HW CI-4 Clustering Algorithms

Computational Intelligence - STRATEGOS UNIGE

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Assignment: Develop Hard and Fuzzy Clustering Algorithms from scratch

We will implement some clustering algorithms from scratch and we will test on two data sets constituted by some 2-dimensional distributions of points.

Then we will apply our algorithms to a real-word data set.

TODO:

1. Generate data sets DS1 (non overlapping blobs), DS2 (overlapping blobs) and load DS3 from the file iris.csv.
2. Implement K-Means, Fuzzy C- Means and Graded Possibilistic C-Means.
3. Implement WTA and the $\alpha - cut$ defuzzifiers of fuzzy partitions.
4. Implement RAND and Jaccard Indeces for hard partition comparison
5. Apply K-Means, Fuzzy C-Means and Graded Possibilistic C-Means to the 3 data sets using a multi-start approach; search for 2, 3, and 4 clusters.
6. Defuzzify the soft partitions of Fuzzy C- Means and Graded Possibilistic C-Means using the WTA (Winner-Takes-All) criterion.
7. Visualize the results on the scatter plot, highlighting the centroids and using a different color for each cluster.
8. Measure the *accuracy* of the hard partitions by comparing them with the ground-truth constituted by the targets of the data sets. For the comparison use RAND and Jaccard indeces.

For the Graded Possibilistic C-Means use a possibilistic degree $\beta = 0.8$ and a value of η (identical for each cluster) comparable with the *standard_dev*^{2} for data sets DS1 and DS2. For DS3 (Iris data set) η must be selected by checking the value of the accuracy (model selection - grid search).

Optional part A: Consensus Matrix

1. Implement the Consensus Matrix technique for partition ensembling.
2. For each data set, take the 9 best hard partitions (3 clusters) obtained for data set DS2 in Part A and construct an ensemble using the tecnique of the consensus matrix.
3. Visualize the results on the scatter plot, highlighting the centroids and using a different color for each cluster.
4. Measure the *accuracy* of the partition induced by the consensus matrix by comparing it with the ground-truth constituted by the targets of the data sets. For the comparison use RAND index. Find the best value for the threshold α.

Optional part B: Study of the Graded Possibilistic C-Means algorithm

see below

Import libraries

In [ ]:

```
from sklearn.datasets import make_blobs
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np
import time  #timing the performances
import copy
```

1 Data sets generation

Data set DS1: Separate blobs

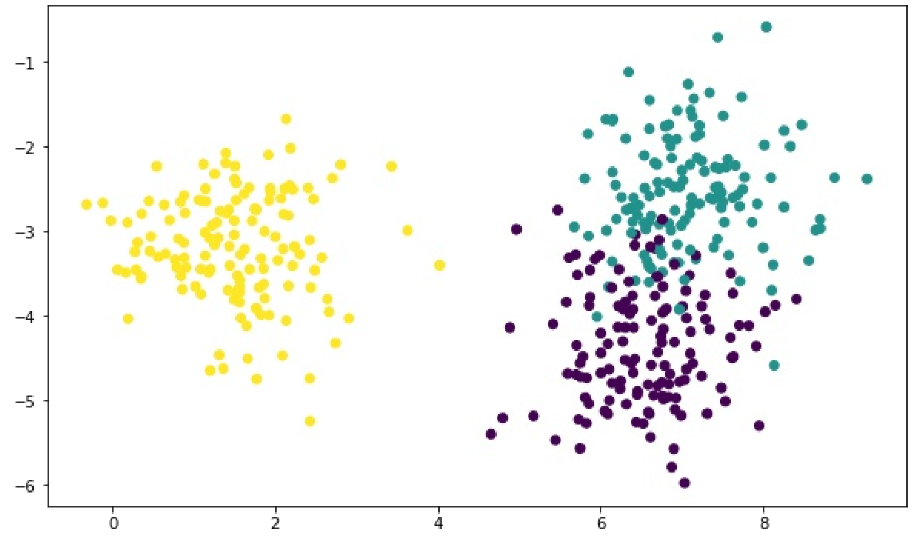
- number of points in the dataset 400
- number of features in the dataset 2
- number of clusters in the dataset 3
- standard deviation of points of a cluster 0.70

In [ ]:

```
# Dataset setup   crea nuovo dataset
number_of_points = 400   # number of points in the dataset
number_of_features = 2    # number of features in the dataset
number_of_clusters = 3    # number of clusters in the dataset
standard_dev = 0.70       # standard deviation of points of a cluster
  # st dev alta mi alza le distanze

features, target = make_blobs(n_samples = number_of_points,
                  n_features = number_of_features,
                  centers = number_of_clusters,
                  cluster_std = standard_dev,
                  shuffle = True)
# il dataset ha features e target
# makeblobs è di sklearn
```

In [ ]:

```
# Create a scatterplot of first two features

#creating array of for c clusters and 400 features


plt.figure(figsize=(10,6))
plt.scatter(features[:,0], features[:,1], c=target)

# View scatterplot
plt.show()
```



In [ ]:

```
x_labels = ['Feature'+str(x) for x in range(features.shape[1])]
y_label = 'target'

feats = pd.DataFrame(features, columns=x_labels)
tgts = pd.Series(target, name=y_label)
dataset1 = pd.concat([feats,tgts],axis=1)
dataset1.head()
```

Out[ ]:

	Feature0	Feature1	target
0	5.702309	-4.698122	0
1	7.340054	-4.161537	0
2	7.410921	-2.245790	1
3	1.314874	-4.465950	2
4	2.742432	-4.326481	2

Data set DS2: Overlapping blobs

- number of points in the dataset 400
- number of features in the dataset 2
- number of clusters in the dataset 3
- standard deviation of points of a cluster 1.70

In [ ]:

```
# Dataset setup
number_of_points = 400    # number of points in the dataset
number_of_features = 2    # number of features in the dataset
number_of_clusters = 3    # number of clusters in the dataset
standard_dev = 1.70       # standard deviation of points of a cluster


features, target = make_blobs(n_samples = number_of_points,
                  n_features = number_of_features,
                  centers = number_of_clusters,
                  cluster_std = standard_dev,
                  shuffle = True)
```

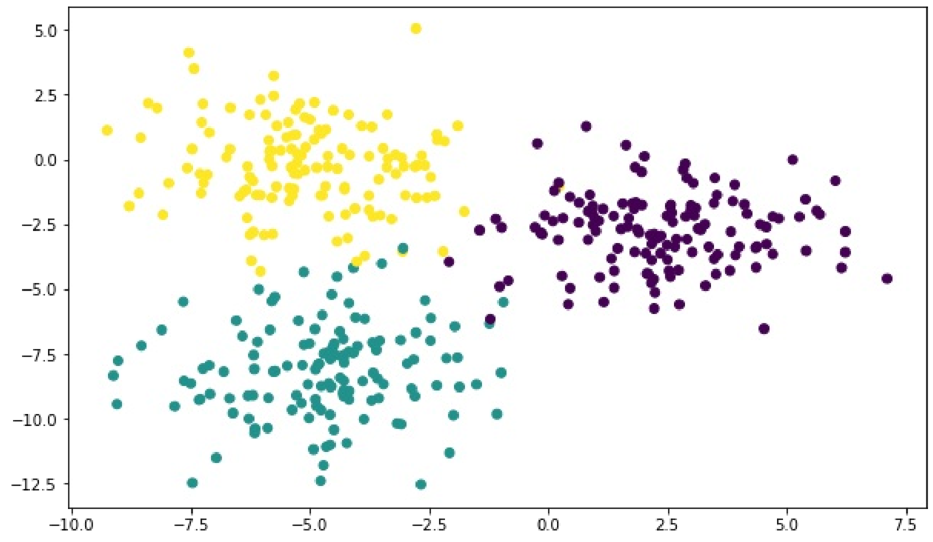
In [ ]:

```
ZeroList = np.zeros((3,400))

#print (ZeroList)
#creating a list of all the zeros for the number of targets we have so that we can run our test later

for i in range(0,len(target)):
    el = target[i]
    ZeroList[el,i] = 1

GT_list= list()
GT_list.append(ZeroList)
print(GT_list)
```

```
[array([[1., 1., 1., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.]])]
```

In [ ]:

```
# Create a scatterplot of first two features
plt.figure(figsize=(10,6))
plt.scatter(features[:,0], features[:,1], c=target)

# View scatterplot
plt.show()
```



In [ ]:

```
x_labels = ['Feature'+str(x) for x in range(features.shape[1])]
feats = pd.DataFrame(features, columns=x_labels)
tgts = pd.Series(target, name='target')
dataset2 = pd.concat([feats,tgts],axis=1)
dataset2.head()
```

Out[ ]:

	Feature0	Feature1	target
0	-7.501660	-8.644862	1
1	-8.207185	1.977507	2
2	-5.692888	1.293990	2
3	4.173844	-2.094026	0
4	-4.227330	-10.947644	1

