Final Proyect: Digital Twin

Departamento de Ingeniería Eléctrica y Electrónica

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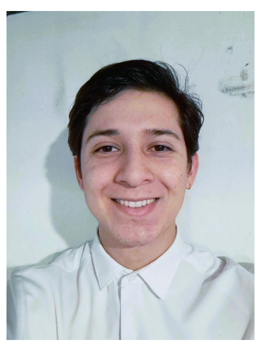
General Information



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Simulation data

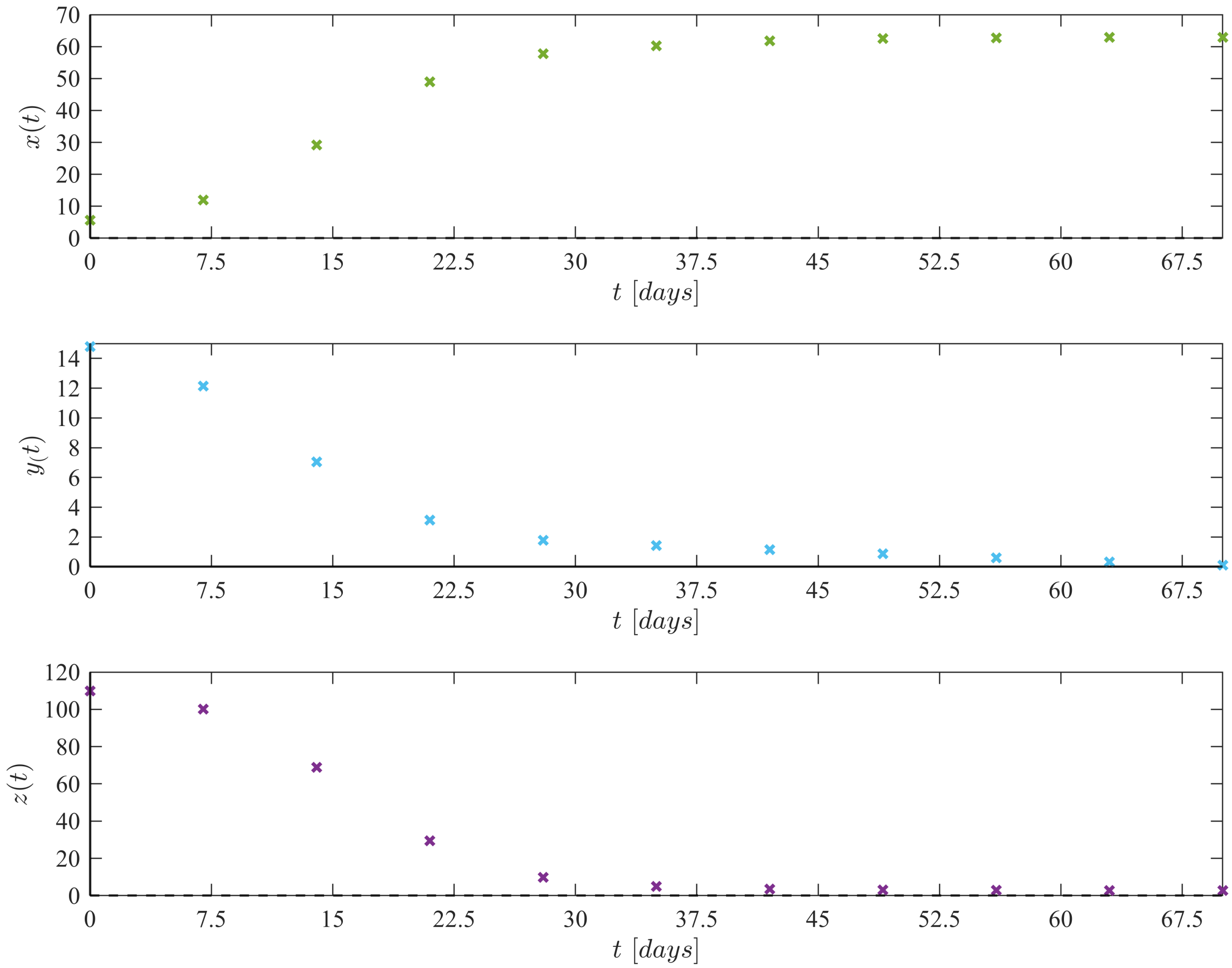
```
clc; clear; close all; warning('off','all')
```

```
filename = 'rawdata.csv';
sys = readmatrix(filename);

t = round(sys(:,1));
x1 = sys(:,2); y1 = sys(:,3); z1 = sys(:,4);

T = array2table([t, x1, y1, z1], ...
    'VariableNames', {'Tiempo', 'x1(t)', 'y1(t)', 'z1(t)', ...
                      });
disp(T)
```

Tiempo	x1(t)	y1(t)	z1(t)
0	5.596	14.8	109.84
7	11.975	12.135	100.18
14	29.188	7.048	68.925
21	48.982	3.126	29.523
28	57.75	1.786	9.812
35	60.279	1.431	4.976
42	61.764	1.158	3.581
49	62.522	0.881	3.064
56	62.732	0.606	2.91
63	62.91	0.321	2.804
70	62.881	0.114	2.73

Raw data plot

```
plotGraficas(t,x1,y1,z1)
exportgraphics(gcf, '1. Datos_en_crudo.pdf', 'ContentType', 'vector');
```

