APA-L3-python

September 6, 2018

1 APA Laboratori 3 - Clustering

```
In [1]: # Uncomment to upgrade packages
        # !pip install pandas --upgrade
        # !pip install numpy --upgrade
        # !pip install scipy --upgrade
        # !pip install statsmodels --upgrade
        # !pip install scikit-learn --upgrade
        %load_ext autoreload
```

```
In [2]: #%matplotlib notebook
        import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        import seaborn as sns
        from collections import Counter
        from IPython.core.interactiveshell import InteractiveShell
        pd.set_option('precision', 3)
        InteractiveShell.ast_node_interactivity = "all"
```

```
In [3]: # Extra imports
        from numpy.random import  uniform,normal
        from sklearn.cluster import KMeans
        from sklearn.metrics import calinski_harabaz_score
        from numpy.random import multivariate_normal
        from sklearn.datasets import make_blobs
        from sklearn.mixture import GaussianMixture
```

```
In [4]: np.random.seed(7)
```

1.1 Example 1. Clustering easy artificial 2D data with k-means

First we create a simple data set:

```
In [5]: N1 = 30
        N2 = 40
        N3 = 50
```

create cluster 1

```
In [6]: x1 = normal (1,0.5,N1)
        y1 = normal (1,0.5,N1)
```

create cluster 2

```
In [7]: x2 = normal (2,0.5,N2)
        y2 = normal (6,0.7,N2)
```

create cluster 3

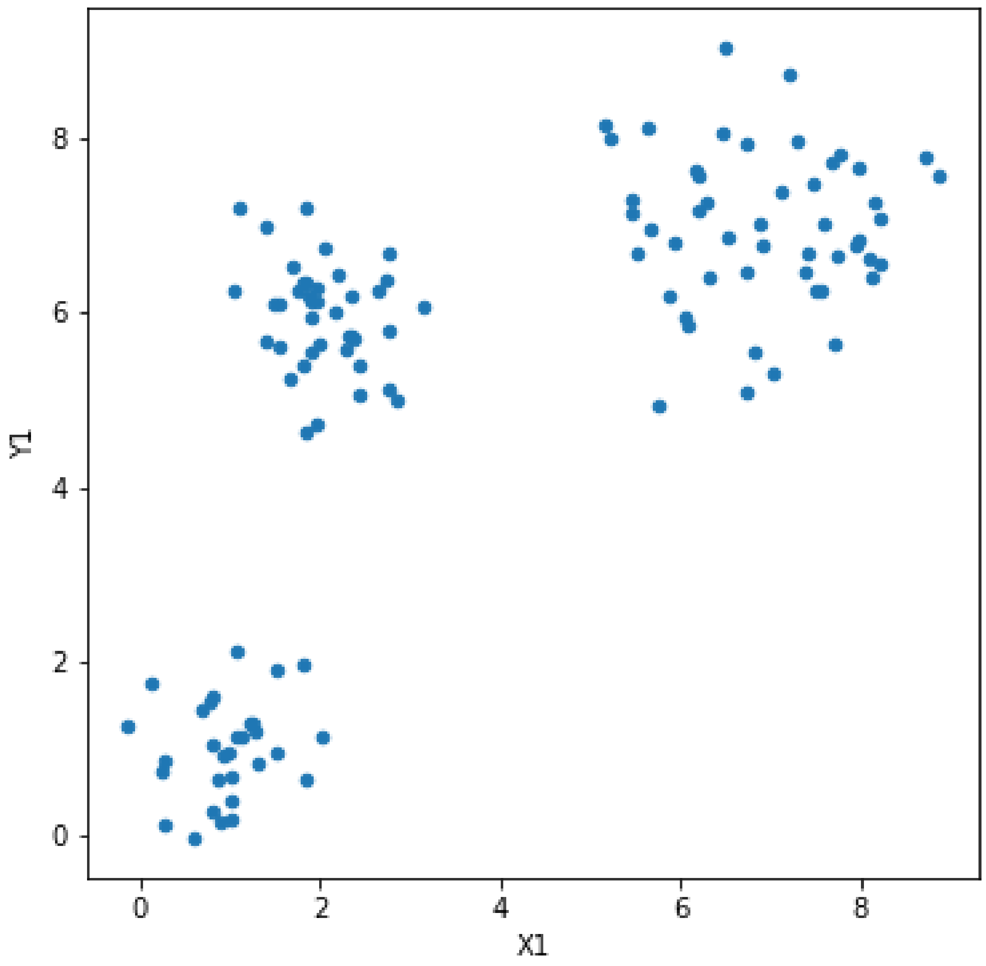
```
In [8]: x3 = normal (7,1,N3)
        y3 = normal (7,1,N3)
```

create the data

```
In [9]: x = np.concatenate((x1,x2,x3))
        y = np.concatenate((y1,y2,y3))
        c = np.array([0] * N1 + [1] * N2 + [2] *N3)
        D = pd.DataFrame({'X1':x, 'Y1':y, 'C':c})
```

