IE 529

COMPUTATIONAL ASSIGNMENT 2

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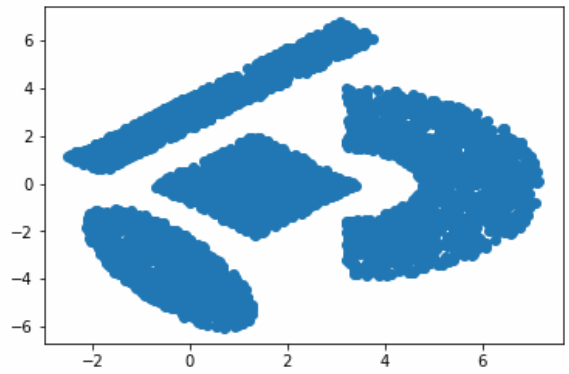
Question 1: Lloyd's Algorithm

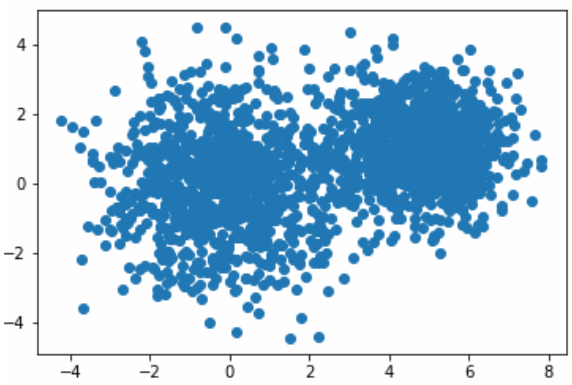
1. Output clustering results for both sets of data
2. Result evaluation for a range of k values-
   We could identify different types of clusters and depending on how many natural clusters, identifying them based on the value of k. In the case of ShapedData.csv, no clustering based on natural clustering was observed. In spite of varying the values of k from 2, the number of apparent clusters being distinguished are varying but the number of natural clusters still remain the same.
3. For the K-means algorithm, how was convergence tested for and why was this chosen as a test.
   The convergence was tested based on the distance function which evaluated the average distance from the cluster centres and as the different values of k were used and the iterations performed, one could test for the convergence criteria.

4. Brief Summary paragraph of findings
   The clustering was done for different values of k and then natural clusters were observed for both the data sets.