Data set DS3: Iris Data set

Read the data set from the file *iris.csv* as done in *HW-CI-3-KNN.ipynb*

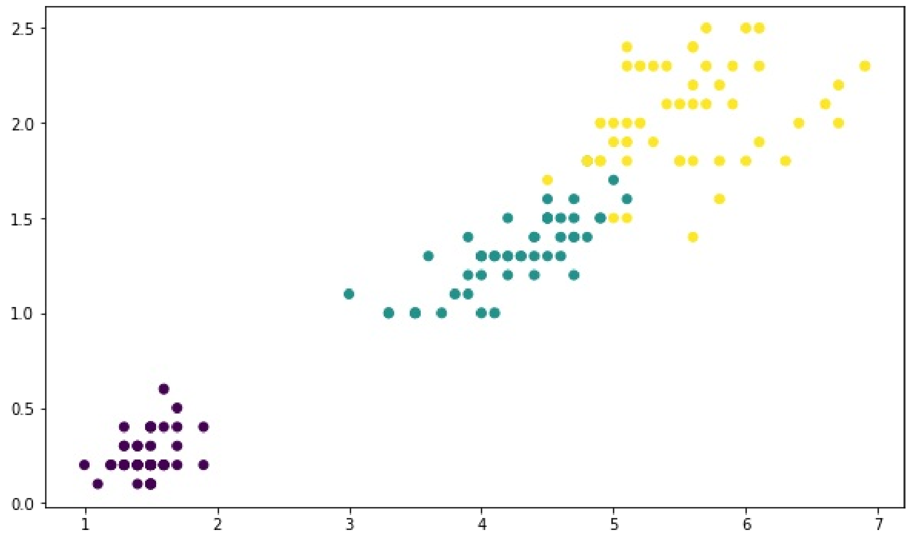
In [ ]:

```
# insert code here
# see DEMO CI3-a kNN classifier

col_names = ['sepal-length', 'sepal-width', 'petal-length', 'petal-width', 'class']
dataset = pd.read_csv('iris.csv', names=col_names)

#print (tgts)
target = 'class'

#creating dataset for petal width and length
x = dataset.get('petal-length')
y = dataset.get('petal-width')

TargetMatrix = dataset.get(target)
ModMatrix = list()
#we will run a loop for every target value and assign number and append to a new column

#identifying each feature with a number 0,1,2
for tgts in TargetMatrix:
    if tgts=='Iris-setosa':
        ModMatrix.append(0)
    if tgts=='Iris-versicolor':
        ModMatrix.append(1)
    if tgts=='Iris-virginica':
        ModMatrix.append(2)

target = pd.Series(ModMatrix, name='target')    #created a new series with the appended data
datasetIris = pd.concat([x,y,target],axis=1)

print(datasetIris)
```

```
     petal-length  petal-width  target
0             1.4          0.2       0
1             1.4          0.2       0
2             1.3          0.2       0
3             1.5          0.2       0
4             1.4          0.2       0
..            ...          ...     ...
145           5.2          2.3       2
146           5.0          1.9       2
147           5.2          2.0       2
148           5.4          2.3       2
149           5.1          1.8       2

[150 rows x 3 columns]
```

In [ ]:

```
# after downloaded the Iris data set uncomment the code in this box

#Create a scatterplot of first two features
plt.figure(figsize=(10,6))
plt.scatter(x,y,c=target)

# View scatterplot
plt.show()
```



In [ ]:

```
GT_iris = np.zeros((3,150), dtype=int)

for i in range(0,len(target)):
    el = target[i]
    GT_iris[el,i] = 1

GT_list.append(GT_iris)
print(GT_list)
```

```
[array([[1., 1., 1., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.]]), array([[1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1
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        1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
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        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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       [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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        1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]]), array([[1, 1, 1, 1, 1, 1, 1, 1, 1,
1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
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       [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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       [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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        1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]]), array([[1, 1, 1, 1, 1, 1, 1, 1, 1,
1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
        1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
        1, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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        1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
        1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
        1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]])]
```

In [ ]:

```
# after downloaded the Iris data set uncomment the code in this box

x_labels = ['Feature'+str(x) for x in range(features.shape[1])]
feats = pd.DataFrame(features, columns=x_labels)
tgts = pd.Series(target, name='target')
dataset2 = pd.concat([feats,tgts],axis=1)
dataset2.head()
```

Out[ ]:

	Feature0	Feature1	target
0	-1.171644	2.434095	0.0
1	5.465683	-1.854309	0.0
2	-1.875120	-5.813020	0.0
3	-2.913915	-7.217382	0.0
4	10.391301	0.238920	0.0

2 Implentation of clustering algoritms

K-Means (aka Hard C-Means)

K-Means minimizes the functional

$$E(X) = \sum_{i=1}^{K} \sum_{\mathbf{x} \in \pi_i} \|\mathbf{x} - \mathbf{v}_i\|^2 = \sum_{ih} u_{ih} \|\mathbf{x}_h - \mathbf{v}_i\|^2, \quad \text{with} \quad u_{ih} = \begin{cases} 1 & if\, \boldsymbol{x}_h \in \pi_i \\ 0 & otherwise \end{cases}$$

where $\mathbf{x}$ is a point of the data set, n is the size of the data set, K is the number of clusters, $\mathbf{v}_i$ are the centroids, and π_i is the subset of the data set belonging to cluster i. Note that $E(X)$ is proportional to the expectation of distortion.

In this implementation we will initialize the cluster centers by selecting at random K points from the data set, and then we will iterate the re-evaluation of all π_i and of $\mathbf{v}_i$, until a STOP CRITERION holds.

The STOP CRITERION can be:

1. *Stop when the variation of $E(X)$ in two subsequent cycles (ΔE) is under an assigned threshold $\tau > 0$.*
2. *Stop when the maximum variation of the centroids $\mathbf{v}_i$ in two subsequent cycles ($\Delta \mathbf{v}$) is under an assigned threshold $\tau > 0$.*
3. *Stop after an assigned number S of iterations.*

We suggest to use the following combined STOP CRITERION: **Stop after an assigned numer S of iterations** AND **Stop when the variation of $<E>=\frac{E(X)}{K \cdot n}$ in two subsequent cycles ($\Delta <E>$) is under an assigned threshold $\tau > 0$**.

In [ ]:

```
# add here the required imports
import sys
import matplotlib.pyplot as plt
import pandas as pd
import numpy as np
from scipy.spatial import Voronoi, voronoi_plot_2d #for voronoi tessellation
```

In [ ]:

```
class KMeans:

    def __init__(self, k=3, tau=0.001, max_iter=300, verbose=False):
        self.k = k # number of centroids
        self.tau = tau # stopping threshold
        self.max_iter = max_iter # maximum number of iterations in case of no convergence
        self.verbose = verbose # detailed printout
        self.cost = list() # service variable to store cost history
        self.centroids = None # centroids after fitting
        self.U = None # membership matrix (for K-Means U is hard, i.e. its element are 0/1)

        # additional variable shared among the various functions
        self.n = 0 # holds the dataset size
        self.prev_error = np.inf # assign initial error as infinite
        self.iteration = None # interation number
        self.error =  None # private variable to hold error E(X)
        self.distances = None # private variable to hold distances
        self.prev_centroids = None
        self.x_map = None
```

```python
    def get_centroids(self):
        return self.centroids

    def get_U(self):
        UU = copy.deepcopy(self.U)
        return UU.transpose()


    def get_cost_history(self):
        return self.cost

    def plot_cost_history(self, size_x = 15, size_y = 6, data=None, label=None):
        if data==None:
            data= self.cost
        if label==None:
            label = 'Cost History'

        # simply plot the cost history
        fig, ax = plt.subplots(figsize=(size_x,size_y))

        ax.plot(data, color='r', label=label)     # cost line
        ax.legend()
        plt.show()
        return ax

    def calc_cost(self):
        # reset distances for items for farther clusters
        # define the cluster index list for data items
        x_map = np.argmin(self.distances,axis=1)

        # define the membership matrix from cluster index list
        # u becomes 1 for items in given cluster and zero for the others
        u = np.zeros_like(self.distances)
        u[np.arange(self.n),x_map] = 1
        # set the distances other than minimal to zero
        dist = np.multiply(self.distances,u) # optimized multiplication
        if self.verbose: sys.stderr.write('dist: {}\n'.format(dist))
        # compute the error - <E> expectation of distortion

        self.error = np.sum(dist)/(self.k*self.n)
        #self.error = np.sum(dist)

        #delta_e = np.abs(self.prev_error - error)
        delta_e = self.prev_error - self.error
        #print ("error= ", error, " delta_error= ", delta_e)
        self.cost.append(self.error)
        self.prev_error = self.error
        return delta_e

    def predict(self,x):
        # checks the test samples and return the list of centroid indexes
        # which each sample belongs to

        if self.verbose: sys.stderr.write('centroids: {}\n'.format(self.centroids))

        # compute distances from centroids
        for j in range(self.n):
            for i in range(self.k):
                #self.distances[j][i] = np.sqrt(np.sum((x[j]-self.centroids[i])**2))
                #self.distances[j][i] = np.sum((x[j]-self.centroids[i])**2)
                    self.distances[j][i] = np.sum(np.dot(x[j]-self.centroids[i],x[j]-self.centroids[i]))

        #print (self.distances)
        # assign the points of the data sets to the k clusters (nearest centroid)
        self.x_map = np.argmin(self.distances,axis=1)
        return self.x_map  # lista delle predizioni

    def get_centroids_distance(self):
        # controllo le distanze da centroidi
        clu_dist = 0
        for c, pc in zip(self.centroids,self.prev_centroids): clu_dist += np.sqrt(np.dot(c-pc,c-pc))
        return clu_dist

    def fit (self, x):
        # performs kmeans clustering on training samples and assign centroids
        self.n = x.shape[0]  # number of training items
        c = x.shape[1]  # number of features

        # initialize the K centroids by selecting at random  K  points from the data_set
        idx = np.random.randint(self.n,size=self.k)
        self.centroids = x[idx].copy()
        self.prev_centroids = self.centroids.copy()
        # initialize the membership matrix with n rows and k columns
        self.U = np.zeros((self.n,self.k), dtype=int)
        # create a distance matrix with the same shape as the membership one
        self.distances = np.zeros_like(self.U,dtype=float)

        # iterate while DELTA E > tau (STOP CRITERION #1) or max_iter not reached
        loop = True
        self.iteration = 0
        while (loop):
            # match training data to the current centroids and update their
            # membership index list
            self.x_map = self.predict(x)
            if self.verbose: sys.stderr.write('x_map: {}\n'.format(self.x_map))

            #   calculate the new k centroids
            for i in range(self.k):
                # perform the average only if the centroid has assigned elements
                # otherwise NaN is assigned and the algorithm has errors
                if (self.x_map == i).any():
                    self.centroids[i] = np.average(x[self.x_map == i],axis=0)

            delta_cost = self.calc_cost()
            self.iteration +=1
            # break the loop if the stopping conditions are met
            clu_dist = self.get_centroids_distance()
            self.prev_centroids = self.centroids.copy()
            if self.verbose:
                  print(self.iteration, "error= ", self.error, " delta_error= ", delta_cost, "tau = ", self.tau)
            loop = (abs(delta_cost) > self.tau) and (self.iteration < self.max_iter)

           #loop = (delta_cost > self.tau) and (clu_dist > self.tau) and (self.iteration < self.max_iter)

        # set the membership matrix for the final configuration
        self.U[np.arange(self.n),self.x_map] = 1

        return self
```

