HW8

October 25, 2020

2

(This problem is based on the cheating-casino hidden Markov model we discussed in class.) Let $X(t)$ be a Markov chain on the state space $\{F, C\}$ (F - fair, C - cheating). Suppose that $X(t)$ changes state with probability $\alpha = .05$ regardless of its current state. Let $Y(t)$ be a r.v. with values from $\{1, 2, 3, 4, 5, 6\}$. ($Y(t)$ corresponds to the t-th role of a die). If $X(t) = F$ then $Y(t)$ is uniformly distributed on $\{1, 2, 3, 4, 5, 6\}$ (a fair die). If $X(t) = C$ then $P(Y(t) = 6) = 1/50$ and all values for $Y(t)$ are equally likely. Assume $X(0) = F$ where π is the stationary distribution of $X(t)$.

a

Write a function, SampleCasino(T) that samples $X(t)$, $Y(t)$ for $t \leq T$.

And so we need to represent the distribution of the data. Do so, we first keep in mind that $X(t)$ is a markov chain and that $Y(t)$ are independent but dependent on the $X(t)$ as shown in the picture above. So:

$$p(X, Y) = p(Y(0) = j_0|X(0) = i_0)p(X(0) = i_0)p(Y(1) = j_1|X(1) = i_1)p(X(1) = i_1|X(0) = i_0)$$
$$p(Y(2) = j_2|X(2) = i_2)p(X(2) = i_2|X(0) = i_0, X(1) = i_1) \dots p(Y(T) = j_T|X(T) = i_T)$$
$$p(X(T) = i_T|X(0) = i_0, X(1) = i_1, \dots, X(T-1) = i_{T-1})$$

$$= p(Y(0) = j_0|X(0) = i_0)p(X(0) = i_0)p(Y(1) = j_1|X(1) = i_1)p(X(1) = i_1|X(0) = i_0)$$
$$p(Y(2) = j_2|X(2) = i_2)p(X(2) = i_2|X(1) = i_1) \dots p(Y(T) = j_T|X(T) = i_T)$$
$$p(X(T) = i_T|X(T-1 = i_{T-1})) \text{ by markov property}$$

$$= p(X(0) = i_0) \prod_{t=1}^{T} p(X(t) = i_t|X(t-1) = i_{t-1}) \prod_{t=0}^{T} p(Y(t) = j_t|X(t) = i_t).$$

Now that we have the joint distribution of the $X(t)$, $Y(t)$, the conditional distribution we are interested in sampling from:

$$p(X(0) = i_0, X(1) = i_1, ..., X(T) = i_T|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$$

$$= \frac{p(X(0)=i_0)\prod_{t=1}^{T} p(X(t)=i_t|X(t-1)=i_{t-1})\prod_{t=0}^{T} p(Y(t)=j_t|X(t)=i_t)}{p(Y(0)=j_0, Y(1)=j_1, ..., Y(T)=j_T)}$$

To sample from the above distribution we will use Metropolis-Hastings. We first consider out sample space, which is $\Omega = \{\omega : \omega \in R^{T+1}, \omega_i \in \{0,1\} \text{ for } i = 1,2,\ldots,T, \omega_0 = 0\}$.

[1]:
```
def SampleCasino(T):
    """
    Args:
        T: scalar
    Returns:
        x, y: matrices of size (T,)

    """
    x_start = 0
    x = [x_start]
    y_start = np.random.choice(range(1,7), p=dist_Y[x[0]])
    y = [y_start]

    for i in range(1, T+1):
        xi = np.random.choice([0, 1], p=P[x[i-1]])
        x.append(xi)
        yi = np.random.choice(range(1,7), p=dist_Y[x[i-1]])
        y.append(yi)

    return x, y
```

b

Use your simulation from part (a) to produce a single realization of $X(t)$ and $Y(t)$ up to time step $T = 200$. Pretend that you don't know the $X(t)$ values, but that you know the $Y(t)$ values generated. Let $(j_0, j_1, ..., j_T)$ be the sequence of $Y(t)$ values you generated. Given a sequence $(i_0, i_1, ..., i_T)$ of states $i \in \{F, C\}$, write an expression for the probability

$$P(X(0)=i_0, X(1)=i_1, ..., X(T)=i_T | Y(0)=j_0, Y(1)=j_1, ..., Y(T)=j_T)$$

Set $\alpha = P(Y(0)=j_0, Y(1)=j_1, ..., Y(T)=j_T)$. Your expression should be a function of α and the i_s, j_s for $s = 0,1,2,...,T$. Provide an expression for α (you can express α through $T+1$ sums).

I am letting Fair= 0 and Cheat= 1.

[2]:
```
import numpy as np
```

[3]:
```
first = np.repeat(1/6,6)
second = np.concatenate((np.repeat((49/50)/5, 5), np.array([1/50])))
```

```
dist_Y = np.concatenate((first, second), axis=0).reshape(2,6)
dist_Y
```

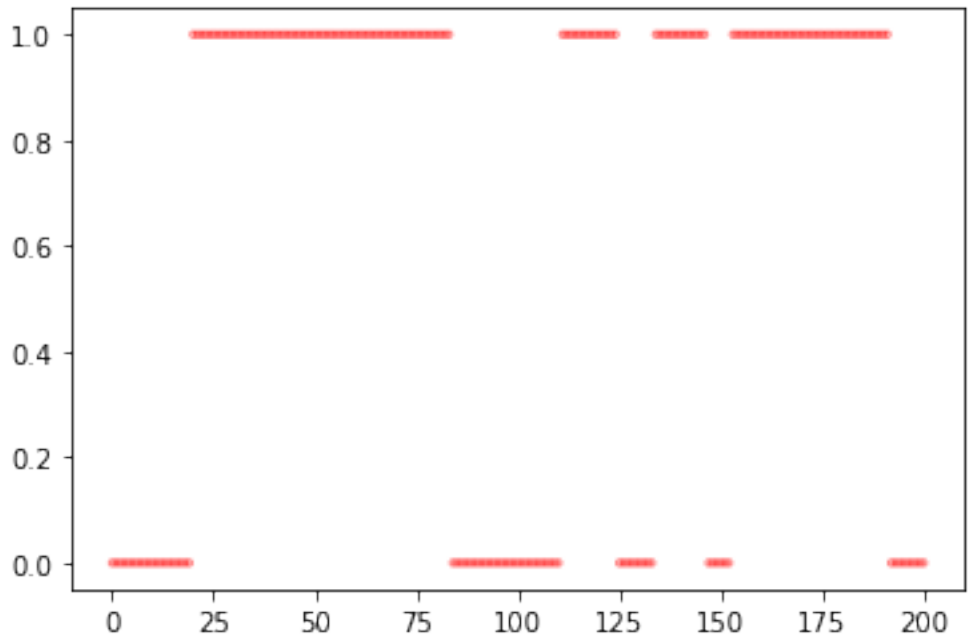
[3]:
```
array([[0.16666667, 0.16666667, 0.16666667, 0.16666667, 0.16666667,
        0.16666667],
       [0.196     , 0.196     , 0.196     , 0.196     , 0.196     ,
        0.02      ]])
```

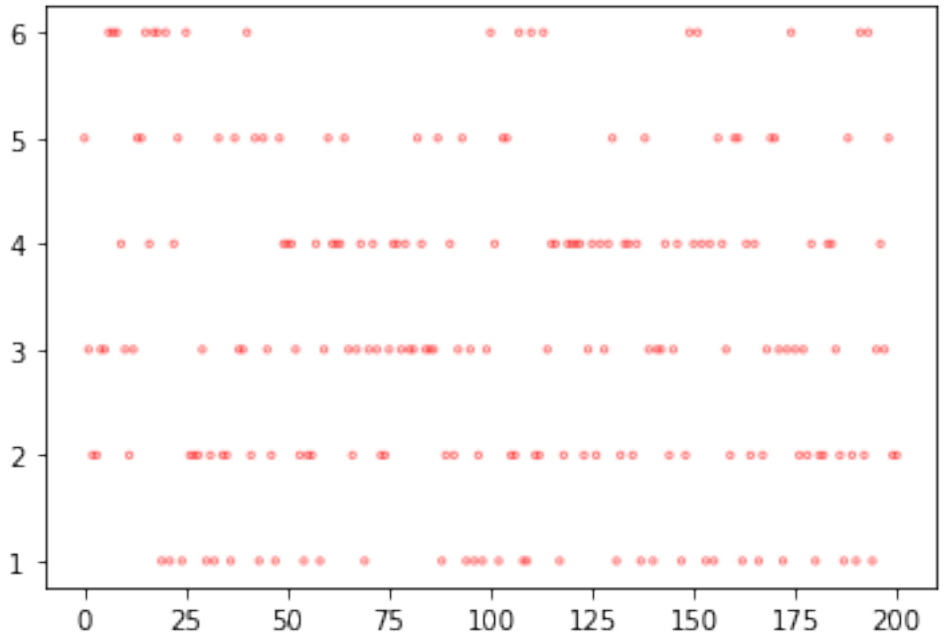
[4]:
```
P = np.array([[0.95,0.05],[0.05,0.95]])
P
```