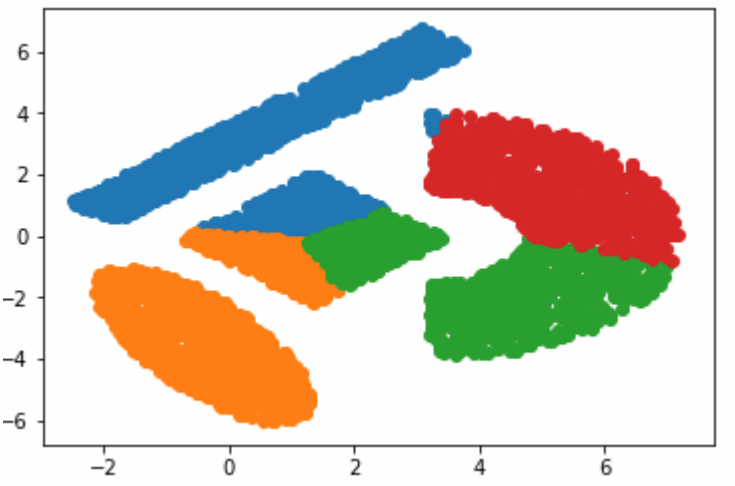
1. Scatter plot of ShapedData.csv



Scatter plot of Clustering.csv

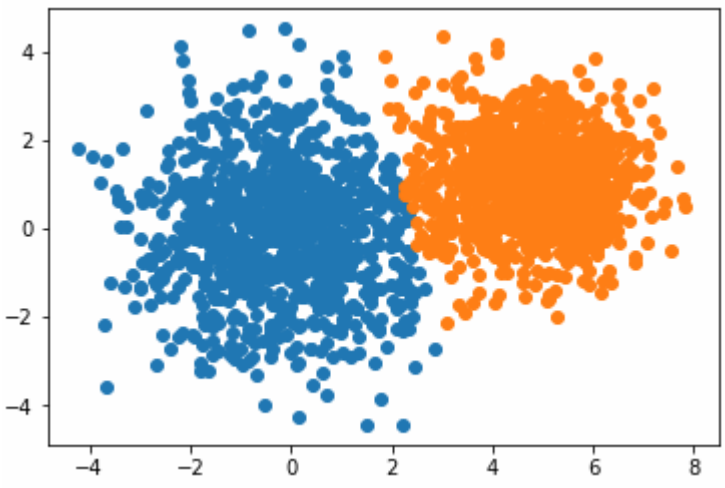


K=4 ShapedData.csv Scatter plot



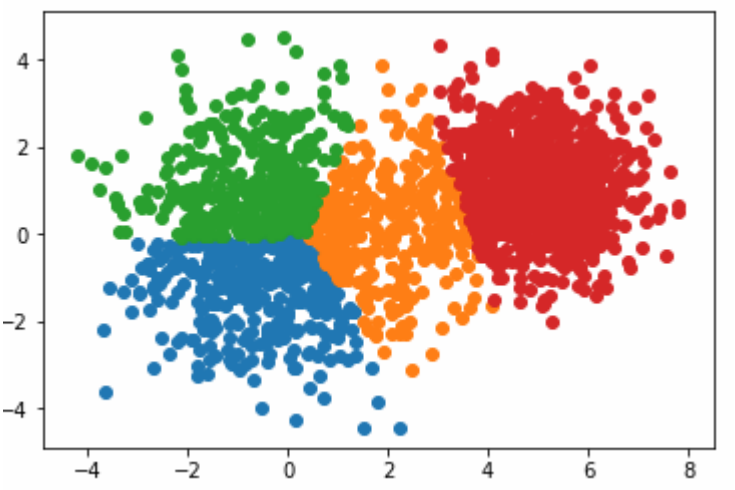
Natural Clusters – 4

K=2 Clustering.csv Scatter plot



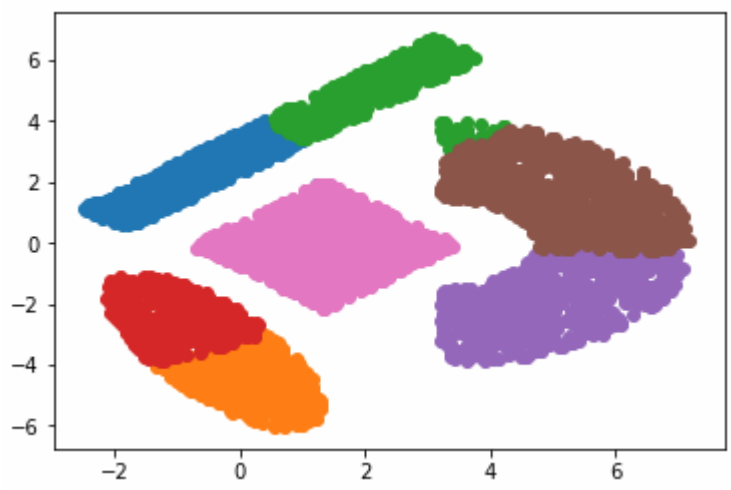
Natural Clusters-2

K=4 Clustering.csv Scatter plot



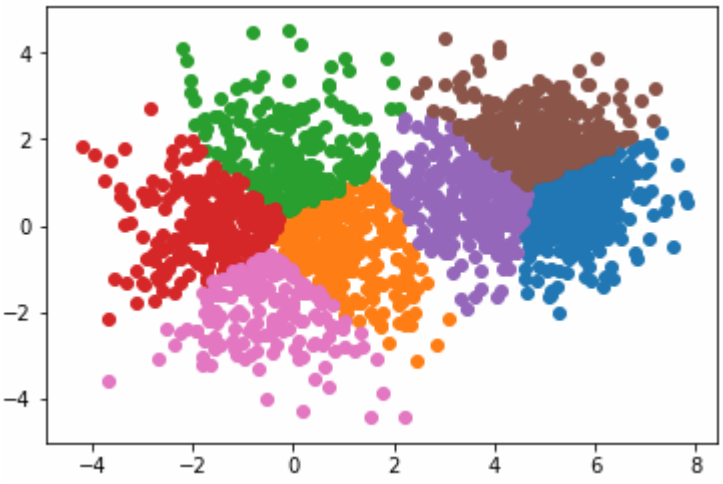
Natural Clusters -2

K=7 ShapedData.csv



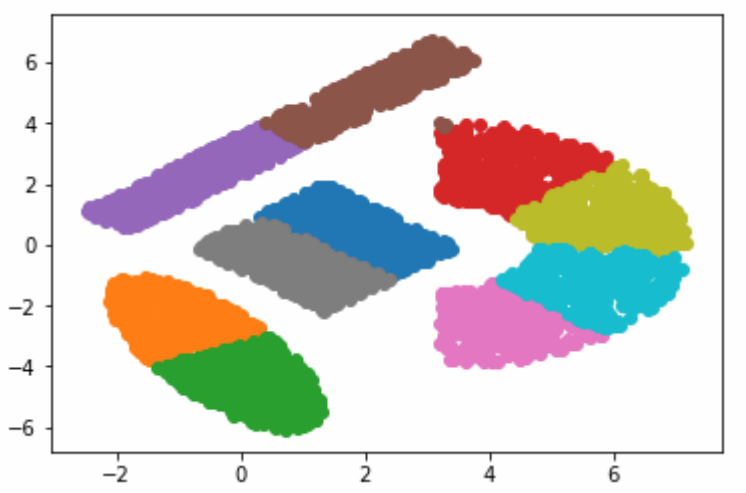
Natural Clusters-4

K=7 Clustering.csv



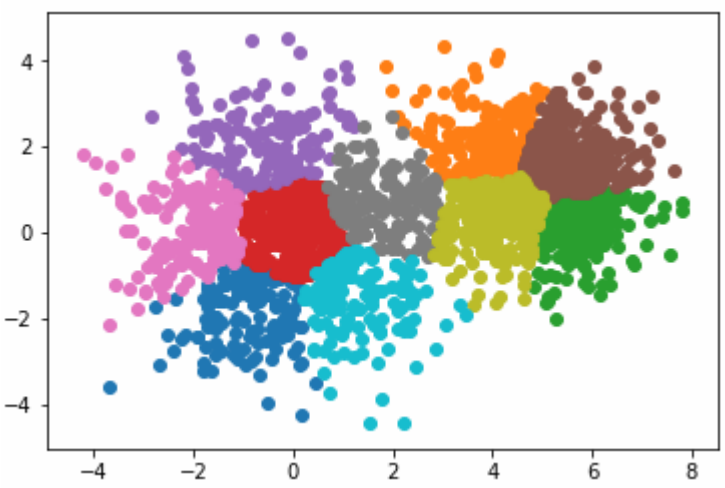
