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EE430 – Final Exam

Q1)

a) The ordinary differential equations of the dynamic model are given below.

$$\frac{d([X])}{dt} = k_2([XY])(t) + k_4([XE])(t) - k_1([X])(t)([Y])(t) - k_3([X])(t)([E])(t) - k_8([YE])(t)([X])(t)$$

$$\frac{d([Y])}{dt} = k_2([XY])(t) + k_6([YE])(t) - k_1([X])(t)([Y])(t) - k_5([Y])(t)([E])(t) - k_7([XE])(t)([Y])(t)$$

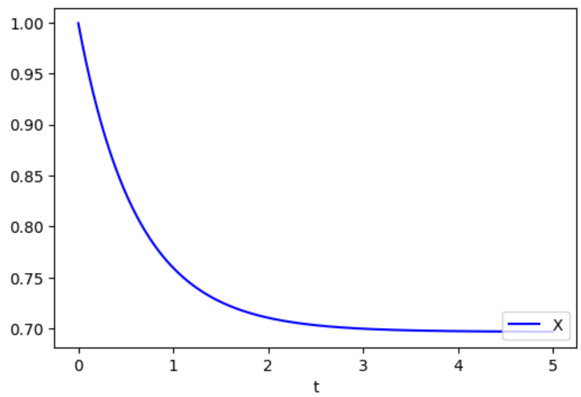
$$\frac{d([E])}{dt} = k_4([XE])(t) + k_6([YE])(t) + k_7([XE])(t)([Y])(t) + k_8([YE])(t)([X])(t) - k_3([X])(t)([E])(t) - k_5([Y])(t)([E])(t)$$

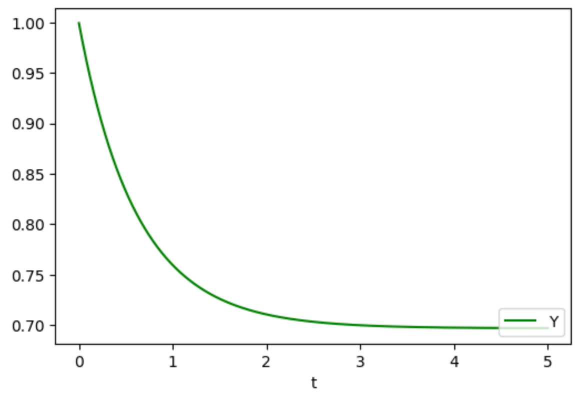
$$\frac{d([XY])}{dt} = k_1([X])(t)([Y])(t)+k_7([XE])(t)([Y])(t) + k_8([YE])(t)([X])(t) - k_2([XY])(t)$$

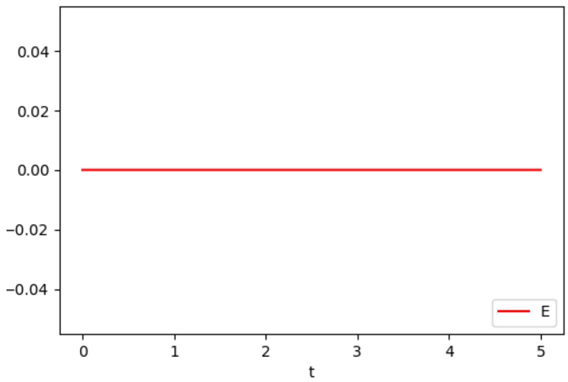
$$\frac{d([XE])}{dt} = k_3([X])(t)([E])(t) - k_4([XE])(t) - k_7([XE])(t)([Y])(t)$$

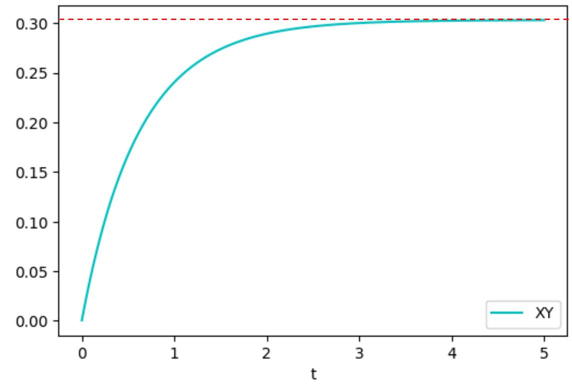
$$\frac{d([YE])}{dt} = k_5([Y])(t)([E])(t) - k_6([YE])(t) - k_8([YE])(t)([X])(t)$$

