EGR102

Final Project Part 4: Fit Actual Data with maximum growth rate, mu\_max

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Due: Wednesday at Midnight April 24th, 2024

The assignment is to simulate a BIOREACTOR WITH SUBSTRATE INHIBITION.

You will be building off this system to

1. Simulate the continuous bioreactor for a time frame with fixed inputs.
2. Simulate the continuous bioreactor with a step response in flow rate.
3. Simulate actual data vs predicted data and calculate mean square error.
4. Fit baseline maximum growth rate, µmax (mu\_max), given set of data.
5. Fit growth kinetics for max growth rate µmax, the Monod Constant, K, and inhibition factor Ki.

EC) Optimize Fin for best production.

Modeling Equations:

Note: growth rate µ(mu) should be in the ODE function file.

% Simulation Parameters

*Obtain from data file: t\_end, delt*

% Initial Conditions:

X(1)= 161.916;% g cells/ L

S(1)= 7.125;% g substrate/ L

P(1)= 80.96;% g protein /L

*Obtain from data file: X\_act*

%Nominal Parameter Values (To Be Fitted):

mu\_max = 0.5;% maximum growth rate h-1

*replace with max, min, and inc values for for loop to fit*

K= 20;% Monod growth constant g substrate/L

Ki= 50;% Substrate inhibition growth constant g substrate/L

% Input

*Obtain from data file: Fin\_act*

% Parameters:

V=1000;% bioreactor volume L

YSX = 1.5;% yield g substrate/ g cells

YPX = 0.5;% yield g protein/ g cells

Xin = 0;% feed biomass concentration g cells/L

Sin = 250;% feed substrate concentration g substrate/L

Pin = 0;% feed protein concentration g protein/L

**Flow Diagram for Brute Optimization Parameter Fit**

A diagram of a flowchart

Description automatically generated

1. Build off the part 3 ic file done earlier. Use the same data file final\_proj\_data.mat. Rename part3 ic so part 4.
   1. Change X(1), S(1), and P(1) to X\_init, S\_init and P\_init. So later when clear X S and P can still reinitialize easily
   2. Remove mu\_max= and replace with
      1. mu\_max\_max=0.7
      2. mu\_max\_min=0.4
      3. mu\_max\_inc=0.05

*Note: make sure that best value is not on an extreme value either a minimum or maximum. Not sure then if best value or not.*

* 1. Make sure Best\_MSE=1E10 as initial value so easily beaten for first experiment MSE.
  2. When new MSE is better than Best\_MSE save Best\_MSE=MSE and save the parameter(s) that caused it eg. Best\_mu\_max=mu\_max.
  3. Keep adjusting ranges and/or increments so find mu\_max to nearest hundredth.

1. Generate one figure with 4 subplots:
   1. Title should be: Final Project Part 4 MSE= “MSE” with best mu max= “mu\_max”, K=”K” , and Ki=”Ki” NOTE:”” are embedded parameters
   2. t vs X as red crosses

t\_act vs X\_act as black diamonds

legend “Predicted” “Actual”

with yaxis “X (g cells/L)”

* 1. t vs S with yaxis “S (g substrate/L)”
  2. t vs P with yaxis “P (g protein/L)”
  3. t vs Fin with yaxis “Fin (L/hr)” and xaxis “Time (hrs)”

Paste here the following:

1. final\_project\_part4\_ic.m file
2. figure generated

Save all files since will be building on these for subsequent parts!

*If done correctly should get figure similar to this if you used the following as starting points for mu\_max*

*mu\_max\_min =0.4;% minimum max growth rate h-1*

*mu\_max\_inc =0.05;% increment max growth rate h-1*

*mu\_max\_max =0.7;% maximum max growth rate h-*

A screenshot of a graph

Description automatically generated

1. final\_project\_part4\_ic.m file

%Bioreactor\_actual/predic\_MSE\_ic%

%Ransford Antwi%

%March 5, 2024%

%Final\_Project\_Part\_4\_main

%blank slate%

clear

clc

% user assigned%

%loading data file

load final\_proj\_3\_data\_file.mat

% Simulation Parameters

% will obtain from data file instead

% Initial Conditions:

X\_init= 161.916;% g cells/ L

S\_init= 7.125;% g substrate/ L

P\_init= 80.96;% g protein /L

%Nominal Parameter Values (To Be Fitted):

