Optimization(CH4020) Course project

Due Date – 6.00 PM, 01.03.2022. Maximum marks - 100

There is a certain dynamic process happening in a bacterial culture whose mathematical model is provided to you. The model when simulated will result in time profiles of M outputs. The experimental data pertaining to this reaction is also provided. The objective of this project is to estimate the optimal values of parameters (rate constants) in the model which will allow it to emulate the experimental data with high accuracy. Formulate the optimization problem to perform the parameter estimation. Note that, the parameters (rate constants) are always positive. Use Mean Square Error (MSE) evaluated over all time points and for all outputs as the objective function. The given model is built for explaining certain specific biological phenomena. However, because of this reason, the model may not converge for any random values of the parameters (rate constants) given by optimizer. Further, being most realistic in nature, the experimental data also possess two issues a) they are very limited in number and b) not all outputs are measured at the same particular instant of time.

With these aforementioned challenges, you are required to utilize the optimization solvers, GA and fmincon of Matlab to estimate the values of the parameters in two case studies described below. Utilize the notes of tutorial session on parameter estimation with ODE models for any help. You may choose to code in a way convenient to you but for project evaluation, you are requested to submit the following for each of the two cases mentioned below.

1. One properly commented matlab script file for ODE solving.
2. One properly commented matlab script file for objective function evaluation.
3. One properly commented matlab script file for nonlinear constraint evaluation (if any).
4. One properly commented matlab script file which will call the optimization solver and hence will be the main file.
5. One properly labelled and legible matlab figure containing the comparison of experimental data (as points) and simulated curves (dashed lines) for all the outputs. Make sure to mention the optimal MSE value in the figure.

Keep all of the above files in 1 folder and name it with corresponding case number. Keep Case 1 and Case 2 folders in another folder and name it with your roll number. Submit the zipped version of this folder to ch17resch11001@iith.ac.in by 6.00 PM on March 1st 2022. Both case studies have equal weightage. Each Script file and figure also has equal weightage. Any zipped folder found empty or not named properly will not be evaluated.

Case study 1

Experimental Data:

SL. No.	Time (t)	Component 1 $[C_1]$	Component 2 $[C_2]$	Component 3 $[C_3]$
1	0	15.0	0.5289	0.0
2	4	14.32	0.8411	0.0
3	8	11.45	2.68	0.8567
4	12	9.21	3.72	1.879
5	16	6.432	4.96	2.567
6	20	4.567	5.86	2.876
7	24	2.734	6.55	2.46
8	28	0.643	6.48	1.576
9	32	0.0	6.11	0.645

Model for simulation: (K_i $\forall$ $i = 1$ to 8 are the parameters)

$$\mu = \frac{K_8[C_1]}{K_1 + [C_1]}$$

$$\frac{d[C_1]}{dt} = -K_4\mu[C_2]$$

$$\frac{d[C_2]}{dt} = \mu[C_2] - \frac{K_2[C_2]}{\exp(10[C_1])} - \frac{K_3[C_2]}{\exp(10[C_2])}$$

$$\frac{d[C_3]}{dt} = K_5\mu[C_2] - \frac{K_6[C_1]}{\exp([C_3])} - \frac{K_7[C_3]}{\exp(10[C_1])}$$

Case study 2

Experimental Data:

SL. No.	Time (t)	Component 1 $[C_1]$	Component 2 $[C_2]$	Component 3 $[C_3]$	Component 4 $[C_4]$
1	0	4.9865	0.6213	0.0	0.0
2	3	4.7459	NA	0.0	0.0
3	4	NA	0.6213	0.0	0.0
4	6	4.6023	NA	0.0	0.0
5	8	NA	0.6213	NA	0.0
6	9	4.5132	NA	0.325	NA
7	12	4.107	0.9847	0.453	0.05
8	15	3.684	NA	0.5372	NA
9	16	NA	1.43	NA	0.35
10	18	3.432	NA	0.6921	NA
11	20	NA	1.56	NA	0.66
12	21	3.16	NA	0.684	NA
13	24	2.659	1.529	0.539	0.85
14	27	2.487	NA	0.321	NA
15	28	NA	1.4	NA	0.93
16	30	2.3048	NA	0	0.88
17	32	NA	1.36	0	NA
18	33	2.12	NA	0	NA

NA – Not available.

Model for simulation: ($K_i \; \forall \; i = 1$ to 11 are the parameters)

$$\mu = \frac{K_{11}[C_1]}{K_1 + [C_1]}$$

$$\frac{d[C_1]}{dt} = -K_4\mu[C_2]$$

$$\frac{d[C_2]}{dt} = \mu[C_2] - K_3[C_2] - \frac{K_2[C_2]}{\exp(10[C_2])}$$

$$\frac{d[C_3]}{dt} = K_5\mu[C_2] - K_6[C_2]\{\exp(10[C_1])\} - K_7[C_3]\{\exp(10[C_4])\}$$

$$\frac{d[C_4]}{dt} = K_8\mu[C_2] - \frac{K_9[C_1]}{\exp(10[C_2])} - K_{10}[C_1]\exp(10[C_4])$$