Homework Assignment Number Eight Solutions

Problem 1.
Perform a single-variable linear regression using the model

$$y = b_0 + b_1 x$$

(a) Report the mean value and standard deviation of the regression coefficients.
(b) Report the measure of fit.
Use the data in the file "file.hw08p01.txt" available on the website.
Note the first column in the data file is *y*. The second column is *x*.

Solution:

I used the code linreg1.m for linear regression with one independent variable.

I wrote the small script hw08p01.m

```
clear all;

M = [15.10065279    1
20.4980324  2
25.56136963 3
...
242.1551242 49
247.5311911 50];

n = 50;
y = M(1:n,1);
x = M(1:n,2);

[b,bsd,MOF] = linreg1(x, y)
```

At the command line prompt, I executed the script

```
>> hw08p01
```

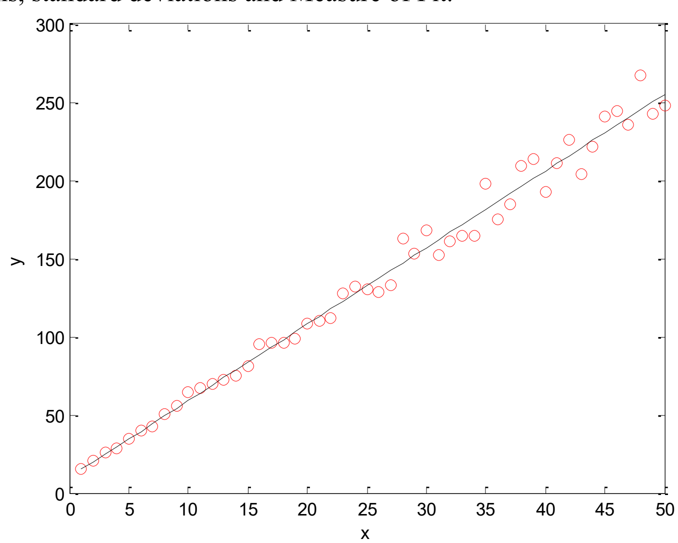
This generated the following output for the means, standard deviations and Measure of Fit.

b =
10.074083107297966
4.896473196043218

bsd =
2.347470564943806
0.080117982695322

MOF =
0.987312123130968

The code also generated a plot.



Problem 2.
Perform a single-variable polynomial regression using the model

$$y = b_0 + b_1 x + b_2 x^2$$

(a) Report the mean value and standard deviation of the regression coefficients.
(b) Report the measure of fit.
Use the data in the file "file.hw08p02.txt" available on the website.
Note the first column in the data file is *y*. The second column is *x*.

Solution:

I used the code linregn.m for linear regression with one independent variable.

I wrote the small script hw08p02.m

```
clear all;

M = [28.60333775    2
61.67477585 4
113.330215  6
...
83236.71749 198
81985.43984 200];

n = 100;
y = M(1:n,1);
x(1:n,1) = M(1:n,2);
x(1:n,2) = x(1:n,1).*x(1:n,1);
[b,bsd,MOF] = linregn(2,x, y)
```

At the command line prompt, I executed the script

```
>> hw08p02
```

This generated the following output for the means, standard deviations and Measure of Fit.

```
b =
  86.579044451471418
   2.860222062350658
   2.015990010806434

bsd =   1.0e+02 *
   3.204973070484634
   0.073237990705217
   0.000351272052967

MOF =   0.998202555108216
```

The code does not generate a plot.

Problem 3.
Perform a multivariate linear regression using the model

$$y = b_0 + b_1 x_1 + b_2 x_2$$

(a) Report the mean value and standard deviation of the regression coefficients.
(b) Report the measure of fit.
Use the data in the file "file.hw08p03.txt" available on the website.
Note the first column in the data file is y. The second column is x_1. The third column is x_2.

Solution:

I used the code linregn.m for linear regression with one independent variable.