Fuzzy C-Means

Fuzzy C-Means minimizes the functional

$$J(U,V) = \sum_{h=1}^{n}\sum_{i=1}^{c}\left(u_{ih}\right)^m \|\mathbf{x}_h - \mathbf{v}_i\|^2 , \qquad \forall h = 1, \dots, n \qquad \forall i = 1, \dots, c$$

with the probabilistic constraint

$$\sum_{i=1}^{c} u_{ih} = 1$$

where $\mathbf{x}_h$ are the point of the data set, c is the number of clusters, $\mathbf{v}_i$ are the centroids, and u_{ih} are the membrships of data points to clusters.

In this implementation we will initialize the cluster centers $\mathbf{v}_i$ by selecting at random c points from the data set, and then we will iterate the re-evaluation of all u_{ih} and of $\mathbf{v_i}$,

$$u_{ih} = \frac{1}{\sum_{j=1}^{c}\left(\frac{\| \mathbf{x}_h - \mathbf{v}_i \|}{\| \mathbf{x}_h - \mathbf{v}_j \|}\right)^{\frac{2}{m-1}}}$$

$$\mathbf{v}_i = \frac{\sum_{h=1}^{n}\left(u_{ih}\right)^m \mathbf{x}_h}{\sum_{h=1}^{n}\left(u_{ih}\right)^m}$$

until a STOP CRITERION holds.

The STOP CRITERION can be either:

1. *Stop when the variation of $J(U,V)$ in two subseguent cycles (ΔJ) is under an assigned threshold $\tau > 0$.*
2. *Stop when the variation of*

   $$E(X) = \sum_{ih} u_{ih}\|x_h - v_i\|^2$$

   in two subseguent cycles (ΔE) is under an assigned threshold $\tau > 0$.
3. *Stop when the maximum variation of the centroids $\mathbf{v}_i$ in two subseguent cycles ($\Delta\mathbf{v}$) is under an assigned threshold $\tau \geq 0$.*
4. *Stop when the maximum variation of the memberships u_{ih} in two subseguent cycles (Δu) is under an assigned threshold $\tau \geq 0$.*
5. Stop after an assigned number S of iterations.

We suggest to use the following combined STOP CRITERION: **Stop after an assigned number S of iterations** AND **Stop when the variation of $<E> = \frac{E(X)}{c \cdot n}$ in two subseguent cycles ($\Delta <E>$) is under an assigned threshold $\tau > 0$**.

In [ ]:

```
class FuzzyCMeans:

    def __init__(self, m=2, k=3, tau=0.001, max_iter=300, verbose=False):
        self.m = m #corresponds to the degree of fuzziness of the solutio
        self.c = k # number of centroids
        self.tau = tau # stopping threshold
        self.max_iter = max_iter # maximum number of iterations in case of no convergence
        self.verbose = verbose # detailed printout
        self.cost = list() # service variable to store cost history

        self.centroids = None # centroids after fitting
        self.U = None # membership matrix (for K-Means U is hard, i.e. its element are 0/1)

        # additional variable shared among the various functions
        self.n = 0 # holds the dataset size
        self.iteration = None # interation number

        self.prev_error = np.inf # assign initial error as infinite
        self.prev_error_j = np.inf # for j parameter
        self.error =  None # private variable to hold error E(X)
        self.errorj = None # for j parameter

        self.distances = None # private variable to hold distances
        self.prev_centroids = None
        self.x_map = None

    def distance(self,vect1, vect2):  # return the square distance of two arrays
                distance=0
                for i in range(len(vect1)):
                    distance = distance + (vect1[i] - vect2[i])**2
                return distance
```

```python
    def calc_U(self, list_x):   # calculate the membership matrix
        # initialize the matrix
        matrix = copy.deepcopy(np.zeros((self.c, self.n)))
        # calculate coeff.
        m_exponent = 2/(self.m -1)
        #modify the centroid by calculating distance amoung each point
        for i in range(0,self.c):        # for all the rows
            for h in range(0, self.n):   # for all the columns
                sum = 0
                for j in range(0,self.c):

                    centroidi = np.array(self.centroids[i])
                    centroidj = np.array(self.centroids[j])
                    dist1 = self.distance(list_x[h],centroidi)
                    dist2 = self.distance(list_x[h], centroidj)
                    if dist2==0: # if element = voronoi
                        sum=sum
                    if dist2!=0 and dist1!=0:
                        sum = sum + (dist1 / dist2)**m_exponent

                if sum!=0:
                    matrix[i][h] = matrix[i][h]+ (1/sum)  # ematrix element
        self.U = matrix.transpose()
        #print(self.U)
        return matrix

    def get_U(self):
        return self.U

    def get_centroids(self):
        return self.centroids

    def get_cost_history(self):
        return self.cost

    def plot_cost_history(self, size_x = 15, size_y = 6, data=None, label=None):
        if data==None:
            data= self.cost
        if label==None:
            label = 'Cost History'

        # simply plot the cost history
        fig, ax = plt.subplots(figsize=(size_x,size_y))
        ax.plot(data, color='r', label=label)     # cost line
        ax.legend()
        plt.show()
        return ax

    def calc_cost(self):

        uj = copy.deepcopy(self.U).transpose()

        # errors
        #if self.verbose: sys.stderr.write('dist: {}\n'.format(dist)) #
        # <E> computation
        dist = np.multiply(self.distances,uj)

        self.error = np.sum(dist)/(self.c*self.n)
        delta_e = abs(self.prev_error - self.error)

        self.cost.append(self.error)
        self.prev_error = self.error
        #----------------------------------------

        # <J> computation
        distj= np.multiply(self.distances,np.power(uj,self.m))
        self.error_j = np.sum(distj)

        if self.iteration>=2:
            delta_j = abs(self.prev_error_j - self.error_j)
        else:
            delta_j = 100

        return [delta_e,delta_j] # compare treshold

    def predict(self,x):
        if self.verbose: sys.stderr.write('centroids: {}\n'.format(self.centroids))
        # compute distances from centroids
        for j in range(self.n):
            for i in range(self.c):
                self.distances[j][i] = np.sum(np.dot(x[j]-self.centroids[i],x[j]-self.centroids[i]))
        # assign the points of the data sets to the k clusters (nearest centroid)

        self.x_map = np.argmin(self.distances,axis=1)
        return self.x_map

    def get_centroids_distance(self):
        # check distance of centroids
        clu_dist = 0
        for c, pc in zip(self.centroids,self.prev_centroids): clu_dist += np.sqrt(np.dot(c-pc,c-pc))
        return clu_dist

    def fit (self, x): #this code was edited
        # performs kmeans clustering on training samples and assign centroids
        self.n = x.shape[0]  # number of training items
        c = x.shape[1] # number of features

        # initialize the K centroids by selecting at random  K  points from the data_set
        idx = np.random.randint(self.n,size=self.c)
        self.centroids = x[idx].copy()
        self.prev_centroids = self.centroids.copy()

        # initialize the membership matrix with n rows and k columns
        self.U = np.zeros((self.n,self.c), dtype=float)                  #
        # create a distance matrix with the same shape as the membership one
        self.distances = np.zeros_like(self.U,dtype=float)
        #-------------------------------------------------------------------------------------

        # iterate while DELTA E > tau (STOP CRITERION #1) or max_iter not reached
        loop = True
        self.iteration = 0
        while (loop):
            # match training data to the current centroids and update their
            # membership index list
            self.x_map = self.predict(x)
            if self.verbose: sys.stderr.write('x_map: {}\n'.format(self.x_map))

            #-----------------------------------
            #   calculate the new k centroids
            #for this we create a loop for each element and calculate the centroid using the formula
            matrix= self.calc_U(x)
            for i in range(0,self.c):
                zero = np.zeros(len(x[0]))   # zero array that will be updated

                numerator = copy.deepcopy(zero)
                denominator = 0
                for h in range(0,self.n):
                    u_ij = matrix[i][h]**self.m  #multiplying it by fuzzy component
                    numerator  = numerator + u_ij*x[h] #calculate the numerator
                    denominator = denominator + u_ij
                self.centroids[i] = numerator/denominator           #centroid is updated everytime
            self.U = matrix
            #------------------------------------

            deltas= self.calc_cost()   # an array of delta_e and delta_j
            self.iteration +=1
            # break the loop if the stopping conditions are met
            clu_dist = self.get_centroids_distance()
            self.prev_centroids = self.centroids.copy()
            if self.verbose:
                print(self.iteration, "error= ", self.error, " delta_error= ", delta_cost, "tau = ", self.tau)
            # condition of loop, that takes delta_e, delta_j and the iterations
            loop = (abs(deltas[0]) > self.tau)  and (abs(deltas[1]) > self.tau)  and(self.iteration < self.max_it
er)

        return self
```

