CMSE 820: Homework #6

Due on October 27, 2019 at 11:59pm

Professor Yuying Xie

Boyao Zhu

Problem 1

Solution

a. Encode training data

We can use ϕ to map the original data matrix to a data matrix $\Phi(X)$ in the feature space, and perform dual PCA on the matrix $\Phi^T\Phi$, i.e.,

$$\Phi^T\Phi = V(\Sigma^2)V^T$$

where $\Phi = U\Sigma V^T$ is the compact SVD of Φ. The first d principal components $Y \in \mathbb{R}^{d\times n}$ are given by

$$Y = \Sigma_d V_d^T$$

where $\Sigma_d \in \mathbb{R}^{d\times d}$ and $V_d \in \mathbb{R}^{n\times d}$ are truncated from Σ and V, respectively.

b. Reconstruct training data

The first d principal component eigenvectors are given by

$$U_d = \Phi V_d(\Sigma_d^{-1})$$

The training data can be reconstructed in the feature space as

$$\tilde{\Phi}(X) = U_d Y = \Phi V_d(\Sigma_d^{-1})Y$$

c. Encode testing example

$$y^* = U_d^T\phi(x^*) = [\Phi V_d(\Sigma_d^{-1}]^T\phi(x^*)$$

d. Reconstruct test example

$$\tilde{\phi}(x^*) = U_d y^* = \Phi V_d(\Sigma_d^{-1})y^*$$

Problem 2

The Algorithm was attached in the following page, developed by Python.

Problem 3

The results were attached in the following page followed by **Problem 2**

Problem 4

The results were attached in the following page followed by **Problem 3**

Problem 5

1. Show that $K \succeq 0$ if and only if its eigenvalues are all nonnegative.

proof Since K is symmetric and hence normal, there exists an orthogonal matrix Q ad a diagonal matrix Λ such that $K = Q\Lambda Q^T$.

$$\begin{aligned} & K \succeq 0 \\ \iff & \forall v \in \mathbb{R}^n, v^TKv = v^TQ\Lambda Q^Tv = (Q^Tv)^T\Lambda(Q^Tv) \geq 0 \\ \iff & \Lambda \succeq 0 \\ \iff & \text{All eigenvalue of} K \text{are nonnegative.} \end{aligned}$$

Problem 5 continued on next page...

2. Show that $d_{ij} = K_{ii} + K_{jj} - 2K_{ij}$ is a squared distance function, i.e., there exists vectors $u_i, u_j \in \mathbb{R}^n$ for $1 \le i, j \le n$ such that $d_{ij} = \|u_i - u_j\|^2$.
proof Let $K = Q\Lambda Q^T$ be the eigenvalue decomposition of K. Define $U = \Lambda^{\frac{1}{2}} Q^T$. In particular, $K = U^T U$, i.e., $\forall i, j, K_{ij} = u_i^T u_j$ where u_i and u_j are the i-th and the j-th columns of U, respectively.

$$d_{ij} = u_i^T u_i + u_j^T u_j - 2u_i^T u_j = (u_i - u_j)^T (u_i - u_j) = \|u_i - u_j\|^2$$

Thus d is a square distance function.

3. Show that $A + B \succeq 0$ and $A \circ B \succeq 0$ (Hadamard product).
proof

$$\forall v \in \mathbb{R}^n, v^T(A+B)v = v^T Av + v^T Bv \ge 0 \Longrightarrow A + B \succeq 0.$$

Let the eigenvalue decompositions of A and B be $A = U\Lambda U^T = \sum_i \lambda_i u_i u_i^T$ and $B = V\Gamma V^T = \sum_i \gamma_i v_i v_i^T$.

$$A \circ B = \sum_{i,j} \lambda_i \gamma_j (u_i u_i^T) \circ (v_j v_j^T) = \sum_{i,j} \lambda_i \gamma_j (u_i \circ v_j)(u_i \circ v_j)^T$$

Note that $\forall x \in \mathbb{R}^T, x^T (u_i \circ v_j)(u_i \circ v_j)^T x = ((u_i \circ v_j)^T x)^T ((u_i \circ v_j)^T x) \ge 0,$ so $\forall i, j, (u_i \circ v_j)(u_i \circ v_j)^T \succeq 0$.
It follows that the nonnegative sum $A \circ B$ of positive semi-definite matrices is also positive semi-definite.

4. Show that the eigen values of AB are all positive given A, B are symmetric positive definite matrix with the same dimension.
proof Let v be an arbitrary eigenvector of AB corresponding to the eigenvalues λ, i.e., $ABv = \lambda v$. Assume $A \succ 0$ and $B \succ 0$.

$$ABv = AB^{\frac{1}{2}} B^{\frac{1}{2}} v = \lambda B^{-\frac{1}{2}} B^{\frac{1}{2}} v \Longrightarrow (B^{\frac{1}{2}} A B^{\frac{1}{2}})(B^{\frac{1}{2}} v) = \lambda (B^{\frac{1}{2}} v).$$

That is, an eigenvalue of AB must be eigenvalue of $B^{\frac{1}{2}} A B^{\frac{1}{2}}$. Note that $\forall x \in \mathbb{R}^n, x^T B^{\frac{1}{2}} A B^{\frac{1}{2}} x = (B^{\frac{1}{2}} x)^T A (B^{\frac{1}{2}} x) > 0$. So all eigenvalues of AB are positive.

