Simulation Assignment 1

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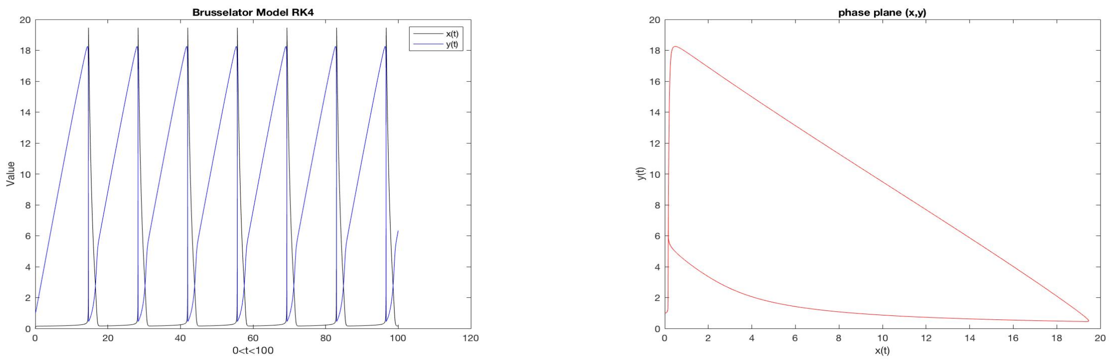
Part A

Question 1

1)Solving model using RK4 approximation with $A = 1.4218, B = 8.7472$

```
clear all
clc
t_init=0;
t_fin=100;
x_init=0;
y_init=1;
h=0.001;
steps=(t_fin-t_init)/h;

A=1.4218;
B=8.7472;

t_vals=zeros(1,steps+1);
x_vals=zeros(1,steps+1);
y_vals=zeros(1,steps+1);
t_vals(1)=t_init;
x_vals(1)=x_init;
y_vals(1)=y_init;

fx=@(t_vals,x_vals,y_vals)(A-B*x_vals+x_vals^2*y_vals-x_vals);
fy=@(t_vals,x_vals,y_vals)(B*x_vals-x_vals^2*y_vals);

for i=2:steps+1
    t_vals(i)=t_vals(i-1)+h;
    k1_x=h*fx(t_vals(i-1),x_vals(i-1),y_vals(i-1));
    k1_y=h*fy(t_vals(i-1),x_vals(i-1),y_vals(i-1));

    k2_x=h*fx(t_vals(i-1)+h/2,x_vals(i-1)+k1_x/2,y_vals(i-1)+k1_y/2);
    k2_y=h*fy(t_vals(i-1)+h/2,x_vals(i-1)+k1_y/2,y_vals(i-1)+k1_y/2);

    k3_x=h*fx(t_vals(i-1)+h/2,x_vals(i-1)+k2_x/2,y_vals(i-1)+k2_y/2);
    k3_y=h*fy(t_vals(i-1)+h/2,x_vals(i-1)+k2_y/2,y_vals(i-1)+k2_y/2);

    k4_x=h*fx(t_vals(i),x_vals(i-1)+k3_x,y_vals(i-1)+k3_y);
    k4_y=h*fy(t_vals(i),x_vals(i-1)+k3_x,y_vals(i-1)+k3_y);
    x_vals(i)=x_vals(i-1)+1/6*(k1_x+2*k2_x+2*k3_x+k4_x);
    y_vals(i)=y_vals(i-1)+1/6*(k1_y+2*k2_y+2*k3_y+k4_y);
end



figure(1)
plot(t_vals,x_vals,'k-')
hold on
plot(t_vals,y_vals,'b-')
title('Brusselator Model RK4')
```

```
xlabel('0<t<100')
ylabel('Value')
legend('x(t)','y(t)')
hold off


figure(2)
plot(x_vals,y_vals,'r-')
title('phase plane (x,y)')
xlabel('x(t)')
ylabel('y(t)')
```