[4]:
```
array([[0.95, 0.05],
       [0.05, 0.95]])
```

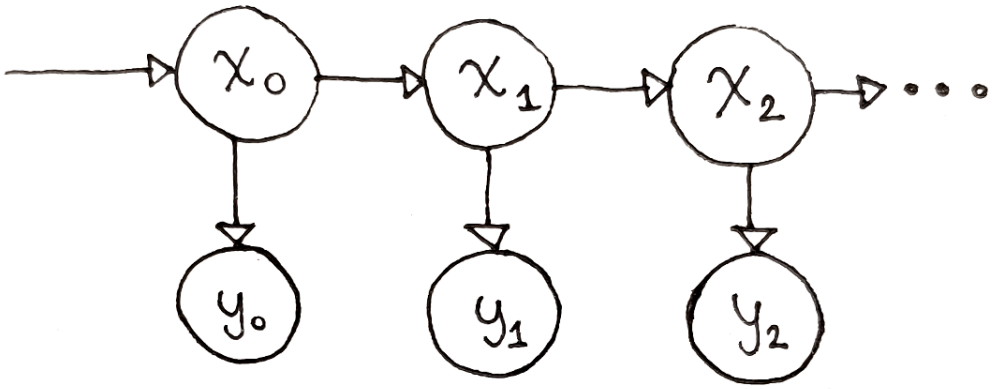
[9]:
```
X, Y = SampleCasino(200)
```

[10]:
```
import matplotlib.pyplot as plt
plt.scatter(range(0, len(X)), X, facecolors='none', edgecolors='red', alpha=0.
 ↪5, s=5)
plt.show()

plt.scatter(range(0, len(Y)), Y, facecolors='none', edgecolors='red', alpha=0.
 ↪5, s=5)
plt.show()
```





Our Markov Model is as follows:



And so we need to represent the distribution of the data. Do so, we first keep in mind that $X(t)$ is a markov chain and that $Y(t)$ are dependent on the $X(t)$ as shown in the picture above. So:

$$p(X(0) = i_0, X(1) = i_1, \ldots, X(T) = i_T, Y(0) = j_0, Y(1) = j_1, \ldots, Y(T) = j_T)$$

$$= p(X(0) = i_0)P(Y(0) = j_0|X(0) = i_0) \prod_{t=1}^{T} p(Y(t) = j_t|X(t) = i_t)p(X(t) = i_t|X(t-1) = i_{t-1}))$$

$$= p(X(0) = i_0) \prod_{t=1}^{T} p(X(t) = i_t | X(t-1) = i_{t-1}) \prod_{t=0}^{T} p(Y(t) = j_t | X(t) = i_t)$$

However, in the context of the problem, $X(0) = 0$ so the above reduces to:

$$= \prod_{t=1}^{T} p(X(t) = i_t | X(t-1) = i_{t-1}) \prod_{t=0}^{T} p(Y(t) = j_t | X(t) = i_t)$$

$$= p(Y(0) = j_0 | X(0) = 0) \prod_{t=1}^{T} p(X(t) = i_t | X(t-1) = i_{t-1}) p(Y(t) = j_t | X(t) = i_t)$$

By letting P be the transition probability matrix and $g_{i_t}(j_t) = P(Y(t) = j_t | X(t) = i_t)$ we get the following form:

$$g_0(j_0) \prod_{t=1}^{T} g_{i_t}(j_t) P_{i_{t-1} i_t}$$

Now that we have the joint distribution of the $X(t)$'s, $Y(t)$'s, the conditional distribution we are interested in sampling from:

$$p(X(0) = 0, X(1) = i_1, ..., X(T) = i_T | Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$$

$$= \frac{g_0(j_0) \prod_{t=1}^{T} g_{i_t}(j_t) P_{i_{t-1} i_t}}{p(Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)}$$

$$= \frac{g_0(j_0) \prod_{t=1}^{T} g_{i_t}(j_t) P_{i_{t-1} i_t}}{\alpha}$$

We can get α by marginalizing the joint distribution, i.e., summing thet joint distribution over all possible values for the $X(t), t = 1, 2, \ldots, T$.

$$p(Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$$

$$= \sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_T=0}^{1} P(X(0) = 0, X(1) = i_1, ..., X(T) = i_T, Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$$

$$= \sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_T=0}^{1} g_0(j_0) \prod_{t=1}^{T} g_{i_t}(j_t) P_{i_{t-1} i_t}$$

c

Let $\nu(i_0, i_1, ..., i_T)$ be the conditional probability given above. Let Z be the r.v. with distribution ν. What is the state space of Z? (We discussed this in class.)

The state space of Z is $\Omega = \{\omega : \omega \in R^{T+1}, \omega_i \in \{0, 1\} \text{ for } i = 1, 2, \ldots, T,\ \omega_0 = 0\}$.

Note ω_0 is 0 since that is what is being assumed in the prompt.

d

Using a Metropolis-Hastings approach, construct a Markov chain $W(s)$ that has Z as its stationary distribution. (Here I'll use s as the time variable so as not to confuse it with the t variable of $X(t)$). Use your sampler to estimate $P(X(t) = C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$ where t is a given value. Using a single long run of $W(s)$, estimate $P(X(t) = C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$, don't forget to include a burn-in time. Do this for all $t \leq 200$. You can use a single long run of $W(s)$ for each value of t. Plot $P(X(t) = C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$ as a function of t and compare the probabilities you computed to the actual state of the casino.

To sample from the conditional distribution,

$$l(\omega) = p(X(0) = 0, X(1) = i_1, ..., X(T) = i_T|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$$
$$= \frac{g_0(j_0)\prod_{t=1}^{T} g_{i_t}(j_t)P_{i_{t-1}i_t}}{\alpha}$$

we will use Metropolis-Hastings.

We first consider our state space, which is $\Omega = \{\omega : \omega \in R^{T+1}, \omega_i \in \{0, 1\} \text{ for } i = 0, 1, 2, \ldots, T, \omega_0 = 0\}$.

Suppose we start with some $\omega_0 \in \Omega$.

Then for $n = 1, 2, \ldots, N$ iterations:

1. We propose ω' by randomly flipping one entry. So our proposal distribution is symmetric, $p(\omega'|\omega) = p(\omega|\omega) = \frac{1}{T}$, and will cancel out in the metropolis-hastings ratio.
2. We accept w' with probability $\min(1, \frac{l(\omega')}{l(\omega)})$

If we accept, $w_{n+1} = \omega'$. Otherwise, $w_{n+1} = \omega$.

We can notice that the metropolis-hastings ratio simplifies significantly because of cancellation. Suppose entry k is randomly chosen to be flipped from i_k to i'_k with $k \neq T$. Then the ratio reduces to:

$$\frac{l(\omega')}{l(\omega)}$$

$$= \frac{p(Y(k) = j_k|X(k) = i'_k)p(X(k) = i'_k|X(k-1) = i_{k-1})p(X(k+1) = i_{k+1}|X(k) = i'_k)}{p(Y(k) = j_k|X(k) = i_k)p(X(k) = i_k|X(k-1) = i_{k-1})p(X(k+1) = i_{k+1}|X(k) = i_k)}$$

If $k = T$ then the ratio is:

$$\frac{l(\omega')}{l(\omega)} =$$

$$\frac{p(Y(k) = j_k|X(k) = i'_k)p(X(k) = i'_k|X(k-1) = i_{k-1})}{p(Y(k) = j_k|X(k) = i_k)p(X(k) = i_k|X(k-1) = i_{k-1})}$$

[11]:
```
def MCMC(w, N, n_indices=1):
    """
    Args:
        w: matrix of size (200, )
        N: scalar
        n_indices: scalar
    Returns:
        samples: list of arrays of size (N, 200)

    """
    def mhr_calc(index, w):
        if index == T:
            num = dist_Y[1-w[index],Y[index]-1]*P[w[index-1],1-w[index]]
            den = dist_Y[w[index],Y[index]-1]*P[w[index-1],w[index]]
        else:
            num =␣
↪dist_Y[1-w[index],Y[index]-1]*P[w[index-1],1-w[index]]*P[1-w[index],w[index+1]]
            den =␣
↪dist_Y[w[index],Y[index]-1]*P[w[index-1],w[index]]*P[w[index],w[index+1]]
        return num/den

    samples = []
    for i in tqdm(range(0, N)):
        index = np.random.choice(range(1, T+1), n_indices).item()
        mhr = mhr_calc(index, w)
        if(np.random.uniform(0,1) < mhr):
            w2 = w.copy()
            w2[index] = 1 - w2[index]
            samples.append(w2)
            w = w2.copy()
        samples.append(w)
    return samples
```

[12]:
```
from tqdm import tqdm
T = 200
w_start = np.concatenate((np.array([0]), np.repeat(1, T)))
samples = MCMC(w_start, 10**7)
```

```
100%|      | 10000000/10000000 [09:01<00:00, 18465.81it/s]
```

To estimate $P(X(t) = C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T)$ for $t \leq 200$ we will invoke the Markov Chain version of the Law of Large Numbers.