5. If $A \succeq 0$ and $c \ge 0$, then $cA \succeq 0$
proof

$$\forall x \in \mathbb{R}^n, x^T cAx = cx^T Ax \ge 0 \Longrightarrow cA \succeq 0.$$

6. If $A \succeq 0$ and C can be written as $C = \{t_{[i]} A_{ij} t_{[j]}\}$ for $\forall t \in \mathbb{R}^n$, then $C \succeq 0$.

$$\forall x \in \mathbb{R}^n, \sum_{i,j} x_i x_j C_{ij} = \sum_{i,j} (x_i t_{[i]}) A_{ij} (x_j t_{[j]}) \ge 0 \Longrightarrow C \succeq 0.$$

7. Show that the Hadamard integral power $A^{\circ p} = \{A_{ij}^p\}$ and $p \in \mathbb{N}$ and Hadamard exponential $\exp(\circ A) = \{\exp(A_{ij})\}$ are p.s.d..
proof By (3),

$$A \succeq 0 \Longrightarrow A^{\circ 2} = A \circ A \succeq 0$$

By induction,

$$\forall p \in \mathbb{N}, A^{\circ p} \succeq 0. \quad \exp(\circ A) = \sum_{p=0}^{\infty} \frac{A^{\circ p}}{p!} \succeq 0.$$

Note that the finite sum $S_n(A) = \sum_{p=0}^{n} \frac{A^{\circ p}}{p!}$ is p.s.d., and $\{S_n\}$ converges uniformly to $\exp(\circ A)$.

Untitled10

October 27, 2019

1 Problem 2

[143]:
```
import numpy as np
from scipy import linalg
import scipy

def GaussianKernel(x,y,sigma):
    G = np.exp((-np.linalg.norm(x-y)**2)/(2*sigma**2))
    return G

def PolynomialKernel(x,y,a):
    P = (x.dot(y))**a
    return P

def KappaMatrix(X,kernel,tunPara):
    row = X.shape[0]
    col = X.shape[1]
    a = np.ones(col).reshape(col,1)
    H = np.identity(col) - np.matmul(a,a.T)/col

    if kernel == "Polynomial":
        X = X.dot(H)

    K = np.zeros((col,col))

    for i in range(col):
        xx = X[:,i]
        for j in range(col):
            yy = X[:,j]
            if kernel == "GaussianKernel":
                K[i,j] = GaussianKernel(xx,yy,tunPara)
            elif kernel == "Polynomial":
                K[i,j] = PolynomialKernel(xx,yy,tunPara)
            else :
                print ("Not valid kernel")
                return
                K[j,i] = K[i,j]
```

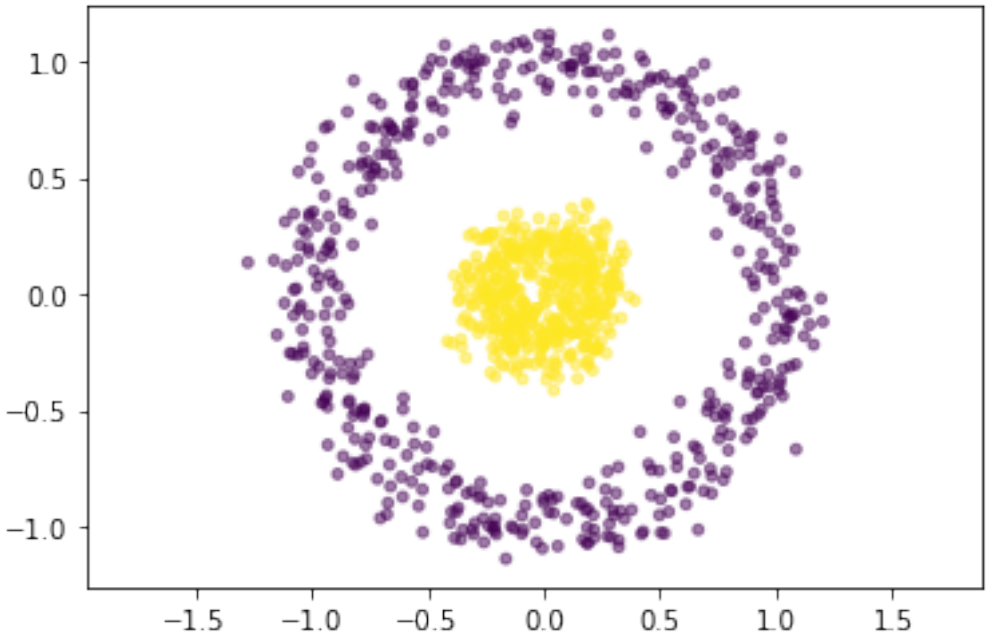
```
    K = H.dot(K.dot(H))
    return K

def KernelPCA(kappa,d):
    u,s,v = np.linalg.svd(kappa)

    Vtmp = v.T[:,0:d]
    s = np.diag(s)
    Sigma = scipy.linalg.sqrtm(s[0:d,0:d])
    Y = np.matmul(Sigma,Vtmp.T)
    return Sigma, Vtmp, Y
```

2 Problem 3

2.0.1 (1)