(a) Brusselator Model

(b) phase plane

Figure 1: images for Brusselator Model in 0 <t <100

the reason with interval [0,50] and $h = 0.001$
The result above shows that x(t) and y(t) seem to be periodic functions depending on the length of time interval, which is around 15. And in the phase plane the graph depicts a limit cycle centered at equilibrium point $(x_{eq}, y_{eq}) = (A, B/A) = (1.4218, 6.1522)$, with A=1.4218 and B=8.7472. Besides, it is clear that periodicity and cycling appears when time increase. And to cover at least one period and to be more precise, I need to choose large time interval and small step size, i.e $0 < t < 100, h = 0.001$

Question 2

From taking different initial values of x_0 and y_0, we can see from the figure that as $t \to \infty$ every initial conditions asymptotically close to the limit cycle. Therefore, system centered at $(x_{eq}, y_{eq}) = (A, B/A) = (1.4218, 6.1522)$ is likely to become a global attractor.

```
% Using initial val as parameter and output are values of x(t),y(t) thourgh RK4 algorithmn
function [x_vals,y_vals]=brusselator(x_init,y_init)
t_init=0;
t_fin=50;
h=0.001;
steps=(t_fin-t_init)/h;
% Could adjust value of A and B for futher investigation
A=1.4218;
B=8.7472;
t_vals=zeros(1,steps+1);
x_vals=zeros(1,steps+1);
y_vals=zeros(1,steps+1);
t_vals(1)=t_init;
x_vals(1)=x_init;
y_vals(1)=y_init;

fx=@(t_vals,x_vals,y_vals)(A-B*x_vals+x_vals^2*y_vals-x_vals);
fy=@(t_vals,x_vals,y_vals)(B*x_vals-x_vals^2*y_vals);
```

```
for i=2:steps+1
    t_vals(i)=t_vals(i-1)+h;
    k1_x=h*fx(t_vals(i-1),x_vals(i-1),y_vals(i-1));
    k1_y=h*fy(t_vals(i-1),x_vals(i-1),y_vals(i-1));

    k2_x=h*fx(t_vals(i-1)+h/2,x_vals(i-1)+k1_x/2,y_vals(i-1)+k1_y/2);
    k2_y=h*fy(t_vals(i-1)+h/2,x_vals(i-1)+k1_y/2,y_vals(i-1)+k1_y/2);

    k3_x=h*fx(t_vals(i-1)+h/2,x_vals(i-1)+k2_x/2,y_vals(i-1)+k2_y/2);
    k3_y=h*fy(t_vals(i-1)+h/2,x_vals(i-1)+k2_y/2,y_vals(i-1)+k2_y/2);

    k4_x=h*fx(t_vals(i),x_vals(i-1)+k3_x,y_vals(i-1)+k3_y);
    k4_y=h*fy(t_vals(i),x_vals(i-1)+k3_x,y_vals(i-1)+k3_y);
    x_vals(i)=x_vals(i-1)+1/6*(k1_x+2*k2_x+2*k3_x+k4_x);
    y_vals(i)=y_vals(i-1)+1/6*(k1_y+2*k2_y+2*k3_y+k4_y);
end

end
```

To plot different initial values in one graph

```
% Various initial values
[x_1,y_1]=brusselator(1,3);
[x_2,y_2]=brusselator(2,4);
[x_3,y_3]=brusselator(3,0);
[x_4,y_4]=brusselator(6,8);
[x_5,y_5]=brusselator(3,2);
% Through defined function to accomplish ploting clearly
plot(x_1,y_1,'b-')
hold on
plot(x_2,y_2,'k--')
plot(x_3,y_3,'r-')
plot(x_4,y_4,'g-')
title('(x(t) against y(t) in different initial values)')
xlabel('x(t)')
ylabel('y(t)')
legend('x1=1,y1=3','x2=2,y2=4','x3=3,y3=0','x4=6,y4=8','x5=3,y5=2')
hold off
```

