Assignment-2

1) a) Zeroth order reaction with FK approximation:-

Finding bifurcation diagram by continuition method:-

$$-\theta + \delta e^{\theta} = 0$$

δ = bifurcation parameter

$$f(\theta, \delta) = -\theta + \delta e^{\theta}$$

$$\frac{\partial f}{\partial \theta} = -1 + \delta e^{\theta}$$

$$\frac{\partial f}{\partial \delta} = e^{\theta}$$

$$\frac{d\theta}{d\delta} = \frac{-f_{\delta}}{f_{\theta}} = \frac{-e^{\theta}}{-1+\delta e^{\theta}}$$

Integrate thisequation to get bifurcation diagram

b) Finding bifurcation diagram by Arc continuition method:

Conside θ and δ are functions of arc length 's'

$$\frac{\partial f}{\partial \delta} = f_{\delta} = e^{\theta}$$

$$\frac{\partial f}{\partial \theta} = f_{\theta} = -1 + \delta e^{\theta}$$

$$\frac{d\theta}{ds} = \frac{f_{\delta}}{\sqrt{f_{\theta}^2 + f_{\delta}^2}} = \frac{e^{\theta}}{\sqrt{(-1+\delta e^{\theta})^2 + e^{2\theta}}}$$

$$\frac{d\delta}{ds} = \frac{-f_{\theta}}{\sqrt{f_{\theta}^2 + f_{\delta}^2}} = \frac{-1+\delta e^{\theta}}{\sqrt{e^{2\theta} + (-1+\delta e^{\theta})^2}}$$

Integrate this two equation simultaneously for getting bifurcation diagram by varying 's'.

Question 2: zeroth order reaction in CSTR without FK approximation

2)

a). continuation method:-

$$f(\theta, \delta) = -\theta + \delta e^{\theta/1+\epsilon\theta}$$

$$\frac{\partial f}{\partial \theta} = -1 + \frac{\partial}{\partial \theta}(\delta e^{\theta/1+\epsilon\theta})$$

$$= -1 + \delta e^{\theta/1+\epsilon\theta} \frac{\partial}{\partial \theta}\left(\frac{1+\cancel{\epsilon\theta-\epsilon\theta}}{(1+\epsilon\theta)^2}\right)$$

$$= -1 + \frac{\delta e^{\theta/(1+\epsilon\theta)}}{(1+\epsilon\theta)^2}$$

$$\frac{\partial f}{\partial \delta} = e^{\theta/1+\epsilon\theta}$$

$$\frac{dx}{d\delta} = -\frac{f_\delta}{f_x}$$

$$= \frac{-e^{\theta/1+\epsilon\theta}}{-1 + \frac{\delta e^{\theta/1+\epsilon\theta}}{(1+\epsilon\theta)^2}}$$

solve this Equation for getting full curve.

b) Arc Length continuation method:-

$$\frac{d\theta}{ds} = \frac{f_\delta}{\sqrt{f_\theta^2 + f_\delta^2}}$$

$$= \frac{e^{\theta/1+\epsilon\theta}}{\sqrt{e^{2\theta/1+\epsilon\theta} + \left(-1 + \frac{\delta e^{\theta/1+\epsilon\theta}}{(1+\epsilon\theta)^2}\right)^2}}$$

$$\frac{d\delta}{ds} = \frac{-f_\theta}{\sqrt{f_\theta^2 + f_\delta^2}} = \frac{[-1 + (\delta e^{\theta/1+\epsilon\theta})/(1+\epsilon\theta)^2]}{\sqrt{e^{2\theta/1+\epsilon\theta} + \left(-1 + \frac{\delta e^{\theta/1+\epsilon\theta}}{(1+\epsilon\theta)^2}\right)^2}}$$