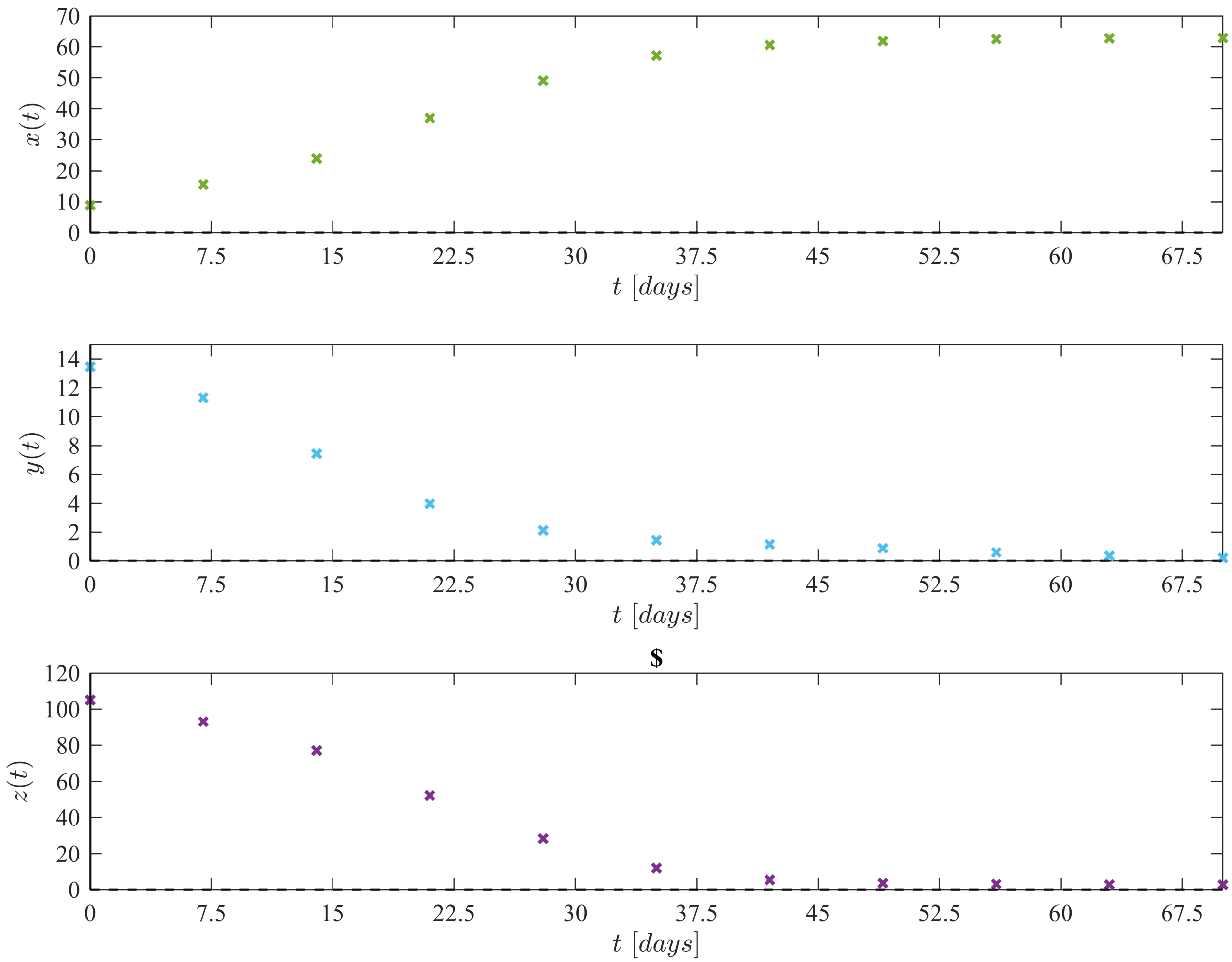


Smooth data

```
sys = readmatrix('rawdata.csv');
t = sys(:,1);
x1 = sys(:,2);
y1 = sys(:,3);
z1 = sys(:,4);

xo =smoothdata(x1);
yo =smoothdata(y1);
zo =smoothdata(z1);


Ts = array2table([t, xo, yo, zo], ...
    'VariableNames', {'Time', 'x(t)', 'y(t)', 'z(t)', ...
                     });
disp(Ts)
```

Time	x(t)	y(t)	z(t)
0	8.7855	13.468	105.01
7	15.586	11.328	92.98
14	23.935	7.4363	77.116
21	36.974	3.9867	52.109
28	49.05	2.1143	28.309
35	57.194	1.4583	11.973
42	60.579	1.1567	5.3582
49	61.824	0.88167	3.6327
56	62.482	0.60267	3.0897
63	62.761	0.347	2.877
70	62.841	0.2175	2.8147

```
writetable(Ts, 'data_smooth.csv');
plotGraficas1(t,xo,yo,zo);
exportgraphics(gcf, '2. Datos_suavizados.pdf', 'ContentType', 'vector');
```