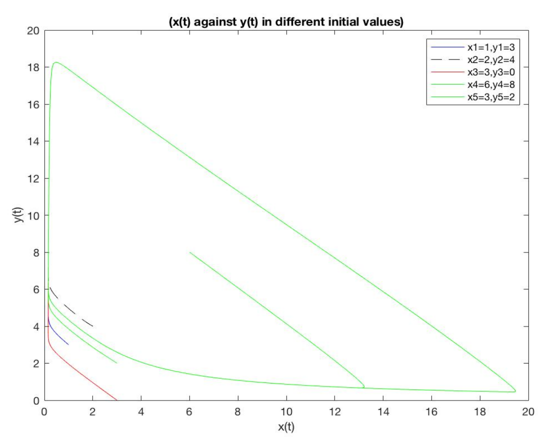


Figure 2: x(t) against y(t) in different initial values

Question 3: SATBILITY OF RK4

RK4 is given by

$$K_1 = h * f(y_n, t_n) \tag{1}$$

$$K_2 = h * f(y_n + \frac{k_1}{2}, t_n + \frac{h}{2}) \tag{2}$$

$$K_3 = h * f(y_n + \frac{k_2}{2}, t_n + \frac{h}{2}) \tag{3}$$

$$K_4 = h * f(y_n + K_3, t_n + h) \tag{4}$$

$$y_{n+1} = y_n + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) \tag{5}$$

To calculate $g_n = \frac{\partial T(y_n,t_n)}{\partial y_n}$,
Let Eq(5),

$$y_{n+1} = y_n + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) = T(y_n, t_n) \tag{6}$$

$$\begin{aligned} g_n &= 1 + \frac{\partial T(y_n,t_n)}{\partial K_1} \times \frac{\partial K_1}{\partial y_n} + \frac{\partial T(y_n,t_n)}{\partial K_2} \times \frac{\partial K_2}{\partial y_n} + \frac{\partial T(y_n,t_n)}{\partial K_3} \times \frac{\partial K_3}{\partial y_n} + \frac{\partial T(y_n,t_n)}{\partial K_4} \times \frac{\partial K_4}{\partial y_n} \\ &= 1 + \frac{1}{6}\frac{\partial K_1}{\partial y_n} + \frac{1}{3}\frac{\partial K_2}{\partial y_n} + \frac{1}{3}\frac{\partial K_3}{\partial y_n} + \frac{1}{6}\frac{\partial K_4}{\partial y_n} \end{aligned}$$

The next step is to calculate partial derivatives separately.

$$\begin{aligned} \frac{\partial K_1}{\partial y_n} &= h * \frac{\partial f(y_n,t_n)}{\partial y_n} \\ \frac{\partial K_2}{\partial y_n} &= h * \frac{\partial f(y_n + \frac{h*f(y_n,t_n)}{2}, t_n + \frac{h}{2})}{\partial y_n} \\ &= h * \frac{\partial f(y_{n+1/2}, t_{n+1/2})}{\partial y_{n+1/2}} * [1 + \frac{h}{2} * \frac{\partial f(y_n,t_n)}{\partial y_n}] \end{aligned}$$

Note: $y_{n+1/2} = y_n + \frac{h}{2} * f(y_n, t_n)$ and use chain rule
For small h we can have

$$\Delta = h * \frac{\partial f(y_n,t_n)}{\partial y_n} \approx h * \frac{\partial f(y_{n+1/2}, t_{n+1/2})}{\partial y_{n+1/2}}$$

Hence,

$$\begin{aligned} \frac{\partial K_1}{\partial y_n} &= \Delta \\ \frac{\partial K_2}{\partial y_n} &= \Delta * [1 + \frac{1}{2}\Delta] = \Delta + \frac{1}{2}\Delta^2 \end{aligned}$$

The same computation can be made for $\frac{\partial K_3}{\partial y_n}$ and $\frac{\partial K_4}{\partial y_n}$

$$\begin{aligned} \frac{\partial K_3}{\partial y_n} &= \Delta[1 + \frac{1}{2}\Delta(1 + \frac{1}{2}\Delta)] = \Delta + \frac{1}{2}\Delta^2 + \frac{1}{4}\Delta^3 \\ \frac{\partial K_4}{\partial y_n} &= \Delta(1 + \Delta + \frac{1}{2}\Delta^2 + \frac{1}{4}\Delta^3) = \Delta + \Delta^2 + \frac{1}{2}\Delta^3 + \frac{1}{4}\Delta^4 \end{aligned}$$

