PHYS 310 Homework 2

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1 Network Laplacian

1.1

The Lagrangian associated with N=10 coupled harmonic oscillators is written as follows. Assuming the oscillators have one degree of freedom along the x - direction:

$$\mathcal{L} = KE - PE$$

$$= \frac{1}{2} \sum_{i=1}^{N} m_i \dot{x}_i^2 - \frac{1}{2} \sum_{i=1}^{N-1} k_i (x_{i+1} - x_i)^2$$

To get the equations of motions, apply the Euler-Lagrangian equation along the x degree of freedom where:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}_i} \right) - \frac{\partial \mathcal{L}}{\partial x_i} = 0$$

$$\sum_{i=1}^{N} m_i \ddot{x}_i - \sum_{i=1}^{N} k_i (x_{i+1} - x_i) = 0$$

1.2

To find the Fiedler Vector, it represents the second eigenvalue of the Netowrk's Laplacian which is calculated via:

$$L = D - A$$

Where D is the degree matrix and A is the Adjacency Matrix.

The following code generates the adjacency and degree matrix for N=10 coupled harmonic oscillators. and computes the Network's Laplacian along with its perspective eigenvalues and vectors. Where v_1 is indeed the identity vector of ones.

The second eigenvector v_2 is graphed with respect to the Node index or network partition. And indeed we see half f the values corresponding to negative weights and the other half to positive weights.

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.linalg import eigh
from scipy.integrate import odeint

# Parameters
N = 10
m = 1
k = 1
A = np.diag(np.ones(N - 1), k=1) + np.diag(np.ones(N - 1), k=-1)

D = np.diag(np.sum(A, axis=1))

L = D - A
```

```
eigenvalues, eigenvectors = eigh(L)

v2 = eigenvectors[:, 1]

# Visualize the Fiedler vector
plt.plot(v2, 'o-', label='Fiedler vector')
plt.xlabel('Node Index')
plt.ylabel('Fiedler Vector Value')
plt.legend()
plt.grid()
plt.show()
```

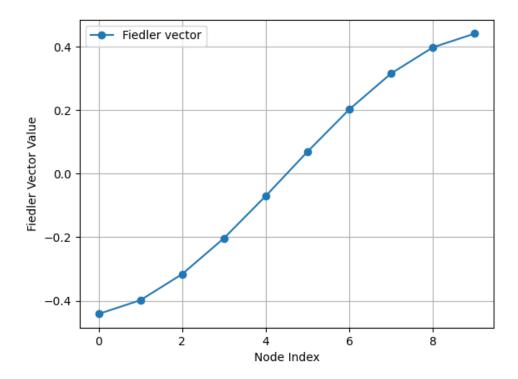


Figure 1: The second eigenvalue with respect to the Node/Network Index

2 Tight-binding

To find the thermodynamical properties of a network depending on which states it is in, the following calculations are carried.

The hamiltonian of the system is defined by the adjacency matrix

$$H = \alpha I + \beta A$$

The associated energies are computed through the eigenvalues of the matrix A

$$E_i = \alpha + \beta \lambda_i$$

Subsequently the problem revolves around computing the following properties of the system depending on the arrangement of the nodes of the network:

- Partition Function: $Z = tr(e^{\beta H}) = \sum_{j} e^{\beta * E_{j}}$
- Entropy $S = -\sum_{j} p_{j} \log(p_{j})$
- Helmholtz Free Energy $F = -\frac{\log Z}{\beta}$
- Gilbert Free Energy $G = F + \frac{\langle E \rangle}{\beta}$

The properties will be computed for the small world, random, and regular models. These will simply change the adjacency matrix generated. The Network package will be used in python to generate the adjacency matrix. Whilst taking the approximation that $\alpha = 0$ and $\beta = \frac{1}{K_B T} = -1$.

The general code that will used to generate the graphs of the partition function, Helmholtz free energy, entropy, and Gilbert free energy as a function of the probabilities is the following:

```
import numpy as np
import matplotlib.pyplot as plt
import networkx as nx
import scipy.sparse
# Define the temperature and other constants
k_B = 1.0 # Boltzmann constant
T = 1.0 # Temperature
# Function to calculate the partition function
def calculate_partition_function(beta, energy_levels):
return np.sum(np.exp(-beta * energy_levels))
# Function to calculate the entropy
def calculate_entropy(probabilities):
return -np.sum(probabilities * np.log(probabilities))
# Function to calculate the Helmholtz free energy
def calculate_helmholtz_free_energy(beta, partition_function):
return -1 / beta * np.log(partition_function)
# Function to calculate the Gibbs free energy
def calculate_gibbs_free_energy(helmholtz_free_energy, average_energy):
return helmholtz_free_energy + 1 / beta * average_energy
for i, p in enumerate(p_values):
```

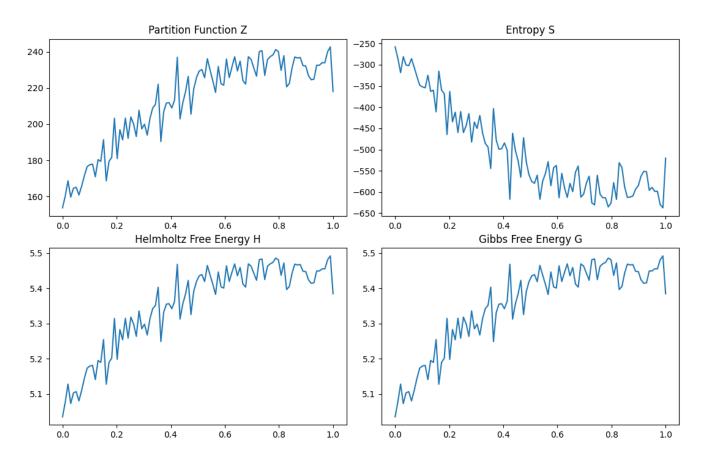
```
adjacency_matrix = ## The code for the adjancey matrix will be given
          \hookrightarrow below
       eigenvalues = np.linalg.eigvals(beta * adjacency_matrix)
       probabilities = np.exp(-beta * (eigenvalues - alpha))
       partition_function= calculate_partition_function(beta, eigenvalues)
       partition_function_values[i] = partition_function
       entropy_values[i] = calculate_entropy(probabilities)
       helmholtz_free_energy_values[i] = calculate_helmholtz_free_energy(beta,
          → partition_function)
       average_energy = np.mean(eigenvalues)
       gibbs_free_energy_values[i] = calculate_gibbs_free_energy(
          → helmholtz_free_energy_values[i], average_energy)
plt.figure(figsize=(12, 8))
plt.grid()
plt.subplot(2, 2, 1)
plt.plot(p_values, partition_function_values)
plt.title('Partition Function Z')
plt.subplot(2, 2, 2)
plt.plot(p_values, entropy_values)
plt.title('Entropy S')
plt.subplot(2, 2, 3)
plt.plot(p_values, helmholtz_free_energy_values)
plt.title('Helmholtz Free Energy H')
plt.subplot(2, 2, 4)
plt.plot(p_values, gibbs_free_energy_values)
plt.title('Gibbs Free Energy G')
plt.tight_layout()
plt.show()
```

What will change throughout the code is how the adjacency matrix is generated for the different models.

2.1 Small-World Network or Watts-Strogatz Model

The code that will generate the adjacency matrix A for the small world model:

The outcome of the code:



2.2 Random Network or Erdos–Renyi Model

The code that will generate the adjacency matrix A for the random network:

```
def generate_random_network(n, p):
    #Same parameters are used in the small world
    G = nx.erdos_renyi_graph(n, p)
    A = nx.adjacency_matrix(G).todense()
    return A
```

The code generates the following graphs:

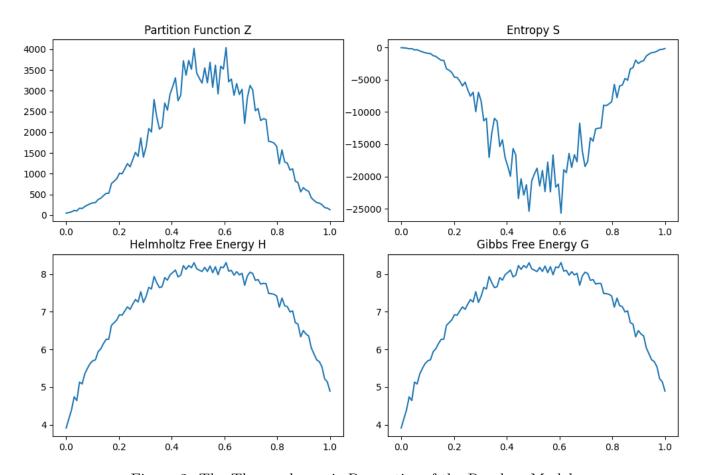


Figure 2: The Thermodynamic Properties of the Random Model

2.3 Regular Network

For Regular networks, the probabilities of neighboring nodes remains the same and the properties remain constant.

The adjancency matrix will be produced as such:

The code outputs a constant measure of the properties that remains constant throughout the network's p.

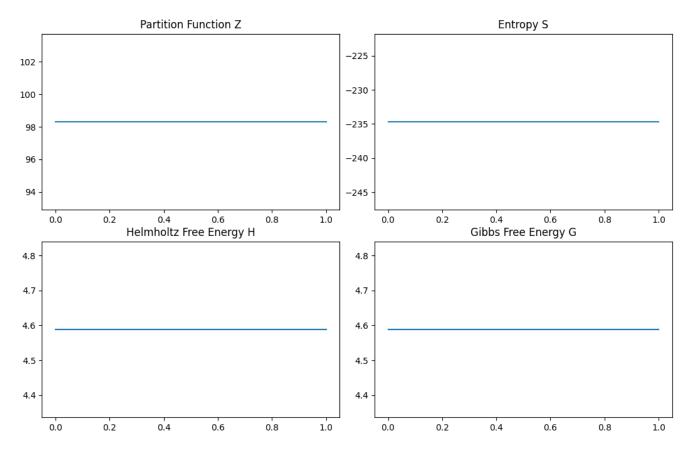


Figure 3: The Thermodynamic Properties of the Regular Model

3 KPZ Universality Class and the Wigner Semi Circle

4 Further Notes

Explored thoroughly!

5 Dynamics

5.1

The Lorenz system of the following function:

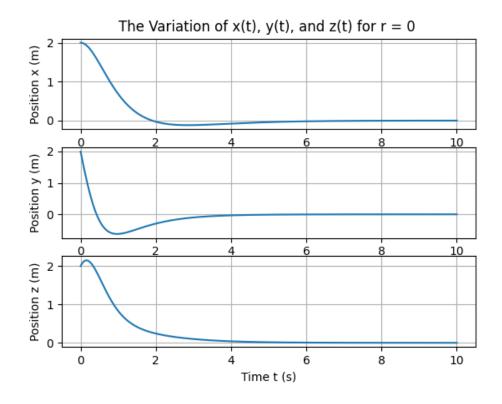
$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = rx - y - xz$$
$$\dot{z} = xy - bz$$

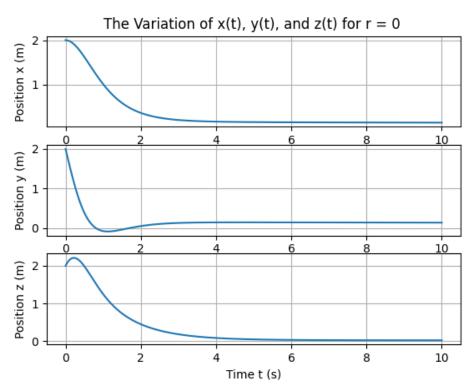
The following code will be used to construct an RK4 approximation to plot x, y, and z in function of time. To assist the code the following parameters were taken: σ , b, r = 1 and the initial conditions of x, y, z = 2.

```
import numpy as np
import scipy as sp
import math
import matplotlib.pyplot as plt
import sympy as sy
# RK 4 Method
\# x' = sigma(y - x)
# y' = rx - y - xz
\# z' = xy - bz
sigma = 1
r = 1
b = 1
def X(x,y,z):
       return sigma*(y - x)
def Y(x,y,z):
       return r*x - y - x*z
def Z(x,y,z):
       return x*y - b*z
t=np.linspace(0,10,100)
xpoints=[]
ypoints=[]
zpoints=[]
h=t[1]-t[0]
x=2
y=2
z=2
for i in range(0,len(t)):
       xpoints.append(x)
       ypoints.append(y)
       zpoints.append(z)
       m1 = h*X(x,y,z)
       k1 = h*Y(x,y,z)
       11 = h*Z(x,y,z)
       m2 = h* X(x+m1/2,y+k1/2,z+11/2)
       k2 = h* Y(x+m1/2,y+k1/2,z+11/2)
       12 = h * Z(x+m1/2,y+k1/2,z+11/2)
       m3 = h* X(x+m2/2,y+k2/2,z+12/2)
       k3 = h* Y(x+m2/2,y+k2/2,z+12/2)
       13 = h * Z(x+m2/2,y+k2/2,z+12/2)
```