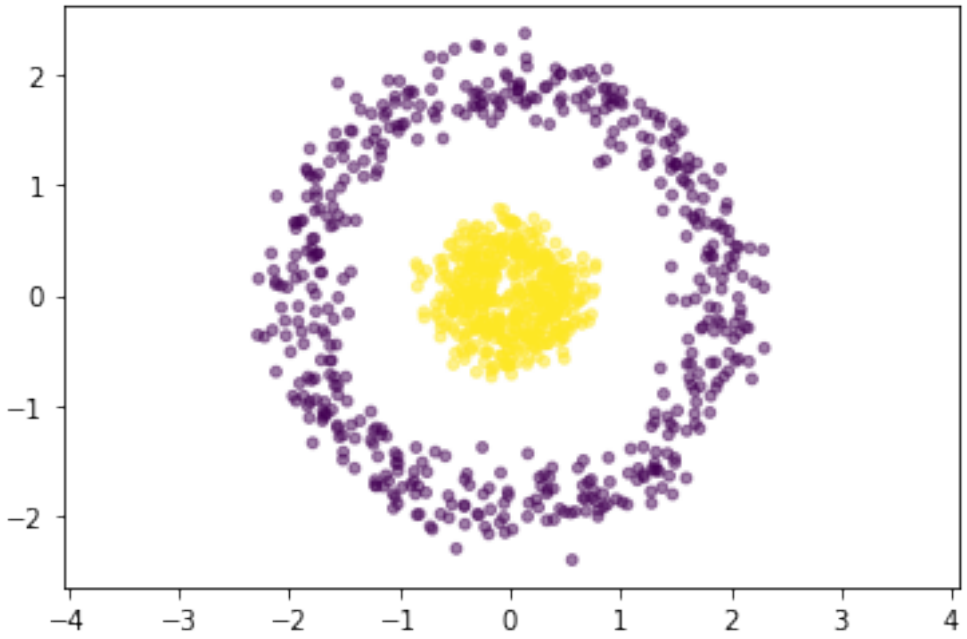
[47]:
```
import csv
import pandas as pd
import matplotlib.pyplot as plt

X = pd.read_csv("HW6_dat.csv").as_matrix()
X12= X[:,0:2]
X1 = X[:,0]
X2 = X[:,1]
y  = X[:,2]

from sklearn import preprocessing

X_scaled = preprocessing.scale(X12)
X1 = X12[:,0]
X2 = X12[:,1]

fig = plt.figure()

plt.scatter(X1,X2,alpha=0.5,c=y,s=15)
plt.axis('equal')
plt.show()
```

```
/Users/boyaozhu/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:5:
FutureWarning: Method .as_matrix will be removed in a future version. Use
.values instead.
  """
```



2.0.2 (2)

[159]:
```
eigval, eigvec = np.linalg.eig(np.cov(X_scaled.T))

Z12 = X_scaled.dot(eigvec)
Z1 = Z12[:,0]
Z2 = Z12[:,1]

fig = plt.figure()

plt.scatter(Z1,Z2,alpha=0.5,c=y,s=15)
plt.axis('equal')
plt.show()
```

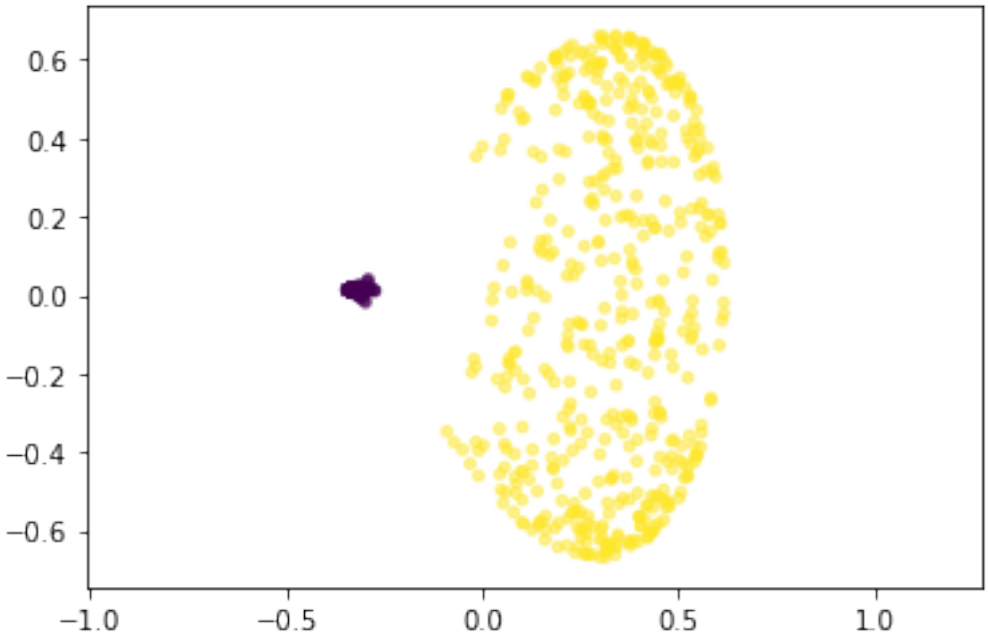


The PCA plot amounts to simply a rotation of the original data plot, and the data points are not linearly separable.

2.0.3 (3)

Gaussian Kernel

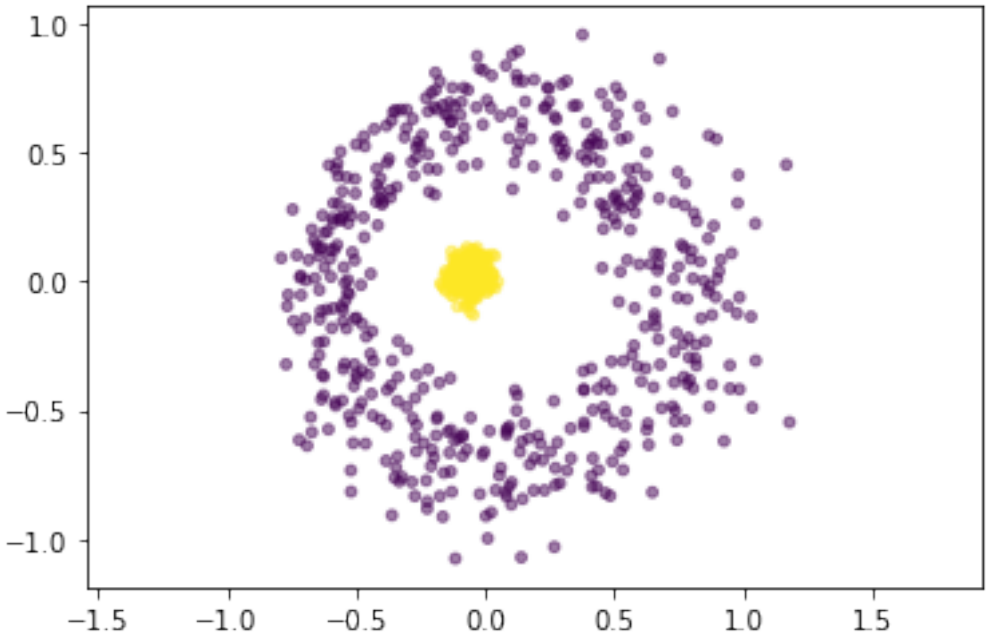
[147]:
```
K = KappaMatrix(X12.T,"GaussianKernel",0.2)

S,V,Y = KernelPCA(K,2)

fig = plt.figure()

Z1 = Y[0,:]
Z2 = Y[1,:]
plt.scatter(Z1,Z2,alpha=0.5,c=y,s=15)
plt.axis('equal')
plt.show()
```