Solve this two equation for getting bifurcation diagram

Q3) Finding Initial value by auxillary function method for zeroth order reaction in CSTR

$$f(x) = -x + s e^{x}$$

→ fix the s

→ lets assume $g(x) = x - a$

→ let construct auxillary function as

$$h(x) = t f(x) + (1-t) g(x)$$

→ at $t=0$, $h(x) = g(x_0) = a$

→ at $t=1$, $h(x) = f(x)$

$$\frac{dx}{dt} = \frac{g(x) - f(x)}{t \frac{\partial f}{\partial x} + (1-t)\frac{\partial g}{\partial x}}$$

$$\frac{\partial f}{\partial x} = -1 + s e^{x}$$

$$\frac{\partial g}{\partial x} = 1$$

$$\frac{dx}{dt} = \frac{(x-a) - (-x + s e^{x})}{t(-1 + s e^{x}) + (1-t)}$$

$$= \frac{2x - a - s e^{x}}{t(-1+s e^{x}) + (1-t)}$$

Integrate this equation until $t=1$. The obtained solution is initial value for 'x' at particular 's'.

please find corresponding Codes & Results below.

Please find corresponding MATLAB codes and results below for all questions.

CH5180: Steady State & Dynamic Analysis of Physiochemical Systems

Assignment 2

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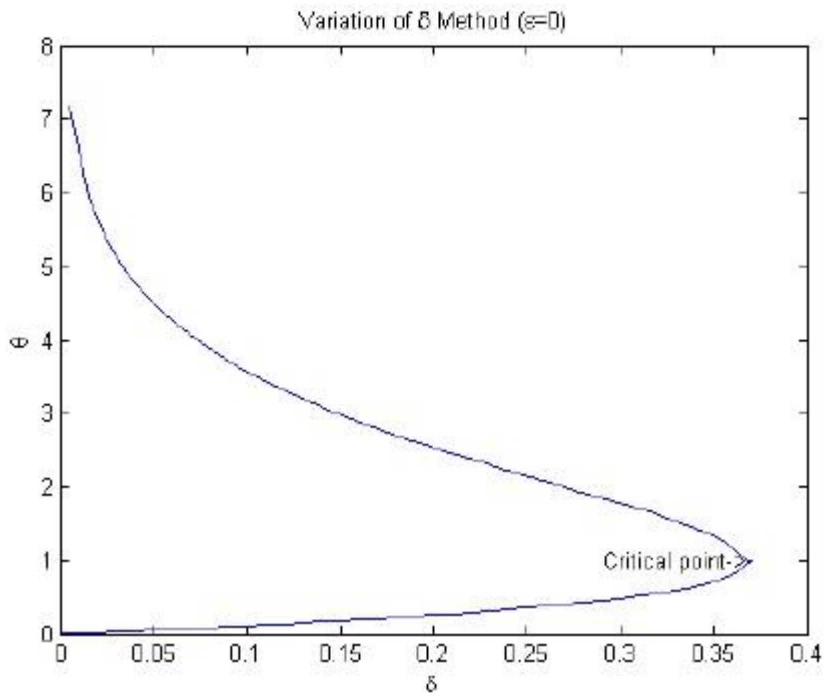
Given below are the MATLAB codes used to generate the bifurcation diagrams of _ varying with _ in di_erent situations, using both the Parameter Variation method and the Arc Length Continuation method.