```
m4 = h* X(x+m3,y+k3,z+13)
              k4 = h* Y(x+m3,y+k3,z+13)
               14 = h * Z(x+m3,y+k3,z+13)
              x += (m1 + 2*m2 + 2*m3 + m4)/6
              y += (k1 + 2*k2 + 2*k3 + k4)/6
               z += (11 + 2*12 + 2*13 + 14)/6
plt.subplot(3,1,1)
plt.plot(t,xpoints)
plt.xlabel('Time t (s)')
plt.ylabel('Position x (m)')
plt.grid()
plt.subplot(3,1,2)
plt.plot(t,ypoints)
plt.xlabel('Time t (s)')
plt.ylabel('Position y (m)')
plt.grid()
plt.subplot(3,1,3)
plt.plot(t,zpoints)
plt.xlabel('Time t (s)')
plt.ylabel('Position z (m)')
plt.grid()
plt.show()
```

The code outputs the following graphs that shows the evolution of x, y, and z in time space. This will be done for three perspective values of the bifurcation coefficient r. It will be done for r = 0, 1, 5





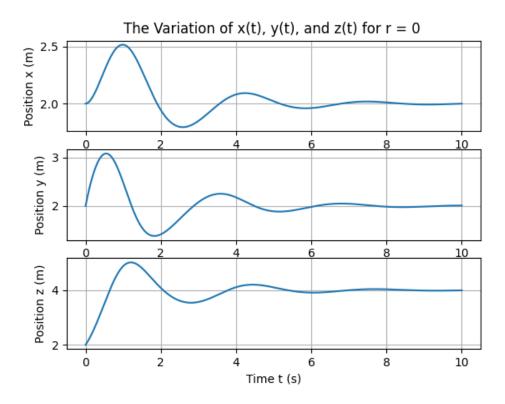


Figure 4: The solution of the Lorenz System done via RK4

If one wants to visualize the Lorenz attractor in 3d projection with the evolution of x, y, and z. The code is executed as such:

Here the literature suggests to choose these parameters: $\sigma = 10, b = 8/3, r = 28$

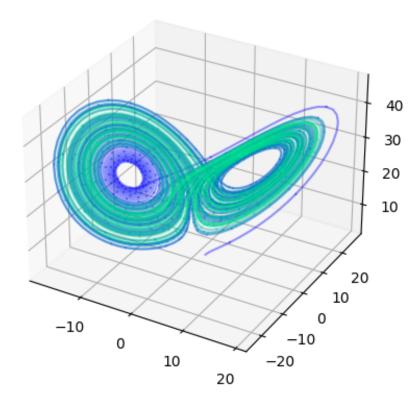


Figure 5: The Lorenz Atrractor plotted in 3d Projection

5.2

To find the fixed points, we import fsolve from scipy.optimize, the code will thus compute the two fixed points numerically.

The code that will execute the operation:

The code outputs the two fixed points: (x = 0, y = 0, z = 0) and (x = 2.008566218225481, y = 2.008566218225481, z = 1.0100387285512362)

These values are consistent even when the parameters σ , b, r are changed.

Setting the bifurcation parameter $r > r_c > 1$, a pair of fixed points points other than the origin emerge. To do so set each derivative to zero.

• $\frac{dx}{dt} = 0 \to \sigma(y - x) = 0 \to x = y$

 $\frac{dz}{dt} = 0 \to x^2 - bz = 0 \to z = \frac{x^2}{b}$

 $\frac{dy}{dt} = 0$ $x(r-1) - xz = 0 \ (\div x)$ (r-1) - z = 0 $-\frac{x^2}{b} + (r-1) = 0 \ (\times -b)$ $x^2 - b(r-1) = 0$

The resulting quadratic equation results in:

$$x^{\pm} = \pm \sqrt{b(r-1)}$$

This corresponds to the following two fixed points:

$$x^* = y^* = \pm \sqrt{b(r-1)}, \ z = r-1$$

To test for stability we compute the Jacobian of the matrix and plug in one of the fixed points.

$$\begin{pmatrix} \frac{d\dot{x}}{dx} & \frac{d\dot{x}}{dy} & \frac{d\dot{x}}{dz} \\ \frac{d\dot{y}}{dx} & \frac{d\dot{y}}{dy} & \frac{d\dot{y}}{dz} \\ \frac{d\dot{z}}{dx} & \frac{d\dot{z}}{dy} & \frac{d\dot{z}}{dz} \end{pmatrix} = \begin{pmatrix} -\sigma & \sigma & 0 \\ r - z & -1 & -x \\ y & x & -b \end{pmatrix} = \begin{pmatrix} -\sigma & \sigma & 0 \\ 1 & -1 & -\sqrt{b(r-1)} \\ \sqrt{b(r-1)} & \sqrt{b(r-1)} & -b \end{pmatrix}$$

To get the stability of the fixed points, take the special values of the parameters σ, b, r and compute the eigenvalues of the Jacobian with the np.linalg.eigvals() function:

