Week 4 exercises, optimization

At each task, visualize the optimized fit by plotting the data and the fit. For uniformity in the plots, use lines for model solutions and circles for data.

1. Fit the model

$$T(t) = \left(T_0 - \frac{k_1 T_w + k_2 T_a}{k_1 + k_2}\right) e^{-(k_1+k_2)t} + \frac{k_1 T_w + k_2 T_a}{k_1 + k_2}$$

   to the data below (given in Matlab form). The unknown parameters are k_1 and k_2. $[T_0\ T_a\ T_w] = [31\ 23\ 5]$

   t_meas = [0 : 60 : 540   840   1020   1320]' ;
   T_meas = [31   28   24   20   17.5   15.5   13.5   12   11   10   8   7   6.5]';

   Use [0.001, 0.0001] as the initial guess for k_1 and k_2.

2. Fit a second-degree polynomial (use Matlab's polyfit and polyval) to the xdata; ydata in data_8.mat. The data values y are positive, and the fitted model values should remain positive, too. Improve the fit by using an exponential form, $y = e^{b0+b1x+b2x^2}$ by making a log-transform to the data y and then performing an LSQ using Matlab backslash. Improve even more by nonlinear fitting with fminsearch (as an initial guess, use the parameter values obtained from fitting with Matlab backslash).

3. Take the $A \to B \to C$ ODE system given in the lecture note. Now, the reaction rates depend on the temperature T, and the dependency is modeled using Arrhenius' equation

$$k_i(T) = k_{i,ref} \exp\left(\frac{E_i}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right), \quad i = (1, 2)$$

   where $k_{i,ref}$ is the reaction rate at the reference temperature T_{ref} , E_i are the activation energies, T is the temperature, and $R = 8.314$ is the gas constant. The goal is to estimate the parameters $\theta = (k_{1,ref}, E_1, k_{2,ref}, E_2)$ using the two batches of data given below, obtained at temperatures T = 282K and T = 313K. You could basically choose the reference temperature; but now use T_{ref} = 300K. Compute the LSQ estimate for the parameters. Hints: reasonable starting values for the LSQ optimization are in the magnitude $k_{i,ref} \approx 1$ and $E_i \approx 10^4$; (for now, use exactly the values provided). Note that now your LSQ function should simulate the model in two different temperatures, with reaction rates computed with the Arrhenius equation, and compare the simulation to the corresponding data.

T = 282K		
time	*A*	*B*
0	1.000	0.000
1	0.504	0.416
2	0.186	0.489
3	0.218	0.595
4	0.022	0.506
5	0.102	0.493
6	0.058	0.458
7	0.064	0.394
8	0.000	0.335
9	0.082	0.309

T = 313K		
time	*A*	*B*
0	1.000	0.000
1	0.415	0.518
2	0.156	0.613
3	0.196	0.644
4	0.055	0.444
5	0.011	0.435
6	0.000	0.323
7	0.032	0.390
8	0.000	0.149
9	0.079	0.222