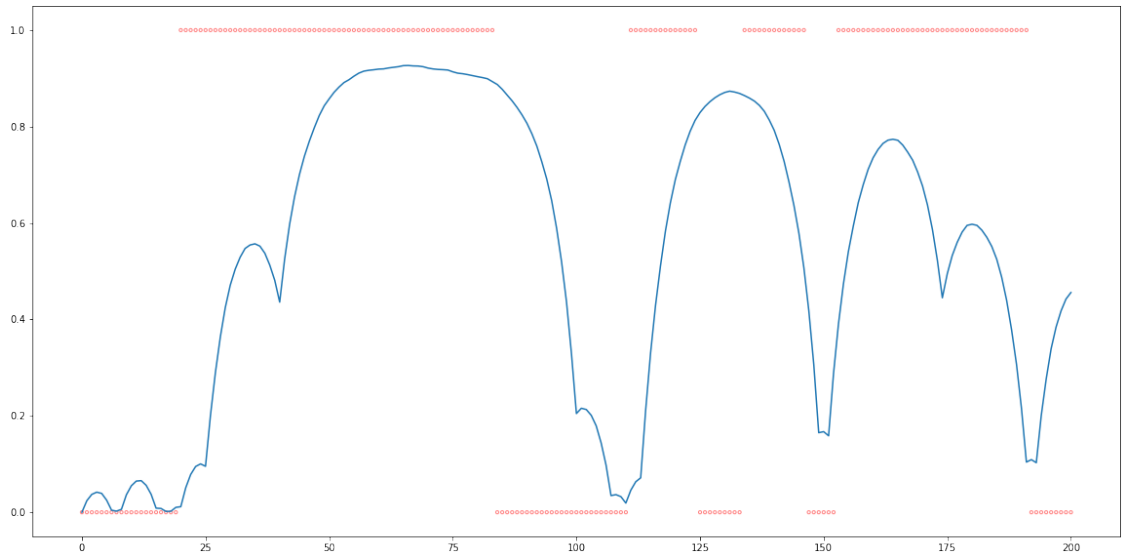
Let H be an indicator random variable that equals 1 if $X(t) = C$ and 0 otherwise.

$$H = \begin{cases} 1 & \text{if } X(t) = C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T \\ 0 & \text{if } X(t) \neq C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T \end{cases}$$

So $E[H] = 1 \cdot P\{X(t) = C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T\} + 0 \cdot P\{X(t) \neq C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T\} = P\{X(t) = C|Y(0) = j_0, Y(1) = j_1, ..., Y(T) = j_T\}$. And so now we can approximate $E[H]$ with $\frac{1}{N}\sum_{n=1}^{N} \mathbb{1}_{\omega_{nt}=C}$ for an appropriate N runs of the Markov Chain, excluding the burn in time. Note ω_{nt} is the t entry of sample n.

[13]:
```
# finding the sample mean
# including burn in at 0.3*N
l = np.mean(samples[int(.3*len(samples)):], axis=0)
```

[14]:
```
import matplotlib.pyplot as plt
plt.figure(figsize=(20,10))
plt.plot(l)
plt.scatter(range(0, len(X)), X, facecolors='none', edgecolors='red', alpha=0.
↪5, s=10)
plt.show()
```



Using a burn in of $0.3 * 10^7$ seems decent enough – one can notice how, for the most part, the probabilites computed are close to 1 (at least greater than 50 percent), when the state of the casino is 1 (cheat), and get close to 0 when the state of the casino is 0 (does not cheat/fair).

2

Attached you will find a R script make_1d_manifold.R that constructs data points $x(i) \in R^{10}$ for $i = 1, 2, ..., 500$ that are localized around a 1-d manifold. The data points produced by the script are in diffusion_maps_data.csv.

1 a

Look at the file diffusion_maps_data.csv. The data points are given in the first 10 columns. The 11th column gives a parameter β discussed in the next subproblem. Can you find a pattern in the data? (The answer will be no, I think.)

[2]:
```
import pandas as pd
data = pd.read_csv("diffusion_maps_data.csv")
data.head()
```

[2]:

	Unnamed: 0	Unnamed: 1	Unnamed: 2	Unnamed: 3	Unnamed: 4	Unnamed: 5	\
0	-0.478914	-0.049141	-0.297305	0.087278	-0.229072	0.515732	
1	-0.469228	-0.058886	-0.295487	0.039958	-0.259343	0.439233	
2	-0.773425	-0.142003	-0.504606	-0.124775	-0.573540	0.447500	
3	-0.723794	-0.105599	-0.461564	-0.000996	-0.448032	0.586690	
4	-0.495562	-0.081031	-0.319431	-0.037716	-0.335130	0.347980	

	Unnamed: 6	Unnamed: 7	Unnamed: 8	Unnamed: 9	beta
0	-0.095343	-0.125465	-0.244472	0.235513	0.000000
1	-0.128250	-0.124088	-0.233148	0.205576	0.002004
2	-0.357173	-0.209389	-0.357601	0.233504	0.004008
3	-0.245723	-0.193004	-0.350866	0.282495	0.006012
4	-0.196559	-0.133088	-0.235042	0.172952	0.008016

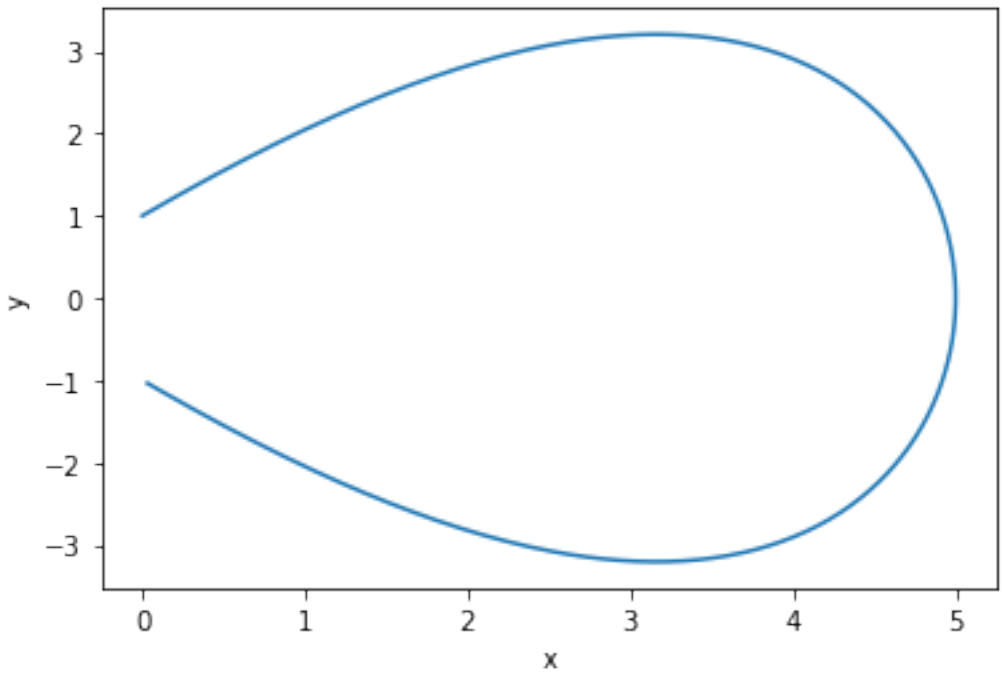
No, I cannot find a pattern in the data.

b

Read the script and describe what the 1-d manifold looks like. Associated with each data point is a scalar $\beta \in [0, 1]$. Explain how β paramatrizes the manifold.

[241]:
```
# ignoring seed because R vs. python
import numpy as np
import matplotlib.pyplot as plt
n = 500
beta = np.arange(0,1,1/500)
x = 5*np.sin(np.pi*beta)
y = 2*(.5-beta) + 20*beta*(1-beta)*np.cos(np.pi*beta)
plt.plot(x,y)
plt.xlabel("x")
plt.ylabel("y")
```

```
plt.show()
```



The manifold looks like a horseshoe as seen above. As we can see from above as well (code), β is used to create the horseshoe structure (it is used inside the sine and cosinse functions to smooth and create a horseshoe structure, and it is used in $2 * (.5 - \beta)$ in the definition of y to create that opening seen at $x = 0$).

c

Reduce the data to R^2 and R using PCA. Plot the data points in the reduced dimension and use color to represent the value of β.

[214]:
```
X = data.iloc[:,:-1].to_numpy()
X.shape
```

[214]: (500, 10)

[215]:
```
# covariance matrix
N = X.shape[0]
cov = (X-X.mean(axis=0)).T.dot(X-X.mean(axis=0))/N
cov.shape
```

[215]: (10, 10)

[216]:
```
# eigen decomposition of the covariance matrix
eig_cov = np.linalg.eig(cov)
# the eigenvalues of the covariance
eig_cov[0]
```

[216]:
```
array([ 5.63757323e+00+0.00000000e+00j,  2.40480288e+00+0.00000000e+00j,
        9.04104221e-16+0.00000000e+00j, -4.24337884e-16+0.00000000e+00j,
        2.83248276e-16+0.00000000e+00j, -1.64893175e-16+0.00000000e+00j,
       -9.45935733e-17+0.00000000e+00j,  2.04444948e-17+1.90693339e-17j,
        2.04444948e-17-1.90693339e-17j,  8.76459000e-17+0.00000000e+00j])
```

[217]:
```
# matrix of two eigenvalues corresponding to two largest eigenvalues
Q = eig_cov[1][:,np.argsort(eig_cov[0])[::-1][:2]]
Q.shape
```