This is the plot of KPCA with Gaussian kernal using the 1st and 2nd principal components. The data points with different colors have distinctly different first principal components. It is possible to separate the two groups by drawing a straight line on the plot.

Polynomial Kernel

[148]:
```
K = KappaMatrix(X12.T,"Polynomial",2)

S,V,Y = KernelPCA(K,2)

fig = plt.figure()

Z1 = Y[0,:]
Z2 = Y[1,:]
plt.scatter(Z1,Z2,alpha=0.5,c=y,s=15)
plt.axis('equal')
plt.show()
```



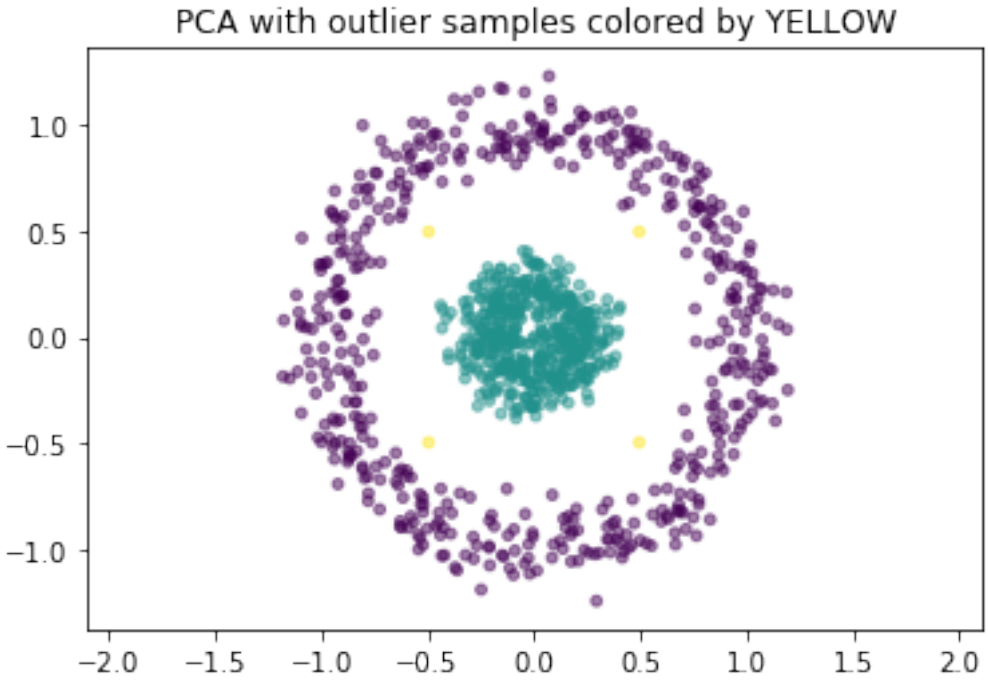
This is the plot of KPCA with polynomial kernel using the 1st and 2nd principal components. The first two principal components are not enough to separate the two groups of data points linearly.

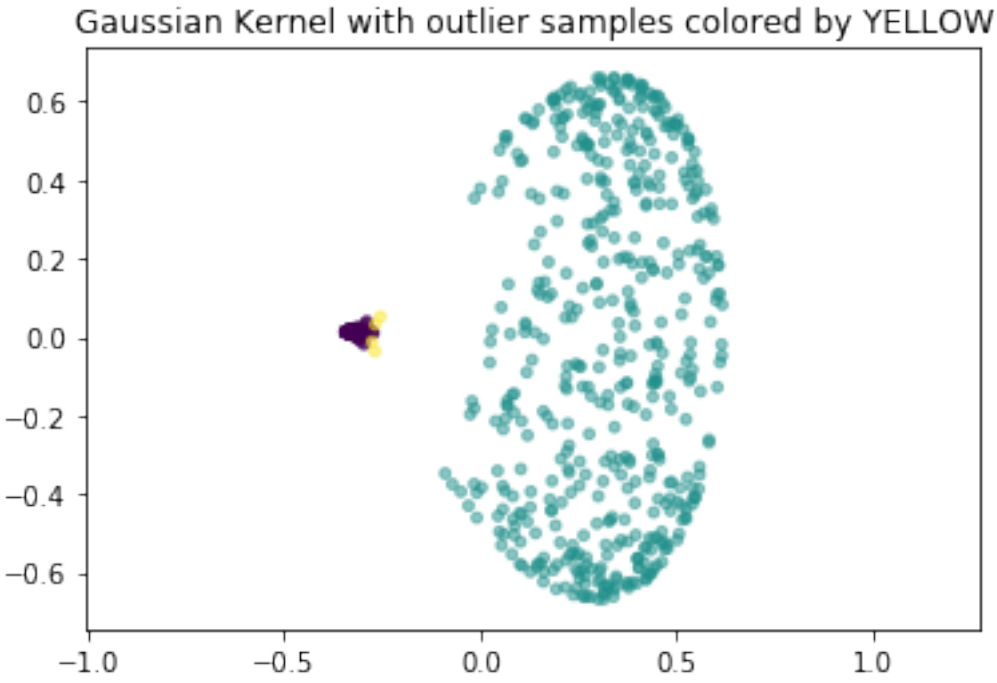
2.0.4 (4)