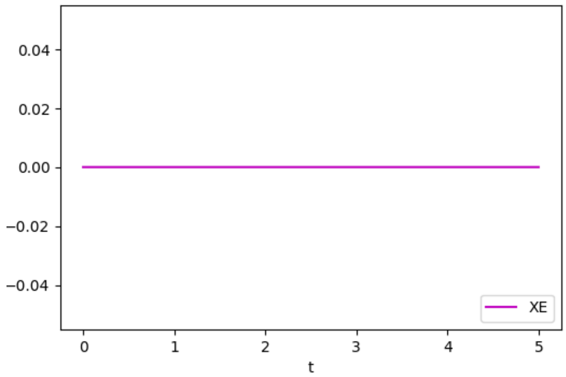
b) The transient behavior of all reactants and moiety groups are given below with initial conditions $[X]|_{t=0} = [Y]|_{t=0} = 1 \; and \; [E]|_{t=0} = [XE]|_{t=0} = [YE]|_{t=0} = [XY]|_{t=0} = 0$.
In addition moeity groups are $G_1 = \{X, XE, XY\}, G_2 = \{Y, YE, XY\}, G_3 = \{E, XE, YE\}$.
Besides, the k values have been chosen experimentally as $k_1 = 0.5, \; k_2 = 0.8, \; k_3 = 0.8, \; k_4 = 1.75, k_5 = 1.2, k_6 = 1.5, k_7 = 2.5, k_8 = 2.2$.
In order to ensure that the XY production in the case of E is greater than in the case of the absence of E, care was taken to ensure that k7 and k8 are greater than the value of k1.