Smooth data plot

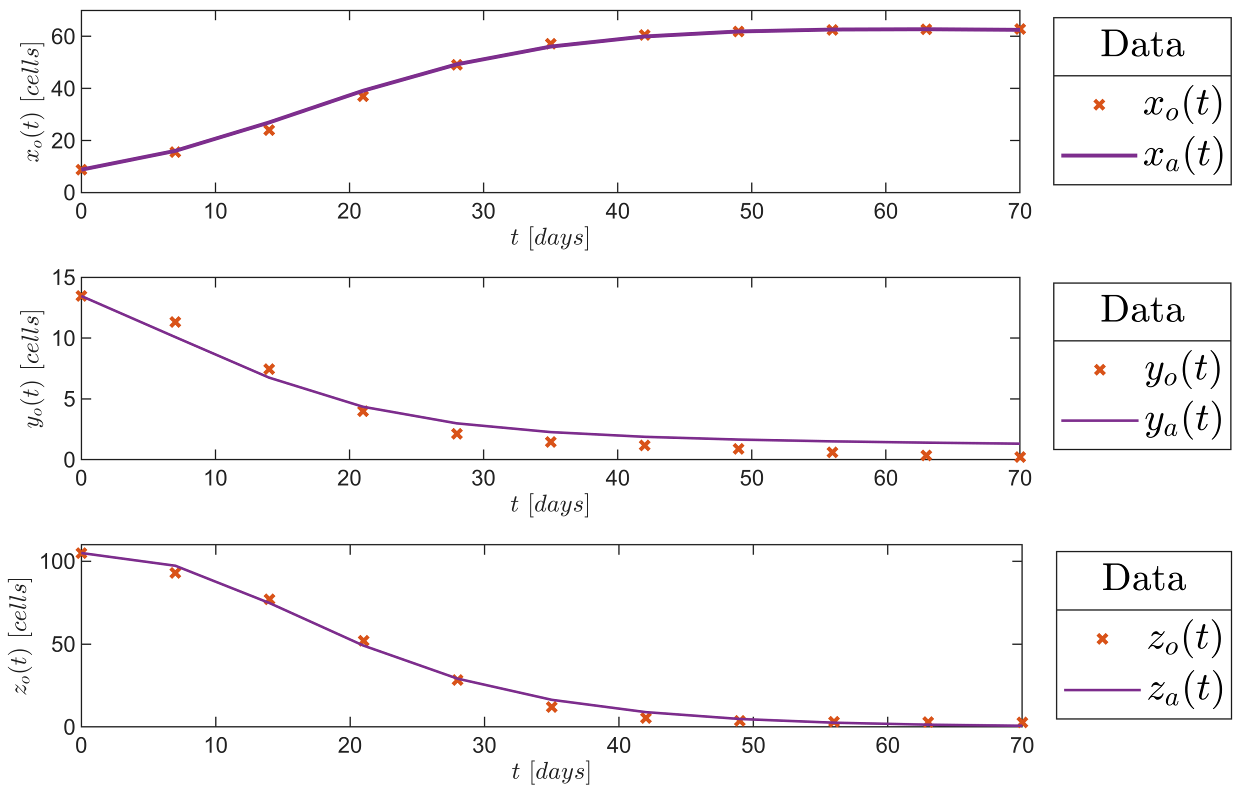
Nonlinear Regression

```
P0 = [0.0009, 0.0040, 0.0150, 0.0001, 0.0050, 0.050];
[mdl, xa, ya, za ] = Model1 (t, xo, yo ,zo, P0); plotModel1(t,[xo,xa],[yo,ya],
[zo,za]);
```

```
Sample size (n): 11
Parameters to be estimated (pars): 6
Degrees of freedom: 27
Significance level (alpha): 0.05
t-Student value: 2.0518
Adjusted R-squared: 0.99624
Corrected AIC (n/pars < 40): 32.0573
```

Parameters	Estimate	SE	MoE	CI95		pvalue
p1	0.00095911	0.00011849	0.00024312	0.00071599	0.0012022	1.0724e-08
p2	0.0010805	0.0011504	0.0023604	0.0012799	0.0034409	0.35592
p3	0.0072501	0.033927	0.069612	0.062362	0.076862	0.83239
p4	2.7553e-05	2.4225e-05	4.9706e-05	2.2153e-05	7.7259e-05	0.26538
p5	0.0077425	0.00094552	0.00194	0.0058024	0.0096825	8.565e-09
p6	0.10239	0.010158	0.020843	0.081542	0.12323	1.1991e-10

```
exportgraphics(gcf, '3. Algoritmo_de_RNL.pdf', 'ContentType', 'vector');
```



Jacobian Matrix and Equilibrium Points

```
syms x y z p1 p2 p3 p4 p5 p6
          dx = p1*x*z - p2*x*y;
          dy = -p3*y - p4*x*y*z;
          dz = p5*y*z - p6*z;

J = jacobian([dx,dy,dz],[x,y,z]);
fprintf('Jacobian matrix of the Lotka-Volterra system: '); disp(J)
```

```
Jacobian matrix of the Lotka-Volterra system:
```

$$\begin{pmatrix} p_1\,z - p_2\,y & -p_2\,x & p_1\,x \\ -p_4\,y\,z & -p_3 - p_4\,x\,z & -p_4\,x\,y \\ 0 & p_5\,z & p_5\,y - p_6 \end{pmatrix}$$

```
edos = solve([dx,dy,dz],[x,y,z]);
fprintf(['the system has ', num2str(length(edos.x)), ' equilibrium points.'])
```

```
the system has 2 equilibrium points.
```

```
X0 = edos.x(1); Y0 = edos.y(1); Z0 = edos.z(1);
X1 = edos.x(2); Y1 = edos.y(2); Z1 = edos.z(2);

syms x0 y0 z0 x1 y1 z1
fprintf('Equilibrium points of the Lotka-Volterra system: ');
```

```
Equilibrium points of the Lotka-Volterra system:
```

```
disp([x0,y0,z0,X0,Y0,Z0]); disp([x1,y1,z1,X1,Y1,Z1]);
```

$$\begin{pmatrix} x_0 & y_0 & z_0 & 0 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} x_1 & y_1 & z_1 & -\frac{p_1\,p_3\,p_5}{p_2\,p_4\,p_6} & \frac{p_6}{p_5} & \frac{p_2\,p_6}{p_1\,p_5} \end{pmatrix}$$

```
eq1 = dx == 0;
eq2 = dy == 0;
eq3 = dz == 0;

equilibria = solve([eq1, eq2, eq3], [x, y, z]);
for i = 1:length(equilibria.x)
    xe(i,1) = simplify(equilibria.x(i));
    ye(i,1) = simplify(equilibria.y(i));
    ze(i,1) = simplify(equilibria.z(i));

    fprintf('Equilibrium point %d:\n', i)
    fprintf('x%d = %s\n', i, char(xe(i,1)));
    fprintf('y%d = %s\n', i, char(ye(i,1)));
    fprintf('z%d = %s\n\n', i, char(ze(i,1)));
end
```

```
Equilibrium point 1:
```

```
x1 = 0
y1 = 0
z1 = 0
Equilibrium point 2:
x2 = -(p1*p3*p5)/(p2*p4*p6)
y2 = p6/p5
z2 = (p2*p6)/(p1*p5)
```

```
p1 = 0.00117;    p2 = 0.00318;    p3 =  0.0118;
p4 = 4.22e-5;    p5 = 0.00631;    p6 = 0.0923;

    x1 = 0;
    y1 = 0;
    z1 = 0;

    x2 = -(p1*p3*p5)/(p2*p4*p6);
    y2 = p6/p5;
    z2 = (p2*p6)/(p1*p5);

    xe = [x1; x2]; ye = [y1; y2]; ze = [z1; z2];
    Eqs = array2table([xe, ye, ze], 'VariableNames', {'x*','y*','z*'});
    disp(Eqs)
```