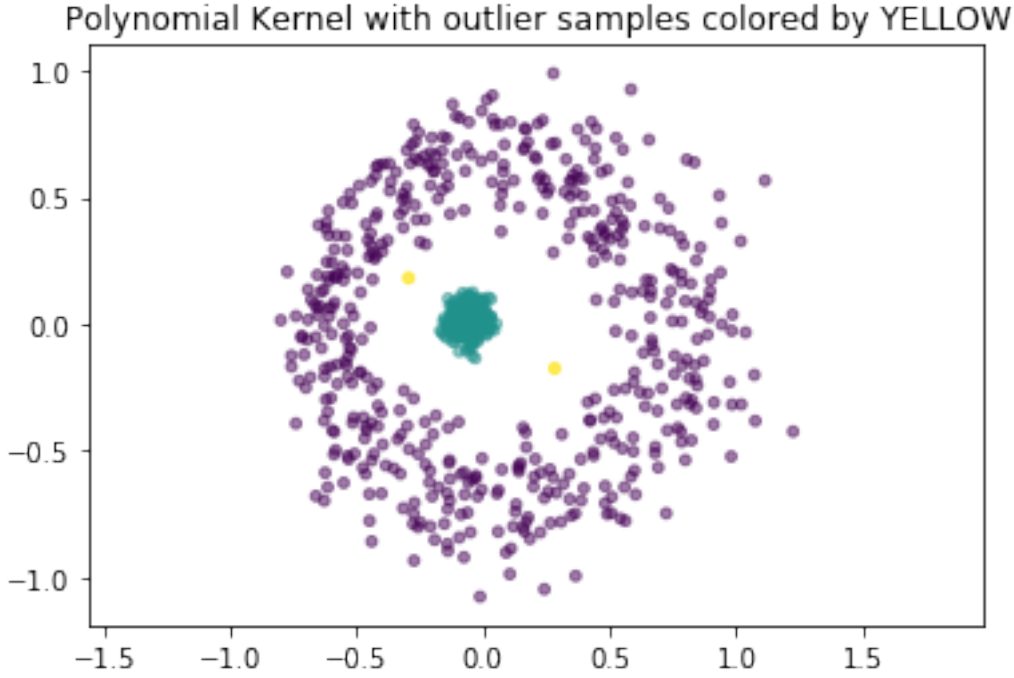
[178]:
```
X = pd.read_csv("HW6_dat.csv").as_matrix()
outPoint = np.array([[0,-0.7,2],[0,0.7,2],[0.7,0,2],[-0.7,0,2]])
yy = outPoint[:,2]
X = np.vstack((X,outPoint))

X12 = X[:,0:2]
y   = X[:,2]
# project first principal component learned from PCA
Comp12 = X12.dot(eigvec)
Comp1 = Comp12[:,0]
Comp2 = Comp12[:,1]

#PCA with outlier sample points colored by yellow
fig = plt.figure()
plt.scatter(Comp1,Comp2,alpha=0.5,c=y,s=15)
plt.axis('equal')
plt.title("PCA with outlier samples colored by YELLOW")
plt.show()
```

```
# Project first two PC learned from Kernel
K = KappaMatrix(X12.T,"GaussianKernel",0.2)
S,V,Y = KernelPCA(K,2)
fig = plt.figure()
Comp1 = Y[0,:]
Comp2 = Y[1,:]
plt.scatter(Comp1,Comp2,alpha=0.5,c=y,s=15)
plt.axis('equal')
plt.title("Gaussian Kernel with outlier samples colored by YELLOW")
plt.show()


# Project first two PC learned from Kernel
K = KappaMatrix(X12.T,"Polynomial",2)
S,V,Y = KernelPCA(K,2)
fig = plt.figure()
Comp1 = Y[0,:]
Comp2 = Y[1,:]
plt.scatter(Comp1,Comp2,alpha=0.5,c=y,s=15)
plt.title("Polynomial Kernel with outlier samples colored by YELLOW")
plt.axis('equal')
plt.show()
```

```
/Users/boyaozhu/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:1:
FutureWarning: Method .as_matrix will be removed in a future version. Use
.values instead.
  """Entry point for launching an IPython kernel.
```




Gaussian Kernel with outlier samples colored by YELLOW
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−1.0
−0.5
0.0
0.5
1.0


Polynomial Kernel with outlier samples colored by YELLOW
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

3 Problem 4

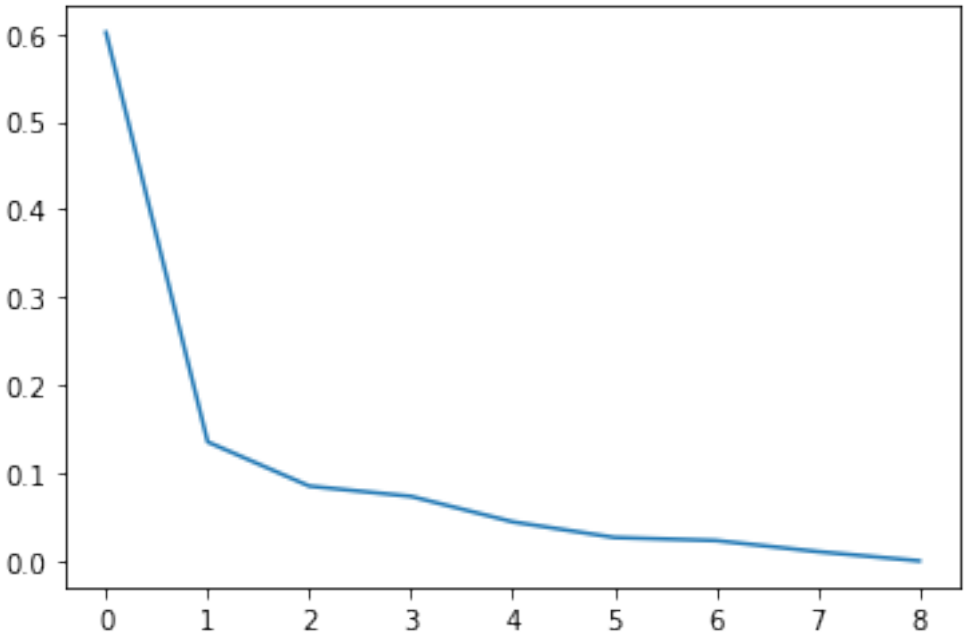
3.0.1 (1)