Question 1

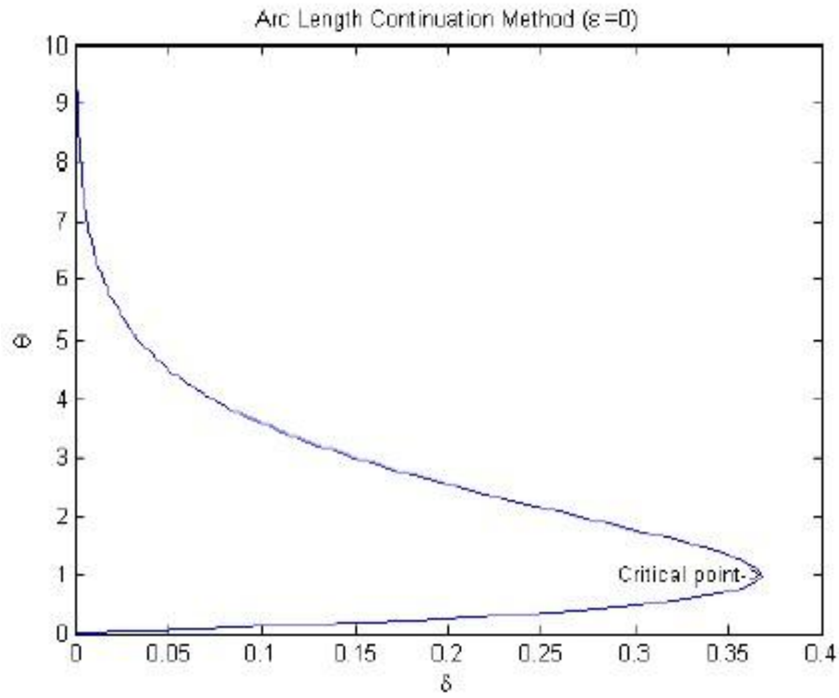
Part (a)

```
clear all;
clc;
pause on;
eps=0;
f=@(t,d) -t+d*exp(t/(1+eps*t)); %steady state function of Theta and delta
dtdd=@(t,d) 1/(exp(-t/(1+eps*t))-d/(1+eps*t)^2); %rate of change of Theta
w.r.t delta
TP=[exp(-1),1; 0.3555,1.2851; -1,1E4; ];
k=1; %set of turning points in graph
step=0.01; %interval size of delta values
n=80; %number of intervals
thet=zeros(n,1); del=zeros(n,1); %creating table
thet(1)=0; del(1)=0; %initial conditions
dir=1; i=2; %determines direction of traversing graph
options=optimset('Display','off'); %To prevent message printing
while i<=n
t=thet(i-1); d=del(i-1);
r=dtdd(t,d); %value of rate of change at given thet,del
if abs(r)*step>1, r=1/step; end %to prevent blowing up
d=d+dir*step; %moving in the appropriate direction
if d<0, break; end
t=t+dir*r*step; %1st order approximate s.s. solution
t=fsolve(@(x) f(x,d),t,options); %s.s. solution for current d
del(i)=d; thet(i)=t; %updating
if dir*(d-TP(k,1))>=0 %When turning point is reached
del(i+1:i+2)=TP(k:k+1,1); thet(i+1:i+2)=TP(k:k+1,2);
i=i+2; k=k+2; dir=-1*dir; %store turning points and reverse direction
end
i=i+1;
end
plot(del(1:i-1),thet(1:i-1));
title('Variation of \delta Method (\epsilon=0)');
xlabel('\delta'); ylabel('\theta');
text(exp(-1),1,'Critical point->','HorizontalAlignment','Right');
```



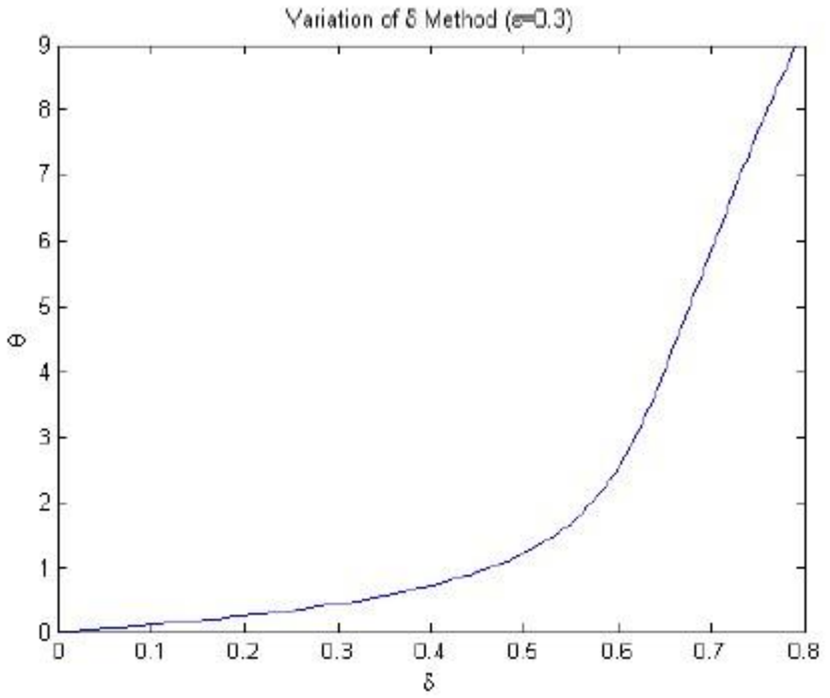
Question 1
Part (b)

```
clear all;
clc;
pause on;
eps=0;
f=@(x,p) -x+p*exp(x/(1+eps*x)); %steady state function
fx=@(x,p) -1+p*exp(x/(1+eps*x))/(1+eps*x)^2; %derivative w.r.t x
fp=@(x,p) exp(x/(1+eps*x)); %derivative w.r.t. p
dxds=@(x,p) (+fp(x,p))/sqrt((fx(x,p))^2+(fp(x,p))^2); %dx/ds
dpds=@(x,p) (-fx(x,p))/sqrt((fx(x,p))^2+(fp(x,p))^2); %dp/ds
ds=0.1; n=100; s=0:ds:n*ds;%determining length of method
par=zeros(n,1); X=zeros(n,1); %creating tables to store values
par(1)=0; X(1)=0; %initial conditions
options=optimset('Display','off'); %to prevent message printing
for i=2:n
par(i)=par(i-1)+ds*dpds(X(i-1),par(i-1)); %1st order approximation of p
X(i)=X(i-1)+ds*dxds(X(i-1),par(i-1)); %1st order approximation of x
par(i)=fsolve(@(p) f(X(i),p),par(i),options); %s.s. solution for given x
end
plot(par,X); %plotting p vs x
title('Arc Length Continuation Method (\epsilon =0)');
xlabel('\delta'); ylabel('\theta');
text(exp(-1),1,'Critical point->','HorizontalAlignment','Right');
```



