

This script was taken from a dissertation submitted to the Indian Institute of Technology Hyderabad: “Mathematical modelling of baculovirus infection process: Kinetic parameter estimation,” by Suraj Kumar Singh (Singh and Giri 2018). It was slightly altered to fit into the scope of our project.

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clc;
close all;
clear all;
global t
% lb=zeros(1,14);
p0 = [5350 535 1000 1200 0.00002 30 100 0.912 500 15 120000 800000 0.00004 2.5
0.009263 4.3 1 0.01 0.076 15 0.01 1.27 0.001 0.5 10 18 1.09 0.002 0.001];
lb = [1000 100 500 600 0.00001 20 50 0.5 200 10 100000 500000 0.00001 1.5
0.005263 1.43 0.5 0.008 0.03 5 0.0006 0.5 0.0008 0.3 8 15 1 0.001 0.0008];
ub = [53500 5350 5000 2000 0.00005 100 300 1.5 1000 30 400000 1000000 0.00008 5
0.02 10 2 0.05 0.1 40 0.05 2.7 0.002 1 12 20 1.11 0.005 0.005];
p = fmincon(@Obj_Complex,p0,[],[],[],[],lb,ub);
tspan = [0 96];
UC = [460000 590000 650000];
y0(2:62) = 0;
y0(63) = p(1);
y0(64) = p(2);
y0(65) = 0;
y0(66) = p(3);
y0(67) = p(4);
y0(68:75) = 0;
VCI = [100 90.8 92.5];
for j=1:3
    y0(1) = UC(j);
    [t,y] = ode23(@(t,y)ODEset_complex(t,y,p),tspan,y0);
    % vd(:,1) = 100 - (y(:,65)./(y(:,1)+y(:,2)+f+g))*100 ;
    ti = [0 24 48 72 96];
    f = 0;
    g = 0;
    for i = 1:30
        d = y(:,i+2);
        f = f + d;
        e = y(:,i+32);
        g = g + e;
    end
    poly = ((f + g)./(f+g+y(:,1)+y(:,2)))*100;
    figure(j)
    plot(t, (y(:,1)+y(:,2)+f+g), 'r');%t,y(:,1),t,y(:,2),t,f,t,g);
    % legend('Cell D','CU','CD','CS','CB')
    % legends_a{j} = char(['ws=',num2str(ws)]); %,' max: ',num2str(Max_c)];
    % legend(char(legends_a),'location','best')
    % hold on;
    % disp(j);

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% end
hold on;
uc = [460000 750000 940000 950000 930000;
590000 1210000 1470000 1510000 1370000;
650000 1010000 1220000 1390000 1290000];
vde = [100 79.55 48.9 17.71 7.03;
90.8 85.6 81.3 77.7 59;
92.5 78.8 71 68.9 48.9];
dead = (y(:,5)./(y(:,1)+y(:,7)))*100 ;
vd = VCI(j) - dead;
title('Infected Cell vs Time'); xlabel('Time (h)'); ylabel('Cell Density');
grid on;
figure(j+5)
plot(t,poly,'g');
hold on;
title('Infected Cell vs Time'); xlabel('Time (h)'); ylabel('% of
Polyhedra/Cell');
grid on;
figure(j+10)
plot(t,vd,'b')
title('Infected Cell vs Time'); xlabel('Time (h)'); ylabel('Cell Viability')
grid on;
end
% figure(4)
% plot(t,y(:,66),t,y(:,67),t,y(:,68))
% legend('Substrate','O2','CO2')
% axis([0,120,0,1200])
%
% figure(5)
% plot(t,y(:,69),t,y(:,70),t,y(:,71),t,y(:,72))
% legend('DNA','RNAe','RNA1','RNAv1')
function [rmse] = Obj_Complex(param)
tspan = [0 24 48 72 96];
UC = [460000 590000 650000];
y0(2:62) = 0;
y0(63) = param(1);
y0(64) = param(2);
y0(65) = 0;
y0(66) = param(3);
y0(67) = param(4);
y0(68:75) = 0;
VCI = [100 90.8 92.5];
Error = 0;
for j=1:3
    y0(1) = UC(j);
    [t,y] = ode23(@(t,y)ODEset_complex(t,y,param), tspan, y0);
    f = 0;
    g = 0;
    for i = 1:30