```
import sympy as sp
import numpy as np
# Define the symbolic variables

sigma = 10
b = 8/3
r = 28
A = np.array([
[-sigma, sigma, 0],
[1, -1, -np.sqrt(b*(r-1))],
[np.sqrt(b*(r-1)), np.sqrt(b*(r-1)), -b]
])

eigenvalues = np.linalg.eigvals(A)

print("Eigenvalues:", eigenvalues)
```

The code outputs the following eigenvalues: Eigenvalues: [-13.85457791 + 0.j], [0.09395562+10.19450522j], and [0.09395562-10.19450522j].

One real and a pair of imaginary eigenvalues. The pitchfork bifurcation usually results in a stable fixed point around the center and a pair of unstable fixed points when the bifurcation parameter is above the bifurcation point. Similar to this case when $r > r_c$ or r > 1.

5.3

To get the Liaponov exponent, we first pick an initial point with coordinates (1, 1, 1). Then we pick a point direct next to it with an additional factor (1 + 1e - 6, 1 + 1e - 6, 1 + 1e - 6). Then we attempt to linearize the equation as such:

$$\delta = \delta_0 e^{\lambda t}$$
$$\ln(\delta) = \lambda t + \ln(\delta)$$

One can plot the variation of the distance between the two points varies with each iteration, then the slope of the linear fit would the exponent. Note that this exponent is unique to the initial conditions, iteration, and parameters chosen. The code to compute the exponent is as such:

For the following conditions: $\sigma = 10, r = 28, b = 8/3, x0 = y0 = z0 = 1$, the code outputs the following Lyaponov exponent: -0.0031681728464301416

5.4

To find the Lorenz Map the following code is executed were the $find_peaks$ function is utilized to find the maxima of z by their perspective indices in the vector. Then a vector is constructed with the maximum points of z and the point directly after it in the vector as such:

```
from scipy.signal import find_peaks
t_values = np.linspace(0, 50, 5000)
z_values = states[:, 2]

maxima_indices, _ = find_peaks(z_values)
#print(maxima_indices)

z_n = z_values[maxima_indices]
z_n_plus_1 = z_values[maxima_indices + 1]

plt.figure(figsize=(8, 6))
plt.plot(z_n, z_n_plus_1, 'o', markersize=2)
plt.title('Lorenz Map')
plt.xlabel('z_n')
plt.ylabel('z_{n+1}')
plt.grid()
plt.show()
```

The output is the following graph. Unfortunately, it doesn't look close to what the literature suggests. I tried varying the parameters, initial conditions, and time scales but the plot looks identical just with more dots on the plot.

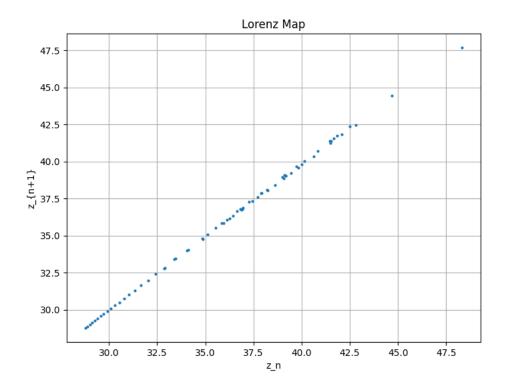


Figure 6: Lorenz Map $\rightarrow z_{n+1}$ vs. z_n

6 Logistic Map

6.1

The Logistic Map is represented by the following iterative function:

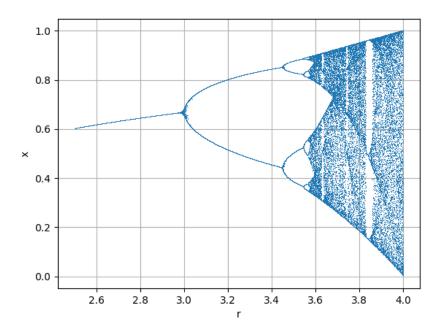
$$x_{n+1} = rx(1 - x_n)$$

To find the chaotic regime, arbitrarily iterate over values of r from 2.5 to 4, the logistic map will be executed as follows:

```
import numpy as np
import scipy as sp
import math
import matplotlib.pyplot as plt
import sympy as sy