Question 2
Part (a): Parameter Method (epsilon=0.3)

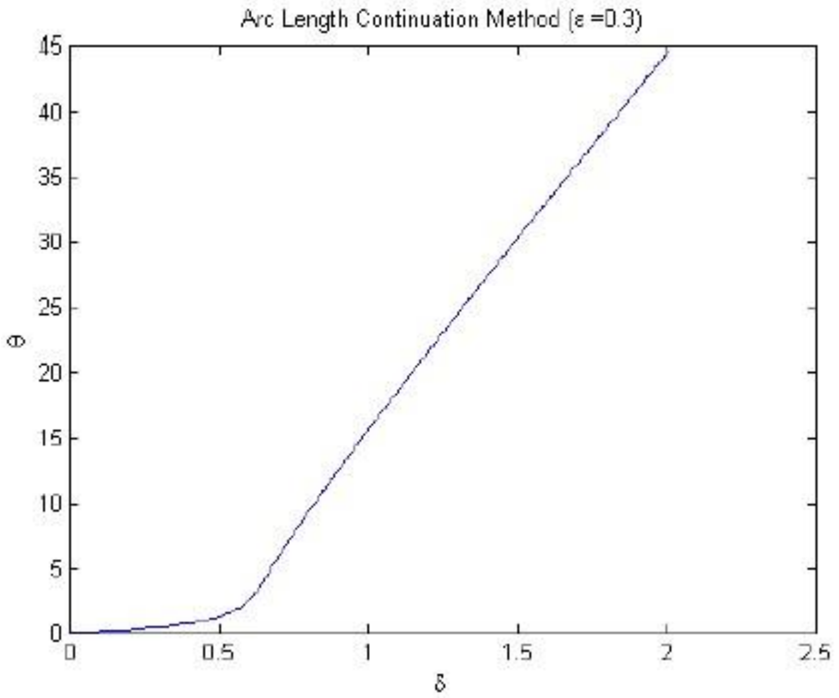
```
clear all;
clc;
pause on;
eps=0.3;
f=@(t,d) -t+d*exp(t/(1+eps*t)); %steady state function of Theta and delta
dtdd=@(t,d) 1/(exp(-t/(1+eps*t))-d/(1+eps*t)^2); %rate of change of Theta
w.r.t delta
step=0.01; %interval size of delta values
n=80; %number of intervals
thet=zeros(n,1); del=zeros(n,1); %creating table
thet(1)=0; del(1)=0; %initial conditions
dir=1; i=2; %determines direction of traversing graph
options=optimset('Display','off'); %To prevent message printing
while i<=n
t=thet(i-1); d=del(i-1);
r=dtdd(t,d); %value of rate of change at given thet,del
if abs(r)*step>1, r=1/step; end %to prevent blowing up
d=d+dir*step; %moving in the appropriate direction
t=t+dir*r*step; %1st order approximate s.s. solution
t=fsolve(@(x) f(x,d),t,options); %s.s. solution for current d
del(i)=d; thet(i)=t; %updating
i=i+1;
end
plot(del,thet);
title('Variation of \delta Method (\epsilon=0.3)');
xlabel('\delta'); ylabel('\theta');
```