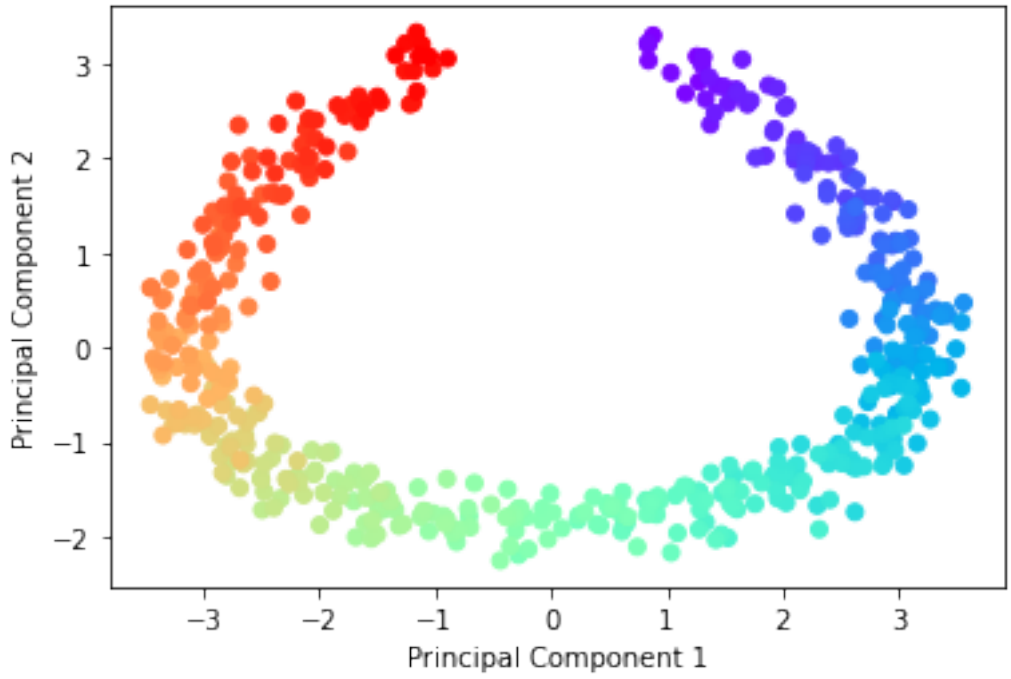
[217]:
```
(10, 2)
```

[218]:
```
# coordinates in R^2
c = (X-X.mean(axis=0)).dot(Q)
c.shape
```

[218]:
```
(500, 2)
```

[222]:
```
import matplotlib.cm as cm
plt.scatter(c[:,0], c[:,1], c=data["beta"], cmap=cm.rainbow)
plt.xlabel("Principal Component 1")
plt.ylabel("Principal Component 2")
plt.show()
```

```
//anaconda3/lib/python3.7/site-packages/numpy/core/_asarray.py:138:
ComplexWarning: Casting complex values to real discards the imaginary part
  return array(a, dtype, copy=False, order=order, subok=True)
```



d

i. The authors of the diffusion maps paper (see Reading above) introduce the diffusion distance between the data points $x^{(i)}, x^{(j)}$,

$$D_t^2(x^{(i)}, x^{(j)}) = \sum_{k=1}^{N} \frac{(P(Z(t) = x^{(k)}|Z(0) = x^{(i)}) - P(Z(t) = x^{(k)}|Z(0) = x^{(j)}))^2}{\pi(x^{(k)})}$$

Explain the intuition behind this distance. How is $Z(t)$ constructed? What is π? Here I'm not looking for any proofs or derivations. Just explain your understanding of the construction.

Let $X \in R^{N \times n}$ be our data. Let $K : X \times X \to R$ be a kernel that satisfies:

- k is symmetric
- k is positive preserving: $k(x, y) \geq 0$

and represents some notion of similarity between the points in X. Because of this, we can think of the data points in X as nodes of a symmetric graph whose weight function is specified by k. And so from the graph defined by (X, k) we can construct a reversible markov chain on X, call it $Z(t)$, with transition probability kernel $p(x, y) = k(x, y)/d(x)$ where $d(x)$ is a normalizing constant guaranteeing $\sum_{y \in \text{state space}} p(x, y) = 1$. For this exercise, $k(x, y)$ will be 500×500 and $p(x, y)$ will be $k(x, y)$ divided by the corresponding row sum. $X(t)$ will depend on the definition of k since it is constructed by the graph defined by (X, k). Since we will be experimenting with a couple of k, we will have a couple of $Z(t)$.

π is the stationary distribution of the markov chain $Z(t)$, detailed above. For this exercise, the stationary distribution of $X(t)$ will $\pi(x^{(i)}) = \frac{d_i}{\sum_{l=1}^{N} d_l}$ where d_i is the sum of the ith row of k.

Lastly, quoting from the paper, D_t defines a distance on X. The notion of proximity it defines reflects the connectivity in the graph of the data. $D_t(x, y)$ will be small if there is a large number of short paths connceting x and y, i.e., if there is a large probability to transition from x to y and viceversa (in t time steps).

ii. The authors describe a mapping from $x(i) \in R^n$ to $y(i) \in R^N$, where $y(i)$ is given by

$$y^{(i)} = \begin{pmatrix} \lambda_1^T r_i^{(1)} \\ \lambda_2^T r_i^{(2)} \\ \vdots \\ \lambda_N^T r_i^{(N)} \end{pmatrix}$$

Explain how to compute the λ and r. What is the formula for $D_t^2(x^{(i)}, x^{(i)})$ in terms of $y^{(i)}, y^{(j)}$? Again, I'm not looking for proofs or step-by-step derivations. Just show my how you would do the computations and state the formula. (The lecture video and paper provide step by step derivations.)

λ are the N eigenvalues (in context of this exercise $N = 500$) of the transition probability matrix P mentioned above, and r are the the 500 right eigenvectors of P. To compute λ, r:

We first create $V = D^{1/2} P D^{-1/2}$, where $D = \text{diag}(\pi(x^{(1)}), \pi(x^{(2)}), \ldots, \pi(x^{(500)}))$. V is a symmetric 500×500 matrix so by the spectral decomposition theorem we can get 500 real eigenvalues, β, with corresponding eigenvectors. Now, $\lambda = \beta$ so the eigenvalues of V are the eigenvalues of P and the right eigenvectors of P can be defined as $r^{(i)} = D^{-1/2} q^{(i)}$ for $i = 1, 2, \ldots, 500$, where $q^{(i)}$ are the eigenvectors of V.

The formula for $D_t^2(x(i), x(j))$ in terms of $y(i), y(j)$ is:

$$D_t^2(x^{(i)}, x^{(i)})$$

$$= ||y^{(i)} - y^{(j)}||^2 =$$

$$|| \begin{pmatrix} \lambda_1^T r_i^{(1)} \\ \lambda_2^T r_i^{(2)} \\ \vdots \\ \lambda_N^T r_i^{(N)} \end{pmatrix} - \begin{pmatrix} \lambda_1^T r_j^{(1)} \\ \lambda_2^T r_j^{(2)} \\ \vdots \\ \lambda_N^T r_j^{(N)} \end{pmatrix} ||^2$$

iii. Describe how we would use diffusion maps to dimensionally reduce the data.

1. We would pick a kernel k of our choice (as long as it conforms with symmetry and positive preserving). (X, k) would gives us our markov chain $Z(t)$ with transition probability matrix P (k with each entry of k divided by its corresponding row sum).

Note, for the exercise, I will pick the family of kernels $K = \{k|k(x^{(i)}, x^{(j)}) = e^{-\frac{||x^{(i)}-x^{(j)}||^2}{\delta}}, \delta > 0\}$.

2. We create $V = D^{1/2}PD^{-1/2}$ and get the eigenvectors and eigenvalues of V to get the eigenvalues and right eigenvectors of P as described in ii.

3. Once we have the eigenvectors and right eigenvectors of P, we map our data $x(i) \in R^10$ to $y(i) \in R^500$, where $y(i)$ is given by

$$y^{(i)} = \begin{pmatrix} \lambda_1^T r_i^{(1)} \\ \lambda_2^T r_i^{(2)} \\ \vdots \\ \lambda_N^T r_i^{(N)} \end{pmatrix}$$

4. Lastly, to map our data to an m dimensional space, we pick the first m entries of $y^{(i)}$ for each $i = 1, 2, \ldots, 500$ (usually ignoring the first entry – so choosing the subsequent m entries of $y^{(i)}$). For this exercise, since we are mapping to a 2 dimensional space we will choose entries $2, 3$ of $y^{(i)}$ (i.e, the first two entries after ignoring the first one).

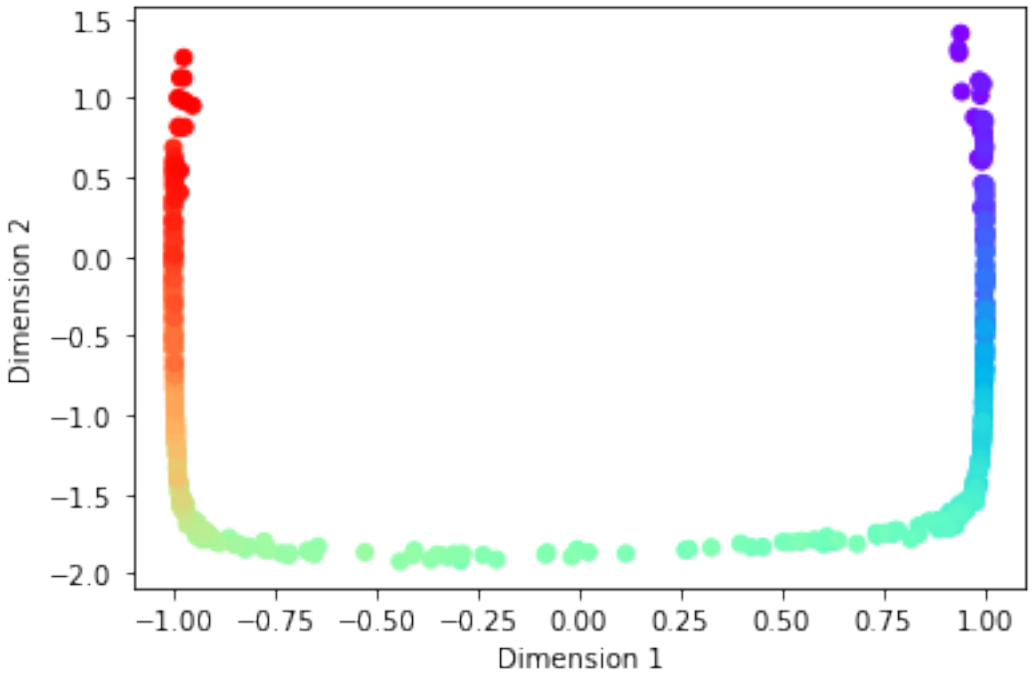
iv. Now repeat (b), but use diffusion maps to dimensionally reduce the data. Experiment with different kernels and different time parameters t in the diffusion maps.