Natural Clusters-2

K=10 ShapedData.csv



Natural Clusters-4

K=10 Clustering.csv



Natural Clusters-2

Pseudocode for K Means Clustering Algorithm

Input: k(The number of clusters)

D(a set of lift ratios)

Output: a set of k clusters

Method:

Arbitrarily choose k objects from D as the initial cluster centers;

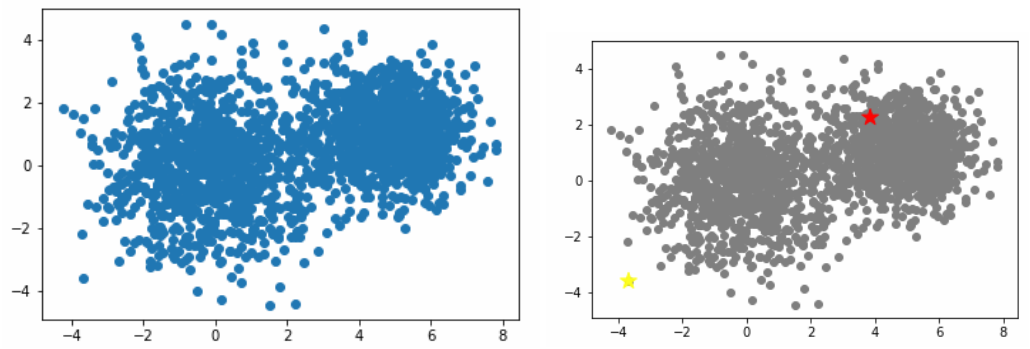
Repeat:

1. (re)assign each object to the cluster to which the object is the most similar, based on the mean value of the objects in the cluster;
2. Update the cluster means, i.e. calculate the mean value of the objects for each cluster