[210]:
```
D1 = np.array([[0     ,850.7 ,393.4 ,1765.9,2593  ,1259.7,187.4 ,2485.5,2694.1],
               [850.7 ,0     ,595.9 ,916.6 ,1742.3,1189.5,713.8 ,1731.2,1853.7],
               [393.4 ,595.9 ,0     ,1490.2,2296.5,927.1 ,206   ,2321.7,2435.7],
               [1765.9,916.6 ,1490.2,0     ,831.9 ,1723.5,1628.9,1016.7,946.6 ],
               [2593  ,1742.3,2296.5,831.9 ,0     ,2333.1,2448.8,959.9 ,342   ],
               [1259.7,1189.5,927.1 ,1723.5,2333.1,0     ,1092.3,2729.9,2588.9],
               [187.4 ,713.8 ,206   ,1628.9,2448.8,1092.3,0     ,2401.7,2567.4],
               [2485.5,1731.2,2321.7,1016.7,959.9 ,2729.9,2401.7,0     ,684.1 ],
               [2694.1,1853.7,2435.7,946.6 ,342   ,2588.9,2567.4,684.1 ,0    ␣
 ↪]])

print (D1)
```

```
[[   0.   850.7  393.4 1765.9 2593.  1259.7  187.4 2485.5 2694.1]
 [ 850.7    0.   595.9  916.6 1742.3 1189.5  713.8 1731.2 1853.7]
 [ 393.4  595.9    0.  1490.2 2296.5  927.1  206.  2321.7 2435.7]
 [1765.9  916.6 1490.2    0.   831.9 1723.5 1628.9 1016.7  946.6]
 [2593.  1742.3 2296.5  831.9    0.  2333.1 2448.8  959.9  342. ]
 [1259.7 1189.5  927.1 1723.5 2333.1    0.  1092.3 2729.9 2588.9]
 [ 187.4  713.8  206.  1628.9 2448.8 1092.3    0.  2401.7 2567.4]
 [2485.5 1731.2 2321.7 1016.7  959.9 2729.9 2401.7    0.   684.1]
 [2694.1 1853.7 2435.7  946.6  342.  2588.9 2567.4  684.1    0. ]]
```

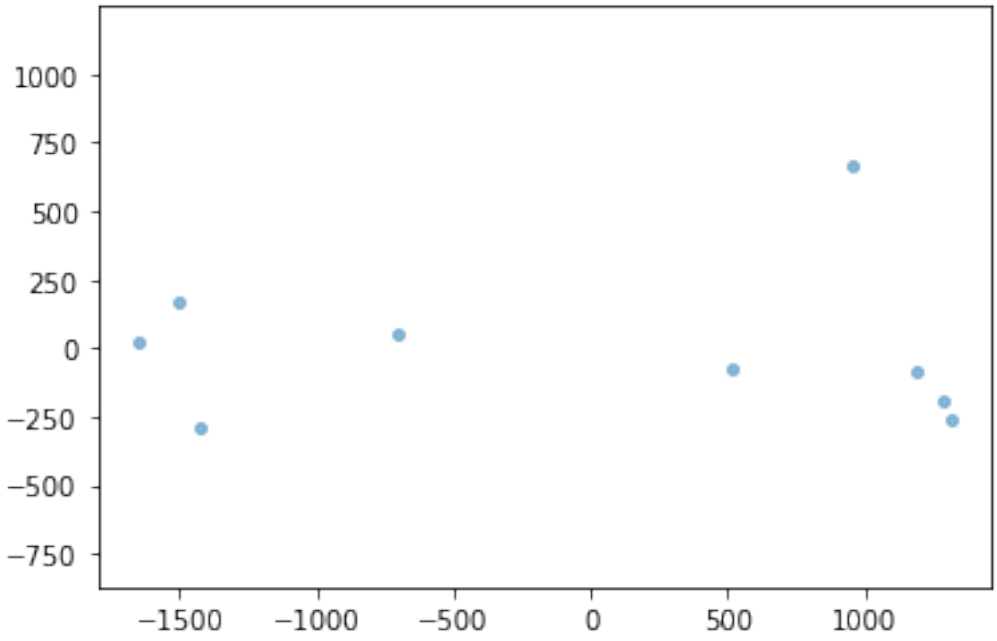
3.0.2 (2)

[234]:
```
identity = np.identity(D1.shape[0])
ones = np.ones(D1.shape[0])
h = identity-np.outer(ones,ones)/D1.shape[0]
b = -1/2*h.dot((D1).dot(h))


eigval, eigvec = np.linalg.eig(b)

eig_scale = np.flip(np.sort(eigval/np.sum(eigval)))

plt.plot(eig_scale)
plt.show()
```



3.0.3 (3)

[235]:
```
PC12 = b.dot(eigvec[:,0:2])
fig = plt.figure()
plt.scatter(PC12[:,0],PC12[:,1],alpha=0.5,s=15)
plt.axis('equal')
plt.show()
```