Question 2

Part (a): Arc Length Continuation Method (epsilon= 0.3)

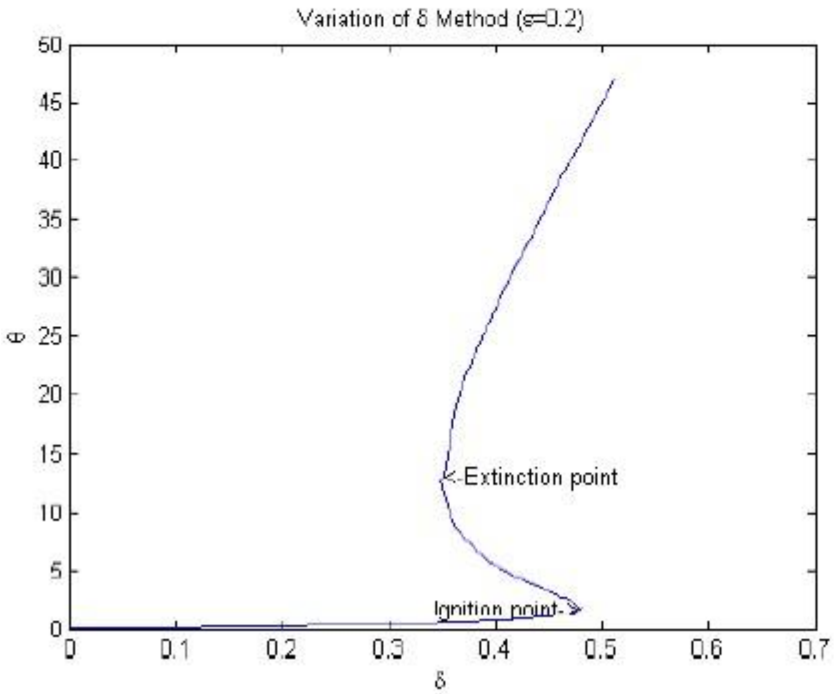
```
clear all;
clc;
pause on;
eps=0.3;
f=@(x,p) -x+p*exp(x/(1+eps*x)); %steady state function
fx=@(x,p) -1+p*exp(x/(1+eps*x))/(1+eps*x)^2; %derivative w.r.t x
fp=@(x,p) exp(x/(1+eps*x)); %derivative w.r.t. p
dxds=@(x,p) (+fp(x,p))/sqrt((fx(x,p))^2+(fp(x,p))^2); %dx/ds
dpds=@(x,p) (-fx(x,p))/sqrt((fx(x,p))^2+(fp(x,p))^2); %dp/ds
ds=0.1; n=450; s=0:ds:n*ds;%determining length of method
par=zeros(n,1); X=zeros(n,1); %creating tables to store values
par(1)=0; X(1)=0; %initial conditions
options=optimset('Display','off'); %to prevent message printing
for i=2:n
par(i)=par(i-1)+ds*dpds(X(i-1),par(i-1)); %1st order approximation of p
X(i)=X(i-1)+ds*dxds(X(i-1),par(i-1)); %1st order approximation of x
par(i)=fsolve(@(p) f(X(i),p),par(i),options); %s.s. solution for given x
end
plot(par,X); %plotting p vs x
title('Arc Length Continuation Method (\epsilon =0.3)');
xlabel('\delta'); ylabel('\theta');
```



