Homework 17

Ch En 263 – Numerical Tools

Due date: 4 Jun 2020

Instructions

- For the handwritten problems, submitted a single pdf file on Learning Suite with the name "LastName_FirstName_HW17.pdf".
- For the problems in Excel, submit a workbook named "LastName_FirstName_HW17.xlsx" where each worksheet tab is named "Problem_1", "Problem_2", etc.
- For the problems in Python, submit a separate file for each problem named "LastName_FirstName_HW17_ProblemXX.py" where XX is the problem number.
- **Please report how long it took you to complete the assignment (in hours) in the "Notes" section on Learning Suite.**

Problems

1. Find the values of A, B, C, D and E in the equation

$$\frac{C_p}{R} = A + BT + CT^2 + DT^3 + ET^4$$

that best fit the C_p/R and T data given in "HW17_Prob1_Data.csv".

   (a) Use a trendline in a scatter plot in Excel to find the coefficients and the value of R^2.

   (b) Use `numpy.polyfit` to find the best-fit coefficients in Python and print the values to the console.

2. The kinetic rates r in the table on the right were collected as a function of temperature, T. We want to fit the model

$$r = kT^m \exp(\frac{-E_a}{RT})$$

to this data where k, m and (E_a/R) are adjustable parameters.

T	r
500.0	105.598
571.43	89.700
642.86	70.768
714.29	66.996
785.71	60.711
857.14	58.992
928.57	55.8328
1000.0	53.420

   (a) Use Solver in Excel to find the best-fit coefficients k, m and E_a/R by minimizing the sum-of-squared error (SSE).

   (b) Use `scipy.optimize.curve_fit` in Python to find the best-fit coefficients and print them to the console. In addition, calculate the value of R^2 in Python and print it to the console.

   (c) Plot the data and the model with the best-fit parameters from part (b) together on the same graph in Python.

3. The data in "HW17_Prob3_Data.csv" contains data for the response of a "first-order system with time delay". Such data is used to create control devices to keep operations running correctly. (You will learn about this in ChEn 436, Process Control and Dynamics.)

   The model for a first-order system with time delay is given by

$$y(t) = 5\left[1 - \exp\left(\frac{-(t-\theta)}{\tau}\right)\right] S(t-\theta)$$

   where

$$S(t-\theta) = \begin{cases} 0, & \text{when } t < \theta \\ 1, & \text{when } t \geq \theta \end{cases}$$

   where τ is a characteristic time of the process and θ is the time delay.

   (a) Use *either Python or Excel* to find the constants, τ and θ, that best fit the model to the process data.

   (b) Determine the R^2-value of the fit and report it.

   (c) Make a plot showing the data (as points) and the fit (as a line).

   Hint: You will need to use an `if` *statement for this problem.*