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The objectives for this assignment are:

1. to gain regression analysis experience for simple linear dynamic, as well as linear and nonlinear algebraic equations,
2. to build some experience using MATLAB and its Optimization Toolbox for performing regression analysis.

You may work together in groups to complete the assignment, but you must hand in your own assignment solution. If you work with a group, please identify the people that you worked with on your solution. Computer printout may be included with your solution as an appendix, but please do not provide these as your entire solution report.

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1. In the file named "che572_assn4q1_2011.mat" on the course web page, you will find data from some step tests for a reactor / cooler system. The data file contains the input flowrate $f$ and the outlet temperature $T$ at each time $t$ during the test. Since there are two vessels in series (*i.e.*, a reactor and an exchanger), you suspect second order dynamics. Using the data, please do / answer each of the following:

   a) Fit a second-order+dead-time transfer function model using linear least squares regression. Do not use any of the built in functions for model fitting or system identification. Show your work where appropriate.

   b) Is the fit satisfactory? If not, what model would you like to attempt to fit? **Explain**.

   c) Try fitting your suggested model form and determine whether it provides a better fit. **Explain**.

2. You have been asked to estimate the heat transfer coefficients in a metal slab re-heating furnace using the data in a file named "che572_assn4q2_2011.mat" on the course web. The metal slabs are reheated by a combination of convective and radiative heat transfer. The data collected from some plant experiments included the heat flux / unit area ($q$), the slab surface temperature ($T$), the radiative source temperature ($T_s$), and the bulk gas temperature ($T_g$). The furnace designers give the radiative and convective heat transfer coefficients as $\sigma = 10^{-10}$ and $U = 2$, respectively. Do / answer each of the following:

   a) Write the equation that represents the heat transfer.

   b) Estimate the radiative and convective heat transfer coefficients.

   c) Calculate the covariance matrix for your parameter estimates.

   d) Do you think that the furnace designers heat transfer coefficients are correct? **Explain**.

3. Your company's laboratory has provided you with some data for the relationship between reaction rate ($r$) in $hr^{-1}$ and concentrations of reactants ($x_1$ and $x_2$) in $g/l$ in one of your reactors. The lab data is contained in a file named "che572_assn4q3_2011.mat" on the course web page. The reaction rate is expected to follow the model:

$$r = \frac{kx_1x_2}{1 + \alpha x_1^2}$$

where $k$ and $\alpha$ are reaction constants. Using the given data, please do / answer each of the following:

a) Estimate $k$ and $\alpha$ using linear least squares regression and an appropriate transformation of the data. (Refer to the text Module 3, Questions 5 and 6 on page 462 for ideas on how you might approach this).

b) Estimate $k$ and $\alpha$ using nonlinear least squares regression. To do this you will have to use the *lsqcurvefit* command in Matlab's Optimization Toolbox. To use the *lsqcurvefit* command, you will also need a function file. This is provided on the course web page and is named "kinetics.m".

c) Compare the results of the two parameter estimation approaches using appropriate plots, the parameter estimates and their covariance matrices. (The actual parameter values are $k = 4$ and $\alpha = 1$). Discuss why transformation / linear least squares approach performed so poorly in comparison to the nonlinear regression.

d) Why do you think the lab chose the grid of compositions used in the experiments? Are there better ways to choose the composition grid? **Briefly explain**.