
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 files named "che572_assn4q1a_2012.mat" and "che572_assn4q1b_2012.mat", which are located on the course web page, you will find some of my cycling training data. This data was taken from two different work-outs. The first was collected very early in the training season and the second was collected several weeks later. The data is organized in an array, as follows:

   - column #1 is the time (seconds),
   - column #2 is the power (watts) that is being exerted during the training effort,
   - column #3 is my heart-rate (beats per minute),
   - column #4 is my cadence (rpm).

   You will be modelling the response of my heart-rate to changes in power. Using the data, please do / answer each of the following:

   a) Fit a first-order model to each data set.

   b) Estimate the gain and time constant for each training session. Do they change from from the first to the second training session? **Justify your answer**.

   c) Can you conclude whether training has had an effect on the physiological response to effort? **Justify your answer**.

   d) Is the sampling time used for collecting the data appropriate? If not, what sampling time would you propose? **Explain**.

   e) Using only the data for the first training session (*i.e.*, from "che572_assn4q1a_2012.mat") develop the linear discrete time model that you think best fits the data. **Explain why you believe that your model is superior to the the other alternative linear, discrete-time models**.

2. In your new role as head engineer for the ACME Chemical Company, you have been asked to develop a fixed temperature *Soave-Redlich-Kwong Equation of State* for one of your company's new products, Factor X. For a fixed temperature, one form of the SRK EOS is:

$$P = \frac{a}{V-b} - \frac{c}{V(V+b)}$$

where: P is pressure (kPA), V is molar volume (m^3), and a, b and c can be considered thermodynamic constants. The apparatus that you will use for determining the values of a, b and c has a very precise temperature controller and uses a set of precision, fixed volume cells. Each experiment is performed by charging a cell with a specified mass of Factor X in liquid form. The cell is sealed and then heated to a specified temperature, which is 500 K in this case. The pressure within the cell is monitored and once it has equilibrated, the pressure is recorded. The pressure sensor is accurate, but P has considerably more error associated with it than does temperature or volume. The data from the experiments is provided in "che572_assn4q2_2012.mat", which is located on the course web page.

   a) Estimate a, b and c using nonlinear least squares regression. To do this you will have to use the *lsqcurvefit* command in Matlab's Optimization Toolbox. Note that choosing the initial guess for the parameters is essential to successfully estimating the actual parameter values.

   b) One of the senior engineers claims that you can use linear least squares regression far more easily and it will give just as good results. He says that you should re-write the SRK EOS as:

   $$PV^3 = \beta PV + \delta V^2 + \epsilon V + \gamma$$

   where $\beta = b^2$, $\delta = a$, $\epsilon = ab - c$ and $\gamma = cb$. Is your colleague correct?

   c) Estimate the values of β , δ , ϵ and γ from the given data. Then calculate the values of a, b, and c.

   c) Compare the results of the two parameter estimation approaches using appropriate plots, the parameter estimates and their covariance matrices. Which approach gave you the best results? Note that the actual values of the parameters are $a = 10$, $b = 1$ and $c = 5$. **Explain**.

   d) If you could run additional experiments, what molar volumes would you like to try? **Explain**.

   e) Is the transformation / linear least squares approach appropriate in this case? **Explain**.