Question 2
Part (b): Parameter Method (epsilon=0.2)

```
clear all;
clc;
pause on;
eps=0.2;
f=@(t,d) -t+d*exp(t/(1+eps*t)); %steady state function of Theta and delta
dtdd=@(t,d) 1/(exp(-t/(1+eps*t))-d/(1+eps*t)^2); %rate of change of Theta
w.r.t delta
TP=[0.47945,1.81; 0.4684,2.6688; 0.3513,13.11; 0.3617,18.6677; 10,1E4; ];
k=1; %set of turning points in graph
step=0.01; %interval size of delta values
n=80; %number of intervals
thet=zeros(n,1); del=zeros(n,1); %creating table
thet(1)=0; del(1)=0; %initial conditions
dir=1; i=2; %determines direction of traversing graph
options=optimset('Display','off'); %To prevent message printing
while i<=n
t=thet(i-1); d=del(i-1);
r=dtdd(t,d); %value of rate of change at given thet,del
if abs(r)*step>1, r=1/step; end %to prevent blowing up
d=d+dir*step; %moving in the appropriate direction
t=t+dir*r*step; %1st order approximate s.s. solution
t=fsolve(@(x) f(x,d),t,options); %s.s. solution for current d
del(i)=d; thet(i)=t; %updating
if dir*(d-TP(k,1))>=0 %When turning point is reached
del(i+1:i+2)=TP(k:k+1,1); thet(i+1:i+2)=TP(k:k+1,2);
i=i+2; k=k+2; dir=-1*dir; %store turning points and reverse direction
end
i=i+1;
```

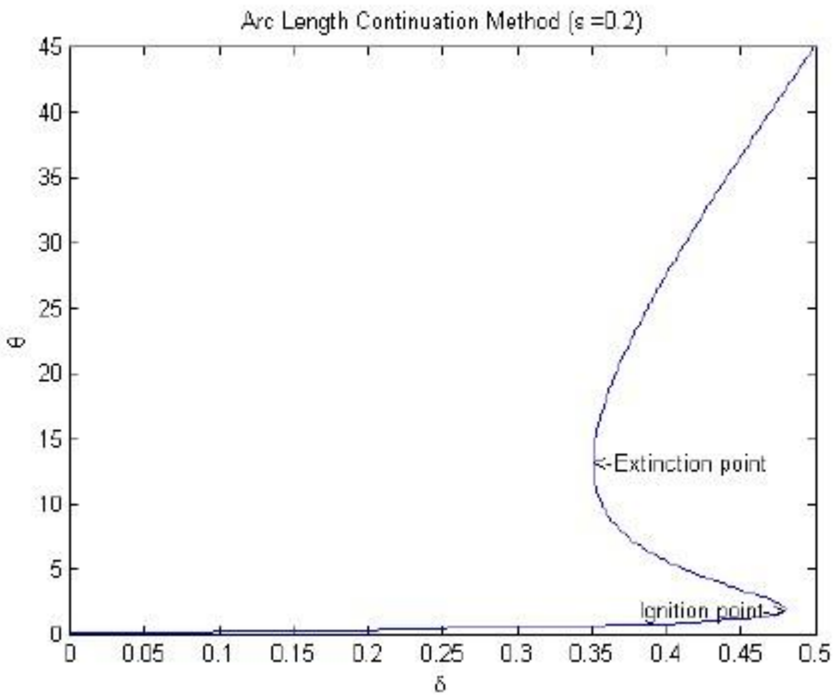
```
end
plot(del,thet);
title('Variation of \delta Method (\epsilon=0.2)');
xlabel('\delta'); ylabel('\theta');
text(0.47945,1.81,'Ignition point->','HorizontalAlignment','Right');
text(0.3513,13.11,'<-Extinction point','HorizontalAlignment','Left');
```



Question 2
Part (b): Arc Length Continuation Method (epsilon= 0.2)

```
clear all;
clc;
pause on;
eps=0.2;
f=@(x,p) -x+p*exp(x/(1+eps*x)); %steady state function
fx=@(x,p) -1+p*exp(x/(1+eps*x))/(1+eps*x)^2; %derivative w.r.t x
fp=@(x,p) exp(x/(1+eps*x)); %derivative w.r.t. p
dxds=@(x,p) (+fp(x,p))/sqrt((fx(x,p))^2+(fp(x,p))^2); %dx/ds
dpds=@(x,p) (-fx(x,p))/sqrt((fx(x,p))^2+(fp(x,p))^2); %dp/ds
ds=0.1; n=450; s=0:ds:n*ds;%determining length of method
par=zeros(n,1); X=zeros(n,1); %creating tables to store values
par(1)=0; X(1)=0; %initial conditions
options=optimset('Display','off'); %to prevent message printing
for i=2:n
par(i)=par(i-1)+ds*dpds(X(i-1),par(i-1)); %1st order approximation of p
X(i)=X(i-1)+ds*dxds(X(i-1),par(i-1)); %1st order approximation of x
```

```
par(i)=fsolve(@(p) f(X(i),p),par(i),options); %s.s. solution for given x
end
plot(par,X); %plotting p vs x
title('Arc Length Continuation Method (\epsilon =0.2)');
xlabel('\delta'); ylabel('\theta');
text(0.47945,1.81,'Ignition point->','HorizontalAlignment','Right');
text(0.3513,13.11,'<-Extinction point','HorizontalAlignment','Left');
```