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    d = y(:,i+2);
    f = f + d;
    e = y(:,i+32);
    g = g + e;
end
poly(:,1) = ((f + g)./(f+g+y(:,1)+y(:,2)))*100;
dead = (y(:,5)./(y(:,1)+y(:,7)))*100 ;
vd = VCI(j) - dead;
uc = [460000 750000 940000 970000 950000;
590000 1210000 1510000 1470000 1370000;
650000 1010000 1220000 1390000 1290000];
vde = [100 79.55 48.9 17.71 7.03;
90.8 85.6 81.3 77.7 59;
92.5 78.8 71 68.9 48.9];
% c_poly_E1=[73.64 76.53 69.10];
% c_poly_E1 = [92.95 92.66 91.48];
inf(:,1) = y(:,1) + y(:,2) + f + g;
sum1=0;
sum2=0;
% error = 0;
for i=1:5
    sum1= sum1 + (uc(j,i)-inf(i,1))^2;
end
for i=1:5
    sum2= (sum2 + (vde(j,i)-vd(i,1))^2);
end
Error = sum1+sum2;
end
[rmse] = sqrt((Error)/15)
end
function dmdt = ODEset_complex(t,y,param)
a= param(5);%0.00002;
b= param(6);%30;
Ks = param(7);%100;
K = param(8);%0.912;
Ko2 = param(9);%500;
Kco2 = param(10);%15;
Ys = param(11);%120000;
Yo2 = param(12);%800000;
kla = param(13);%0.00004;
kdna = param(14);%2.5;
kdeg = param(15);%0.009263;
krna = param(16);%4.3;
Kpoly = param(17);%1;
Kfp = param(18);%0.01;
kpe = param(19);%0.076;
Krna = param(20);%15;
ktrans = param(21);%0.01;
Ostar = param(22);%1.27;

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alpha = param(23);%0.0001;
beta = param(24);%0.5;
mumax = param(27);%1.1;
kd1 = param(28);%0.002;
kstar = param(29);%0.001;
mul = mumax*(y(66)/(y(66) + Ks));
O2 = (y(67)/(y(67) + Ko2));
CO2 = (K/(y(68)+ Kco2));
mu = mul*O2*CO2;
for i = 1:30
    if i <=param(25)
        z(i) = 1;
    else
        z(i) = 0;
    end
end
for i = 1:30
    if i <=param(26)
        p(i) = 0;
    else
        p(i) = alpha*exp(beta*(i-param(26)));
    end
end
kd3 = kstar*log(y(69));
if t< 24
    kd = kd1;
else
    kd = kd1+kd3;
end
dydt(1) = mu*y(1) - a*(y(63)+y(64))*y(1) - kd1*y(1);
dydt(2) = mu*y(2) + a*y(64)*y(1) -a*y(63)*y(2) - kd*y(2);
dydt(3) = a*y(63)*y(1) + ktrans*y(75) - y(3) - y(3)*p(1) -a*y(3)*y(64)*z(1) -
kd*y(3);
for i = 4:31
    dydt(i) = y(i-1) + ktrans*y(75) - y(i) -y(i)*p(i-2) - a*y(i)*y(64)*z(i-2) -
kd*y(i);
end
dydt(32) = y(31)+ ktrans*y(75) - y(32)*p(30) - a*y(32)*y(64)*z(30) - kd*y(32);
sumes = 0;
for i = 1:30
    v = y(i+2)*z(i);
    sumes = sumes + v;
end
dydt(33) = ktrans*y(75)+ a*y(64)*sumes +a*y(63)*y(2)- y(33) - y(33)*p(1) -
kd*y(33);
for i = 34:61
    dydt(i) = ktrans*y(75)+ (y(i-1) - y(i)) - y(i)*p(i-32) - kd*y(i);
end
dydt(62) = ktrans*y(75) + y(61) - y(62)*p(30)- kd*y(62);

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r = 0;
s = 0;
for i = 1:30
    v = y(i+2)*p(i);
    r = r + v;
    x = y(i+32)*p(i);
    s = s + x;
end
dydt(63) = b*r*y(73) - a*y(63)*sum(y(1:62));
dydt(64) = b*s*y(73) - a*y(64)*sum(y(1:62));
dydt(65) = kd1*y(1) + kd*sum(y(2:62));
dydt(66) = -mul*((sum(y(1:62))/Ys));
dydt(67) = kla*(Ostar - y(67)) - ((sum(y(1:62))/Yo2)) ;
dydt(68) = ((sum(y(1:62))/Yo2));
if 6<t && t <= 20
    f1 = 1 - ((t-6)/14);
else
    f1 = 0;
end
if 1<t && t <= 6
    f2 = 1 - ((t-1)/5);
else
    f2 = 0;
end
if 6<t && t <= 15
    f3 = 1 - ((t-6)/9);
else
    f3 = 0;
end
if 15<t && t <= 48
    f4 = 1 - ((t-15)/33);
else
    f4 = 0;
end
dydt(69) = f1*a*y(63) + kdna*y(69)*f1 - kdeg*y(69);
dydt(70) = f2*krna*y(63) - kdeg*y(70); %RNA early
dydt(71) = f3*krna*y(69) - kdeg*y(71); %RNA late
dydt(72) = f4*krna*y(69) - kdeg*y(72);
dydt(73) = f2*kpe*(y(70)/(y(70) + Krna))*sum(y(2:62)) - kdeg*y(73); %gp64
protein
dydt(74) = f3*kpe*(y(71)/(y(71) + Krna))*(1/(Kfp + y(74)))*sum(y(2:62)) -
kdeg*y(74); %fp25k protein
dydt(75) = f4*kpe*(y(72)/(y(72) + Krna))*(y(74)/(y(74)+Kpoly))*sum(y(2:62)) -
kdeg*y(75); %ODE protein
dmdt = dydt';
end

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