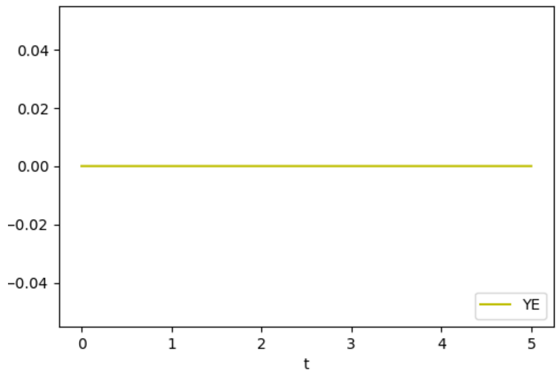


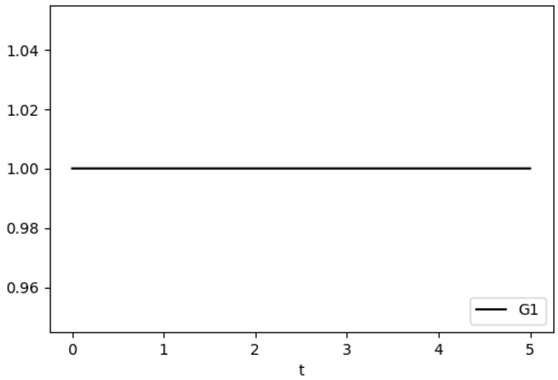


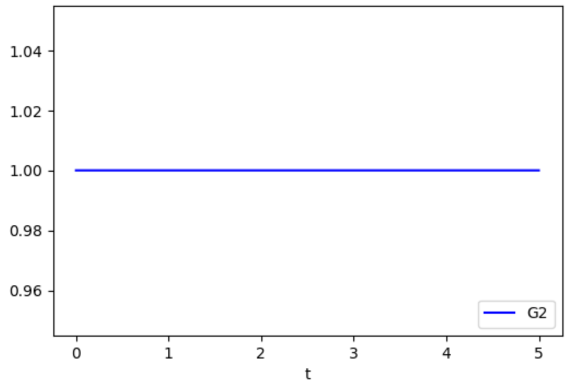


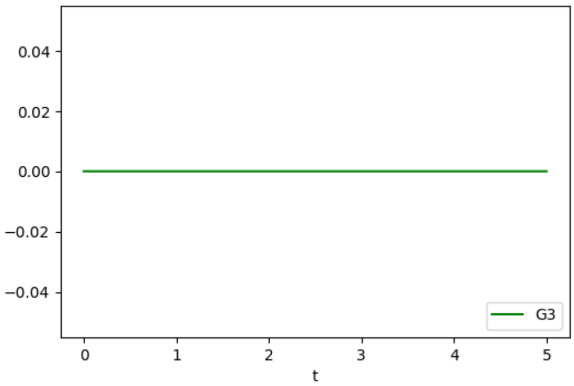






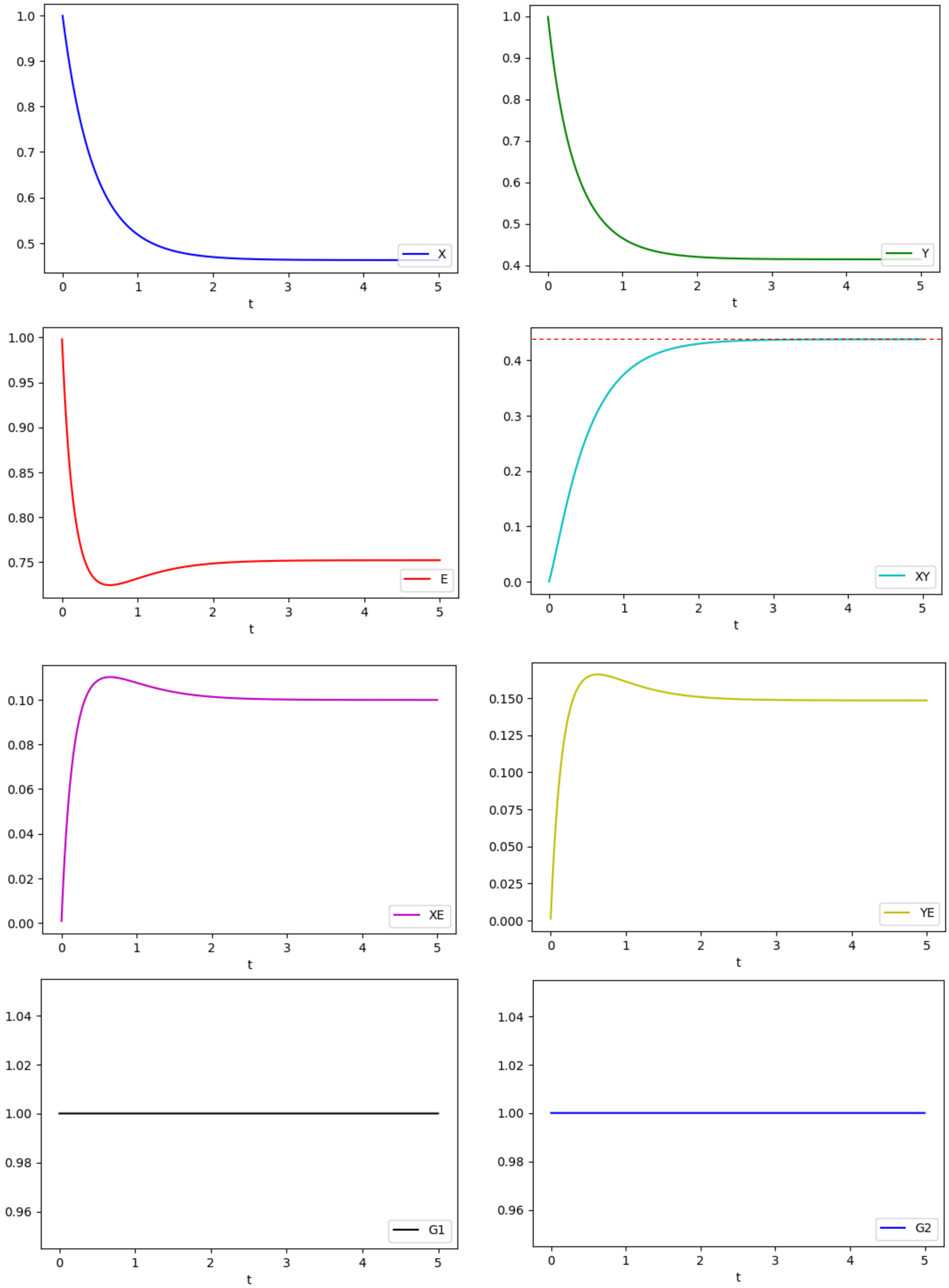


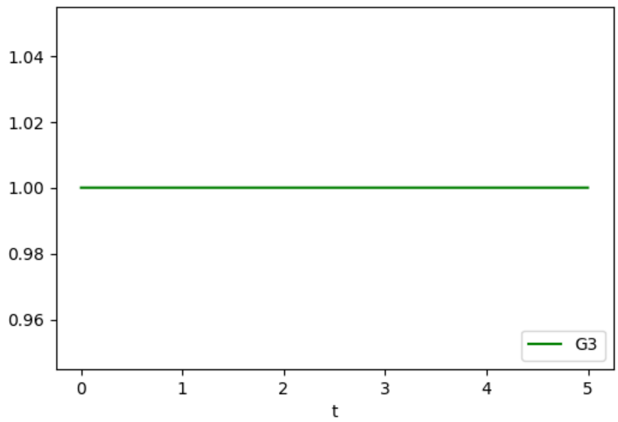




It has been observed that XE, YE are not produced due to the absence of E. The concentration of XY is about 0.30

c) The transient behavior of all reactants and moiety groups are given below with initial conditions $[X]|_{t=0} = [Y]|_{t=0} = [E]|_{t=0} = 1 \; and \; [XE]|_{t=0} = [YE]|_{t=0} = [XY]|_{t=0} = 0$.