For the Parameter Variation method, the position of the turning points, as well as at least one point succeeding them, are required to be know a priori to plotting the graph.
For the Arc Length Continuation method, no a priori information is required.
Hence, the Arc Length Continuation method is superior to the Parameter Variation method for plotting a bifurcation diagram.

Q3) Auxillary function

The following is the MATLAB code:

Main file :

```
clc
clear all
%close all

a(1) = 0 ;     % The root for g(x)
a(2) = 0 ;     % Initial time

[t,x] = ode45(@q23func,[0 1],a);

plot(t,x(:,1),'g');
hold on
```

function file:

```
function dy = q23func(t,y)

dy = zeros(2,1);

a = 0;
del = 0.25;

dy(1) = (-(y(1) - a) + y(1) - del*exp(y(1)))/(y(2)*(-1 + del*exp(y(1))) -
(1-y(2)));
dy(2) = 1;
```

Results:

To find the solution for

$$f(x) = -x + \delta e^{x}$$

We define

$$g(x) = x - a$$

And

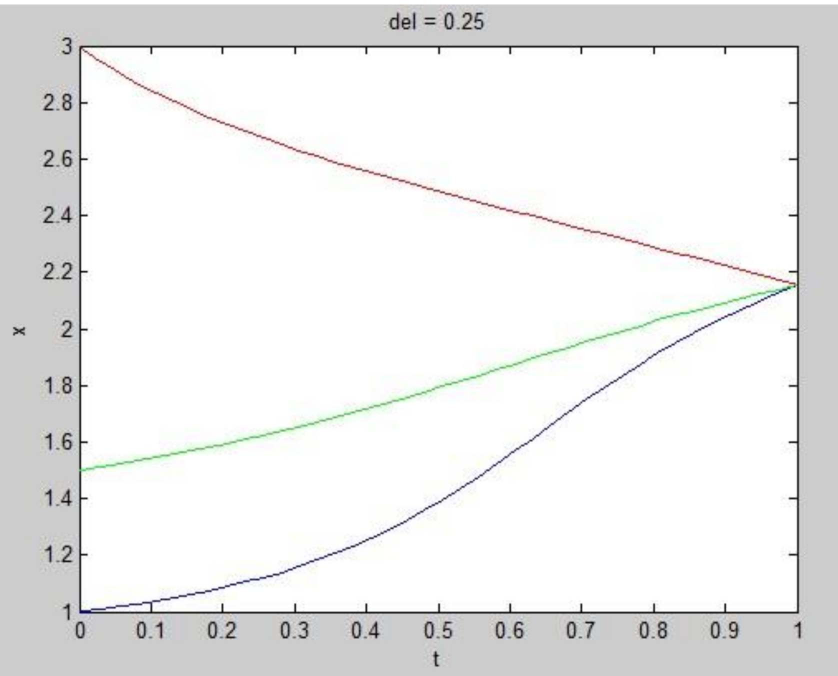
$$h(x,t) = t * f(x) + (1-t) * g(x)$$

To find solution for F(x) we integrate the following equation

$$\frac{dx}{dt} = \frac{g(x) - f(x)}{t\left(\frac{\partial f}{\partial x}\right) + (1-t)\left(\frac{\partial g}{\partial x}\right)}$$