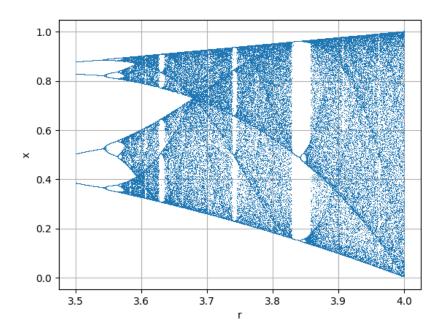
xpoints = [] # Storing the x points
R = np.linspace(3.5,4,100000)

for r in R:
```



6.2

The obvious chaotic regime is seen to be around the values of r between 3.5 and 4. To zoom in to that regime and to find its constituents, the zoomed in figure is as such:

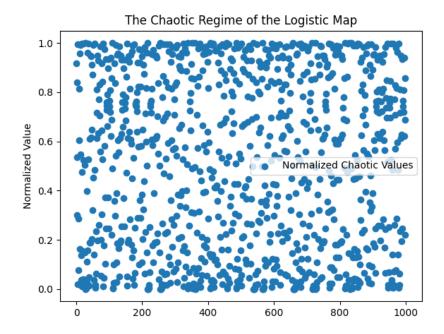


The values of function around r=4 show proper chaos that the values can be used as a random number generator.

To do that, first one needs to normalize the values.

The Chaotic regime is developed by:

The given plot is of the following:



Randomly picking a value from these x values will generate a random number that is normalized between 0 and 1.

6.3

To compute the $\delta = \frac{\Delta_{n+1}}{\Delta_n}$ and $\alpha = \frac{d_{n+1}}{d_n}$ values, we require to know at which value of r the period doubles. The following code will compute at what values of r we experience the first period doubling:

```
import numpy as np
import scipy as sp
import math
import matplotlib.pyplot as plt
import sympy as sy
xpoints = np.zeros((1000,3))
bifurcation_points = []
R = np.linspace(2.85, 3.15, 1000)
for i in range(len(R)):
       xpoints[i,0] = R[i]
       x = np.random.random()
       x_points = []
       for j in range(500):
              x = R[i]*x*(1-x)
               x_points.append(x)
               if round(x_points[197],2) != round(x_points[198],2):
               bifurcation_points.append(R[i])
```

Which shows that at r = 2.9794294294294295 The first period doubling takes place. Unfortunately I couldn't figure out how to write a code that will break when another period doubling takes place. Thus x will oscillate between 4 different values rather than 2. The if statement wouldn't work to break when 4 different values of x are detected.

7 What do 1D maps have to do with Science?

7.1

The Rossler system that constitutes the following PDEs:

$$\dot{x} = -y - z$$

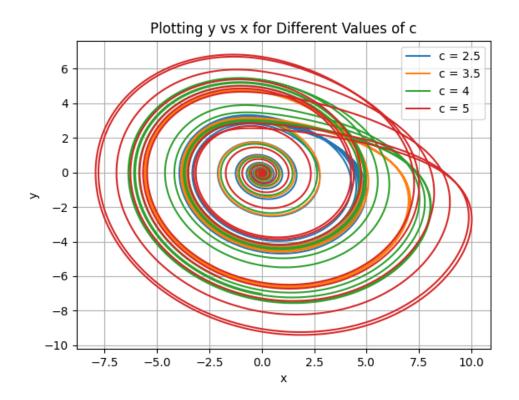
$$\dot{y} = x + ay$$

$$\dot{z} = b + z(x - c)$$

The system will be solved using scipy package and $solve_ivp$ function

```
return [X,Y,Z]
#Initial conditions
xyz0 = [1,1,1]
def solve_rossler(c):
       # Initial conditions
       xyz0 = [0, 0, 0]
       t=(0,100)
       # Solve the system
       sol = solve_ivp(rossler, t, xyz0, args=(c,), dense_output=True)
       return sol
for c in c:
       sol = solve_rossler(c)
       t_eval = np.linspace(0, 100, 10000)
       xyz = sol.sol(t_eval)
       plt.plot(xyz[0], xyz[1], label=f'c = {c}')
plt.title('Plotting y vs x for Different Values of c')
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
plt.grid()
plt.show()
```

The code outputs the evolution of y with respect to x for different values of c. The evolution is a bunch of circles evolving around the origin. The greater is c is the bigger and wider the circular path is.



7.2

To find the successive maxima of x for c = 5, the following function is written:

```
def find_maxima(t, y):
    maxima_indices = (y[:-2] < y[1:-1]) & (y[2:] < y[1:-1])
    return t[1:-1][maxima_indices], y[1:-1][maxima_indices]

sol = solve_rossler(5)
maxima_t, maxima_x = find_maxima(sol.t, sol.y[0])

plt.figure(figsize=(8, 6))
plt.plot(maxima_x[:-1], maxima_x[1:], '.', markersize=2)
plt.title('Successive Maxima Plot for c = 5')
plt.xlabel('$x_n$')
plt.ylabel('$x_n$')
plt.grid()
plt.show()</pre>
```

The outcome of the code didn't show the logistic map but it showed something similar I found online for the progression of y_{n+1} vs. y_n

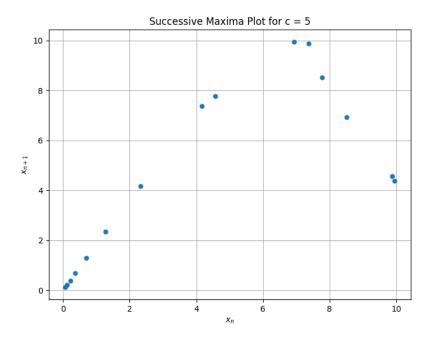


Figure 7: Evolution of x_{n+1} vs. x_n for c=5

7.3

To find the Maxima representing the period variation of the system, as we vary c, the following code is done:

```
plt.xlabel('c')
plt.ylabel('Maxima')
plt.grid()
plt.show()
```

The fig tree diagram showing the Maxima as c is varied is the following:

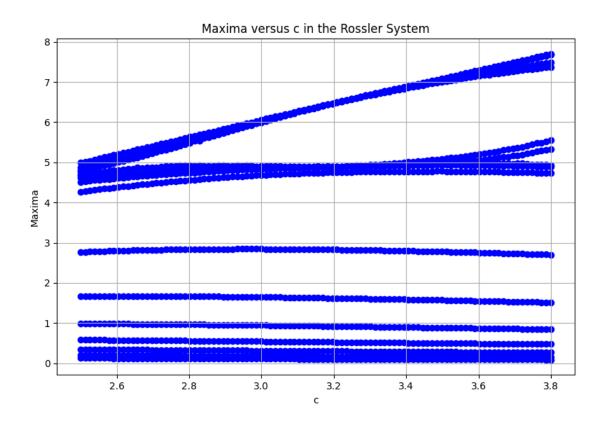


Figure 8: The evolution of the Maxima vs. c

8 SVD and Lagragian coherent Structures

To solve the following system:

$$\psi(x, y, t) = A \sin(\pi f(t)) \sin(\pi y)$$
$$f(x, t) = a(t)x^{2} + b(t)x$$
$$a = \epsilon \sin(\omega t)$$
$$b = 1 - 2\epsilon \sin(\omega t)$$

Taking the following parameters:

$$A = 0.25, \ \epsilon = 0.1, \ \omega = \frac{2\pi}{10}$$

The velocity field is defined over:

$$u = -\frac{\partial \psi}{\partial y}$$
$$v = -\frac{\partial \psi}{\partial x}$$

8.1

The code that will compute the evolution of the velocity fields in 200 time frames and in the domain $x \in [0, 2]$ and $y \in [0, 1]$

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.linalg import svd
from scipy.integrate import odeint
from matplotlib.animation import FuncAnimation
A = 0.25
epsilon = 0.1
omega = 2 * np.pi / 10
x_range = np.linspace(0, 2, 100)
y_range = np.linspace(0, 1, 50)
t_frames = 200
dt = 0.1
u_frames = np.zeros((t_frames, len(y_range), len(x_range)))
v_frames = np.zeros((t_frames, len(y_range), len(x_range)))
for t in range(t_frames):
       a = epsilon * np.sin(omega * t * dt)
       b = 1 - 2 * epsilon * np.sin(omega * t * dt)
       f = lambda x: a * x**2 + b * x
       psi = A * np.sin(np.pi * f(x_range)) * np.sin(np.pi * y_range[:,
          → None])
       u_frames[t] = -1 * np.gradient(psi, axis=1) # Partial derivative
          \hookrightarrow with respect to y
       v_frames[t] = np.gradient(psi, axis=0) # Partial derivative with
          \hookrightarrow respect to x
sample_frame_index = 20
plt.quiver(x_range, y_range, u_frames[sample_frame_index, :, :], v_frames
   → [sample_frame_index, :, :])
plt.title('Velocity field for 200 time frames')
plt.xlabel('x')
```

```
plt.ylabel('y')
plt.show()
```

The velocity field scatter of x and y in time frames 200:

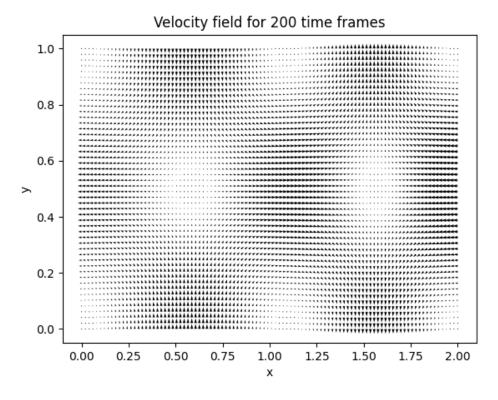


Figure 9: Y and X position for 200 frames in the domain [0,2] and [0,1]

8.2

To reshape the vectors in a D matrix with dimensions $(2 \times N \times M) \times t$.