Graded Possibilistic C-Means (GPCM)

Graded Possibilistic C-Means (GPCM)

In this implementation we will initialize the cluster centers $\mathbf{v}_i$ by selecting at random c points from the data set, and then we will iterate the re-evaluation of all u_{ih} and of $\mathbf{v_i}$,

$$u_{hi} = \frac{\backslash\mathrm{O}_m atrix_{hi}}{Z_h}, \quad \backslash\mathrm{O}_m atrix_{hi} = e^{-\|\mathbf{x}_h - \mathbf{v}_i\|^2/\eta_i}, \quad Z_h = \left(\sum_{i=1}^{c} \backslash\mathrm{O}_m atrix_{hi}\right)^{\beta}, \quad \beta \in [0, 1]$$

$$\mathbf{v}_i = \frac{\sum_{h=1}^{n} u_{ih}\mathbf{x}_h}{\sum_{h=1}^{n} u_{ih}}$$

until until a STOP CRITERION holds.

$\beta \in [0, 1]$ is the *possibilistic degree* and establishes the grade between possibilistic and probabilistic clustering.

$\eta_j > 0$ is the spread of clusters. It can be set a-priori or estimated by using

$$\eta_i = \gamma \frac{\sum_{h=1}^{n} u_{ih} \|\mathbf{x}_h - \mathbf{v}_i\|^2}{\sum_{i=1}^{n} u_{ih}}$$

after an initialization with a Fuzzy C-Means algorithm ($\gamma > 0$, try $\gamma \approx 1$).

The STOP CRITERION for the GPCM can be either:

1. *Stop when the variation of*

   $$E(X) = \sum_{ih} u_{ih} \|\boldsymbol{x}_h - \boldsymbol{v}_i\|^2.$$

   in two subseguent cycles (ΔE) is under an assigned threshold $\tau > 0$.
2. *Stop when the maximum variation of the centroids $\mathbf{v}_i$ in two subseguent cycles ($\Delta \mathbf{v}$) is under an assigned threshold $\tau \geq 0$.*
3. *Stop when the maximum variation of the memberships u_{ih} in two subseguent cycles (Δu) is under an assigned threshold $\tau \geq 0$.*
4. Stop after an assigned number S of iterations.

We suggest to use the following combined STOP CRITERION: **Stop after an assigned number S of iterations** AND **Stop when the variation of $< E >= \frac{E(X)}{c \cdot n}$ in two subseguent cycles ($\Delta < E >$) is under an assigned threshold $\tau > 0$**.

In [ ]:

```python
class GPCM:

    def __init__(self, k=3, tau=0.001, max_iter=300, eta=[0.1,0.1,0.1],gamma=1, beta=0.4, verbose=False):

        self.c = k # number of centroids
        self.tau = tau # stopping threshold
        self.max_iter = max_iter # maximum number of iterations in case of no convergence
        self.eta = eta     # eta array
        self.gamma = gamma # gamma value
        self.beta = beta   # beta value
        self.verbose = verbose # detailed printout
        self.cost = list() # service variable to store cost history

        self.centroids = None # centroids after fitting
        self.U = None # membership matrix

        # additional variable shared among the various functions
        self.n = 0 # holds the dataset size
        self.iteration = None # interation number

        self.prev_error = np.inf # assign initial error as infinite
        self.error =  None # private variable to hold error E(X)
        self.distances = None # private variable to hold distances
        self.prev_centroids = None
        self.x_map = None

    def distance(self,vect1, vect2):  # return square distance
        dist=0
        for i in range(len(vect1)):
            dist = dist + (vect1[i] - vect2[i])**2
        return dist


    def calc_U(self, x):
        # calculation of the membership matrix
        matrix = copy.deepcopy(np.zeros((self.n, self.c)))
        matrix = copy.deepcopy(np.zeros((self.n, self.c)))
        O_matrix  = copy.deepcopy(np.zeros((self.n, self.c)))


        for h in range(0,self.n):
            sum_O_matrix = 0
            for i in range (0,self.c):
                O_matrix[h][i]= np.exp( (-1)*(self.distance(x[h], self.centroids[i])) / self.eta[i])
                sum_O_matrix = sum_O_matrix + O_matrix[h][i]
            Z = sum_O_matrix**self.beta

            for i in range(0,self.c):
                matrix[h][i] = O_matrix[h][i]/ Z
        self.U = matrix
        return matrix

    def get_U(self):
        UU = copy.deepcopy(self.U)

        return UU.transpose()

    def get_centroids(self):
        return self.centroids


    def get_cost_history(self):
        return self.cost

    def plot_cost_history(self, size_x = 15, size_y = 6, data=None, label=None):
        if data==None:
            data= self.cost
        if label==None:
            label = 'Cost History'
        # simply plot the cost history
        fig, ax = plt.subplots(figsize=(size_x,size_y))
        ax.plot(data, color='r', label=label)     # cost line
        ax.legend()
        plt.show()
        return ax

    def calc_cost(self):

        x_map = np.argmin(self.distances,axis=1)
        # define the membership matrix from cluster index list
        # u becomes 1 for items in given cluster and zero for the others
        u = np.zeros_like(self.distances)
        u[np.arange(self.n),x_map] = 1

        #u = copy.deepcopy(self.U)
        dist= np.multiply(self.distances,u)
        # set the distances other than minimal to zero
        #dist = np.multiply(self.distances,u) # fa la mltpliczione in modo semplice
        if self.verbose: sys.stderr.write('dist: {}\n'.format(dist))
        # compute the error - <E> expectation of distortion
        self.error = np.sum(dist)/(self.c*self.n)
        #self.error = np.sum(dist)

        #delta_e = np.abs(self.prev_error - error)
        delta_e = self.prev_error - self.error
        #print ("error= ", error, " delta_error= ", delta_e)
        self.cost.append(self.error)
        self.prev_error = self.error
        return delta_e


    def predict(self,x):
        if self.verbose: sys.stderr.write('centroids: {}\n'.format(self.centroids))
        # compute distances from centroids
        for j in range(self.n):
            for i in range(self.c):
                self.distances[j][i] = np.sum(np.dot(x[j]-self.centroids[i],x[j]-self.centroids[i]))
        # assign the points of the data sets to the k clusters (nearest centroid)
        self.x_map = np.argmin(self.distances,axis=1)
        return self.x_map  # lista delle predizioni

    def get_centroids_distance(self):
        # check centroids distance
        clu_dist = 0
        for c, pc in zip(self.centroids,self.prev_centroids): clu_dist += np.sqrt(np.dot(c-pc,c-pc))
        return clu_dist

    def fit (self, x):
        # performs kmeans clustering on training samples and assign centroids
        self.n = x.shape[0]  # number of training items
        c = x.shape[1]  # number of features
        # initialize the K centroids by selecting at random  K  points from the data_set
        idx = np.random.randint(self.n,size=self.c)
        self.centroids = x[idx].copy()
        self.prev_centroids = self.centroids.copy()

        # initialize the membership matrix with n rows and k columns
        self.U = np.zeros((self.n,self.c), dtype=float)                  # <==== perchè di nuovo ?
        # create a distance matrix with the same shape as the membership one
        self.distances = np.zeros_like(self.U,dtype=float)
        #--------------------------------------------------------------------------------------

        # iterate while DELTA E > tau (STOP CRITERION #1) or max_iter not reached
        loop = True
        self.iteration = 0
        while (loop):
            # match training data to the current centroids and update their
            # membership index list
            self.x_map = self.predict(x)   # da qua escono gli indici di cluster
            if self.verbose: sys.stderr.write('x_map: {}\n'.format(self.x_map))

            #-----------------------------------
            #   calculate the new k centroids
            #omega needs to be calculated
            matrix= self.calc_U(x).transpose()      # now is a 3 x 9
            for i in range(0,self.c):

                zero = np.zeros(len(x[0]))   # then will update
                numerator = copy.deepcopy(zero)

                denominator = 0
                for h in range(0,self.n):
                    u_ij = matrix[i][h]
                    numerator  = numerator + u_ij*x[h]
                    denominator = denominator + u_ij
                self.centroids[i] = numerator/denominator
            self.U = matrix.transpose()
            #--------------------------------------

            # calculate self.eta array
            matrix = copy.deepcopy(self.U).transpose()
            eta= np.zeros(self.c)

            for i in range(0,self.c):
                numerator = 0
                denominator = 0


                for h in range(0, self.n):
                    u_ij = matrix[i][h]
                    numerator  = numerator + u_ij* self.distance(x[h], self.centroids[i]) #updated as according t
o GPCM formula
                    denominator = denominator + u_ij
                eta[i]=self.gamma * (numerator / denominator)


            if eta[0]>0 and eta[1]>0 and eta[2]>0: #control loop
                self.eta=eta
            #---------------------------------------
            delta= self.calc_cost()
            self.iteration +=1
            # break the loop if the stopping conditions are met
            clu_dist = self.get_centroids_distance()
            self.prev_centroids = self.centroids.copy()
            if self.verbose:
                print(self.iteration, "error= ", self.error, " delta_error= ", delta_cost, "tau = ", self.tau)
            # loop conditions
            loop = (abs(delta) > self.tau) and (self.iteration < self.max_iter)

        return self
```

