**ChE 310 Problem Set 8 Due Wed 3/27/19**

Collect all m-files in a single .zip file and upload the .zip file to the course webpage by midnight on Wednesday, March 27, 2019. Please note any collaborations in comments. Each student must upload their own unique copy of the work.

**8\_1 Regression (use a method of your choice)**

1. Problem 15.18 from the textbook. Be sure to report the correct units on your calculated coefficients A1 and A2. (The units of “R” should probably be presented as 82.05 mL\*atm/K, to be dimensionally consistent with the other terms.)
2. Problem 15.23 from the textbook. Report cs, kmax, and the requested growth rate, with correct units.

**8\_2 Linear vs. nonlinear regression**

Solve Chapra problem 14.31. Determine B and D using both a linear regression technique (after linearizing the model) and using a nonlinear regression technique on the original model equation. Plot the corresponding best-fit functions along with the original data. Ensure your plot is labeled (axes, legend); the plot is the only necessary output. Keep in mind that Andrade’s equation takes temperatures in K, while the table provides temperatures in .

**8\_3**

The kinetic rate of a chemical equation is dependent on temperature (). The Arrhenius equation is used to show this dependence and when properly fitted also shows the activation energy () of the reaction:

where is the rate constant, is the pre-exponential factor, and is the universal gas constant.

Eleven experiments were conducted to determine the activation energy of the following reaction:

The data from these experiments are contained in the ‘kinetics’ zipped folder. Each experiment is its own \*.csv file with the first column = temperature (K) and the second column = reaction rate or k(T) in cm3/(molecule\*s) (Note: units matter!). Plot the raw data with the model fits (one subplot for each of the 11 experiments). Determine the activation energy (kJ/mole) for each experiment and report the average over all 11 experiments along with the associated 95% confidence interval; assume a normal distribution applies to the activation energy data.

For this problem you can linearize the equation or solve in the non-linear form. Which is better? Note: you can automate reading in the file name with the help of the num2str and strcat commands for the file name.

**8\_4 Multivariable regression**

***Background***. As part of Dr. Roling’s postdoctoral research, he used linear regression to parameterize the energies of metal atoms in nanoparticles.[[1]](#footnote-1) These models fit 20 parameters corresponding to 20 independent variables in a 140-point alloy data set; this was done for each of 21 bimetallic combinations. Here, we’ll focus on a smaller subset of data.

In this model, each bond formed by a metal atom is considered to have its own unique energy. The total energy of nanoparticle is then determined by the sum of all its bond energies . For example, a metal dimer (two isolated bonded atoms) is composed of two atoms, each with a single bond; the energy of a metal dimer is therefore calculated as . A triangular arrangement of three atoms (each bound to two other atoms) has an energy calculated as .

***Problem Statement****.* We seek a model to calculate the energy of a small cluster of metal atoms as:

where are parameters and are independent variables denoting the number of each type of bond in a configuration. The following data were collected using density functional theory calculations for Pt clusters:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Geometry Type |  |  |  | (kJ/mol) |
| dimer | 2 | 0 | 0 | -255.3 |
| 3-atom triangle | 3 | 3 | 0 | -603.2 |
| 3-atom line | 3 | 1 | 0 | -475.0 |
| 5-atom line | 5 | 3 | 0 | -865.6 |
| 4-atom tetrahedron | 4 | 4 | 4 | -969.7 |
| 4-atm trigonal planar | 4 | 1 | 1 | -655.2 |
| 4-atom square | 4 | 4 | 0 | -858.7 |
| 4-atom diamond | 4 | 4 | 2 | -911.5 |
| 6-atom rectangle | 6 | 6 | 2 | -1481.9 |
| 6-atom pair of triangles | 6 | 6 | 2 | -1333.4 |

Use linear regression to find the best-fit values of , , and ; also report the corresponding R2 value.

1. L. T. Roling, T. Choksi, F. Abild-Pedersen, “A coordination-based model for transition metal alloy nanoparticles”, *Nanoscale* 11, 4438-4452 (2019), <https://dx.doi.org/10.1039/C9NR00959K> [↑](#footnote-ref-1)