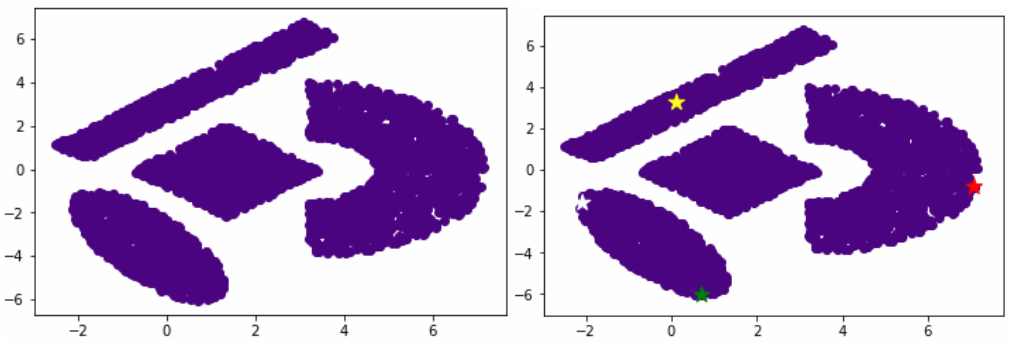
Until no change;

Question 2:

Scatter plot of Data 1(Clustering.csv)

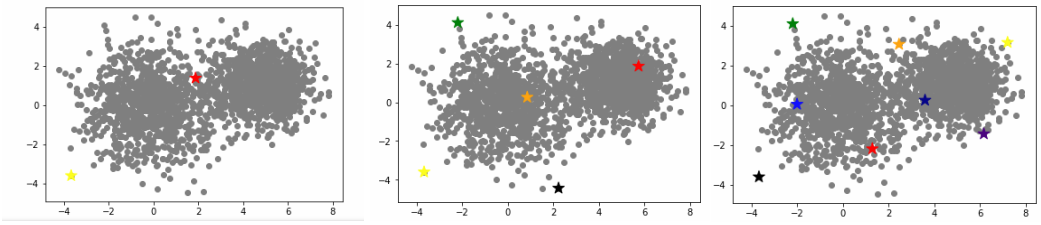


Scatter plot of Data2(ShapedData.csv)



Plots for k =2, 5 and 8

```
Centers:          0       1
13    1.8697  1.3846
641 -3.6773 -3.5965
Cost: 6.00669092514
```



Natural Clusters-2

Pseudocode for Greedy Algorithm

Input: Metric space $(V, d), k \in \mathbb{N}$.
Output: $F \subseteq V, |F| = k$, with minimum max distance to elements of V.

$F \leftarrow \{u\}$, for $u \in V$ arbitrary
while $|F| < k$ **do**
  Let $u \in V \setminus F$ be the element maximizing $d(u, F)$.
  $F \leftarrow F \cup \{u\}$
end while
return F

- Pick an arbitrary point $\bar{c}_1$ into C_1
- For every point $p \in \mathbf{P}$ compute $d_1[p]$ from $\bar{c}_1$
- Pick the point $\bar{c}_2$ with highest distance from $\bar{c}_1$. (This is the point realizing $r_1 = \underset{p \in P}{max}\, d_1[p]$)
- Add it to the set of centers and denote this expanded set of centers as C_2. Continue this till k centers are found

  - Choose the first centre arbitrarily.
  - At every step, choose the vertex that is furthest from the current centre to become a centre.
  - Continue until k centres are chosen

Pseudocode for Single Swap:

BEGIN FUNCTION SWAP

INPUT x, y

OUTPUT x, y (values switched)

t = x

x = y

y = t

RETURN

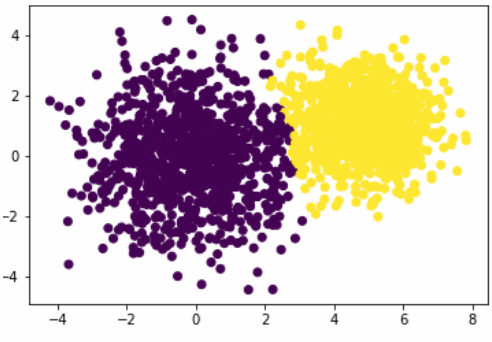
END FUNCTION swap

Pseudocode for Spectral Clustering:

1. project your data into R^n
2. define an A*ffinity* matrix A , using a Gaussian Kernel K or say just an Adjacency matrix (i.e. $A_{i,j} = \delta_{i,j}$)
3. construct the Graph Laplacian from A (i.e. decide on a normalization)
4. solve an Eigenvalue problem , such as $Lv = \lambda v$ (or a Generalized Eigenvalue problem $Lv = \lambda Dv$)
5. select k eigenvectors $\{v_i, i = 1, k\}$ corresponding to the k lowest (or highest) eigenvalues $\{\lambda_i, i = 1, k\}$, to define a k-dimensional subspace $P^t LP$
6. form clusters in this subspace using, say, k-means

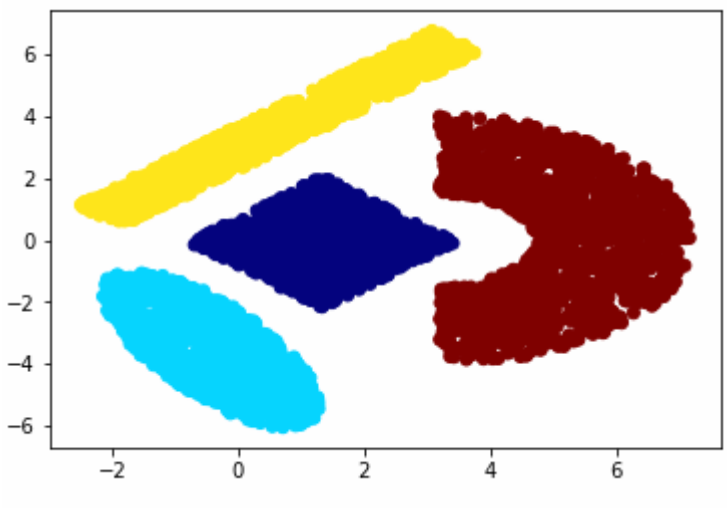
QUESTION 3: Spectral Clustering

Scatter plot for Clustering.csv



Natural clusters - 2

Scatter Plot of Shapeddata.csv



Natural clusters - 4

SHORT ANALYSIS OF THE COMPUTATIONAL EFFORT

Short analysis:
Lloyd's algorithm: The computational complexity of each iteration is O(Nkd) , complexity of the worst case is : $O(\mathrm{n}^{Kd+1}\log n)$
Greedy K Centers algorithm: The computational complexity of each iteration is O(Nkd)
Single-swap algorithm: The algorithm will terminate within $\binom{N}{K}$ steps.
Spectral clustering: The computational complexity of the similarity matrix is $O(d^2N^2)$, and the complexity of eigenvalues and eigenvectors is $O(N^3)$
Expectation Maximization: The computational complexity should be $O(mN^3)$, where m is the number of iterations.

The single swap algorithm is the most time consuming one.

Appendix[]:

Question 1: Lloyd's Algorithm and K-Means Clustering code

```
import random
import math
import numpy as np
```

```
def random_centers(data,k):
data_ = np.array(data)
centres_list = []
for x in range(0,k):
temp_rand = np.random.randint( 0,high = 1999)
temp = data_[temp_rand]
centres_list.append(temp)
data_ = np.delete(data_,temp,axis = 0)
return((centres_list))
def assign_data_centers(data, k,centres):
thePartition = [[] for _ in range(0,k)] # list of k empty lists
c = np.array(centres)
dp = np.array(data)
for a in dp:
temp_norm = np.linalg.norm((c-a),axis =1 )
minn = temp_norm.min()
temp_list = list(temp_norm)
thePartition[temp_list.index(minn)].append(a)
return thePartition
def revalaute_centres(data_with_centres,k):
data = data_with_centres
new_centres=[]
for x in data:
temp = np.array(x)
temp_m = temp.mean(axis = 0)
new_centres.append(temp_m)
return(new_centres)
```

```
import pandas as pd
data = pd.read_csv('ShapedData.csv',header = None)
```

```
k = 4
C = random_centers(data,k)
D_C_2 = assign_data_centers(data,k,C)
tol = 1
while tol > 0.00001:
N_C = revalaute_centres(D_C_2,k)
D_C_1 = D_C_2
D_C_2 = assign_data_centers(data,k,N_C)
temp_sum = 0
tol = tol/10
```

```
import matplotlib.pyplot as plt
plt.plot()
for i in D_C_2:
plt.scatter(pd.DataFrame(i)[0],pd.DataFrame(i)[1])
plt.show()
```

```
import pandas as pd
data_2 = pd.read_csv('clustering.csv', header=None)
```

```
k = 4
C = random_centers(data_2,k)
D_C_2 = assign_data_centers(data_2,k,C)
tol = 1
while tol > 0.00001:
N_C = revalaute_centres(D_C_2,k)
D_C_1 = D_C_2
```

```
D_C_2 = assign_data_centers(data_2,k,N_C)
temp_sum = 0
tol = tol/10

import matplotlib.pyplot as plt
plt.plot()
for i in D_C_2:
plt.scatter(pd.DataFrame(i)[0],pd.DataFrame(i)[1])
plt.show()
```