x*	y*	z*
0	0	0
-7.0332	14.628	39.757

Local Stability

```
close all; warning('off','all')
p1 = 0.00095911;
p2 = 0.0010805;
p3 = 0.0072501;
p4 = 2.7553e-05;
p5 = 0.0077425;
p6 = 0.10239;

syms x y z
    dx = p1*x*z - p2*x*y;
    dy = -p3*y - p4*x*y*z;
    dz = p5*y*z - p6*z;
edos = solve([dx,dy,dz],[x,y,z]);
x0 = double(edos.x(1)); y0 = double(edos.y(1)); z0 = double(edos.z(1));
x1 = double(edos.x(2)); y1 = double(edos.y(2)); z1 = double(edos.z(2));


clear x y z
x = [x0;x1]; y = [y0;y1]; z= [z0;z1];
var = {'(x0,y0,z0) '; '(x1,y1,z1) '};
Equilibria = table(x,y,z,'RowNames',var);
```

```
Equilibria.Properties.VariableNames = {'xe','ye','ze'};
fprintf('Equilibrium points of the system:\n'); disp(Equilibria)
```

Equilibrium points of the system:

	xe	ye	ze
(x0,y0,z0)	0	0	0
(x1,y1,z1)	-17.662	13.224	14.898

```
L = zeros(length(x),3);
for i = 1:length(x)
     J = [ (p1*z(i) - p2*y(i)), (-p2*x(i)), (p1*x(i));
          (-p4*y(i)*z(i)), (-p3 - p4*x(i)*z(i)), (-p4*x(i)*y(i));
          0, (p5*z(i)), (p5*y(i) - p6) ];
      L(i,:) = eig(J);
end
L1 = L(:,1); L2 = L(:,2); L3 = L(:,3);
Lambdas = table(L1,L2,L3,'RowNames',var);
disp('Eigen values of the Jacobian matrix evaluated at each equilibrium point:');
disp(Lambdas);
```

Eigen values of the Jacobian matrix evaluated at each equilibrium point:

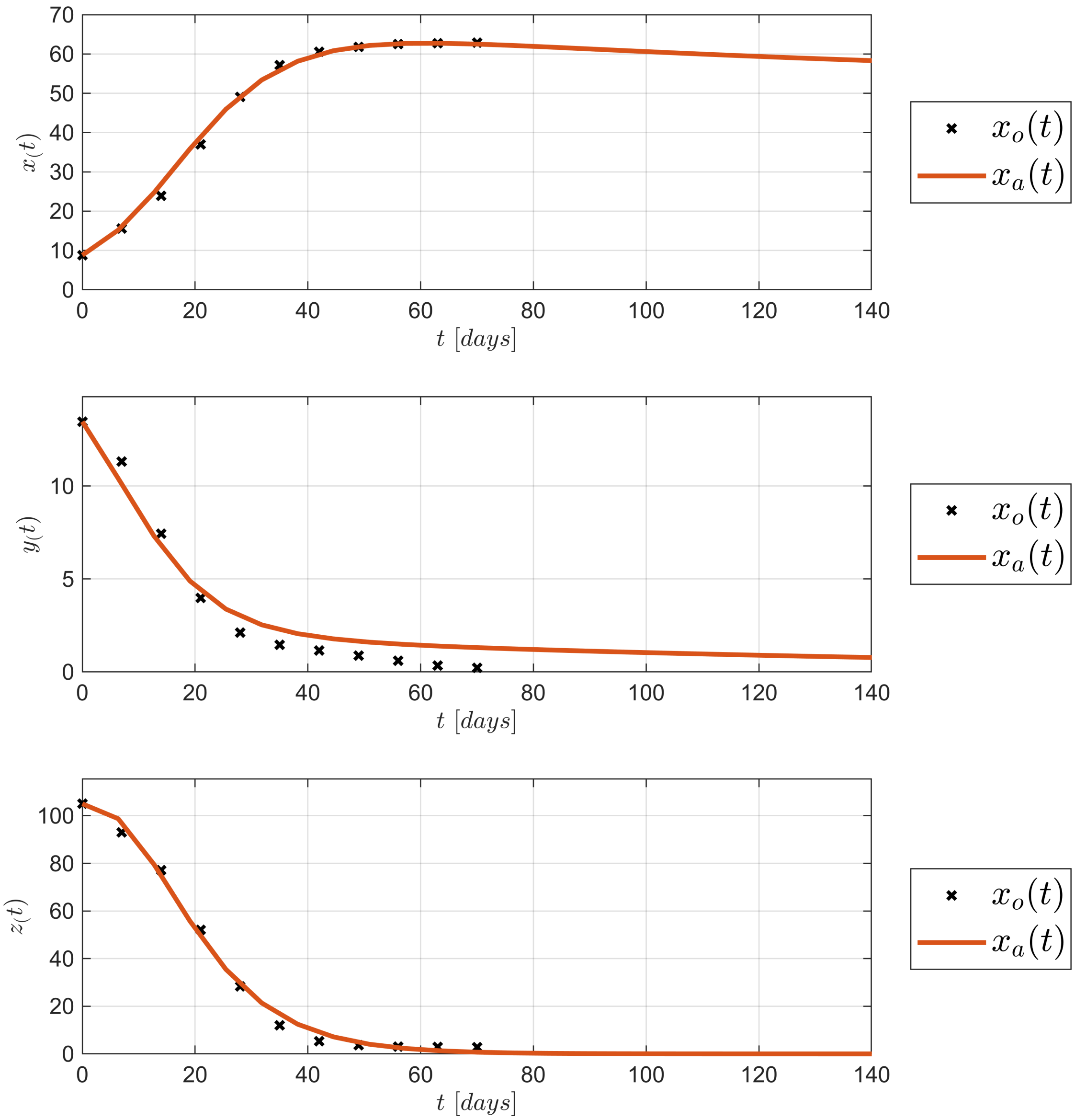
	L1	L2	L3
(x0,y0,z0)	-0.10239+0i	-0.0072501+0i	0
(x1,y1,z1)	-0.015636+0.0097319i	-0.015636-0.0097319i	0.031272

```
minx = min(xo);
maxx = max(xo);
xonormalizado = (xo - minx) / (maxx - minx);
miny = min(yo);
maxy = max(yo);
yonormalizado = (yo - miny) / (maxy - miny);
minz = min(zo);
maxz = max(zo);
zonormalizado = (zo - minz) / (maxz - minz);
```