I wrote the small script hw08p03.m

```
clear all;

M = [-0.981903982   2   10
-11.36111514    4   10
-17.92444528    6   10
...
188.825984  18  100
181.0279417 20  100];

n = 100;
y = M(1:n,1);
x(1:n,1) = M(1:n,2);
x(1:n,2) = M(1:n,3);
[b,bsd,MOF] = linregn(2,x, y)
```

At the command line prompt, I executed the script

```
>> hw08p03
```

This generated the following output for the means, standard deviations and Measure of Fit.

```
b =
 -19.426169012360049
  -4.968806248543629
   2.990195728881456

bsd =
   1.109461283774494
   0.066903032685564
   0.013380606537113

MOF =    0.998235942566897
```

The code does not generate a plot.

Problem 4.

Consider the isomerization reaction:

$$A \rightarrow B$$

The reaction rate is given by

$$rate = C_A k_o e^{-\frac{E_a}{RT}} \quad \text{[moles/liter/minute]}$$

where

concentration of A: C_A [moles/liter]
prefactor: k_o [1/minute]
activation energy for reaction: E_a [Joules/mole]
constant: $R = 8.314$ [Joules/mole/K]
temperature: T [K]

Determine the rate constants, k_o and E_a, from experimental data. The reaction is measured at a constant concentration of A, C_A=0.1 mol/liter, over a variety of temperatures. The rate is recorded. The rate as a function of temperature is given in tabular form in the file "file.hw08p04.txt" (containing 108 data points).

Convert the data into the form necessary for a linear regression.

$$ln(rate) - ln(C_A) = -\frac{E_a}{RT} + ln(k_o)$$

This equation is of the form: $y = b_1 x + b_0$ where

$y = ln(rate) - ln(C_A)$, $b_1 = E_a$, $x = -\frac{1}{RT}$, and $b_0 = ln(k_o)$.

Solution:

I used the code linreg1.m for linear regression with one independent variable.

I wrote the small script hw08p04.m

```
clear all;

%Temperature     rate of A loss
%K               mole/liter/min

M = [275    24.19186881
280 23.66394411
285 26.15820944
...
805 90.60688637
810 94.70386442];

R = 8.314; % J/mol/K
CA = 0.1; % mol/liter
n = 108;
for i = 1:1:n
    x(i) = -1.0/(R*M(i,1));
    y(i) = log(M(i,2)) - log(CA);
end
[b,bsd,MOF] = linreg1(x, y)
Ea = b(2)
ko = exp(b(1))
```

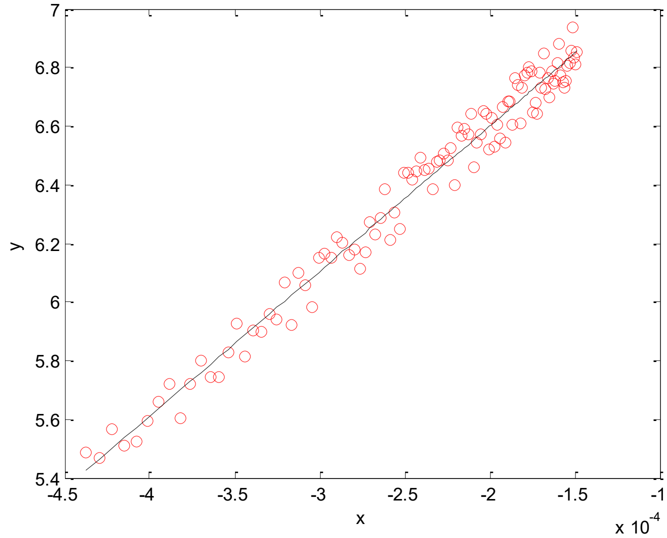
At the command line prompt, I executed the script

```
>> hw08p04
```

This generated the following output for the means, standard deviations and Measure of Fit.

```
b =   1.0e+03 *
   0.007590882856898
   4.952404881054963

bsd =
   0.018538702614459
  72.525898202990689

MOF =    0.977772149142637

Ea =      4.952404881054963e+03

ko =      1.980060852689931e+03
```

The activation energy was 4950 J/mol.
The rate constant was 1980 1/min.