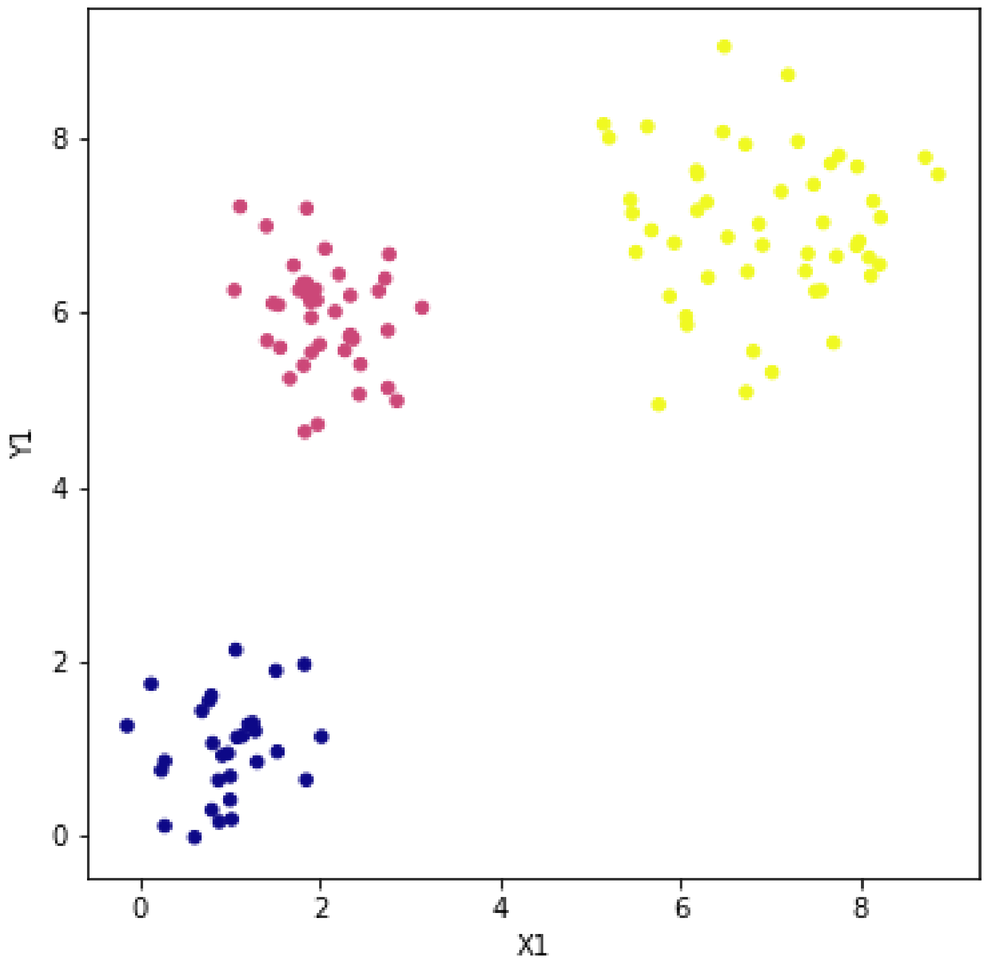
this is your data

```
In [10]: D.plot.scatter(x='X1', y='Y1',figsize=(6,6));
```



and these are the true clusters

```
In [11]: D.plot.scatter(x='X1',
                        y='Y1',
                        c='C',
                        colormap='plasma',
                        figsize=(6,6),colorbar=False);
```