Substitute all derivatives back to equation g_n and get

$$g_n = 1 + \Delta + \frac{1}{2}\Delta^2 + \frac{1}{6}\Delta^3 + \frac{1}{24}\Delta^4 \tag{7}$$

The next step would be to determine the locations in theΔ-plane of the stability boundary (i.e. where$|g| = 1$). The following is the Matlab code which produces the stability region for the RK4 in complex plane.

```
% Specify x range and number of points
clear all
x_init= -3;
x_end =  3;
num_x = 301;
% Specify y range and number of points
y_init = -3;
y_end =  3;
num_x = 301;
% Construct mesh
x_vals  = linspace(x_init,x_end,num_x);
y_vals  = linspace(y_init,y_end,num_x);
[x,y] = meshgrid(x_vals,y_vals);
% Calculate z
DET = x + i*y;
% 4th order Runge-Kutta growth factor
g_n = 1 +DET + 0.5*DET.^2 + (1/6)*DET.^3+(1/24)*DET.^4;
% Calculate magnitude of g
gmag = abs(g_n);
% Plot contours of gmag
contour(x,y,gmag,[1 1],'k-');
hold on
contour(x,y,gmag,[1 1],'k-');
axis([x_init,x_end,y_init,y_end]);
axis('square');
xlabel('Real \Delta r');
ylabel('Imag \Delta i');
title('Stability region for RK4')
hold off
grid on;
```

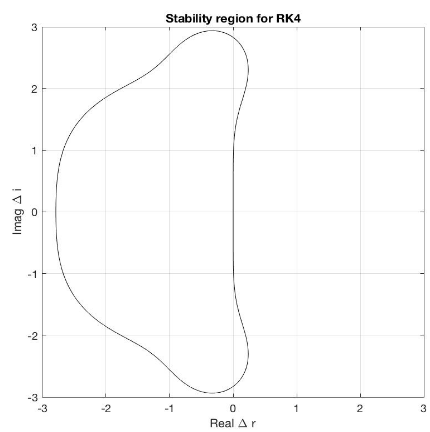


Figure 3: stable within the boundaries

Question 4: ACCURACY OF RK4

I decide to use RK2 algorithm with second order accuracy to verify the accuracy of RK4.
The general idea is built on:

- GTE=$Ch^p = O(h^p)$, where p is the order of the method and h is the step size, C is constant.
- RK2 has 2-nd accuracy for sure.
- If RK4 is 4-th order accuracy then by controlling error in the same level with RK2, approximation at the end of time interval is roughly the same when defining smaller step size for RK2.

Here are some assumptions to make:

- time interval $0 < t < 50$
- error of RK4 $\epsilon_4 = C_4(h_4)^4$, error of RK2 $\epsilon_2 = C_2(h_2)^2$
- control error in the same level $\epsilon_2 \approx \epsilon_4 \approx\ C * 10^{-8}$

Use the above assumptions to determine h_4 and h_2 for RK4 and RK2 considering $p_4 = 4$ and $p_2 = 2$

$$\text{RK4: } \epsilon_4 = C_4 * 10^{-8} \Rightarrow \mathrm{h}_4 = 0.01 = 10^{-2}$$

$$\text{RK2: } \epsilon_2 = C_2 * 10^{-8} \Rightarrow \mathrm{h}_2 = 0.0001 = 10^{-4}$$

Note: it seems reasonable because based on knowledge have learnt, RK2 is 2-nd accuracy which means requiring small step size to make more accuracy.
The next step is to use Matlab code to verify whether the approximation at the end of interval is roughly the same. If it does, then RK4 is 4-th accuracy