ALTERNATIVELY the Distance function in the K Means Algorithm may also be written as follows:

```
def k_means(data, centres, k, tol):
    """
    Kmeans algorihtm
    input data
    output: new clusters, centres

    """
    n = data.shape[0]
    e = 100
    c = 0
    for epoch in range(0,e):
        #calculated distances
        print (centres.shape)

        dist = distance_cal (data, centres)
        #assign cluster labels
        cluster_labels = np.argmin(dist, axis = 1) # n*1
        #new centroids
        centres_updates = np.zeros(shape = centres.shape)

        for j in range(0, k):
            points = []
            if sum(cluster_labels == j) == 0:
```

```
            centres_updates[j] = centres[j]
        else:
          # print (data[0])
           for d,label in zip(data, cluster_labels):
              if label == j:
                 points.append(list(d))

           centres_updates[j] = np.mean(points,axis = 0)
           np.mean(data[cluster_labels == j, :], axis=0)

    if (np.mean(np.amin(euclidean_distances(centres, centres_updates), axis = 1)) <= tol):
       print ("Convergence, iterations:", c)
       break
    c+=1
    centres = centres_updates

  return({"Iterations":c,    "Centroids": centres,
       "Labels": cluster_labels, "Cost": (np.mean(np.amin(euclidean_distances(data, centres), axis =
1))))})
```