The code also generated a plot.

Problem 5.
On the project page of the course website, there is a zip file containing data for the "Data Wrangling with Carbon Fiber Mechanical Properties". This file contains the results from many tensile test experiments on carbon fibers. For the first experiment in the first data set **only**, determine
(a) strain at fracture
(b) ultimate tensile strength
(c) modulus average and standard deviation
(d) report the limits in terms of strain that you chose for your regression and justify.
(e) provide a plot of the entire raw data
(f) provide a plot of the relevant data to (a), (b) and (c) and indicate strain at fracture, ultimate tensile strength and modulus regression on the plot.

Solution
To perform this task, I wrote a script, hw10_p5_driver.m, provided below.

*** start hw10_p5_driver.m ***

```
clear all;
close all;

%
%  open file
%
cfiber_script_1fileonly;
% number of data points in stress and strain vectors
ndata = length(strain);

%
%  task 1. determine strain at failure
%
```

```
%  scan through data and look for first abrupt decrease in stress
%
% threshold = fractional relative change drop in stress that constitutes
% failure, a value of 0.9 means stress must drop 90%
% threshold is an adjustable parameter
threshold = 0.2;
% ifoundit is 1 if you have found the strain at failure, 0 if otherwise
ifoundit = 0;
% icount = data point counter
icount = 1;
while (ifoundit == 0 && icount < ndata)
    icount = icount + 1;
    deltastress = (stress(icount) - stress(icount-1))/stress(icount-1);
    if (deltastress < -threshold)
        ifoundit = 1;
    end
end
% save information about strain at fracture point
indexfrac = icount;
strainfrac = strain(icount);
stressfrac0 = stress(icount-1);
stressfrac1 = stress(icount);
fprintf(1, 'Strain at failure occurs at point %i with strain %e where the stress changes from %e
to %e MPa \n',indexfrac,strainfrac,stressfrac0, stressfrac1);

%
%  task 2. determine ultimate tensile stress
%
% set range over which to search for UTS
indexlo = 1;
indexhi = indexfrac;
% use max function to find UTS and save information
[stressuts,indexuts] = max(stress(indexlo:indexhi));
strainuts = strain(indexuts);
fprintf(1, 'Ultimate Tensile Stress occurs at point %i with strain %e where the stress is %e MPa
\n',indexuts,strainuts,stressuts);

%
%  task 3.  determine modulus
%
% set range over which to perform regression
indexreglo = 1;
indexreghi = indexuts;
% perform linear regression
[b,bsd,MOF] = linreg1(strain(indexreglo:indexreghi),stress(indexreglo:indexreghi));
% save information regarding regression
modulusav = b(2);
modulussd = bsd(2);
intercept = b(1);
fprintf(1, 'Elastic modulus is %e +/- %e with MOF = %f.\n',modulusav,modulussd,MOF);

%
%  plot results
%
figure(2)
LineWidthValue = 2;
plot(strain,stress,'k-','LineWidth',LineWidthValue);
hold on;
ylabel('stress (MPa)');
xlabel('strain');
%
%  set reasonable axis limits
%
temp = axis;
[stressmin,indexmin] = min(stress(indexlo:indexhi+10));
ylo = min(0,stressmin);
yhi = stressuts*1.1;
axis([0 strainfrac*1.1 ylo yhi]);
%
% add line corresponding to strain at fracture
%
```

```
strainfracx(1) = strainfrac;
strainfracx(2) = strainfrac;
strainfracy(1) = ylo;
strainfracy(2) = yhi;
plot(strainfracx,strainfracy,'r:','LineWidth',LineWidthValue);
%
% add point corresponding to ultimate tensile stress
%
plot(strainuts,stressuts,'ro','LineWidth',LineWidthValue);
%
% add regression line
%
yhatx(1) = strain(indexreglo);
yhatx(2) = strain(indexreghi);
yhaty(1) = modulusav*yhatx(1)+intercept;
yhaty(2) = modulusav*yhatx(2)+intercept;
plot(yhatx,yhaty,'b-','LineWidth',LineWidthValue);
lgd = legend('data','strain at fracture','ultimate tensile stress','modulus regression');
lgd.Location = 'northwest';
```