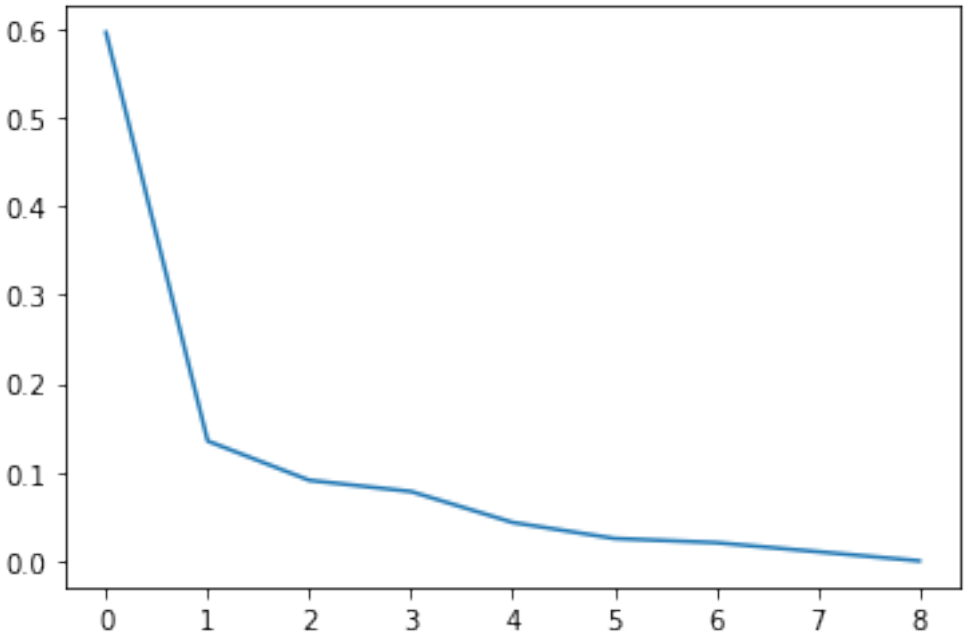


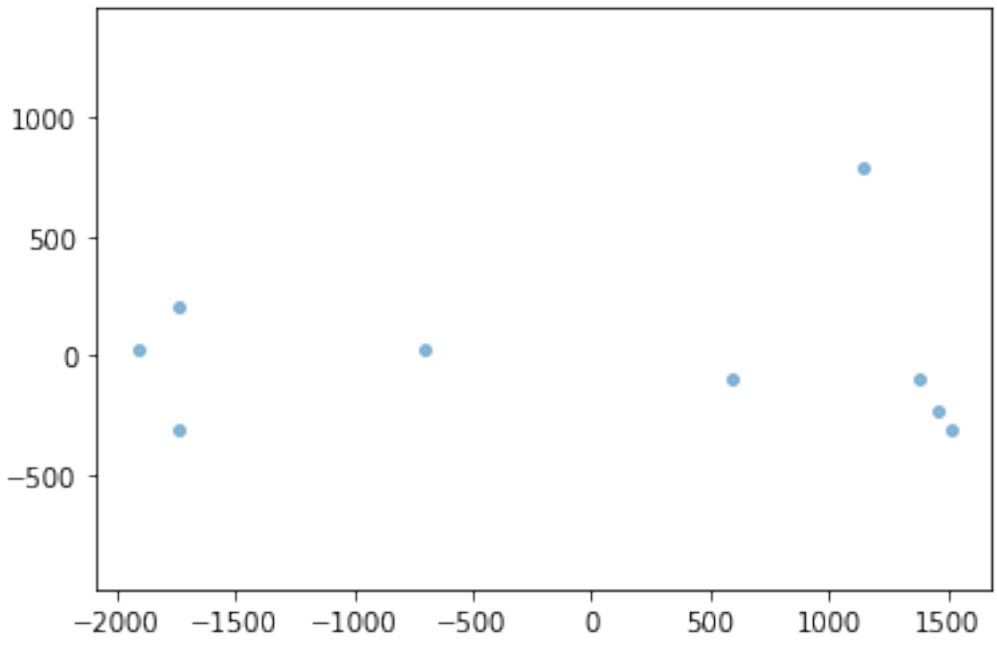
The relative positions and distances of the cities are well recovered.

3.0.4 (4)

[237]:
```
D1 = np.array([[0   ,983 ,441 ,1970,2983,1500,220 ,3054,3095],
               [983 ,0   ,699 ,1002,2015,1377,789 ,2064,2127],
               [441 ,699 ,0   ,1672,2669,1052,225 ,2767,2811],
               [1970,1002,1672,0   ,1017,2065,1779,1371,1255],
               [2983,2015,2669,1017,0   ,2734,2790,1135,382 ],
               [1500,1377,1052,2065,2734,0   ,1278,3300,3075],
               [220 ,789 ,225 ,1779,2790,1278,0   ,2861,2902],
               [3054,2064,2767,1371,1135,3300,2861,0   ,808 ],
               [3095,2127,2811,1255,382 ,3075,2902,808 ,0   ]])


identity = np.identity(D1.shape[0])
ones = np.ones(D1.shape[0])
h = identity-np.outer(ones,ones)/D1.shape[0]
b = -1/2*h.dot((D1).dot(h))


eigval, eigvec = np.linalg.eig(b)

eig_scale = np.flip(np.sort(eigval/np.sum(eigval)))
```

```
plt.plot(eig_scale)
plt.show()


PC12 = b.dot(eigvec[:,0:2])
fig = plt.figure()
plt.scatter(PC12[:,0],PC12[:,1],alpha=0.5,s=15)
plt.axis('equal')
plt.show()
```