3 Defuzzification of fuzzy partitions

The output of a fuzzy clustering algorithm is a soft (fuzzy) partition of the data set defined by the partition matrix U.

To transform a soft partition of data set in a hard partition, we must apply the winner take all (WTA) or the α-cut rules:

- the winner take all (WTA) rule for each data point finds the clustering with higher membership value and change this value to 1 and set the memberships to the other clusters to 0;
- the α-cut rule compares the membership of each data point to a cluster and if it is larger than α change it to 1, otherwise set it to 0.

In [ ]:

```
def WTA(U): # Winner Take All rule. U is the membership matrix
            # U matrix [num_cluster x el_dataset]
            # take one column: look for higher value and then set 1

    def Column_largest(rows):
        # find the position of largest inside array
        max_pos= 0
        maxm= rows[0] #initize the rows
        #loop till the maximum position is found
        for i in range(0,len(rows)):
            if rows [i] > maxm:
                max_pos = i
                maxm = rows[i]
        return max_pos

    #------------------------------
    size = np.shape(U)
    # initialize W matrix with same rows/columns as U
    W= np.zeros((size[0], size[1]))

    #create a loop for all the rows
    for h in range(0, size[1]):           # every columns
        position= Column_largest(U[:,h]) # every positions of the higher value
        for i in range(0, size[0]):
            if i!= position:
                W[i][h] = 0
            else:
                W[i][h] = 1
    return W
```

In [ ]:

```
def alpha_cut(U, alpha):   # alpha-cut rule. U is the membership matrix, alpha is the threshold

#calcualte the size of the shape
    size =np.shape(U)
    #create number of 0's according to size
    matrix= np.zeros((size[0], size[1]))
    for i in range(0, size[1]):    # for every columns
        for j in range(0, size[0]):

            if U[j,i] > alpha: #if row and column and greater than alpha then append 1 to the matrix
                matrix[j,i] = 1
    return matrix
```

4 Partition similarity indeces

Rand Index

Given two hard partitions A and B of a data set Z, we call

- n_{11} number of pairs of data points in Z both in the same cluster in A and in the same cluster in B
- n_{00} number of pairs of data points in Z both in different clusters in A and in different clusters in B
- n_{01} number of pairs of data points in Z both in different clusters in A and in the same cluster in B
- n_{10} number of pairs of data points in Z both in the same cluster in A and in different clusters in B

the Rand index is defined as

$$r(A,B) = \frac{n_{00} + n_{11}}{n_{00} + n_{11} + n_{01} + n_{10}}$$

NOTE: If A and B are identical $r(A, B) = 1$.

In [ ]:

```
import numpy as np
from scipy.special import comb

def rand(actual,pred):
    # Uih are matrix i x h   or j x h con j>i

#define Rand index function
#code source from internet i tried to implement but it was creating an error, however i have understood the follo
wing code and can implement on my own

    tp_plus_fp = comb(np.bincount(actual), 2).sum()
    tp_plus_fn = comb(np.bincount(pred), 2).sum()
    A = np.c_[(actual, pred)]
    tp = sum(comb(np.bincount(A[A[:, 0] == i, 1]), 2).sum()
             for i in set(actual))
    fp = tp_plus_fp - tp
    fn = tp_plus_fn - tp
    tn = comb(len(A), 2) - tp - fp - fn
    return (tp + tn) / (tp + fp + fn + tn)
```

Jaccard Index

Given the same definitions as for the Rand Index, the Jaccad Index is defined as:

$$J(A,B) = \frac{n_{11}}{n_{11} + n_{01} + n_{10}}$$

In [ ]:

```
def jaccard(U1,U2):
    # each is a ixh matrix

    #Calculate hard matrix using the WTA
    A = WTA(U1)
    B = WTA(U2)

    # hard matrix conversion
    A1= np.shape(U1)
    rowsA = A1[0]
    columns = A1[1]

    #Return the shape of U2
    B1= np.shape(U2)
    #append 0
    rowsB = B1[0]

    A_Vector= np.zeros(columns) # array that will be updated
    B_Vector= np.zeros(columns) # when will find the element 1 in matrix

    for h in range(0,columns):
        A_Vector[h]= h
        for i in range(0,rowsA):
            u1 = A[:,h]
            if u1[i]== 1:
                A_Vector[h] = i

        for i in range(0,rowsB):
            u2 = B[:,h]
            if u2[i]== 1:
                B_Vector[h] = i

    #------------
    # permutations
    # the different values:
    #intialize the values
    n11 = 0
    n01 = 0
    n10 = 0

    for h in range(0,columns):
        A_element= A_Vector[h]  # fixed elements in the following loop
        B_element= B_Vector[h]
  #calculate AnB and AUB to compute the index

        for i in range(h,columns):   # for permutations
            if h!= i:
                notA= A_Vector[i]  # elements that change during the loop
                notB= B_Vector[i]

                if A_element==notA and B_element==notB:
                    n11+=1
                if A_element==notA and B_element!=notB:
                    n01+=1
                if A_element!=notA and B_element==notB:
                    n10+=1

    SUM = n11+n01+n10 #sum of all the numbers
    r= n11/SUM #using the formula

    return r
```

Clustering Accuracy

Accuracy of a clustering algo can be evaluated as similarity of the obtained partition to a known labeling of the data.

Rand and Jaccard indeces can be used to evaluate clustering accuracy.

5, 6, 7, 8 Experiments

Note: Depending on the initialization, a clustering algorithm could trap in alocal minimum. **Multi-start euristics** consists in multiple num_iter of the algorithm with random inizializations and in the selection of the best one, on the basis ,e.g., of the minimum evaluation of $<E>$ after training.

5, 7, 8 - Experiments with K-Means

In [ ]:

```
U_ds1 = list()
U_ds2 = list()
U_Iris = list()

#create 3 for data to store

def multi_start(x,k=3,tau=.0001, num_iter=10):
    # constants assignement
    precision = 4
    #create E constant
    E = np.inf

    runs = num_iter  # number of re-starts
    #initiate a cluster k
    clusters=k
    #initate value of tau
    tau_val=tau


    #calculate the running time of the code
    t_before = time.time()
    for i in range(num_iter):
      #loop for until number of iteration is compeleted
      #call k mean algorithm
        km = KMeans(k=clusters, tau=tau_val, verbose=False)
        #fit algorithm will assign centroids
        # performs kmeans clustering on training samples and assign centroids
        km.fit(x)

        EE= km.error
        Niter= km.iteration
        #print("run = {} - <E> = {:.{}f} ".format(i, EE, precision))
        print("run = {} - iterations = {} - <E> = {:.{}f} ".format(i, Niter-1, EE, precision))

        if EE < E:
            # store the best instance of trained model
            #
            kmi = km
            E=EE
            best_run=i

    print ('\n best run = {} - <E> = {:.{}f}'.format(best_run, E, precision))
    t_after = time.time()
    ## Compute training time
    t_training = t_after - t_before
    print("Time for multi-start training (seconds): {:.{}f} - runs = {}\n".format(t_training, precision, runs))

    return kmi, E, best_run
```

In [ ]:

```
from scipy.spatial import Voronoi, voronoi_plot_2d
import matplotlib.pyplot as plt
def plot_clustered_data(x,y,c,preds):
    size_x = 16
    size_y = 6
#call voronoi which is imported from the library Voronoi diagram is a partition of a plane into regions close to
each of a given set of objects
    vor = Voronoi(c)
#create plots, sub plotting graphs
    fig, (ax1, ax2) = plt.subplots(1,2,figsize=(size_x,size_y))
    ax1.scatter(x[:,0], x[:,1], c=y, alpha=0.5)
    ax1.set_title('Original Data')
    #ax1.legend()
#plot data for Predictions and showing centroids
    ax2.scatter(x[:,0], x[:,1], c=preds, alpha=0.5, label='Predictions')
    ax2.scatter(c[:,0], c[:,1], marker='P', c='red', label='Centroids')
    ax2.set_title('Clustered Data')
    ax2.legend()
#plotting a voronoi 2d plot
    voronoi_plot_2d(vor, ax2, show_points=False, line_width=1, show_vertices=False)
    ax2.set_xlim(min(x[:,0])-1,max(x[:,0])+1)
    ax2.set_ylim(min(x[:,1])-1,max(x[:,1])+1)

    plt.show()
```