8.3

To perform the SVD, we utilize the built-in function svd from Scipy:

```
from scipy.linalg import svd
U, S, Vt = svd(D)
```

8.4

To find the highest singular values:

```
plt.plot(S)
plt.title('Singular Values')
plt.xlabel('Index')
plt.ylabel('Magnitude')
plt.show()
```

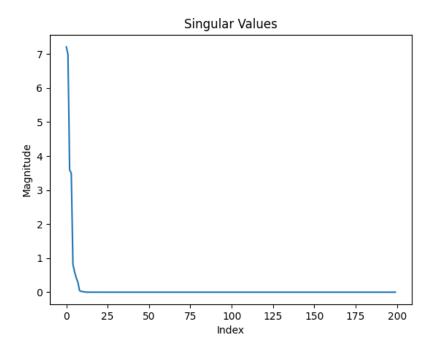


Figure 10: The highest Singular Values and their index

8.5

The simulation that computes the finite time lyapunov exponent and animates the flow:

```
num_modes = 5
num_frames = 200
N=100
M=50
temporal_basis = U[:, :num_modes]

FTLE = np.log(S[:num_modes]).reshape((num_modes, 1)) / num_frames

from matplotlib.animation import FuncAnimation
fig, ax = plt.subplots()
def update(frame):
```

The video showing the animation of the phase portrait will be uploaded in GitHub under "Q8."

9 PDEs

To solve the Turning reaction diffusion model of the following system of equations:

$$\frac{\partial a}{\partial t} = d_a \nabla^2 a + F(a, b)$$
$$\frac{\partial b}{\partial t} = d_b \nabla^2 b + G(a, b)$$

Where d_a and d_b are the diffusion coefficient of a and b respectively. By setting a certain equation to the diffusion equation F(a, b) and F(a, b), by doing the finite element to find the diffusion patterns in both the reactions.

The equations can be written in this format to achieve:

• Spots:

$$F(a,b) = u - v * a + a^2b$$
$$G(a,b) = -a^2b$$

• Strips

$$F(a,b) = u - v * a - a^2b$$
$$G(a,b) = +a^2b$$

Where u and v are arbitrary numbers that represent different diffusion parameters.

The following code is implemented in MATLAB to achieve a simulation of the diffusion of both u and v. The video will be recorded and attached in GitHub.

```
da = 0.1;
db = 0.05;
u = 0.2;
v = 0.1;

L = 40;
Nx = 100;
Nt = 5000;
dt = 0.01;
```

```
dx = L / (Nx - 1);
x = linspace(0, L, Nx);
[X, Y] = meshgrid(x, x);
a = 1 - 0.1 * rand(Nx, Nx);
b = 0.1 * rand(Nx, Nx);
for t = 1:Nt
       laplace_a = del2(a, dx);
       laplace_b = del2(b, dx);
       % For spots
       f_{spots} = u - v * a + a.^2 .* b;
       g_{spots} = -a.^2 .* b;
       % For strips
       f_{strips} = u - v * a - a.^2 .* b;
       g_{strips} = a.^2 .* v;
       dadt = da * laplace_a + f_strips;
       dbdt = db * laplace_b + g_strips;
       a = a + dt * dadt;
       b = b + dt * dbdt;
       % To plot the simulation
       if \mod(t, 100) == 0
               subplot(1, 2, 1);
               contourf(X, Y, a, 20, 'LineStyle', 'none');
               title(['a at t = ' num2str(t * dt)]);
               subplot(1, 2, 2);
               contourf(X, Y, b, 20, 'LineStyle', 'none');
               title(['b at t = ' num2str(t * dt)]);
               pause(0.001)
               hold on
       end
end
```

The simulation video shows the creation of spots in u and v, with very quick diffusion for v and slow diffusion in u. I tried to play with the parameters to fix the simulation but MATLAB kept crashing and my laptop couldn't handle the simulation. Unfortunately as well I couldn't achieve the diffusion of strips even after changing the additional terms in the differential equation of F(a, b) and G(a, b). I will include the outcome in the videos titled "Q9 Strips" and "Q9 Spots."