CBE 31358 Junior Lab

Statistics Quiz # 6

Due in class on 4/29/11

Note: This is open book and open notes, however **don't** discuss this quiz with your classmates!

Answer the following question with a **MATLAB PROGRAM** . Turn in both your source code and your output.

You are tasked with analyzing the results from a second order irreversible dimerization reaction, given by 2A -> B. The concentration C_A is governed by the rate expression:

$dC_A/dt = - k\, C_A^2$

We are interested in using a set of measured concentrations as a function of time to get the rate constant k. Using the data given below, solve the following problems:

1). Solve the differential equation for $C_A(t)$. This will be a function of two unknowns: C_{A0} and the rate constant k.

2). Linearize the model so that the expression is linear in two new unknown parameters x_1 and x_2, and show how these are related to the unknowns from part 1.

3). Using the data below, and unweighted linear regression, determine the rate constant k.

4). It is asserted that this linearization improperly weights the data, and that the errors in the measured concentrations are really what are both independent and of the same magnitude. Using this, develop a linearized weighted regression scheme that calculates the rate constant k and determines its 95% confidence interval, comparing it to the value obtained using unweighted regression. Hint: you can easily get the relative weighting of each data point by error propagation!

5). Do the problem again, only this time use unweighted non-linear regression, similar to the approach used in the example problem. This is easy to do if you take in the unknown fitting parameters as a vector, calculate the residual in the function for the observed data, and then use fminsearch to determine the optimal values. Error calculation is likewise simple: take the script you wrote above (which determines fitting parameters for a set of measured concentrations) and then turn it into a vector *function* of the concentration data array. You can then easily calculate the dependence of the fitting parameters on the data numerically (e.g., change the data points one by one to get the gradient) and do error propagation the usual way. Compare these results to that of part 4.

6). Plot up the observed concentrations as a function of time, and the unweighted linearized, weighted linearized, and non-linear regression model predictions.

Data:

t	C_A
1.0000	0.6895
2.0000	0.5310
3.0000	0.4277
4.0000	0.3182
5.0000	0.2946
6.0000	0.2682
7.0000	0.2007
8.0000	0.2040
9.0000	0.1971
10.0000	0.1409