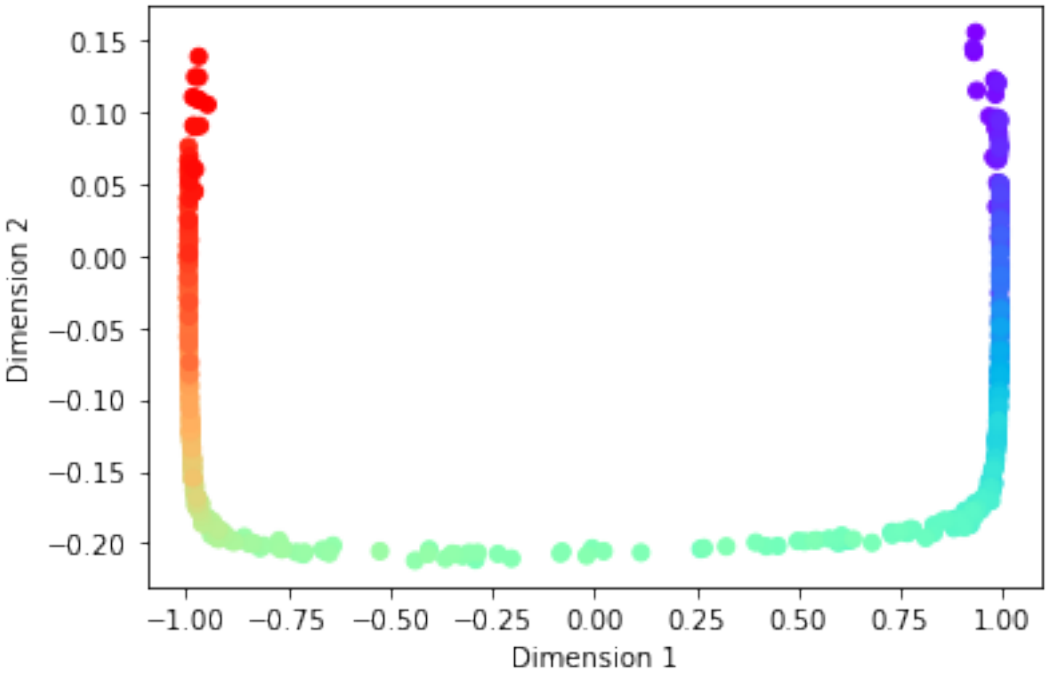
Lets create a function that does the above mentioned 4 steps.

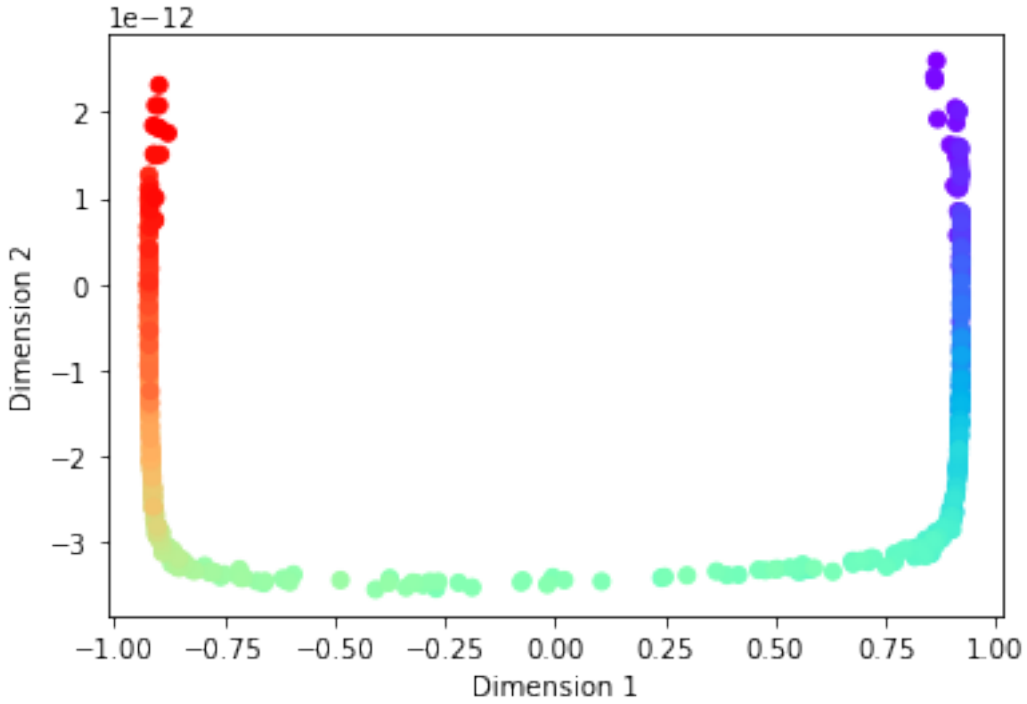
[200]:
```
def diffusion_map(T, delta):
    """Reduces data to 2 dimensional
    Args:
        T: Markov Chain time steps, positive scalar
        delta: bandwidth parameter in kernel function, positive scalar

    Returns:
        c: matrix of shape (500, 2)

    """
    # Kernel matrix, probability transition matrix, and
    # stationary distribution of P
    K = np.exp(-X.dot(X.T)/delta)
    d = np.diag(K.sum(axis=1))
    P = np.linalg.inv(d).T.dot(K)
    D = d/d.sum()

    V = np.sqrt(D).dot(P).dot(np.sqrt(np.linalg.inv(D)))
    eig_V = np.linalg.eig(V)
    Q = eig_V[1][:,np.argsort(abs(eig_V[0]))[::-1][1:3]]

    # right eigenvectors of P corresponding to
    # 2nd and 3rd most dominant eigenvalues of P
    R = np.sqrt(np.linalg.inv(D)).dot(Q).real
    e = np.sort(abs(eig_V[0]))[::-1][1:3].real
```

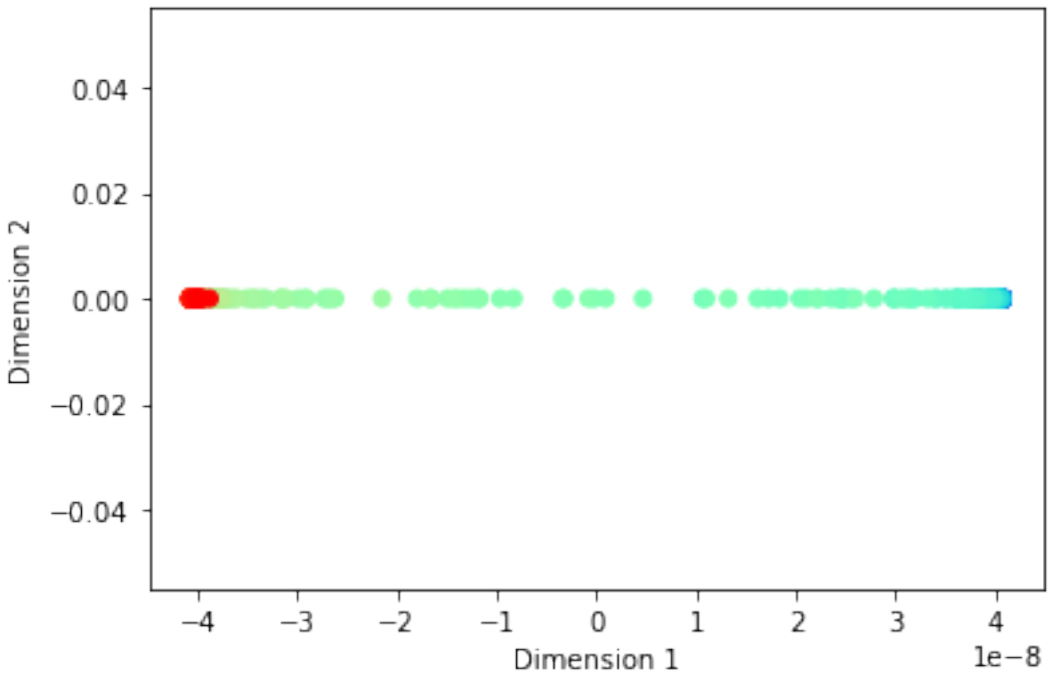
```
    # coordinates in R^2
    c = (e**T)*R

    return c
```

[227]:
```
times = [1, 5, 50, 10000]
for t in times:
    c = diffusion_map(t, 1)
    plt.scatter(c[:,0],c[:,1], c=data["beta"], cmap=cm.rainbow)
    plt.xlabel("Dimension 1")
    plt.ylabel("Dimension 2")
    plt.show()
```