Prediction 2t

```
p1ajustado = 0.00095911;
p2ajustado = 0.0010805;
p3ajustado = 0.0072501;
p4ajustado = 2.7553e-05;
p5ajustado = 0.0077425;
p6ajustado = 0.10239;



toriginalmax = max(t);
tpredict = 0:(toriginalmax/length(t)):1000;
initialconditions = [xo(1); yo(1); zo(1)];
```

```
options = odeset('RelTol',1e-6,'AbsTol',1e-9);
[tsol, xsol] = ode45(@(t, X) myODESystem(t, X, ...
                                    p1ajustado, p2ajustado, p3ajustado, ...
                                    p4ajustado, p5ajustado, p6ajustado), ...
                       tpredict, initialconditions, options);
xpredict = xsol(:,1);
ypredict = xsol(:,2);
zpredict = xsol(:,3);

 plotprediction(t, xo, yo, zo, tsol, xpredict, ypredict, zpredict);
 exportgraphics(gcf, '5. Predicción_a_2t.pdf', 'ContentType', 'vector');
```

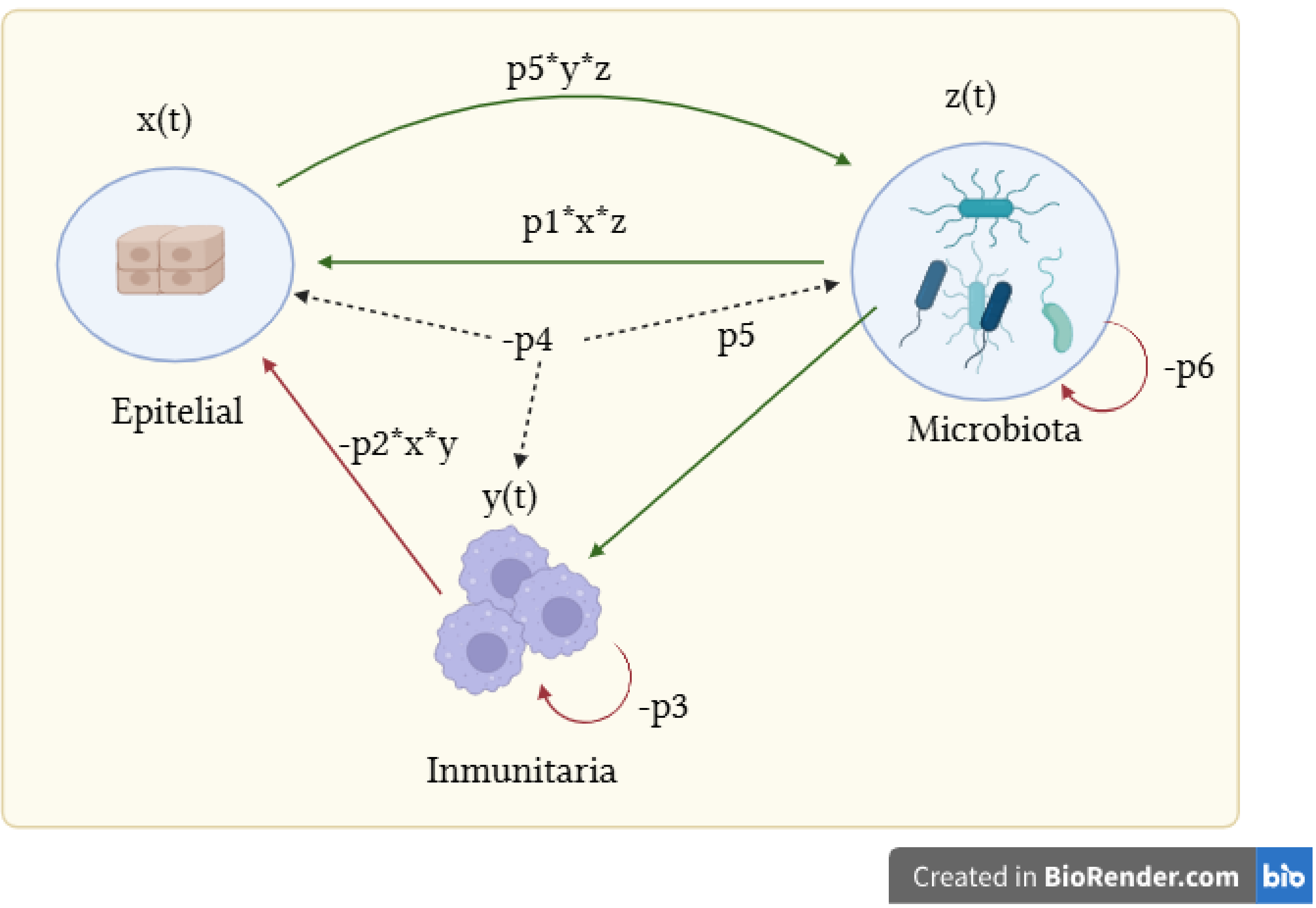


Conclusion.