Question 2[]:

```
#Importing libraries
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import random as rd

from sklearn.metrics.pairwise import euclidean_distances
data1 = pd.read_csv("C:/Users/Karthik/Desktop/IE_529/clustering.csv", header = None)
data2 = pd.read_csv("C:/Users/Karthik/Desktop/IE_529/ShapedData.csv", header = None)
def greedy_kcenters( data1, k ):
```

```
    copy = data1.copy()
    Init_center = copy.sample( 1 )
    copy.drop(Init_center.index,inplace = True)
    copy.index = list(range( copy.shape[0] ) )

    while Init_center.shape[0] < k:

        #Get index of data point that has maximum minimum distance from any centre
        ind = np.argmax(np.amin( euclidean_distances(copy, Init_center), axis=1 ))

        #Append data in temp_df at index ind into C
        Init_center = Init_center.append( copy.loc[ind] )

        #Remove that row from temp_df
        copy.drop(ind,inplace = True)
        #and change indices to 0,1,2,...,n-1
        copy.index = list( range( copy.shape[0] ) )
    del copy
    return( Init_center, np.amax(np.amin(euclidean_distances( data1, Init_center ), axis=1 )) )
plt.scatter(data1[0],data1[1])
plt.show()
centers, dist_cost = greedy_kcenters( data1, 2 )
print("Centers:", pd.DataFrame(centers))
print("Cost:", dist_cost)
plt.scatter(data1[0], data1[1], color = 'grey')
plt.scatter(centers[0],centers[1], marker = "*", color = ['red', 'yellow'], s =180)
plt.show()
plt.scatter(data1[0], data1[1], color = 'grey')
plt.scatter(centers[0],centers[1], marker = "*", color = ['red', 'yellow'], s =180)
plt.show()
centers2, dist_cost2 = greedy_kcenters( data2, 4 )
print("Centers:", pd.DataFrame(centers2))
print("Cost:", dist_cost2)
norm = plt.Normalize()
plt.scatter(data2[0], data2[1], color = 'indigo')
plt.scatter(centers2[0],centers2[1], marker = "*", color = ['yellow', 'green','red','white'], s =150)
```

```
plt.show()
k = [2,4,5,7,8,9]
for i in k:
    centers, dist_cost = greedy_kcenters( data1, i )
    print("Centers:", pd.DataFrame(centers))
    print("Cost:", dist_cost)
    plt.scatter(data1[0], data1[1], color = 'grey')
    plt.scatter(centers[0],centers[1], marker = "*", color = ['red', 'yellow','green','black', 'orange','indigo', 'blue', 'darkblue', 'lightgreen', 'purple'], s =180)
    plt.show()
def sswap_centers( data, k ):

    centers,dist = greedy_kcenters( data, k )

    C0 = pd.DataFrame(euclidean_distances( data, centers )).min(axis=1).sum()
    print("Gk centers cost= ", C0)

    counter = centers.shape[0]

    beginning = False

    while counter > 0:

        for i in range( centers.shape[0] ):
            if beginning == True:
                beginning = False
                break

            #Create a copy of the dataframe df without the centers Q
            copy = pd.concat( [data,centers] )
            copy.drop_duplicates(keep=False)
            copy.index = list( range( copy.shape[0] ) )

            #Swap
            while copy.shape[0] != 0:
                centers_new = pd.concat( [ centers.drop(centers.index[i]), copy.loc[[0]] ] )
```

```
            #Get cost of new centers
            Cost_new =  pd.DataFrame(euclidean_distances( data, centers_new )).min(axis=1).sum()

            #Check for reduced cost of more than gamma(which is taken to be 0.05)
            if Cost_new <= 0.95 * C0:
                print('1')
                centers = centers_new.copy()
                print("SS_cost= ", Cost_new)
                copy = pd.concat( [data,centers] )
                copy.drop_duplicates(keep=False)
                copy.index = list( range( copy.shape[0] ) )
                beginning = True
                counter = centers.shape[0]
                break
            else:
                copy.drop(0, inplace=True)
                copy.index = list( range( copy.shape[0] ) )
        if beginning == False:
            print(counter)
            counter -= 1

    #Return the centers
    return( centers )
sscenters = sswap_centers(data1,2)
plt.scatter(data1[0], data1[1], color = 'grey')
plt.scatter(sscenters[0],sscenters[1], marker = "*", color = ['red', 'yellow'], s =180)
plt.show()
sscenters2 = sswap_centers(data2,2)
plt.scatter(data2[0], data2[1], color = 'grey')
plt.scatter(sscenters2[0],sscenters2[1], marker = "*", color = ['red', 'yellow'], s =180)
plt.show()
```