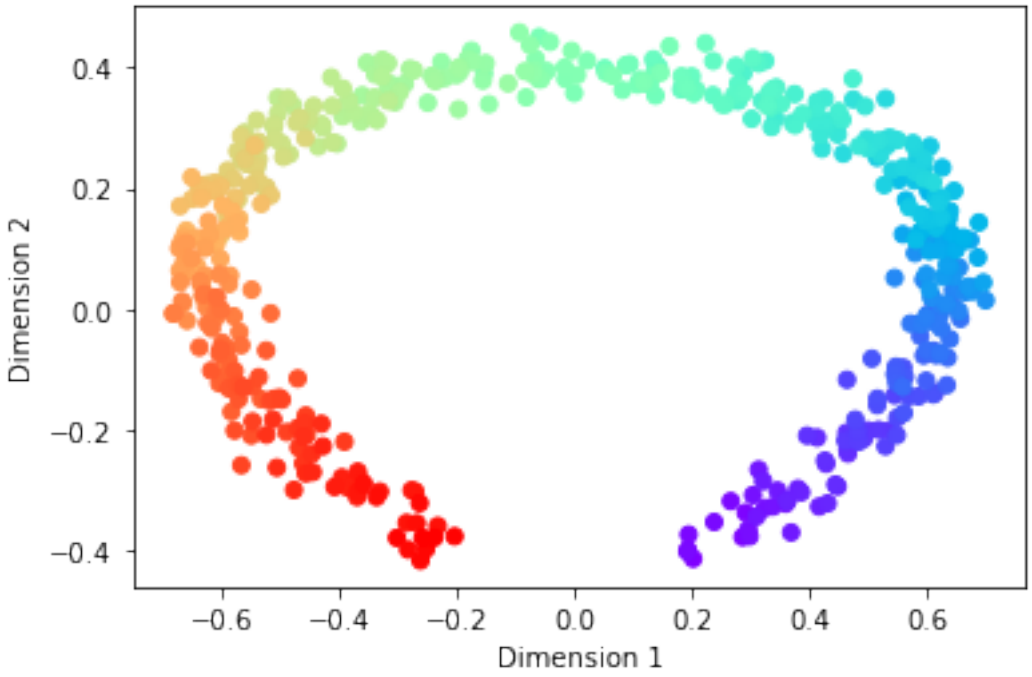


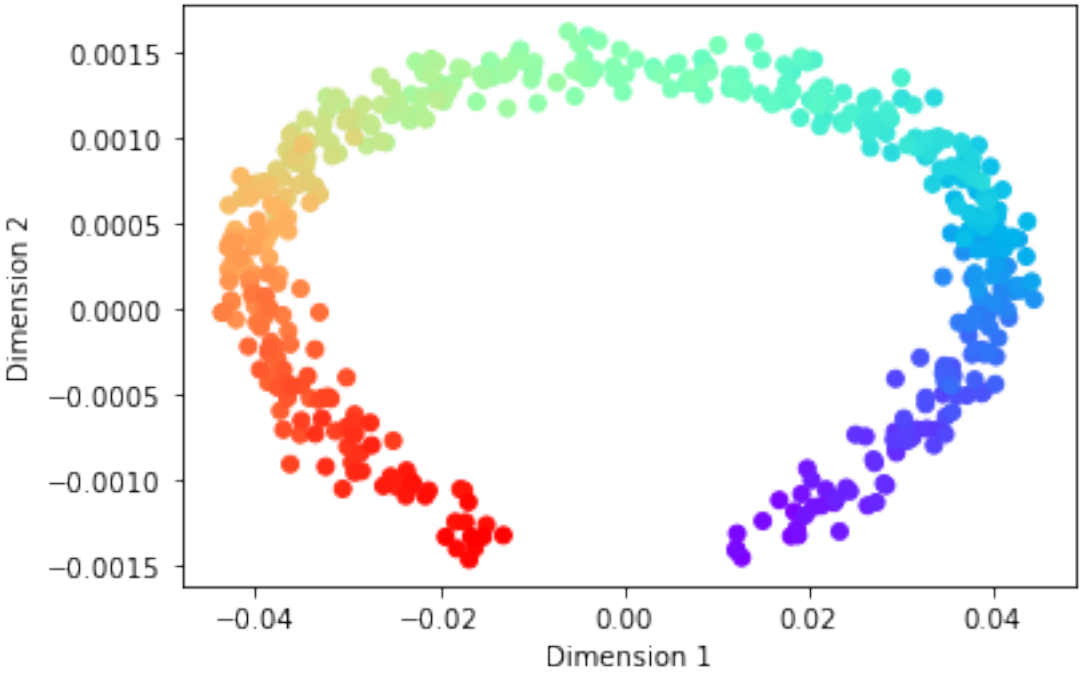

0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20
Dimension 2
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
Dimension 1

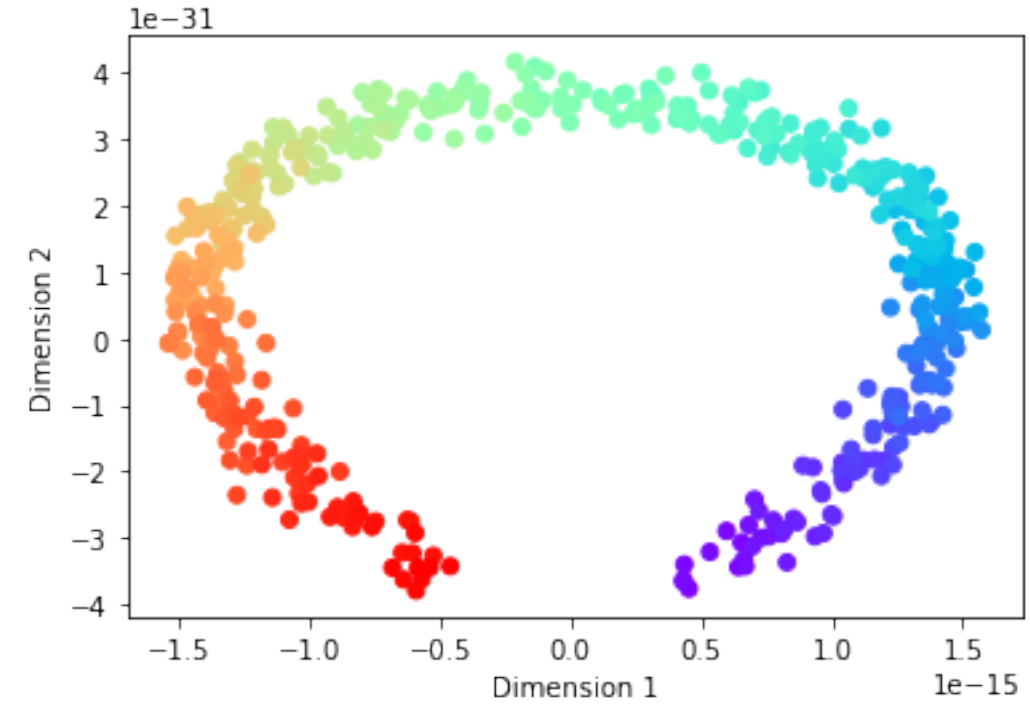

1e−12
2
1
0
−1
−2
−3
Dimension 2
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
Dimension 1

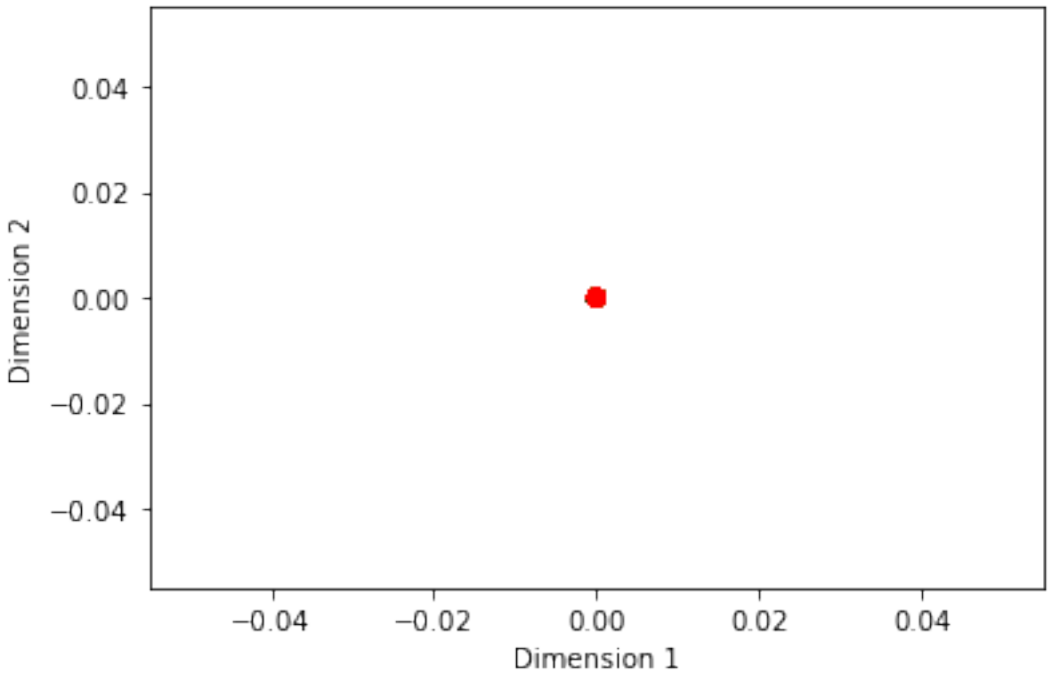


[225]:
```
for t in times:
    c = diffusion_map(t, 10)
    plt.scatter(c[:,0], c[:,1], c=data["beta"], cmap=cm.rainbow)
    plt.xlabel("Dimension 1")
    plt.ylabel("Dimension 2")
    plt.show()
```

