Homework Assignment Number Six

Problem (1) Single Variable Linear Regression
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.hw06p01.txt" available on the website.
Note the first column in the data file is *y*. The second column is *x*.

Problem 2. Single Variable Polynomial Regression.
Perform a single-variable linear 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.hw06p02.txt" available on the website.
Note the first column in the data file is *y*. The second column is *x*.

Problem 3. Multivariate Linear Regression
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.hw06p03.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.

Problem 4. Reaction Rate Constants
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.hw06p04.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 $b_0 = \ln(k_o)$.

Problem (5) Multivariate Nonlinear Optimization

Consider the rate equation

$$rate = k_o e^{-\frac{E_a}{RT+C}} \qquad \text{[mol/s]}$$

where

prefactor: k_o [mol/sec]
activation energy for reaction: E_a [Joules/mole]
non-Arrhenius parameter: C [Joules/mole]
constant: $R = 8.314$ [Joules/mole/K]
temperature: T [K]

Determine the rate constants, E_a, k_o and C, from experimental data. The rate as a function of temperature is given in tabular form in the file "file.hw06p05.txt".

For initial guesses, use the knowledge that E_a should be on the order of 10,000 J/mol, k_o should be on the order of 100,000 mol/s and C should be on the order of 1000 J/mol.
Use whatever method you prefer. If you use the amoeba method, set the initial volume space to 50% of the initial guess and set your tolerance for both x and f to 10^{-8} or less. Use the RMS (root-mean-square error) as the objective function.

$$f_{obj} = \sqrt{\frac{1}{n_{data}} \sum_{i=1}^{n_{data}} \left(rate_i^{\exp} - rate_i^{\text{mod}} \right)^2}$$

Problem (6) Fast Fourier Transforms

Using the Fast Fourier Transform, identify the frequencies present in the data file hw06p06.txt.