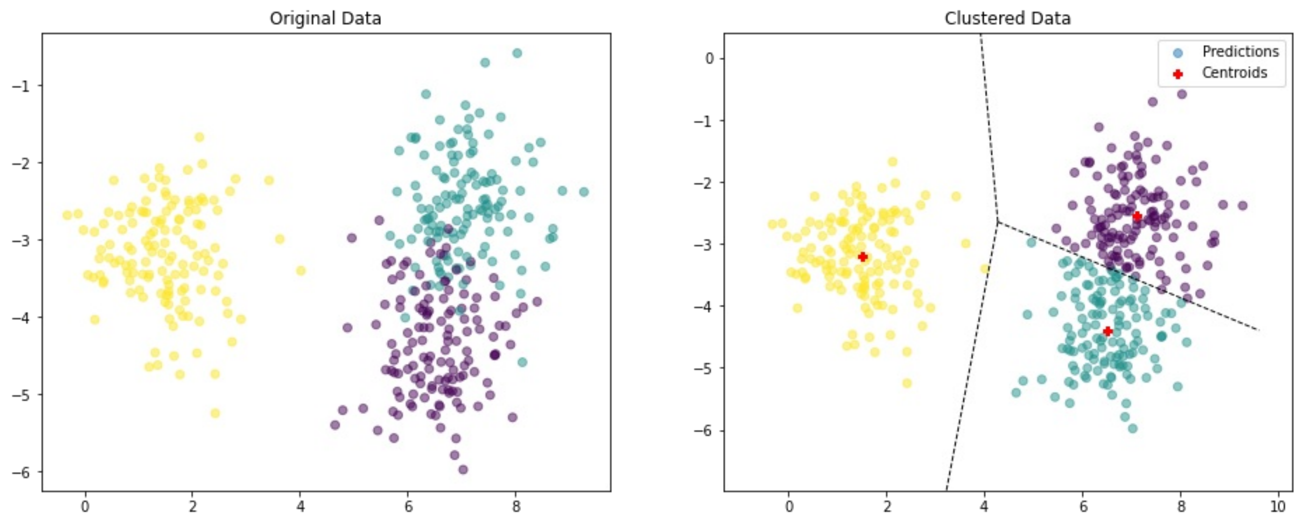
In [ ]:

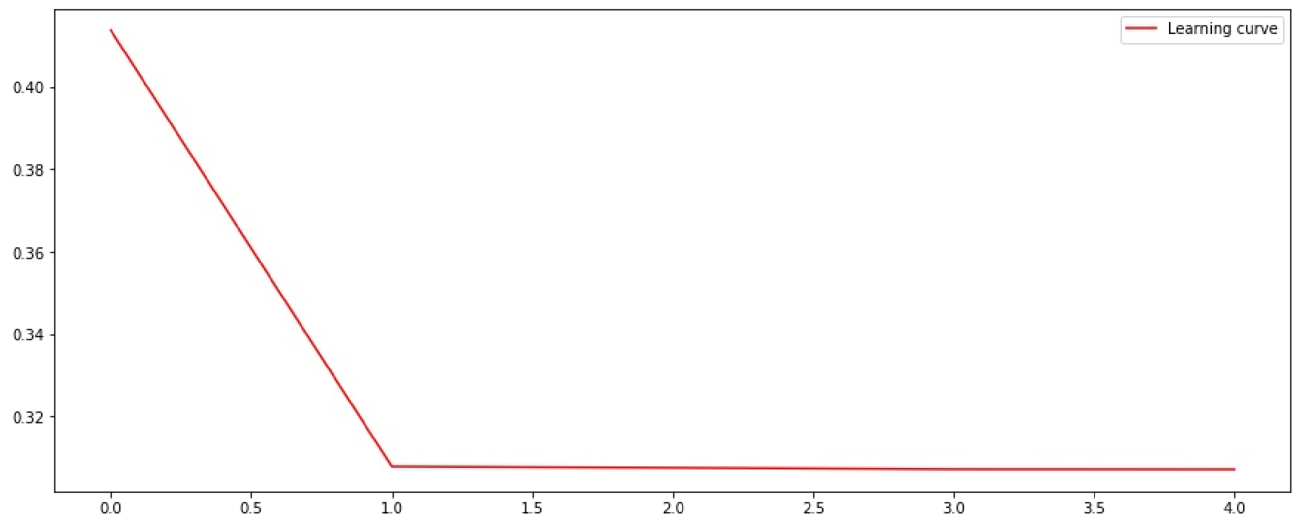
```
# simplified test datasets (for debugging aims)
simpleTest = False
if simpleTest:
    d1a = [[-1.0,-1.0],[-1.1,-1.2],[-1.2,-1.1],[1.0,1.0],[1.1,1.2],[1.2,1.1],[-1.0,1.0],[-1.1,1.2],[-1.2,1.1]]
    target = [0,0,0,1,1,1,2,2,2]
    feats = pd.DataFrame(d1a, columns=x_labels)
    tgts = pd.Series(target, name=y_label)
    dataset1 = pd.concat([feats,tgts],axis=1)
    d2a = [[-0.3,-0.2],[-0.2,-0.25],[-0.35,-0.3],[0.3,0.25],[0.2,0.2],[0.35,0.3],[-0.3,0.2],[-0.35,0.2],[-0.2,0.2
5],[-0.25,-0.2],[0.3,0.2],[-0.3,0.25]]
    target = [0,0,0,1,1,1,2,2,2,0,1,2]
    feats = pd.DataFrame(d2a, columns=x_labels)
    tgts = pd.Series(target, name=y_label)
    dataset2 = pd.concat([feats,tgts],axis=1)
```

In [ ]:

```
ds = dataset1
print("Data set DS")
print()
x = np.array(ds[x_labels].copy())
y = np.array(ds[y_label].copy())
#calling all the function to initiate k mean algorithm
km, E, best_run = multi_start(x, num_iter=10) #3 clusters
c = km.get_centroids()
U = km.get_U()
hist = km.get_cost_history()
p = km.predict(x)
#calling jaccard and rand function and print
print( '\n RandIndex:', (GT_list[0], U),'  ','jaccard index:',jaccard(GT_list[0], U))
U_ds1.append(U)
#plotting the iris data to visualize and show the clusters and centroid in the image
plot_clustered_data(x,y,c,p)
#plot a line graph that shows the learning curve, the less the learning curve the better it is
km.plot_cost_history(data=hist, label="Learning curve")
```

```
Data set DS

run = 0 - iterations = 6 - <E> = 0.3072
run = 1 - iterations = 6 - <E> = 0.3073
run = 2 - iterations = 9 - <E> = 0.3073
run = 3 - iterations = 3 - <E> = 0.4779
run = 4 - iterations = 8 - <E> = 0.3073
run = 5 - iterations = 4 - <E> = 0.3072
run = 6 - iterations = 5 - <E> = 0.4830
run = 7 - iterations = 9 - <E> = 0.3073
run = 8 - iterations = 5 - <E> = 0.3073
run = 9 - iterations = 7 - <E> = 0.3072

 best run = 5 - <E> = 0.3072
Time for multi-start training (seconds): 1.4347 - runs = 10


 RandIndex: (array([[1., 1., 1., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.]]), array([[0, 0, 1, ..., 0, 0, 0],
       [1, 1, 0, ..., 0, 1, 1],
       [0, 0, 0, ..., 1, 0, 0]]))    jaccard index: 0.2696279213850549
```