The extended Lotka-Volterra model, although not all of its parameters were individually significant, achieved an excellent fit to the smoothed data, validating its ability to represent population dynamics. Analysis of the equilibrium points revealed two scenarios. The point (0,0,0) represents the extinction of all populations, a biologically plausible outcome. However, the second equilibrium point yielded a negative value for population x*, indicating a biological impossibility. This suggests that, under the modeled interactions, the system does not tend toward a stable and positive state of coexistence for the three populations. The instability of this point, confirmed by a positive eigenvalue, reinforces that the system would move away from it under any perturbation, leading to continuous dynamics of population change. Long-term simulations (up to 1000 days) illustrate this instability, showing that two populations (y(t) and z(t)) tend toward extinction, while one (x(t)) stabilizes, suggesting exclusion or dominance dynamics. The formulated mathematical model demonstrated high validity in its ability to approximate the experimental data and predict its short-term dynamics. The extremely high Rfit is the main evidence that the model faithfully reproduces the observed variability. The fitted parameters, although not all individually statistically significant, together allow the system of differential equations to replicate biological behavior.

The predictive capacity of the model is a fundamental characteristic of this digital twin. By integrating the system of ODEs with the fitted parameters, the model allows the simulation and projection of future population dynamics beyond the original data range. This extrapolation, while not guaranteeing perfect accuracy over the very long term without additional validation, provides a robust tool for understanding and anticipating trends in the biological system over relevant timeframes.

In conclusion, this digital twin offers an accurate representation of the biological system, validated by its outstanding data fit and predictive capacity. Although the biological inviability of some equilibrium points indicates a lack of coexistence stability in the model, its usefulness lies in the simulation and anticipation of population dynamics.