QUESTION 3: SPECTRAL CLUSTERING

```
import pandas as pd
import numpy as np
```

```
import matplotlib.pyplot as plt
from sklearn.metrics.pairwise import euclidean_distances
import warnings
warnings.filterwarnings("ignore")
#This cell is for Lloyds Algorithm
def cluster_index( U, Y ):

    #Get the distance matrix which measures euclidean distance between rows of U and Y
    distanceMatrix = euclidean_distances( U, Y )

    #Return the index of the column that has minimun value as this would identify the closest centroid
    #and the average distance
    return ( np.argmin( distanceMatrix, axis=1 ), np.mean( np.amin( distanceMatrix, axis=1 ) ) )

def lloyds_kmean( U, k, tol ):

    #Convert U to pandas dataframe
    U = pd.DataFrame( U )

    #Initialization
    Y = U.sample( k )    #samples k points from df uniformly and stores them into Y
    Y.index  = list( range( len( Y.index ) ) )    #Replacing index values with regular 0,1,2,3,..,k-1

    #Initializing D to have very large value and D_ to have value less than D - tolerance to allow looping
    D = 1e5
    D_ = D - (tol + 7)

    while D - D_ > tol:
        D = D_
```

```
        #Assigning cluster index to each row of U and getting average distance
        C, D_ = cluster_index( U, Y )

        #Update Y with new centroids by calculating means of clusters
        for i in Y.index:
            Y.loc[i] = U.loc[U.index[C == i]].mean()

    #Return Y, C and D_
    return( Y, C, D_ )
#This function returns a matrix with Gaussian similarity between rows of dataframe
def gaussian_similarity_matrix( df ):

    #Ask the user for a sigma value
    sigma = float( input( "Please input a value for sigma:\nRemember that the parameter sigma controls the width of the neighborhoods" ) )

    #Create Euclidean distance matrix
    distance_Matrix = euclidean_distances( df, df )

    #Modify distance matrix to represent Gaussian similarity matrix
    distance_Matrix = np.exp( -np.square(distance_Matrix) / ( 2 * np.square(sigma) ) )

    #Return the gaussian-similarity matrix
    return distance_Matrix

#This function returns a matrix where each row has binary values and 1 representing that the row has that row as its nearest neighbor
def k_Nearest_Neighbor_matrix( df ):

    #Ask the user to input a value for k
    k = int( input( "Please input a value for k") )

    #Create a numpy array of zeros of size no. of rows in df x no. of rows in df
```

```
    k_NN_structure = np.zeros((df.shape[0],df.shape[0]))

    #Fill in 1 at all k nearest neighbors of each row
    k_NN_structure[np.array([np.arange(df.shape[0])]).T,\
                np.array(list(map( lambda x: np.argsort(euclidean_distances( x, df ))[:,1:k+1][0], np.array(df) )))] = 1

    #Ask the user what kind of undirected k-Nearest Neighbor structure does he/she want
    structure_type = input("What kind of undirected structure do you desire?\n" \
                    + "Press M for 'Mutual Nearest Neighbor Graph' which means that " \
                    + "vertices vi and vj are connected if both vi is among the k-nearest" \
                    + "neighbors of vj and vj is among the k-nearest neighbors of vi\n" \
                    + "Press S to simply ignore the directions of the edges, that is " \
                    + "connect vi and vj with an undirected edge if vi is among" \
                    + "the k-nearest neighbors of vj or if vj is among the k-nearest neighbors of vi.")

    if structure_type == 'M':
        k_NN_structure = k_NN_structure * k_NN_structure.T
    elif structure_type =='S':
        k_NN_structure[k_NN_structure + k_NN_structure.T > 0] = 1

    #Return the k-Nearest Neighbor structure matrix
    return k_NN_structure
def adjacency_matrix_creation( df ):

    #Next two lines not required. Remove later
    #Ask the user what kind of similarity function would they like
    #similarity_type = input( "Please select smilarity type of the graph:\nType G for the Gaussian Similarity function\nType K for the k-nearest neighborhood structure\n")

    #Get the k Nearest Neighbor Structure
    k_nearest_neighbor_structure = k_Nearest_Neighbor_matrix( df )
```

```
    #Get the Gaussian Similarity matrix
    gaussian_similarity = gaussian_similarity_matrix( df )

    #Multiply the two together to get the Weighted adjacency matrix W
    W = k_nearest_neighbor_structure * gaussian_similarity

    #Return the Weighted adjacency matrix W
    return W
#This function performs un-normalized graph Laplacian Spectral Clustering
def spectral_clustering( path, k ):

    #Read the data
    df = pd.read_csv( path, header = None )

    #W = adjacency matrix
    W = adjacency_matrix_creation( df )

    #Get the degree matrix D
    D = np.diag( np.sum( W, axis = 1 ) )

    #Get the graph Laplacian matrix
    L = D - W

    #Get the eigen values and eigen vectors of L
    w, v = np.linalg.eig( L )

    #Sort the eigen vectors based on ascending order of the eigen values
    v = v[ : , np.argsort( w ) ]

    #Ask the user to input a value of K which would help us get the first K eigen vectors
    K = int(input( "Please input a value for K to select the first K eigen vectors: "))
```

```
    #Store the first K eigen vectors in U
    print(v.shape)
    U = v[:,:K]


    #Ask the user to input a value for tolerance for Lloyds Algorithm
    tol = float(input( "Please input a value for tolerance for Lloyds Algorithm" ))


    #Run the Lloyds k-Means algorithm to return centers, cluster index vector and the
objective function cost
    return lloyds_kmean( U, k, tol )
centers, Cluster_index, cost = spectral_clustering( "clustering.csv", 2 )
trial_df = pd.read_csv("clustering.csv", header=None)
plt.scatter(trial_df[0], trial_df[1], c=Cluster_index)
plt.show()
centers, Cluster_index, cost = spectral_clustering( "ShapedData.csv", 4 )
trial_df = pd.read_csv("ShapedData.csv", header=None)
norm = plt.Normalize()
plt.scatter(trial_df[0], trial_df[1],  c = plt.cm.jet(norm(Cluster_index)))
plt.show()
print(np.square(1.22474487139), \
np.square(0.894427191))
```