Define $A = 1, B = 1.8$ with $x_0 = 0, y_0 = 1$. The following is the RK2 method using matlab code.

```matlab
clear all
t_init=0;
t_fin=50;
x_init=0;
y_init=1;
h=0.01;
steps=(t_fin-t_init)/h;

A=1;
B=1.8;

t_vals_RK2=t_init:h:t_fin;
t_vals_half_RK2=t_init+h/2:h:t_fin-h/2;

x_vals_RK2=zeros(1,steps+1);
x_vals_half_RK2=zeros(1,steps);

y_vals_RK2=zeros(1,steps+1);
y_vals_half_RK2=zeros(1,steps);

x_vals_RK2(1)=x_init;
y_vals_RK2(1)=y_init;

fx=@(t_vals_RK,x_vals_RK,y_vals_RK)(A-B*x_vals_RK+x_vals_RK^2*y_vals_RK-x_vals_RK);
fy=@(t_vals_RK,x_vals_RK,y_vals_RK)(B*x_vals_RK-x_vals_RK^2*y_vals_RK);

for i=2:steps+1

    x_vals_half_RK2(i-1)=x_vals_RK2(i-1)+(h/2)*fx(t_vals_RK2(i-1),x_vals_RK2(i-1),y_vals_RK2(i-1));
    y_vals_half_RK2(i-1)=y_vals_RK2(i-1)+(h/2)*fy(t_vals_RK2(i-1),x_vals_RK2(i-1),y_vals_RK2(i-1));

    x_vals_RK2(i)=x_vals_RK2(i-1)+h*fx(t_vals_half_RK2(i-1),x_vals_half_RK2(i-1),y_vals_half_RK2(i-1));
    y_vals_RK2(i)=y_vals_RK2(i-1)+h*fy(t_vals_half_RK2(i-1),x_vals_half_RK2(i-1),y_vals_half_RK2(i-1));
end

digits(25)
c=x_vals_RK2(end);
d=y_vals_RK2(end);
c_RK2=vpa(c)
D_RK2=vpa(d)
```

By using code I can find the last value of x(t),y(t) in this time interval for both algorithm.

- $x_{RK2}(end) = 1.00343793415757587261794, y_{RK2}(end) = 1.79802667499869883727114 9$
- $x_{RK4}(end) = 1.00430494074452369979155 7, y_{RK4}(end) = 1.79809131126009580370350 7$

It can be seen that for x and y values the approximation is quite similar. Then RK4 is 4-th accurate.

Part B

The stability of Brusselator model can be evaluated through the Jacobian at equilibrium point of first order ODE system.

$$J= \begin{pmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{pmatrix} = \begin{pmatrix} B-1 & A^2 \\ -B & -A^2 \end{pmatrix}$$

In order to evaluate the stability of the stationary state (A, $\frac{B}{A}$), the eigenvalue equation of the Jacobian matrix is expressed as

$$det(J - \lambda I) = 0$$

whereλ is eigenvalue and I is identity matrix. Arranging equation gives characteristic equation

$$\lambda^2 - M\lambda + det(J) = 0 \tag{1}$$

where $M = (B - 1 - A^2)$ and $det(J) = A^2$ just for convenience. The eigenvalues have the form

$$\lambda_{1,2} = \tfrac{1}{2}(M \pm \sqrt{\Delta})$$

where $\Delta = M^2 - 4 * det(J) = (B - 1 - A^2)^2 - 4A^2$

The next step is to discuss value of M which determines the position of characteristic equation, i.e the roots of function, whether real roots or conjugate roots.

case 1:$\Delta > 0, (B - 1 - A^2)^2 - 4A^2 > 0$

There are two eigenvalues and eigenvectors that are real and have same sign. The largest eigenvalue defines the direction in which orbits asymptotically converge or not. Hence, further discussion can be based on the sign of eigenvalues. And there are two cases:
(i) $M < 0, det(J) > 0$
when $M < 0, -\frac{b}{2a} = \frac{M}{2} < 0$ which means both eigenvalues are negative real numbers, i.e $\lambda_2 < \lambda_1 < 0$.In the sketch of orbit,the trajectories directs to equilibrium point and this point is called sink which also shows **asymptotically stable**.Any perturbation to this steady state will monotonically decrease and disappear. Then the equilibrium point is an attractor.

