4. Curve fitting and parameter estimation in Matlab

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Course 28864: Introduction to Matlab programming

The purpose of this exercise is to get familiar with the Matlab curve fitting functions. Fitting a curve to experimental data can be achieved using the 'fminsearch' function in Matlab, which can be used to minimize the difference between the curve and the measured data.

Parameter estimation in fed-batch fermentation model

The model from last week consisted of the following reactions taking place in a CSTR:

(1) $A \rightarrow I$ $r_1 = k_1 C_A$
(2) $A \rightarrow B$ $r_2 = k_2 C_A$
(3) $I + D \rightarrow P$ $r_3 = k_3 C_I C_D$
(4) $B + D \rightarrow S$ $r_4 = k_4 C_D C_B^2$

In which the mass balance equation for the component *j* can be written as:

$$V.\frac{dC_j}{dt} = q\left(C_{j,in} - C_j\right) + Vr_j$$

Where;
C_j the concentration of component j in the reactor
$C_{j,in}$ the concentration of component j in the inflow
q the flowrate of the inflow and outflow
r the net reaction rate of component j
V the volume of the reactor

The same parameter values as last week are used in the model:

Table 1. Parameters for the model

Parameter	Value	Unit
k_1	-	min^{-1}
k_2	-	min^{-1}
k_3	0.265	$m^3\ mol^{-1}\ min^{-1}$
k_4	0.15	$m^6\ mol^{-2}\ min^{-1}$
Volume	800	L
q	0.032	$L\ sec^{-1}$
$C_{A,in}$	0.012	$mol\ L^{-1}$
$C_{D,in}$	0.020	$mol\ L^{-1}$

Initial conditions were set to 1.252 mol m^{-3} for *A*, 3.131 mol m^{-3} for *B* and 6.52 mol m^{-3} for *I*. The initial concentrations of all other components are set to 0.

In the file "data_ex4.mat" you will find data of the concentrations of all the components with the corresponding sampling time.

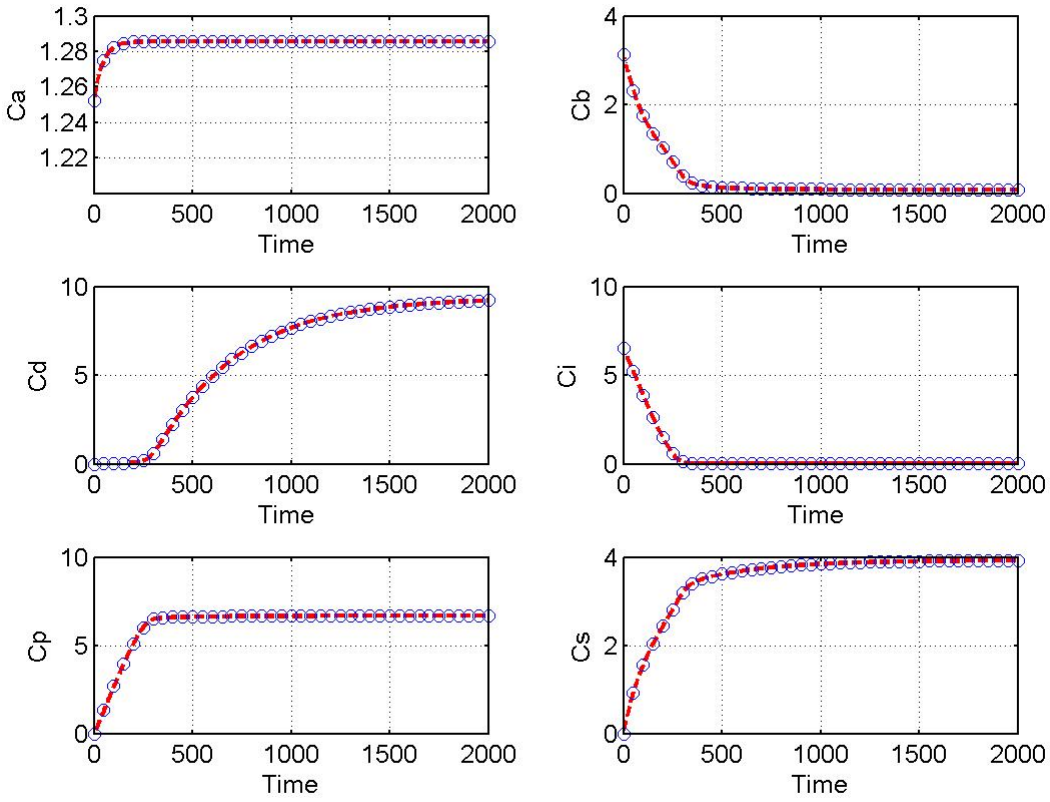
Write a script that allows you to obtain values for k_1 and k_2 for this system, based on the given component A concentration data (A_data).
You will do this by defining a cost function – or objective function – that is to be minimized. This cost function is defined in a separate m-file, in which you solve the ODE system from last week to get the C_A concentration. Then you subtract the data supplied to you from the simulated C_A concentration data, and you calculate the sum of squared errors. It is recommended that you use the solver "ode15s", since this solver is good at dealing with stiff problems like this one.

In your script you will minimize the cost function by using the build in 'fminsearch' function to estimate the parameter values.
Note that you can try to estimate other parameters and/or fit the model to another model output (any other component concentration).
Attention: Please define the following options for the function `fminsearch`.

```
options = optimset('display', 'iter','maxfunevals', 1000);
```

This line has to be inserted before the line where you call the 'fminseach' function. Also, in the function call you should replace `[]` with `options`. It allows you to display the number of iterations that 'fminsearch' has reached in the Command Window, and also defines the maximum number of times the function is evaluated and therefore influences the curve-fitting quality. Note that 'fminsearch' is sensitive to the initial values of the parameters to be estimated. Do therefore select initial guesses carefully. If you do not reach a satisfactory model fit, it is often a good idea to try again with a new set of initial parameter guesses.

Besides performing the model fit on the given data and displaying the estimated parameter values, the script should also plot the data and the resulting model fit in one graph. Data points should appear in the graph as blue open circles. If you plot every 50th point of your data points, both lines will be visible. The model fitted to the data should appear in the graph as red dashed lines with a line-width of 2.0. The X and Y axis of the graph should be labelled. If you did everything correctly your results should look like this:



Handing in:

The solution consists of 3 m-files. The script and the two functions (the ODEs and the cost function) should be sent as e-mail attachments to kvg@kt.dtu.dk before March 4th at 4 pm.

In the e-mail, you clearly list the names and student numbers of the members of your group (maximum 2 persons per group). To allow automatic sorting of the emails containing your solutions, the subject line of the email should be: 28864-F2015-E4. For help or questions: dsem@kt.dtu.dk or kvg@kt.dtu.dk .