*** end hw10_p5_driver.m ***

This main script calls another script and a function. The script is cfiber_script_v01.m, which is included in the zip file where the data is located. The script is modified to read only the first file from the first data set.

The script also calls the function, linreg1.m, which performs linear regression of the experimental data to a first order polynomial model. This function is used without modification from its form on the course website.

The results of the script are provided below.

(a) strain at fracture

Strain at failure occurs at point 717 with strain 2.350000e-03 where the stress changes from 4.773658e+01 to 3.153238e+01 MPa

(b) ultimate tensile strength

Ultimate Tensile Stress occurs at point 714 with strain 2.340000e-03 where the stress is 5.685883e+01 MPa

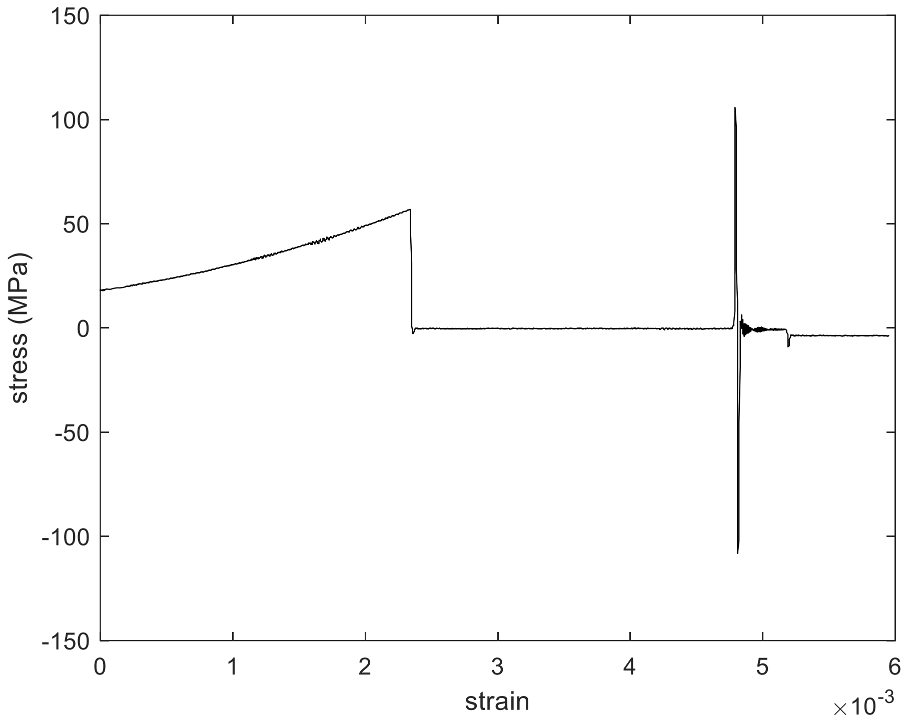
(c) modulus average and standard deviation

Elastic modulus is 1.641727e+04 +/- 7.551521e+01 with MOF = 0.985159.

(d) report the limits in terms of strain that you chose for your regression and justify.

I used the first point to the point corresponding to UTS. This seemed reasonable given that there was some curvature through-out the data and no clear perfectly linear region.

(e) provide a plot of the entire raw data



(f) provide a plot of the relevant data to (a), (b) and (c) and indicate strain at fracture, ultimate tensile strength and