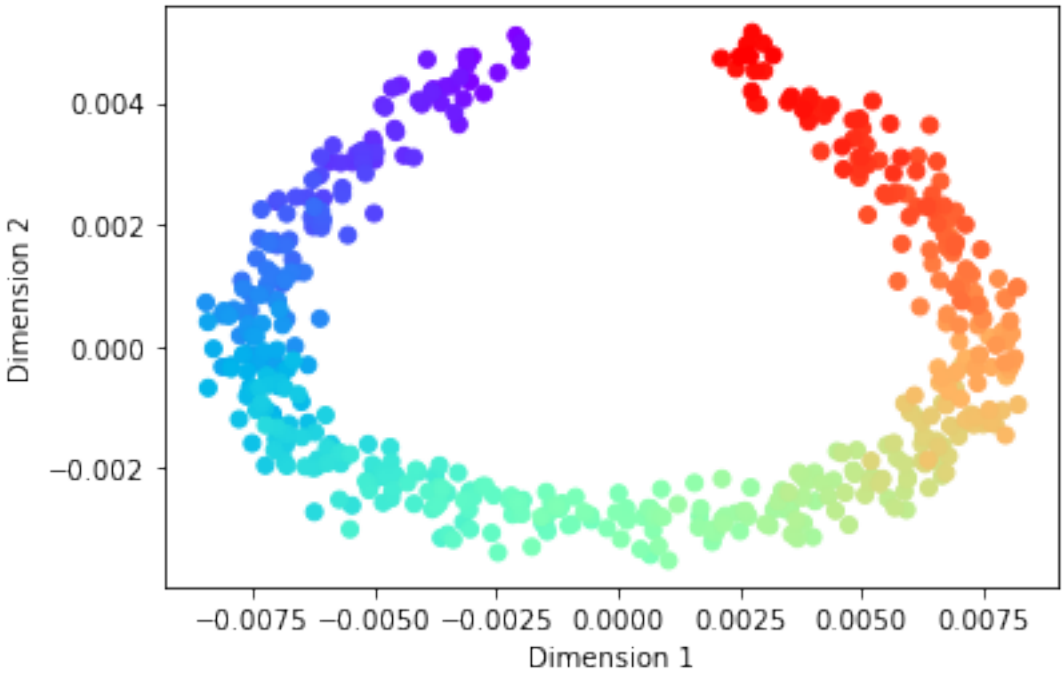

0.4
0.2
0.0
−0.2
−0.4
Dimension 2
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6
Dimension 1

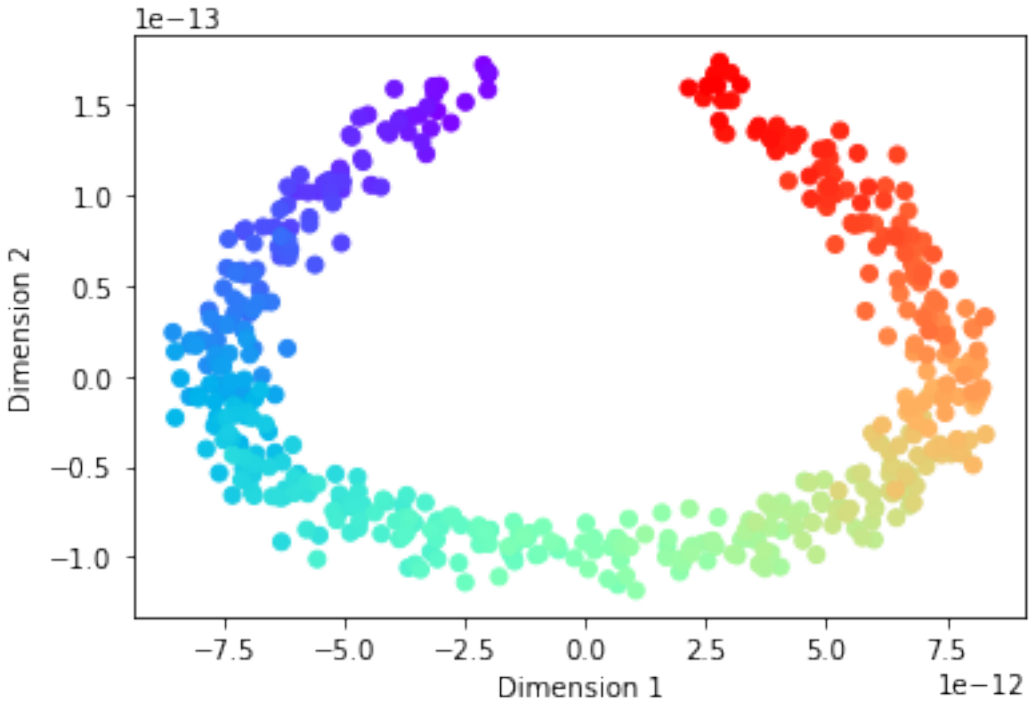

0.0015
0.0010
0.0005
0.0000
−0.0005
−0.0010
−0.0015
Dimension 2
−0.04
−0.02
0.00
0.02
0.04
Dimension 1

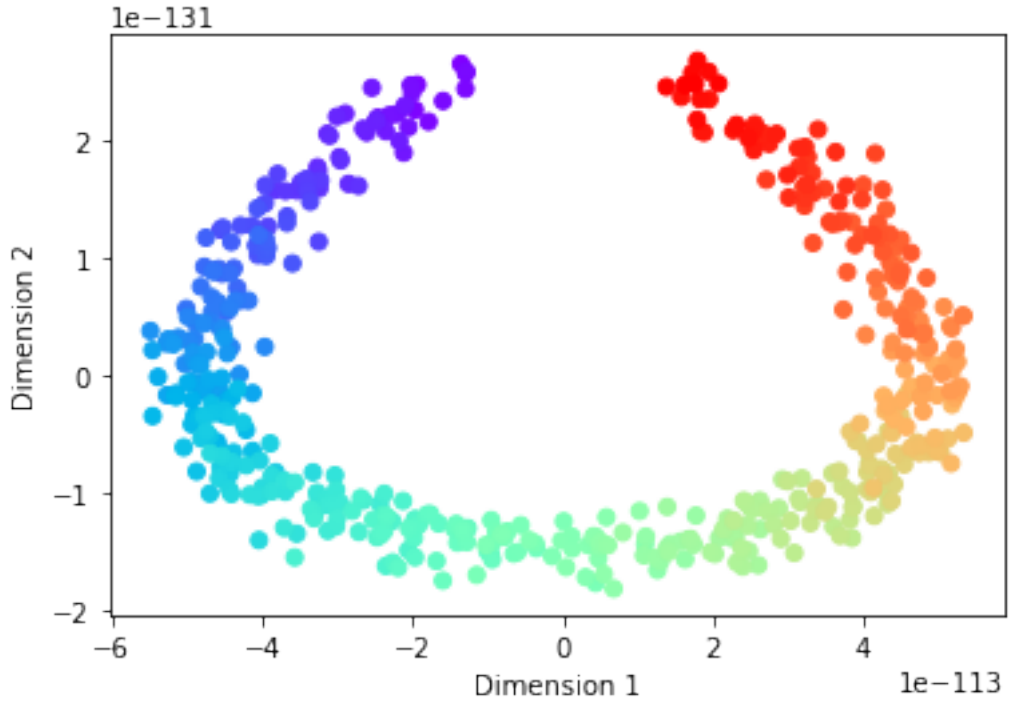

1e−31
4
3
2
1
0
−1
−2
−3
−4
Dimension 2
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
Dimension 1
1e−15

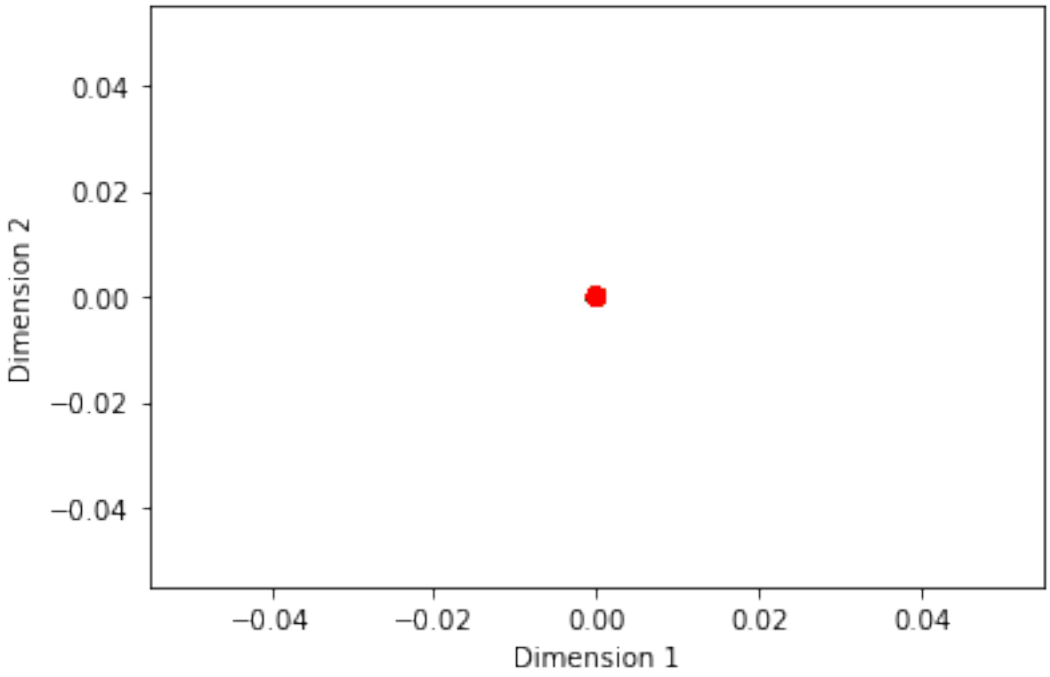

0.04
0.02
0.00
−0.02
−0.04
Dimension 2
−0.04
−0.02
0.00
0.02
0.04
Dimension 1

[226]:
```
for t in times:
    c = diffusion_map(t, 1000)
    plt.scatter(c[:,0],c[:,1], c=data["beta"], cmap=cm.rainbow)
    plt.xlabel("Dimension 1")
    plt.ylabel("Dimension 2")
    plt.show()
```