Functions (Plots)

```
function plotGraficas(t, x1, y1, z1)
    figure('Position', [100, 100, 800, 600]);
    rd = [0.6350 0.0780 0.1840];
    cy = [0.3010 0.7450 0.9330];
    gr = [0.4660 0.6740 0.1880];
    pr = [0.4940 0.1840 0.5560];
    or = [0.8500 0.3250 0.0980];

    subplot(3,1,1)
    set(gca,'FontName','Times New Roman','FontSize',10)
    hold on; box on; grid off;
    plot(t, x1, 'x', 'MarkerSize',5, 'LineWidth',1.5, 'Color', gr)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$x(t)$','Interpreter','latex')
    xlim([0 70]); xticks(0:7.5:70)
    ylim([0 70]); yticks(0:10:70)
    xline(0,'','LineWidth',1,'Color','k')
    yline(0,'--','LineWidth',1,'Color','k')
    title('','Interpreter','latex')


    subplot(3,1,2)
    set(gca,'FontName','Times New Roman','FontSize',10)
    hold on; box on; grid off;
    plot(t, y1, 'x', 'MarkerSize',5, 'LineWidth',1.5, 'Color', cy)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$y_(t)$','Interpreter','latex')
    xlim([0 70]); xticks(0:7.5:70)
    ylim([0 15]); yticks(0:2:15)
    xline(0,'','LineWidth',1,'Color','k')
    yline(0,'','LineWidth',1,'Color','k')
    title('','Interpreter','latex')

    subplot(3,1,3)
    set(gca,'FontName','Times New Roman','FontSize',10)
    hold on; box on; grid off;
    plot(t, z1, 'x', 'MarkerSize',5, 'LineWidth',1.5, 'Color', pr)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$z(t)$','Interpreter','latex')
    xlim([0 70]); xticks(0:7.5:70)
    ylim([0 120]); yticks(0:20:120)
    xline(0,'','LineWidth',1,'Color','k')
    yline(0,'--','LineWidth',1,'Color','k')
    title('','Interpreter','latex')
```

```
end

function plotGraficas1(t, xo, yo, zo)
figure('Position', [100, 100, 800, 600]);
    rd = [0.6350 0.0780 0.1840];
    cy = [0.3010 0.7450 0.9330];
    gr = [0.4660 0.6740 0.1880];
    pr = [0.4940 0.1840 0.5560];
    or = [0.8500 0.3250 0.0980];

    subplot(3,1,1)
    set(gca,'FontName','Times New Roman','FontSize',10)
    hold on; box on; grid off;
    plot(t, xo, 'x', 'MarkerSize',5, 'LineWidth',1.5, 'Color', gr)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$x(t)$','Interpreter','latex')
    xlim([0 70]); xticks(0:7.5:70)
    ylim([0 70]); yticks(0:10:70)
    xline(0,'','LineWidth',1,'Color','k')
    yline(0,'--','LineWidth',1,'Color','k')
    title('','Interpreter','latex')


    subplot(3,1,2)
    set(gca,'FontName','Times New Roman','FontSize',10)
    hold on; box on; grid off;
    plot(t, yo, 'x', 'MarkerSize',5, 'LineWidth',1.5, 'Color', cy)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$y(t)$','Interpreter','latex')
    xlim([0 70]); xticks(0:7.5:70)
    ylim([0 15]); yticks(0:2:15)
    xline(0,'','LineWidth',1,'Color','k')
    yline(0,'--','LineWidth',1,'Color','k')
    title('','Interpreter','latex')

    subplot(3,1,3)
    set(gca,'FontName','Times New Roman','FontSize',10)
    hold on; box on; grid off;
    plot(t, zo, 'x', 'MarkerSize',5, 'LineWidth',1.5, 'Color', pr)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$z(t)$','Interpreter','latex')
    xlim([0 70]); xticks(0:7.5:70)
    ylim([0 120]); yticks(0:20:120)
    xline(0,'','LineWidth',1,'Color','k')
    yline(0,'--','LineWidth',1,'Color','k')
    title('$','Interpreter','latex')
end

function plotModel1(t,x,y,z)
    set(figure(),'Color','w')
```

```
    set(gcf,'Units','Centimeters','Position',[2,2,20,12])
    set(gca,'FontName','Times New Roman')
    fontsize(12,'points')
    c1 = [0.8500, 0.3250, 0.0980];
    c2 = [0.4940, 0.1840, 0.5560];
    c3 = [0.4660, 0.6740, 0.1880];

    subplot(3,1,1)
    hold on; box on; grid off;
    plot(t,x(:,1),'x','MarkerSize',5,'LineWidth',1.5,'Color',c1)
    plot(t,x(:,2),'-','LineWidth',1.5,'Color',c2)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$x_o(t)$ $[cells]$','Interpreter','latex')
    L = legend ('$x_o(t)$','$x_a(t)$');
    set(L,'Interpreter','latex','FontSize',15,'Location','EastOutside','Box','On')
    title(L,'Data')
    xlim([min(t) max(t)])
    ylim([0 70])

    subplot(3,1,2)
    hold on; box on; grid off;
    plot(t,y(:,1),'x','MarkerSize',5,'LineWidth',1.5,'Color',c1)
    plot(t,y(:,2),'-','LineWidth',1,'Color',c2)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$y_o(t)$ $[cells]$','Interpreter','latex')
    L = legend ('$y_o(t)$','$y_a(t)$');
    set(L,'Interpreter','latex','FontSize',15,'Location','EastOutside','Box','On')
    title(L,'Data')
    xlim([min(t) max(t)])
    ylim([0 15])

    subplot(3,1,3)
    hold on; box on; grid off;
    plot(t,z(:,1),'x','MarkerSize',5,'LineWidth',1.5,'Color',c1)
    plot(t,z(:,2),'-','LineWidth',1,'Color',c2)
    xlabel('$t$ $[days]$','Interpreter','latex')
    ylabel('$z_o(t)$ $[cells]$','Interpreter','latex')
    L = legend ('$z_o(t)$','$z_a(t)$');
    set(L,'Interpreter','latex','FontSize',15,'Location','EastOutside','Box','On')
    title(L,'Data')
    xlim([min(t) max(t)])
    ylim([0 110])
end

function plotNormalizadas(t, xo_normalizado, yo_normalizado, zo_normalizado)
figure('Position', [100, 100, 800, 600]);

cy = [0.3010 0.7450 0.9330];
gr = [0.4660 0.6740 0.1880];
pr = [0.4940 0.1840 0.5560];
```

```
subplot(3,1,1);
set(gca,'FontName','Times New Roman','FontSize',10);
hold on; box on; grid off;
plot(t, xo_normalizado, '-', 'MarkerSize', 5, 'LineWidth', 1.5, 'Color', gr);
xlabel('$t$ $[days]$', 'Interpreter', 'latex');
ylabel('$x_{norm}(t)$', 'Interpreter', 'latex');
xlim([0 70]); xticks(0:7.5:70);
ylim([0 1]); yticks(0:0.2:1);
xline(0, '', 'LineWidth', 1, 'Color', 'k');
yline(0, '--', 'LineWidth', 1, 'Color', 'k');
title('', 'Interpreter', 'latex');

subplot(3,1,2);
set(gca,'FontName','Times New Roman','FontSize',10);
hold on; box on; grid off;
plot(t, yo_normalizado, '-', 'MarkerSize', 5, 'LineWidth', 1.5, 'Color', cy);
xlabel('$t$ $[days]$', 'Interpreter', 'latex');
ylabel('$y_{norm}(t)$', 'Interpreter', 'latex');
xlim([0 70]); xticks(0:7.5:70);
ylim([0 1]); yticks(0:0.2:1);
xline(0, '', 'LineWidth', 1, 'Color', 'k');
yline(0, '--', 'LineWidth', 1, 'Color', 'k');
title('', 'Interpreter', 'latex');

subplot(3,1,3);
set(gca,'FontName','Times New Roman','FontSize',10);
hold on; box on; grid off;
plot(t, zo_normalizado, '-', 'MarkerSize', 5, 'LineWidth', 1.5, 'Color', pr);
xlabel('$t$ $[days]$', 'Interpreter', 'latex');
ylabel('$z_{norm}(t)$', 'Interpreter', 'latex');
xlim([0 70]); xticks(0:7.5:70);
ylim([0 1]); yticks(0:0.2:1);
xline(0, '', 'LineWidth', 1, 'Color', 'k');
yline(0, '--', 'LineWidth', 1, 'Color', 'k');
title('', 'Interpreter', 'latex');

sgtitle('', 'Interpreter', 'latex', 'FontSize', 14);

end

function plotprediction(t, xo, yo, zo, t_sol, x_predict, y_predict, z_predict)

figure('Position', [100, 100, 800, 800]);

c_original = [0 0 0];
c_predict = [0.8500 0.3250 0.0980];

subplot(3,1,1);
hold on; box on; grid on;
```

```
plot(t, xo, 'x', 'MarkerSize', 5, 'LineWidth', 1.5, 'Color', c_original);
plot(t_sol, x_predict, '-', 'LineWidth', 2, 'Color', c_predict);
xlabel('$t$ $[days]$', 'Interpreter', 'latex');
ylabel('$x_(t)$', 'Interpreter', 'latex');
title('', 'Interpreter', 'latex');
L = legend ('$x_o(t)$','$x_a(t)$');
    set(L,'Interpreter','latex','FontSize',15,'Location','EastOutside','Box','On')
xlim([0 140]);

ylim_x_min = 0;
ylim_x_max = max(max(xo), max(x_predict));
if ylim_x_max < 70
    ylim_x_max = 70;
end
ylim([ylim_x_min ylim_x_max]);


subplot(3,1,2);
hold on; box on; grid on;
plot(t, yo, 'x', 'MarkerSize', 5, 'LineWidth', 1.5, 'Color', c_original);
plot(t_sol, y_predict, '-', 'LineWidth', 2, 'Color', c_predict);
xlabel('$t$ $[days]$', 'Interpreter', 'latex');
ylabel('$y_(t)$', 'Interpreter', 'latex');
title('', 'Interpreter', 'latex');
L = legend ('$x_o(t)$','$x_a(t)$');
    set(L,'Interpreter','latex','FontSize',15,'Location','EastOutside','Box','On')
xlim([0 140]);
ylim_y_min = 0;
ylim_y_max = max(yo)*1.1;
if ylim_y_max < 1
    ylim_y_max = 1;
end
ylim([ylim_y_min ylim_y_max]);


subplot(3,1,3);
hold on; box on; grid on;
plot(t, zo, 'x', 'MarkerSize', 5, 'LineWidth', 1.5, 'Color', c_original);
plot(t_sol, z_predict, '-', 'LineWidth', 2, 'Color', c_predict);
xlabel('$t$ $[days]$', 'Interpreter', 'latex');
ylabel('$z_(t)$', 'Interpreter', 'latex');
title('', 'Interpreter', 'latex');
L = legend ('$x_o(t)$','$x_a(t)$');
    set(L,'Interpreter','latex','FontSize',15,'Location','EastOutside','Box','On')
xlim([0 140]);
ylim_z_min = 0;
ylim_z_max = max(zo)*1.1;
if ylim_z_max < 1
    ylim_z_max = 1;
end
```

```
ylim([ylim_z_min ylim_z_max]);


sgtitle('', 'Interpreter', 'latex', 'FontSize', 14);

end
```