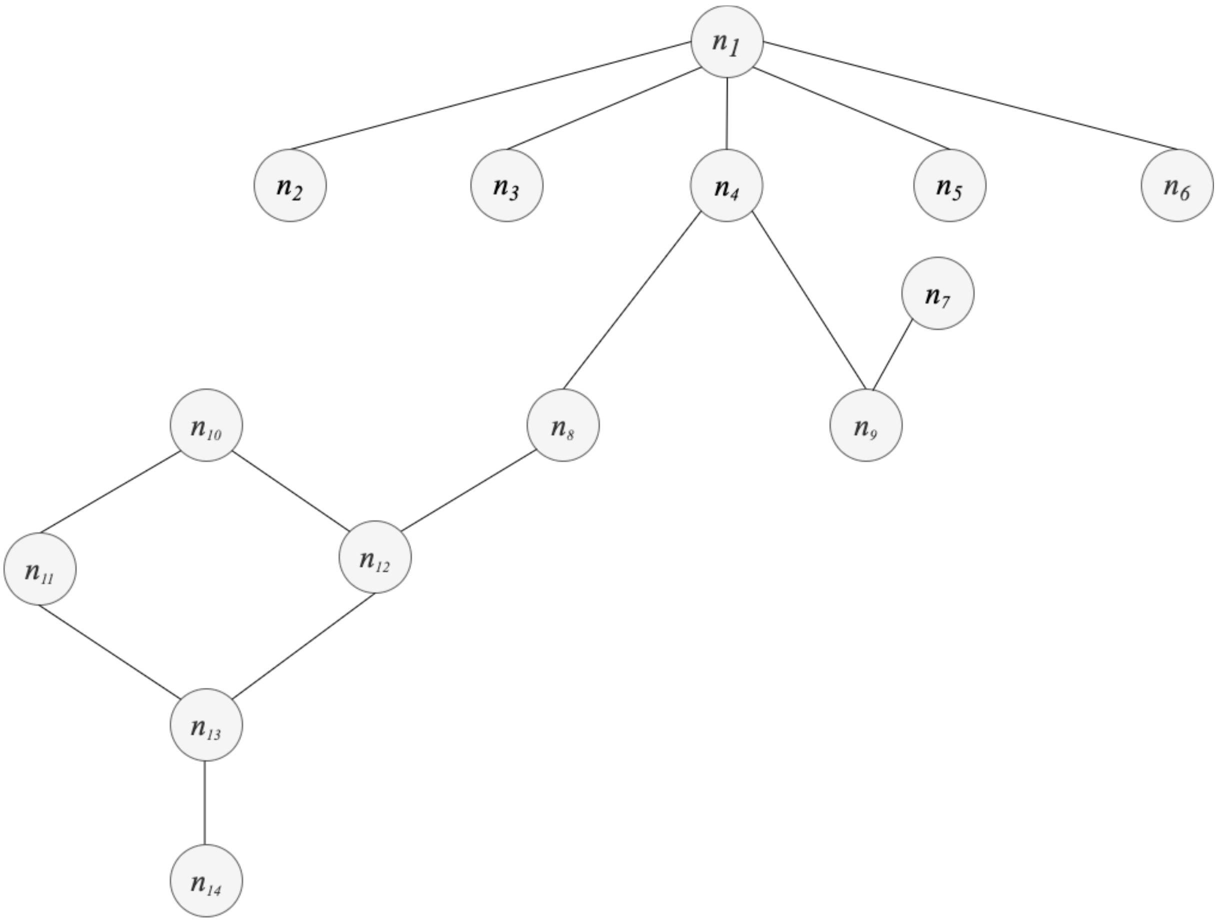




In the case of E, the XY concentration is about 0.44. In the presence of E, the concentration of XY is greater than in the absence of it.

Q2)

a) The graph of the undirected network is given below.



b) Degrees and cluster coefficients were calculated by counting the edges as in below.

$$\deg(n_1) = 5, \deg(n_2) = 1, \deg(n_3) = 1, \deg(n_4) = 3, \deg(n_5) = 1,$$

$$\deg(n_6) = 1, \deg(n_7) = 1, \deg(n_8) = 2, \deg(n_9) = 2,$$

$$\deg(n_{10}) = 2, \deg(n_{11}) = 2, \deg(n_{12}) = 3, \deg(n_{13}) = 3, \deg(n_{14}) = 1.$$

$$C_1 = C_2 = C_3 = C_4 = C_5 = C_6 = C_7 = C_8 = C_9 = C_{10} = C_{11} = C_{12} = C_{13} = C_{14} = 0$$

The value of *e* is 0 for all nodes since there is no edge between the neighbors of the nodes. If the value of e in the cluster coefficient formula given below is 0, the cluster coefficients for all nodes are 0.

$$C = 2\frac{e}{\deg(n_i)(\deg(n_i) - 1)}$$

c) The adjacency matrix of the system id given below.

$$A = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

To get the eigenvector centrality of the graph, computer algorithms were used.(Appendix 2). For the maximum eigenvalue, the eigenvectors are given in below.

$$v = \begin{bmatrix} 0.531 \\ 0.218 \\ 0.218 \\ 0.424 \\ 0.218 \\ 0.218 \\ 0.086 \\ 0.294 \\ 0.209 \\ 0.190 \\ 0.172 \\ 0.292 \\ 0.229 \\ 0.094 \end{bmatrix}$$

Here are the nodes in a decreasing order of centrality;

$$n_4, n_{12}, n_2, n_3, n_5, n_6 n_{11}, n_{14}, n_7, n_{10}, n_9, n_{13}, n_8, n_1.$$