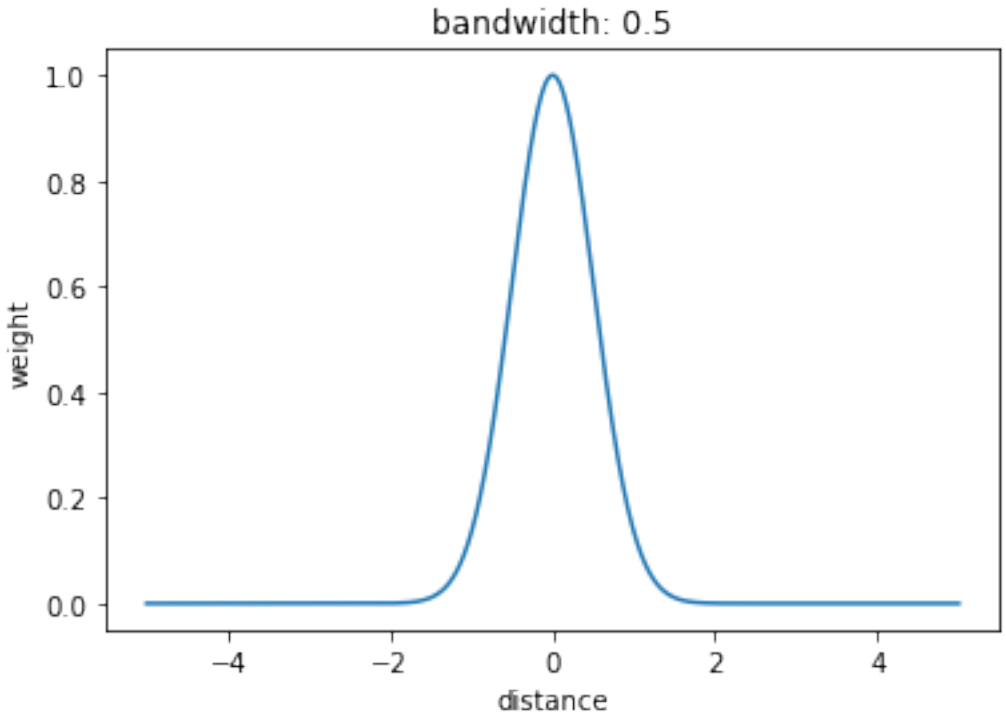

1e−13
1.5
1.0
0.5
0.0
−0.5
−1.0
Dimension 2
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
Dimension 1
1e−12

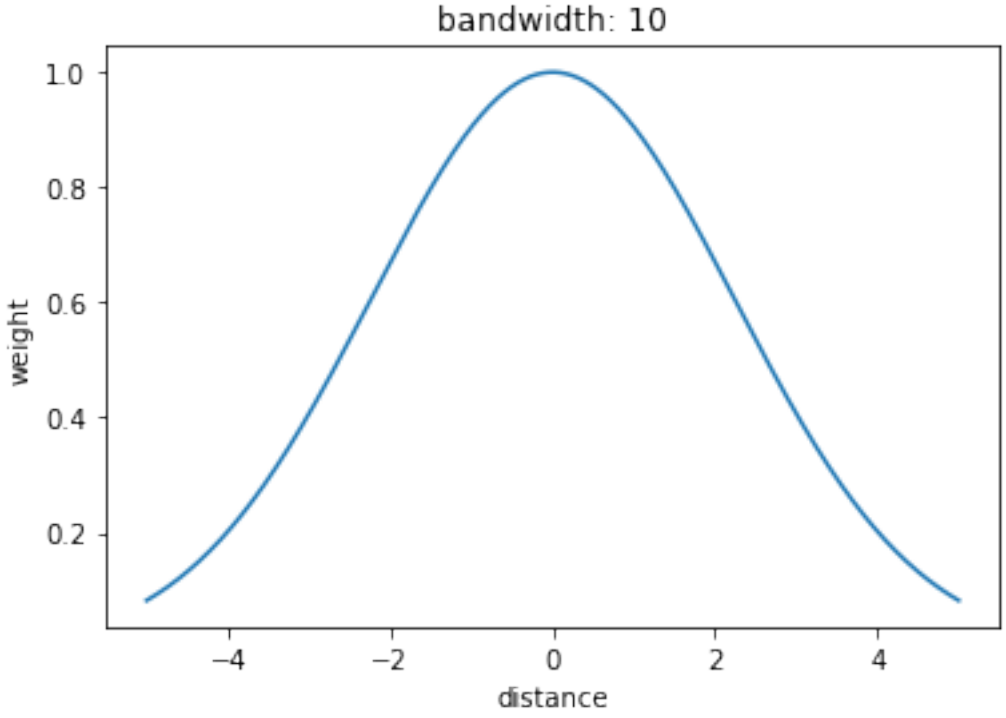

1e−131
2
1
0
−1
−2
Dimension 2
−6
−4
−2
0
2
4
Dimension 1
1e−113

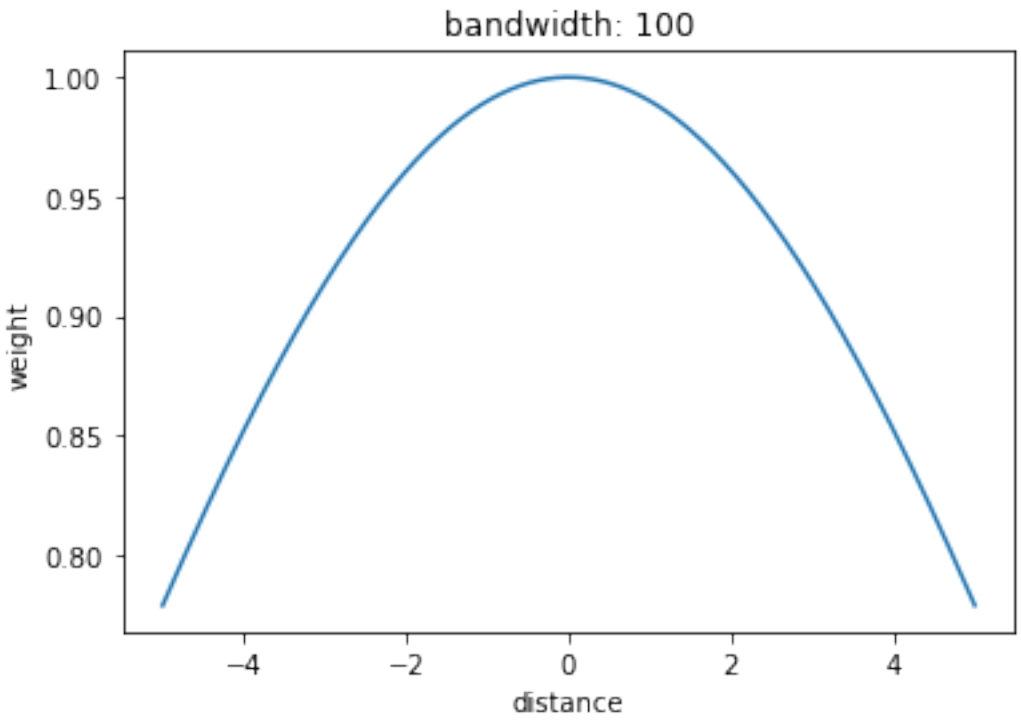


The greater the bandwidth, the higher weights you will be assigning to points further away (by definition of k) as can seen below in the plots. From the above plots, it seems like a bandiwth of 10 works well, and T doesn't make much of a difference until it becomes very big (for ex: $T = 10000$), in which case you loose information regarding the geometry of points as said in the lecture.

[211]:
```
def kernel(delta):
    return np.exp(-(0-x)**2/delta)
x = np.arange(-5, 5, 0.001)
for delta in [0.5, 10, 100]:
    y = kernel(delta)
    plt.plot(x, y)
    plt.title(f"bandwidth: {delta}")
    plt.xlabel("distance")
    plt.ylabel("weight")
    plt.show()
```


bandwidth: 0.5
1.0
0.8
0.6
0.4
0.2
0.0
weight
−4
−2
0
2
4
distance


bandwidth: 10
1.0
0.8
0.6
0.4
0.2
weight
−4
−2
0
2
4
distance


bandwidth: 100
1.00
0.95
0.90
0.85
0.80
weight
−4
−2
0
2
4
distance