Out[ ]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x7fca0aa84e50>
```

5, 6, 7, 8 - Experiments with Fuzzy C-Means

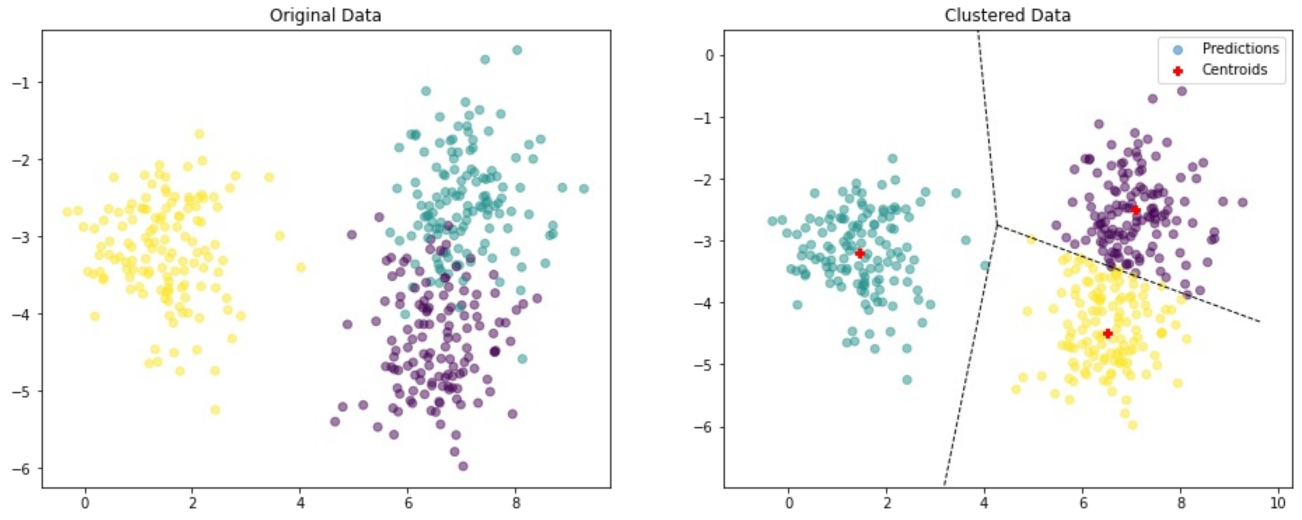
In [ ]:

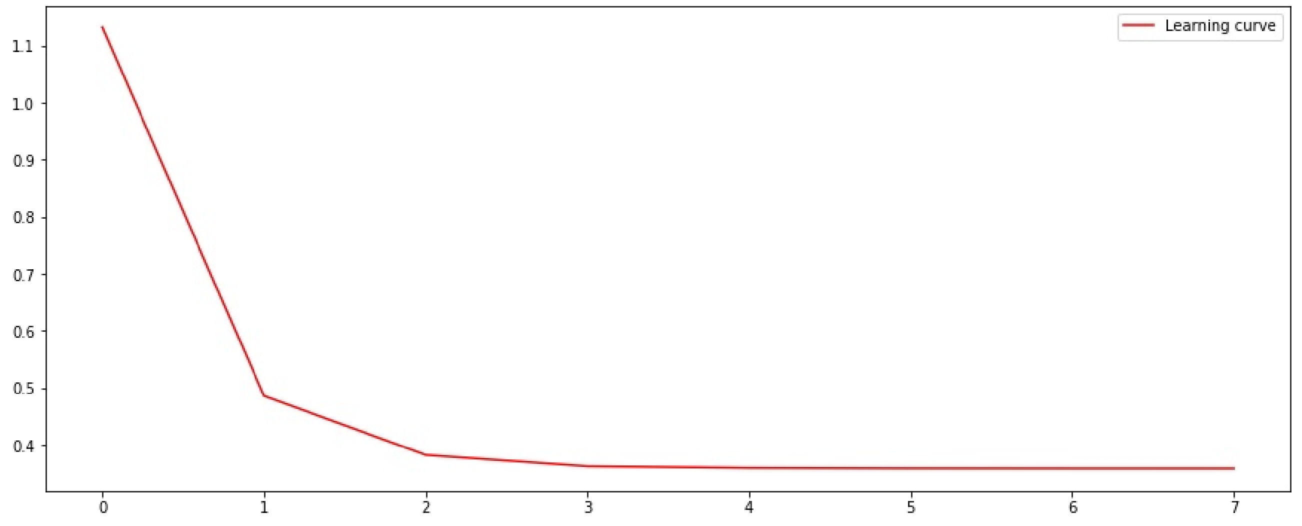
```
# to do
def multi_startFuzzyCMeans(x, k=3,tau=.0001, num_iter=10):
    #-----------------------------------
    # constants assignement
    precision = 4
    E = np.inf
    num_iter = num_iter  # number of re-starts
    clusters=k
    tau_val=tau
    #-----------------------------------
    t_before = time.time()
    #run until number of iterations are done
    for i in range(num_iter):
      #call Cmean functions to intiate
        km = FuzzyCMeans( k=clusters,  tau=tau_val, verbose=False)
        #fit will compute the predicted centroid
        km.fit(x)
        EE= km.error
        Niter= km.iteration
        #print("run = {} - <E> = {:.{}f} ".format(i, EE, precision))
        print("run = {} - iterations = {} - <E> = {:.{}f} ".format(i, Niter-1, EE, precision))

        if EE < E:
            # store the best instance of trained model
            kmi = km
            E=EE
            best_run=i

    print ('\n best run = {} - <E> = {:.{}f}'.format(best_run, E, precision))
    t_after = time.time()
    ## Compute training time
    t_training = t_after - t_before
    #print("Time for multi-start training (seconds): {:.{}f} - num_iter = {}\n".format(t_training, precision, num
_iter))

    return kmi, E, best_run
```

In [ ]:

```
ds_l=dataset1
#dataset of iris is dataset1
print("Data set DS 1")
print()
#create 2 copies of arrays and copy rows of dataset in to a new array
x = np.array(ds_l[x_labels].copy())
y = np.array(ds_l[y_label].copy())
#run the cmean algorthm
km, E, best_run = multi_startFuzzyCMeans(x,k=3, num_iter=10)
#calculate the centroids
c = km.get_centroids()
U = km.get_U()
hist = km.get_cost_history()
p = km.predict(x)
#print(U,'\n',p)
#run the rand and jaccard index code to calculate the accuracy
print( '\n rand index:',(GT_list[0], U),'  ','jaccard index:',jaccard(GT_list[0], U))
U_ds1.append(U)
plot_clustered_data(x,y,c,p)
km.plot_cost_history(data=hist, label="Learning curve")
```

```
Data set DS 1

run = 0 - iterations = 6 - <E> = 0.3585
run = 1 - iterations = 6 - <E> = 0.3585
run = 2 - iterations = 8 - <E> = 0.3585
run = 3 - iterations = 6 - <E> = 0.3585
run = 4 - iterations = 7 - <E> = 0.3585
run = 5 - iterations = 6 - <E> = 0.3585
run = 6 - iterations = 6 - <E> = 0.3585
run = 7 - iterations = 6 - <E> = 0.3585
run = 8 - iterations = 6 - <E> = 0.5630
run = 9 - iterations = 12 - <E> = 0.5630

 best run = 4 - <E> = 0.3585

 rand index: (array([[1., 1., 1., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.]]), array([[1.04309152e-02, 6.98825339e-02, 9.99234430e-01, ...,
        1.60385953e-04, 1.02247610e-04, 1.63961764e-03],
       [1.19556987e-03, 4.60146136e-04, 1.90739357e-05, ...,
        9.99602171e-01, 1.89931423e-06, 4.97795927e-05],
       [9.88373515e-01, 9.29657320e-01, 7.46496127e-04, ...,
        2.37443191e-04, 9.99895853e-01, 9.98310603e-01]]))    jaccard index: 0.2697994663912557
```





Out[ ]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x7fca0aeb1d50>
```

5, 6, 7, 8 - Experiments with Graded Possibilistic C-Means

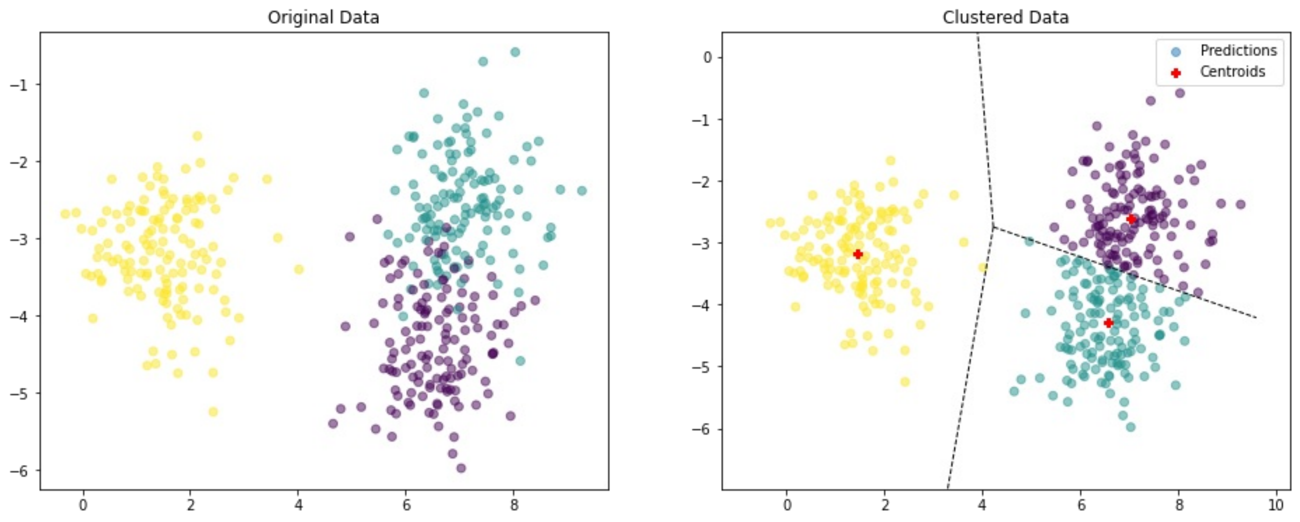
In [ ]:

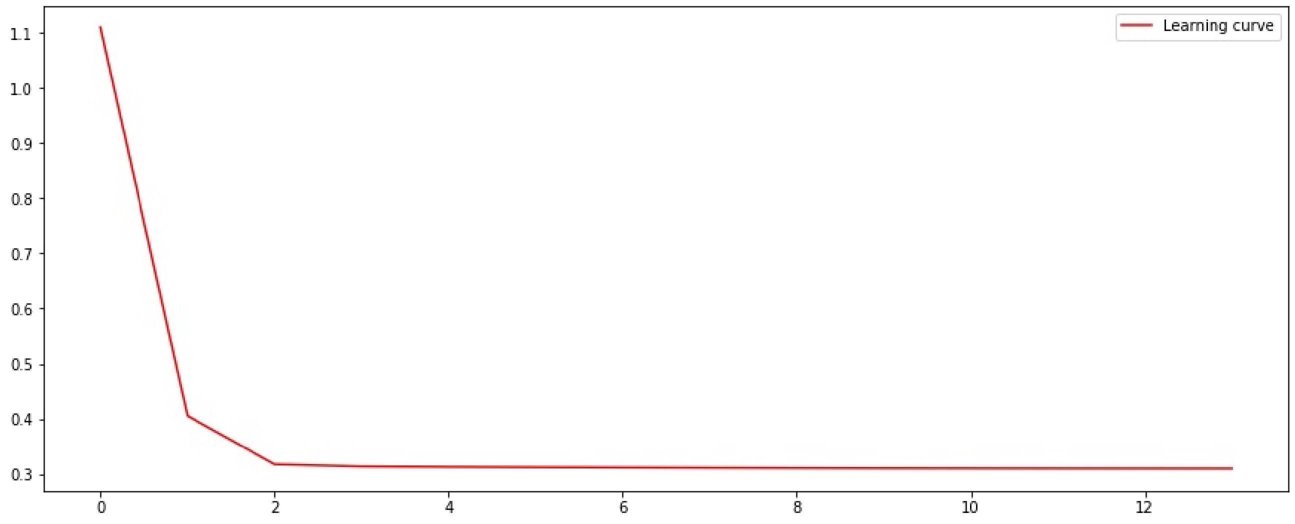
```
# to do
def multi_startGPCM(x, k=3,tau=.0001,num_iter=10, eta_array=[0.1,0.1,0.1] ,gamma_value=1, beta_value=0.8):
    #---------------------------------
    # constants assignement
    #initialze the params required
    precision = 4
    E = np.inf
    num_iter = num_iter  # number of re-starts
    clusters=k
    eta= eta_array
    gamma= gamma_value
    beta= beta_value
    clusters=k
    tau_val=tau
    #----------------------------------
    t_before = time.time()
    for i in range(num_iter):
      #run GPCM code using the given params
        km = GPCM(k=3, tau=tau_val, eta=eta_array,gamma=1, beta=0.8, verbose=False)
        #run the fit algorithm to calculate the centroids
        #In central clustering data objects are points or vectors in data space, and c clusters are represented b
y means of their “central” points or centroids yj . The
#Graded Possibilistic model is a soft central clustering method, implying that cluster membership can be partial.
This is usually represented by means of cluster
#indicators (or membership functions) which are real-valued rather than integer.
        km.fit(x)
        EE= km.error
        Niter= km.iteration
        #print("run = {} - <E> = {:.{}f} ".format(i, EE, precision))
        print("run = {} - iterations = {} - <E> = {:.{}f} ".format(i, Niter-1, EE, precision))

        if EE < E:
            # store the best instance of trained model
            kmi = km
            E=EE
            best_run=i

    print ('\n best run = {} - <E> = {:.{}f}'.format(best_run, E, precision))
    t_after = time.time()
    ## Compute training time
    t_training = t_after - t_before
    #print("Time for multi-start training (seconds): {:.{}f} - num_iter = {}\n".format(t_training, precision, num
_iter))

    return kmi, E, best_run
```

In [ ]:

```
ds_l = dataset1

print("Data set DS 1")
print()
x = np.array(ds_l[x_labels].copy())
y = np.array(ds_l[y_label].copy())
km, E, best_run = multi_startGPCM(x, k=3, eta_array=[0.7,0.7,0.7],num_iter=10)
c = km.get_centroids()
U = km.get_U()
hist = km.get_cost_history()
p = km.predict(x)
#print(U,'\n',p)
print( '\n rand index:',(GT_list[0], U),'  ','jaccard index:',jaccard(GT_list[0], U))
U_ds1.append(U)
plot_clustered_data(x,y,c,p)
km.plot_cost_history(data=hist, label="Learning curve")
```

```
Data set DS 1

run = 0 - iterations = 13 - <E> = 0.3101
run = 1 - iterations = 18 - <E> = 0.4850
run = 2 - iterations = 7 - <E> = 0.4888
run = 3 - iterations = 13 - <E> = 0.4839
run = 4 - iterations = 19 - <E> = 0.4850
run = 5 - iterations = 16 - <E> = 0.3102
run = 6 - iterations = 19 - <E> = 0.4850
run = 7 - iterations = 68 - <E> = 1.8294
run = 8 - iterations = 18 - <E> = 0.3107
run = 9 - iterations = 11 - <E> = 0.3106

 best run = 0 - <E> = 0.3101

 rand index: (array([[1., 1., 1., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.],
       [0., 0., 0., ..., 0., 0., 0.]]), array([[8.10355186e-04, 6.26308251e-02, 9.29560519e-01, ...,
        1.88032396e-22, 1.15042962e-02, 2.32515663e-03],
       [8.05191449e-01, 8.15198867e-01, 4.14516610e-03, ...,
        1.42705360e-17, 9.81288112e-01, 9.18684919e-01],
       [1.48097945e-11, 4.21381216e-20, 1.32952731e-20, ...,
        8.77622065e-01, 9.31488499e-17, 5.03111261e-18]]))    jaccard index: 0.27043689403984916
```





Out[ ]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x7fca0ad7bd50>
```

Optional Part A

Clustering Ensembling

Partition Diversity

We exploit **clustering algorithms diversity** to obtain ensemble models with high stability

Possible strategies to increase diversity:

- Different clustering algorithms and weak clustering algos, e.g., only few iterations of k-means to avoid convergence;
- Randomizing using different initializations; different n. of clusters to look for;
- Different data sets: resampling with replacement (bagging); resampling without replacement;
- Different feature subsets (random subspace method).

A1 - Consensus Matrix implementation

A1

A popular use of the Consensus Matrix:

- Given data set $Z = z_1, \ldots, z_N$ with N elements.
- Pick the ensemble size L and the number of clusters c.
- Generate L hard partitions of Z in c clusters.
- Form a co-association matrix for each partition, $M(k) = m_{ij}(k)$ of size $N \times N$, $k = 1, \ldots, L$, where

$$m_{ij}(k) = \begin{cases} 1, & \text{if } z_i \text{ and } z_j \text{ are in the same cluster in partition } k, \\ 0, & \text{if } z_i \text{ and } z_j \text{ are in different clusters in partition } k. \end{cases}$$

- Form a final co-association matrix M (consensus matrix) by averaging the L co-association matrices M(k).
- Derive the final clustering using this matrix by applying an α-cut rule.

In [ ]:

```
def coassoc_matrix(U):
    #input: hard membership matrix
    #output: co-association matrix

    # insert code here

    return C

def cons_matr(CC, alpha):
      # input: CC list of L co-association matrices representing L partitions,
      # alpha threshold
      # output ensemble co-association matrix

    # insert code here

    # consensu matrix C as average the L co-association matrices in CC
    # compare the elements of C with threshold alpha.
                    #If larger set the element to 1 otherwise to 0
    # tranform C in an hard membership matrix
    return C
```

A2, A3, A4 - Experiments on Consensus Matrix ensembling

- **A2**. For each data set, take the 9 hard best partitions obtained for data set DS2 in Part A and construct an ensemble using the tecnique of the consensus matrix.
- **A3**. Visualize the results on the scatter plot, highlighting the centroids and using a different color for each cluster.
- **A4**. Measure the *accuracy* of the partition induced by the consensus matrix by comparing it with the ground-truth constituted by the targets of the data sets. For the comparison use RAND index. Find the best value for the threshold α.

In [ ]:

```
#For each data set, take the 9 hard partitions obtained for data set DS2 in Part A

# insert code here

# using coassoc-matrix obtain the 9 co-association matrices

# insert code here

# using cons_matr (with alpha=.4) obtain the ensemble co-association matrix


# insert code here


# Create a scatterplot of first two features



# insert code here


# display learning curve



# insert code here



# Measure the accuracy of the hard partitions (GT is the ground-truth)

# insert code here
```

Optional Part B: Study of the Graded Possibilistic C-Means algorithm

Implement a soft transition from probabilistic clustering to possibilistic clustering:

- Define a scheduling for β, e.g. $(1, .8, .6, .4, .2, 0)$ and for any value of β run the GPCM starting from the results obtained in the previous run.
- After each run evalutate the accuracy.
- Test on the 3 data sets.

In [ ]:

```

```

(h) Discussion

- What are the best results?

K-Means Clustering is a hard clustering algorithm Fuzzy C-Means clustering is a soft clustering approach, where each data point is assigned a likelihood or probability score to belong to that cluster Fuzzy c-means clustering has can be considered a better algorithm compared to the k-Means algorithm. Unlike the k-Means algorithm where the data points exclusively belong to one cluster, in the case of the fuzzy c-means algorithm, the data point can belong to more than one cluster with a likelihood. Fuzzy c-means clustering gives comparatively better results for overlapped data sets.

In our above results we also find out that
K mean jaccard index: 0.2700055092624475
Cmean jaccard index: 0.2696279213850549
GPCM jaccard index: 0.27043689403984916

My results shows that GPCM turns out to be most accurate representations of the clusters

- Additional discussion here