$$M < 0 \Rightarrow B - 1 - A^2 < 0 \Rightarrow B < 1 + A^2$$

(ii) $M > 0, det(J) > 0$
when $M > 0, -\frac{b}{2a} = \frac{M}{2} > 0$ which means both eigenvalues are positive real numbers, i.e $\lambda_2 > \lambda_1 > 0$. So the state is **unstable** and trajectories directs outside. Any perturbation will grow exponentially away from the steady state. Because of the fundamental set of solutions $x(t) = c_1 e^{\lambda_1 t}\eta_1 + c_2 e^{\lambda_2 t}\eta_2$.

$$M > 0 \Rightarrow B - 1 - A^2 > 0 \Rightarrow B > 1 + A^2$$

case 2:$\Delta < 0, (B - 1 - A^2)^2 - 4A^2 < 0$

Since $\Delta < 0$,Eq(1) can only have complex roots, i.e eigenvalues are complex conjugate pairs, and x(t) against y(t) is oscillations. Depending on the sign of real parts of roots, there are 3 subcases to be discussed.
(i)$M > 0, det(J) > 0$
The real parts of eigenvalues are positive.The system diverges from equilibrium point as time increases, and amplitude is large. This is an **unstable focus**.
(ii) $M < 0, det(J) > 0$
The real parts of eigenvalues are negative. In the system,x(t) and y(t) oscillate as it decays back to the equilibrium state. And the system is **asymptotically stable**.
(ii)$M > 0, det(J) > 0$
The real parts of eigenvalues are negative. The system diverges from equilibrium point. This is an **unstable focus**.
(iii)$M = 0, det(J) > 0$
In this case, the eigenvalues are purely imaginary.Orbits around the vortex neither converge nor diverge, but oscillate around it with constant amplitude.It's a stable state.

case 3:$\Delta = 0, (B - 1 - A^2)^2 - 4A^2 = 0$

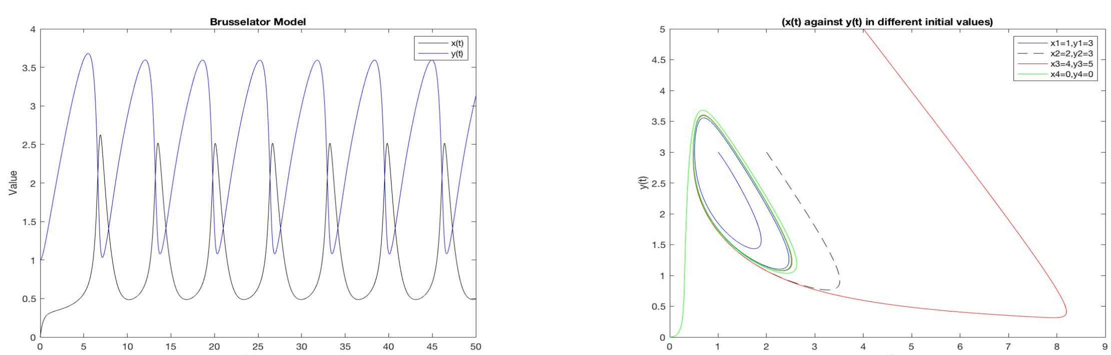
The eigenvalues are both real and equal, $\lambda_1 = \lambda_2 = \lambda$. If $J \neq \lambda I$, only one eigenvector can be determined. It is a straight line, along which the **system asymptotically converges** to equilibrium when the eigenvalue is negative, or **diverges** from equilibrium when the eigenvalue is positive. If $J = \lambda I$, Jcobian becomes diagonal.The equilibrium point is called star point.

