Parameter Estimation in Dynamic Systems

The (system) of ordinary differential equations

$$\hat{y}_i = g(a_0, a_1 \ldots a_n, x_{1,i}, x_{2,i}, \ldots x_{n,i})$$

is used to model the data by finding the values of the parameters a_0, a_1 … a_n that minimize the squares of the errors

$$S = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Solution of such problems requires the integration of the differential equations in an inner loop in order to obtain the $\hat{y}_i$ values and minimizing S as function of a_0, a_1 … a_n in an outer loop.

A solved example is available in the Cutlip and Shacham (2007) book (Prob. 6.9)

ESTIMATING MODEL PARAMETERS INVOLVING ODE'S USING FERMENTATION DATA

When the microorganism *Penicillium Chrysogenum* is grown in a batch fermentor under carefully controlled conditions, the cells grow at a rate which can be modeled by the logistic law:

$$\frac{dy_1}{dt} = b_1 y_1 \left(1 - \frac{y_1}{b_2}\right)$$

where y_1, is the concentration of the cell expressed as percent dry weight. In addition, the rate of production of penicillin has been mathematically quantified by the equation:

$$\frac{dy_2}{dt} = b_3 y_1 - b_4 y_2$$

Use the experimental data to find the values of the parameters b_1, b_2, b_3 and b_4 which minimize the sum of squares of the differences between the calculated and experimental concentrations (y_1 and y_2).

METHOD OF SOLUTION

Time h	Cell concentration, percent dry weight (y_1)	Penicillin concentration , units/mL (y_2)
0	0.18	0
10	0.12	0
22	0.48	0.0089
34	1.46	0.0642
46	1.56	0.2266
58	1.73	0.4373
70	1.99	0.6943
82	2.62	1.2459
94	2.88	1.4315
106	3.43	2.0402
118	3.37	1.9278
130	3.92	2.1848
142	3.96	2.4204
154	3.58	2.4615
166	3.58	2.283
178	3.34	2.7078
190	3.47	2.6542

$$\frac{dy_1}{dt} = b_1 y_1 \left(1 - \frac{y_1}{b_2}\right)$$

$$\frac{dy_2}{dt} = b_3 y_1 - b_4 y_2$$

d(y1)/d(t) = b1 * y1 * (1 - y1 / b2)
d(y2)/d(t) = b3 * y1 - b4 * y2
b1 = 0.1
b2 = 4
b3 = 0.02
b4 = 0.02
(b1–b4: Initial estimates)
y1(0) = 0.18
y2(0) = 0
t(0) = 0
t(f) = 190 10, 22, 34….

Stop and restart the integration at t = 10, 22, 34 …..190 h for the specified parameter values. Introduce the resultant y values into the objective function

$$\min S = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Calculation of the Sum of Squares of Errors

```
function dYfuncvecdt = ODEfun(t,Yfuncvec,Beta);
y1 = Yfuncvec(1);
y2 = Yfuncvec(2);
b1=Beta(1);
b2=Beta(2);
b3=Beta(3);
b4=Beta(4);
dy1dt = b1 * y1 * (1 - y1 / b2);
dy2dt = b3 * y1 - b4 * y2 ;
dYfuncvecdt = [dy1dt; dy2dt];
```

Add **ß to** the input parameters

```
function sum=SumSqr(Beta,data)
global Feval SumSave
Feval=Feval+1;
time=data(:,1);
ym=data(:,2:end); % ym – Measured data
yc(1,:)=ym(1,:);
[nr,nc]=size(ym); % nr - number of data points;
              % nc - number of dependent variables
tspan = [time(1) time(2)]; % Range for the independent variable
y0 = ym(1,:); % Initial values for the dependent variables
for i=2:nr
   [t,y]=ode45(@ODEfun,tspan,y0,[],Beta);
   yc(i,:)=y(end,:);  % Put final values of y in the current interval into yc
   if i<nr
      tspan = [time(i) time(i+1)];  % Move forward the time interval
      y0 = yc(i,:);  % Put the final values from the previous interval into y0
   end
end
sum=0;
for ic=1:nc
   sum=sum+(ym(:,ic)-yc(:,ic))'*(ym(:,ic)-yc(:,ic));
end
if sum< SumSave*0.9
   disp([' Function evaluation No. ' num2str(Feval) '  Sum of Squres ' num2str(sum)]);
   SumSave=sum;
end
```

$$\min S = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Minimization of the Sum of Squares of Errors and Display of the Results

```
global Feval SumSave
load Run2.txt  % Load experimental data as a text file.
Beta=[0.1 4 0.02 0.02]; % Initial estimate for parameter values
Feval=0;
SumSave=realmax;
[BetaOpt,Fval]=fminsearch(@SumSqr,Beta,[],Run2);  % Find optimal β values
disp(' ');
disp('Optimal Results ');
disp(' Parm. No.  Value')
for i=1:size(Beta,2)
   disp([i BetaOpt(i)]);
end
disp([' Final Sum of Squares ' num2str(Fval) '  Function evaluations  ' num2str(Feval)]);
tspan = [Run2(1,1) Run2(end,1)];
y0=[Run2(1,2) Run2(2,2)];
[t,y]=ode45(@ODEfun,tspan,y0,[],BetaOpt);
for i=1:size(y,2)
   hold off
    plot(t,y(:,i));
   title([' Plot of dependent variable y' int2str(i)]);
   xlabel(' Independent variable (t)');
   ylabel([' Dependent variable y' int2str(i)]);
   hold on
   plot(Run2(:,1),Run2(:,i+1),'*')
   pause
 end
```

Display numerical results

Plot experimental data and calculated curve

ESTIMATING MODEL PARAMETERS INVOLVING ODE'S USING FERMENTATION DATA

Data

Time h	Cell Concentration Percent Dry Weight y_1	Penicillin Concentration Units/mL y_2
0	0.18	0
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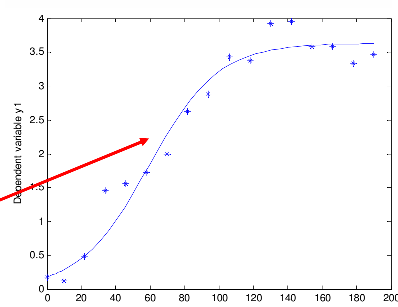
Function evaluation No. 1 Sum of Squares 36.1271
Function evaluation No. 63 Sum of Squares 1.5582

Optimal Results	
Parameter Number	Value
1	0.049875
2	3.634
3	0.020459
4	0.02652

Final Sum of Squares 1.4358 Function evaluations 268

Parameter values



Plot of experimental vs. calculated