Functions (Fitting_model)

```
function [mdl,xa,ya,za] = Model1(to,xo,yo,zo,P0)
    x0 = xo(1); y0 = yo(1); z0 = zo(1);
    to = [to;to;to];
    fo = [xo;yo;zo];

    function fi = model(p,t)
        p1 = p(1); p2 = p(2);
        p3 = p(3); p4 = p(4);
        p5 = p(5); p6 = p(6);


        dt = 1E-3;
        t = reshape (t,[],3); t = t(:,1);
        time = (0:dt:max(t))';
        n = round(max(t)/dt);
        x = zeros(n+1,1); x(1) = x0;
        y = zeros(n+1,1); y(1) = y0;
        z = zeros(n+1,1); z(1) = z0;

        for i = 1:n
            [fx,fy,fz] = f(x(i),y(i),z(i));
            xn = x(i) + fx*dt;
            yn = y(i) + fy*dt;
            zn = z(i) + fz*dt;
            [fxn,fyn,fzn] = f(xn,yn,zn);

            x(i+1) = x(i) + (fx + fxn)*dt/2;
            y(i+1) = y(i) + (fy + fyn)*dt/2;
            z(i+1) = z(i) + (fz + fzn)*dt/2;
        end

        function [dx,dy,dz] = f(x,y,z)
            dx = p1*x*z - p2*x*y;
            dy = -p3*y - p4*x*y*z;
            dz = p5*y*z - p6*z;
        end

        xi = zeros(length(t),1);
        yi = zeros(length(t),1);
        zi = zeros(length(t),1);
```

```
        for j = 1:length(t)
            k = abs(time-t(j)) < 1E-9;
            xi(j) = x(k);
            yi(j) = y(k);
            zi(j) = z(k);
        end

        fi = [xi;yi;zi];
    end

    mdl = fitnlm(to,fo,@model,P0);

    fa = mdl.Fitted;
    fn = reshape(fa,[],3);
    xa = fn(:,1); ya = fn(:,2); za = fn(:,3);

    Estimate = table2array(mdl.Coefficients(:,1));
    SE = table2array(mdl.Coefficients(:,2));
    pvalue = table2array(mdl.Coefficients(:,4));
    alpha = 0.05;
    CI95OG = coefCI(mdl,alpha);
    CI95 = abs(CI95OG);
    dof = mdl.DFE;
    tval = tinv(1-alpha/2,dof);
    MoE = SE*tval;
    Parameters = ['p1';'p2';'p3';'p4';'p5';'p6'];
    Results = table(Parameters,Estimate,SE,MoE,CI95,pvalue);

    fprintf(['\nSample size (n): ', num2str(numel(xo))])
    fprintf(['\nParameters to be estimated (pars): ', num2str(numel(P0))])
    fprintf(['\nDegrees of freedom: ', num2str(dof)])
    fprintf(['\nSignificance level (alpha): ', num2str(alpha)])
    fprintf(['\nt-Student value: ', num2str(tval)])
    fprintf(['\nAdjusted R-squared: ', num2str(mdl.Rsquared.Adjusted)])
    fprintf(['\nCorrected AIC (n/pars < 40): 32.0573 ','\n\n'])
    disp(Results)

end
```

Prediction 2t

```
function dxdt = myODESystem(t, X, p1, p2, p3, p4, p5, p6)
x = X(1);
y = X(2);
z = X(3);
dx = p1*x*z - p2*x*y;
dy = -p3*y - p4*x*y*z;
dz = p5*y*z - p6*z;
dxdt = [dx; dy; dz];
```

```
end
```