K= 20;% Monod growth constant g substrate/L

Ki= 50;% Substrate inhibition growth constant g substrate/L

% mu\_max\_max = 0.593;% maximum growth rate h-1

% mu\_max\_min = 0.591;% maximum growth rate h-1

% mu\_max\_inc=0.001;%increament

mu\_max\_max = 0.59;% maximum growth rate h-1

mu\_max\_min = 0.58;% maximum growth rate h-1

mu\_max\_inc=0.001;%increament

%input added

Fin=Fin\_act;

%Parameters

V=1000;% bioreactor volume L

Ysx = 1.5;% yield g substrate/ g cells

Ypx = 0.5;% yield g protein/ g cells

Xin = 0;% feed biomass concentration g cells/L

Sin = 250;% feed substrate concentration g substrate/L

Pin = 0;% feed protein concentration g protein/L

%main program

%[xdot]=lorenz\_ode\_2(t,x,opts,sigma,r,b)

%intialization

X(1)=X\_init;

S(1)=S\_init;

P(1)=P\_init;

x0=[X(1);S(1);P(1);];

%unpacking to various parameters

param(1)=V;

param(2)=Ysx;

param(3)=Ypx;

param(4)=Xin;

param(5)=Sin;

param(6)=Pin;

param(7)=K;

param(8)=Ki;

%initial time

t(1)=0;

%number of samples in for loop

N=ceil(t\_end/delt);

%best MSE

Best\_MSE= 1E10;

for mu\_max=mu\_max\_min:mu\_max\_inc:mu\_max\_max

% Initial Sum of Square Error

SSE=(X\_act(1)-X(1))^2;

%This is my experimental loop!!!!!

for i=2:N

t(i)=t(i-1)+delt;

%[xdot]=vdv\_fxn(t,x,opts,param,u)

[~,Xout]=ode45('Bioreactor\_fxn',[t(i-1) ,t(i)],x0,[],param,Fin(i-1),mu\_max);

%unpack Xout to common notation for states

X(i)=Xout(end,1);

S(i)=Xout(end,2);

P(i)=Xout(end,3);

% ba reinitialization vector

x0=[X(i);S(i);P(i)];

%BA call sum of sq error

SSE=SSE+(X\_act(i)-X(i))^2;

end

%Mean square error divide total by numebr sample

MSE=SSE/N;

if MSE<Best\_MSE

Best\_MSE=MSE; % save current MSE as the new best one

Best\_mu\_max=mu\_max; % save the current paramater used as the new best one.

end

% Clean up and Reset Experiment 7. BA

clear t X S P % always clear the time vector and states

% Reinitialize

t(1)=0; % reinitialize time vector

X(1)=X\_init; % 2. set first CA and T to init values

S(1)=S\_init;

P(1)=P\_init;

x0=[X(1);S(1);P(1)];% ba initialization vector

end %end o loop for Mu\_max

% Set parameter(s) to Best ones found! and rerun simulation 8. BA

mu\_max=Best\_mu\_max;

%experimental loop

% Initial Sum of Square Error

SSE=(X\_act(1)-X(1))^2;

for i=2:N

t(i)=t(i-1)+delt;% BA time vector

%[xdot]=vdv\_fxn(t,x,opts,param,u)

[~,Xout]=ode45('Bioreactor\_fxn',[t(i-1) ,t(i)],x0,[],param,Fin(i-1),mu\_max);

%unpack Xout to common notation for states

X(i)=Xout(end,1);

S(i)=Xout(end,2);

P(i)=Xout(end,3);

% ba reinitialization vector

x0=[X(i);S(i);P(i)];

%BA call sum of sq error

SSE=SSE+(X\_act(i)-X(i))^2;

end

MSE=SSE/N; % mean square error divide total by number samples

%Graphing

%ploting subplot

figure(1);

subplot(4,1,1);plot(t,X,'rx',t,X\_act,'kd')

ylabel('X(g cells/L')

legend('Predicted','Actual')

title(['Final Project Part 4 MSE=',num2str(MSE),' with the best mu max=',num2str(mu\_max),'K=',num2str(K),'and Ki=',num2str(Ki)])

subplot(4,1,2);plot(t,S)

ylabel('S(g substrate/L')

subplot(4,1,3);plot(t,P)

ylabel('P(g Protein/L')

subplot(4,1,4);plot(t,Fin)

ylabel('Fin(g L/hr)')

xlabel('Time(hrs)')

1. figure generated