From t = 0 to 1

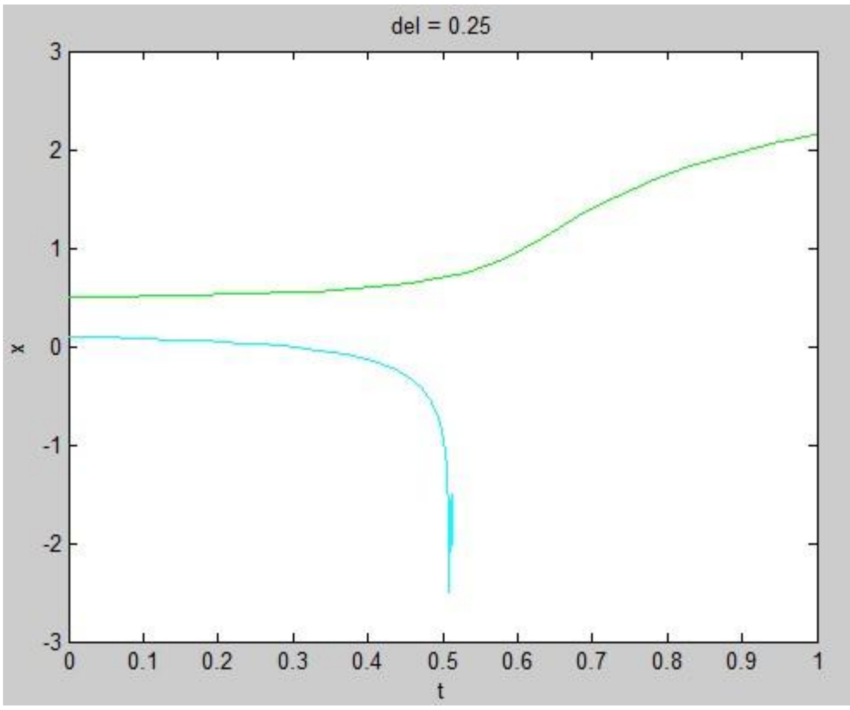
For different values of a we get the following result.



Therefore x = 2.16 is a solution for f(x) = 0

But we know that f(x) has two solutions for del > 0 (and < e^{-1})

If we try a different initial condition

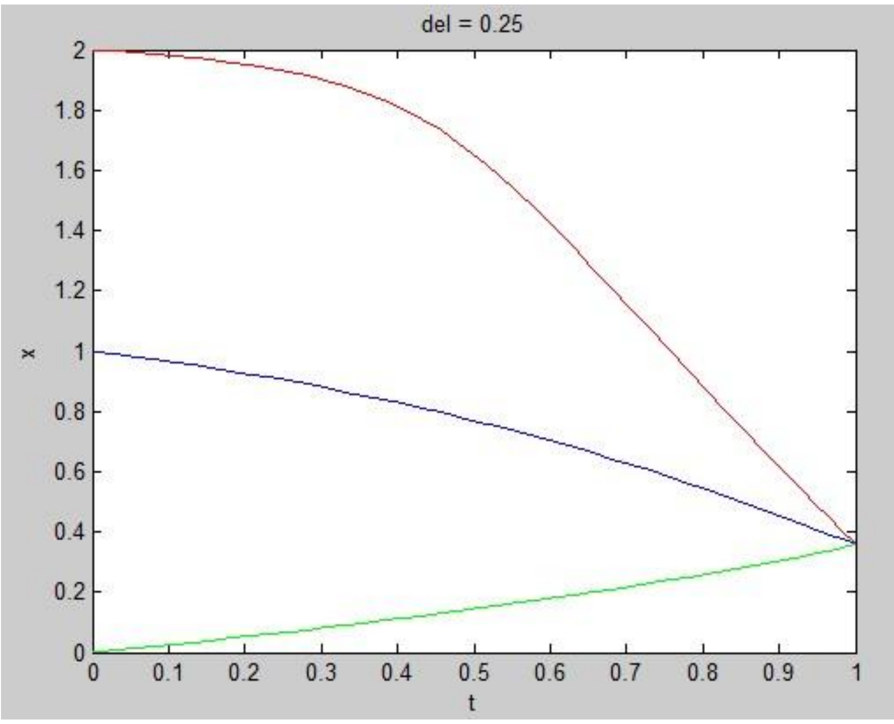


Clearly, it is not giving the second solution, but this issue can be solved by redefining g(x)

Let,

$$g(x) = a - x$$

Now if we solve the equation we get



Therefore the second solution is x = 0.38