Appendix I

```
import numpy as np
import math
import matplotlib.pyplot as plt

dt = 0.001
t = np.arange(0,5,dt)

X = np.ndarray((len(t)))
Y = np.ndarray((len(t)))
E = np.ndarray((len(t)))
XY = np.ndarray((len(t)))
XE = np.ndarray((len(t)))
YE = np.ndarray((len(t)))
G1 = np.ndarray((len(t)))
G2 = np.ndarray((len(t)))
G3 = np.ndarray((len(t)))

k1 = 0.5
k2 = 0.8
k3 = 0.8
k4 = 1.75
k5 = 1.2
k6 = 1.5
k7 = 2.5
k8 = 2.2

X_i = 1.0
Y_i = 1.0
E_i = 0.0
XY_i = 0.0
XE_i = 0.0
YE_i = 0.0

cind = 0

for ct in t:
  dXdt = k2*XY_i + k4*XE_i - k1*X_i*Y_i - k3*X_i*E_i - k8*YE_i*X_i
  dYdt = k2*XY_i + k6*YE_i - k1*X_i*Y_i - k5*Y_i*E_i - k7*XE_i*Y_i
  dEdt = k4*XE_i + k6*YE_i + k7*XE_i*Y_i + k8*YE_i*X_i - k3*X_i*E_i -
k5*Y_i*E_i
  dXYdt = k1*X_i*Y_i + k7*XE_i*Y_i + k8*YE_i*X_i - k2*XY_i
  dXEdt = k3*X_i*E_i - k4*XE_i - k7*XE_i*Y_i
  dYEdt = k5*Y_i*E_i - k6*YE_i - k8*YE_i*X_i

  X_n = X_i + dt * dXdt
  Y_n = Y_i + dt * dYdt
  E_n = E_i + dt * dEdt
```

```
    XY_n = XY_i + dt * dXYdt
    XE_n = XE_i + dt * dXEdt
    YE_n = YE_i + dt * dYEdt


    X[cind] = X_n
    Y[cind] = Y_n
    E[cind] = E_n
    XY[cind] = XY_n
    XE[cind] = XE_n
    YE[cind] = YE_n

    G1[cind] = format(X_n + XY_n + XE_n, '.2f')
    G2[cind] = format(Y_n + XY_n + YE_n, '.2f')
    G3[cind] = format(E_n + XE_n + YE_n, '.2f')


    X_i = X_n
    Y_i = Y_n
    E_i = E_n
    XY_i = XY_n
    XE_i = XE_n
    YE_i = YE_n

    cind +=1


plt.figure(dpi=100)
plt.plot(t, X, 'b', label='X')
plt.xlabel('t')
plt.legend(loc='lower right')
plt.show()

plt.figure(dpi=100)
plt.plot(t, Y, 'g', label='Y')
plt.xlabel('t')
plt.legend(loc='lower right')
plt.show()

plt.figure(dpi=100)
plt.plot(t, E, 'r', label='E')
plt.xlabel('t')
plt.legend(loc='lower right')
plt.show()

plt.figure(dpi=100)
plt.plot(t, XY, 'c', label='XY')
plt.xlabel('t')
plt.legend(loc='lower right')
```

```python
plt.show()

plt.figure(dpi=100)
plt.plot(t, XE, 'm', label='XE')
plt.xlabel('t')
plt.legend(loc='lower right')
plt.show()

plt.figure(dpi=100)
plt.plot(t, YE, 'y', label='YE')
plt.xlabel('t')
plt.legend(loc='lower right')
plt.show()

plt.figure(dpi=100)
plt.plot(t, G1, 'k', label='G1')
plt.xlabel('t')
plt.legend(loc='lower right')
plt.show()

plt.figure(dpi=100)
plt.plot(t, G2, 'b', label='G2')
plt.xlabel('t')
plt.legend(loc='lower right')
plt.show()


plt.figure(dpi=100)
plt.plot(t, G3, 'g', label='G3')
plt.xlabel('t')
plt.legend(loc='lower right')
plt.show()
```

Appendix II

```
import numpy as np
from numpy import linalg as LA
a=[[0,1,1,1,1,1,0,0,0,0,0,0,0,0], [1,0,0,0,0,0,0,0,0,0,0,0,0,0],
[1,0,0,0,0,0,0,0,0,0,0,0,0,0], [1,0,0,0,0,0,0,1,1,0,0,0,0,0],
[1,0,0,0,0,0,0,0,0,0,0,0,0,0], [1,0,0,0,0,0,0,0,0,0,0,0,0,0],
[0,0,0,0,0,0,0,0,1,0,0,0,0,0], [0,0,0,1,0,0,0,0,0,0,0,1,0,0],
[0,0,0,1,0,0,1,0,0,0,0,0,0,0], [0,0,0,0,0,0,0,0,0,0,1,1,0,0],
[0,0,0,0,0,0,0,0,0,1,0,0,1,0], [0,0,0,0,0,0,0,1,0,1,0,0,1,0],
[0,0,0,0,0,0,0,0,0,0,1,1,0,1], [0,0,0,0,0,0,0,0,0,0,0,0,1,0]]
a = np.array(a, dtype=np.float32)
value, vector = LA.eig(a)

max_index = np.argmax(value)
print(vector[:,max_index])
```