From above discussion, we can clearly see that relation between parameter A and B determines the stability of system. I will divide relations into 3 states with various initial values and time interval $0 < t < 50$

Plotting graphs with various A and B

(i) $B > A^2 + 1, A = 1, B = 2.5$

- 2 complex roots with positive real are obtained.$\lambda_{1,2} = 0.25 \pm 0.968i$.
- It's a unstable state
- X and Y against t leading to oscillations.
- Graph of X(t) against Y(t) leading to attractor.



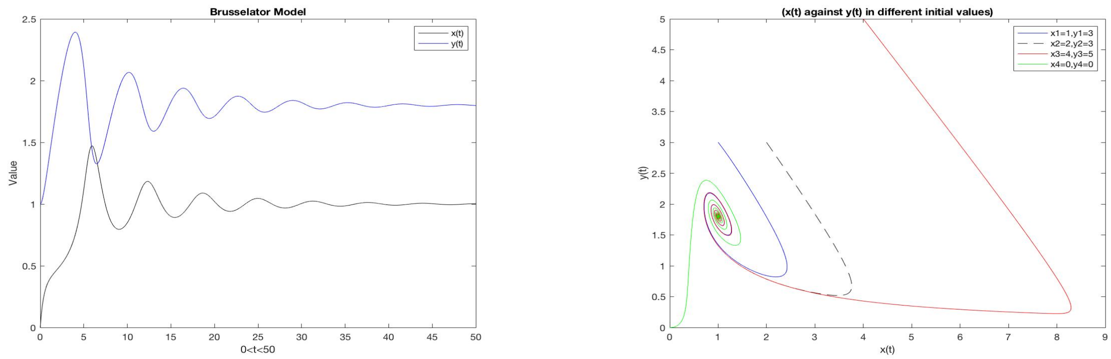
(a) oscillations

(b) phase plane leading to attractor

Figure 4: $A = 1, B = 2.5$

(ii)$B < A^2 + 1, A = 1, B = 1.8$

- 2 complex roots with negative real parts are obtained.$\lambda_{1,2} = -0.1 \pm 0.0.995i$.
- system is asymptotically stable
- X and Y against t leading to damped oscillations.
- Graph of X(t) against Y(t) asymptotically closes to a fixed point



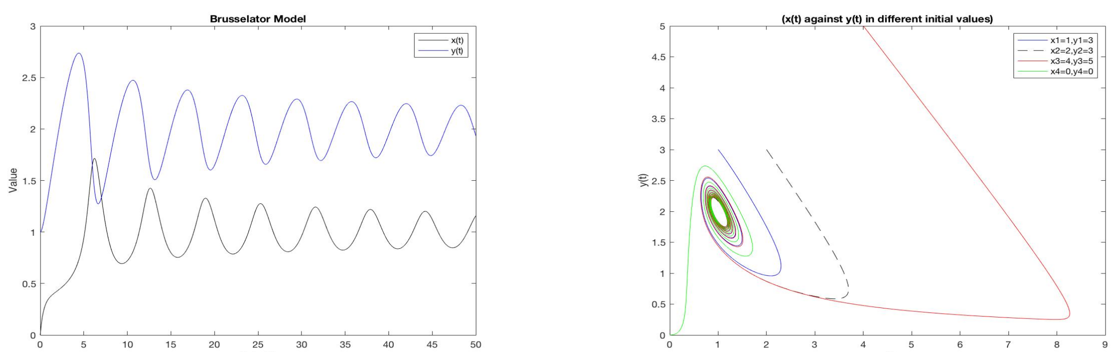
(a) damped oscillations

(b) phase plane approach to equilibrium point

Figure 5: $A = 1, B = 1.8$

(iii)$B = A^2 + 1, A = 1, B = 2$

- 2 complex roots only with imaginary parts are obtained.$\lambda_{1,2} = \pm 1i$.
- system is stable
- X and Y against t leading to damped oscillations.
- Graph of X(t) against Y(t) leading to a limit cycle



(a) damped oscillations

(b) phase plane leading to limit cycle

Figure 6: $A = 1, B = 2$