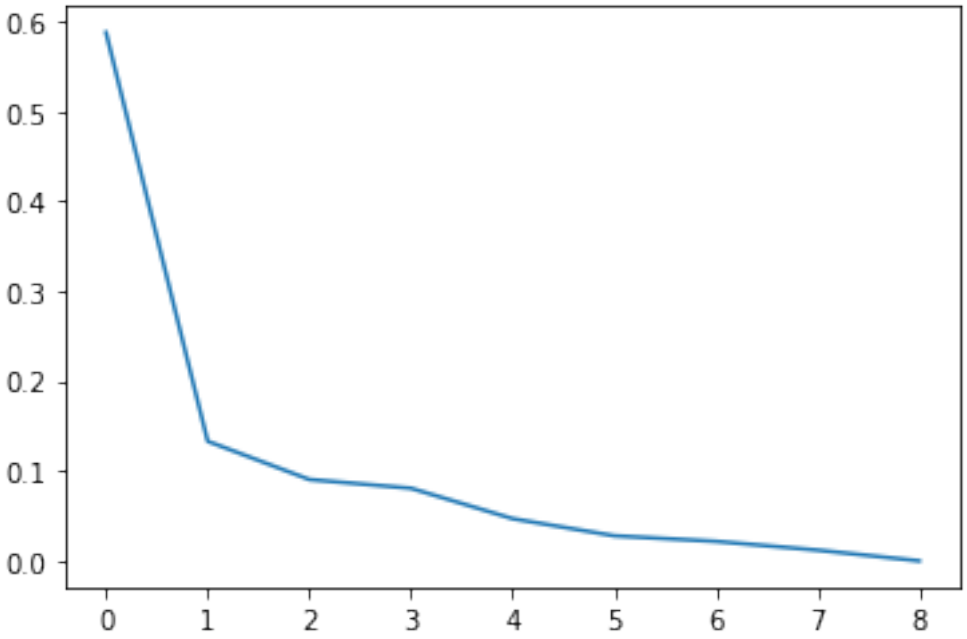


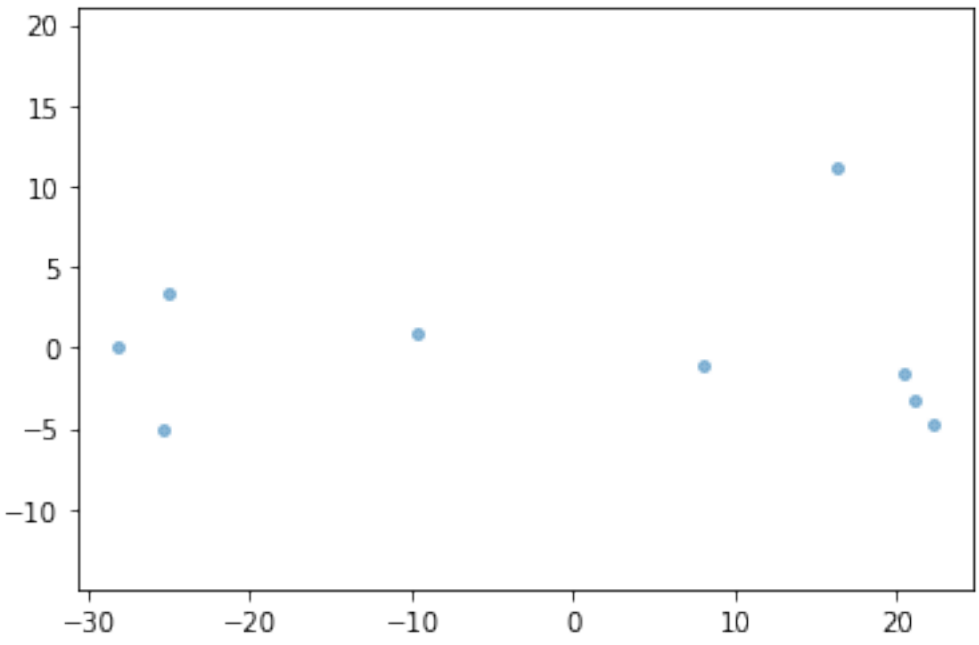
The relative positions and distances of the cities are well recovered. And we can see this is same as that of the air.

3.0.5 (5)

[238]:
```
D1 = np.array([[0   ,15   ,7.07 ,29   ,44   ,21.9 ,3.78 ,45   ,46   ],
               [15  ,0    ,10.9 ,14.87,29   ,19.82,12.6 ,30   ,31   ],
               [7.07,10.9 ,0    ,25   ,40   ,15.3 ,3.88 ,41   ,42   ],
               [29  ,14.87,25   ,0    ,15.83,29   ,26   ,20.4 ,19.18],
               [44  ,29   ,40   ,15.83,0    ,39   ,40   ,17.63,5.95 ],
               [21.9,19.82,15.3 ,29   ,39   ,0    ,18.6 ,48   ,45   ],
               [3.78,12.6 ,3.88 ,26   ,40   ,18.6 ,0    ,43   ,43   ],
               [45  ,30   ,41   ,20.4 ,17.63,48   ,43   ,0    ,12.28],
               [46  ,31   ,42   ,19.18,5.95 ,45   ,43   ,12.28,0    ]])

identity = np.identity(D1.shape[0])
ones = np.ones(D1.shape[0])
h = identity-np.outer(ones,ones)/D1.shape[0]
b = -1/2*h.dot((D1).dot(h))


eigval, eigvec = np.linalg.eig(b)

eig_scale = np.flip(np.sort(eigval/np.sum(eigval)))
```

```
plt.plot(eig_scale)
plt.show()


PC12 = b.dot(eigvec[:,0:2])
fig = plt.figure()
plt.scatter(PC12[:,0],PC12[:,1],alpha=0.5,s=15)
plt.axis('equal')
plt.show()
```





The relative positions and distances of the cities are well-recovered.

The three scatter plots of cities using classical MDS with different kinds of distances are very similar to one another, and the results agree very well with the actual geographical distances and positions. This is because all the distances used here are very close to the Euclidean distance on a 2D map.

[ ]: