2.826 \\ 1.489 \\ 0.398 \end{bmatrix}$.