so we have 3 very clean clusters ...
Let's execute k-means

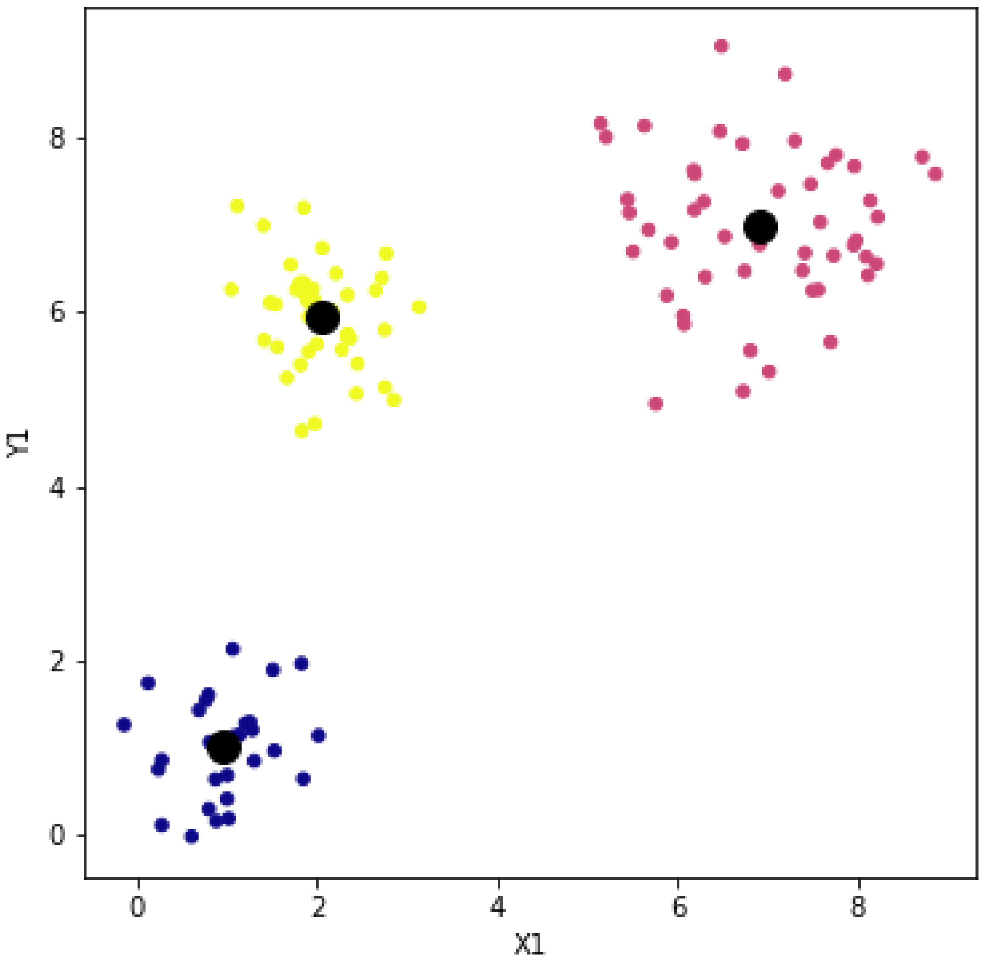
```
In [12]: K = 3 # yeah, this is tricky, why 3?
```

execute k-means with a maximum of 100 iterations

```
In [13]: kmeans_3 = KMeans(n_clusters=K,max_iter=100)
         kmeans_3.fit(D.loc[:,['X1','Y1']]);
```

plot and paint the clusters (according to the computed assignments) and plot the cluster centers

```
In [14]: D.plot.scatter(x='X1',
                        y='Y1',
                        c=kmeans_3.labels_,
                        colormap='plasma',
                        figsize=(6,6),
                        colorbar=False)
         plt.plot(kmeans_3.cluster_centers_[:,0],
                  kmeans_3.cluster_centers_[:,1],
                  'ko', markersize=12);
```



clustering quality as measured by the Calinski-Harabasz index (recommended)

This index measures the dispersion of the data points within the clusters (SSW) and between the clusters (SSB)

A good clustering has small SSW (compact clusters) and large SSB (separated cluster centers)

There is also a correction for the number of clusters

The CH index is then:

$CH = \frac{SSB/(K-1)}{SSW/(N-K)}$

where N is the number of data points and K is the number of clusters

```
In [15]: CH_3 = calinski_harabaz_score(D.loc[:,['X1','Y1']],
                                        kmeans_3.labels_ )

         CH_3
```

```
Out[15]: 728.0901256606564
```

now let's not be tricky ##

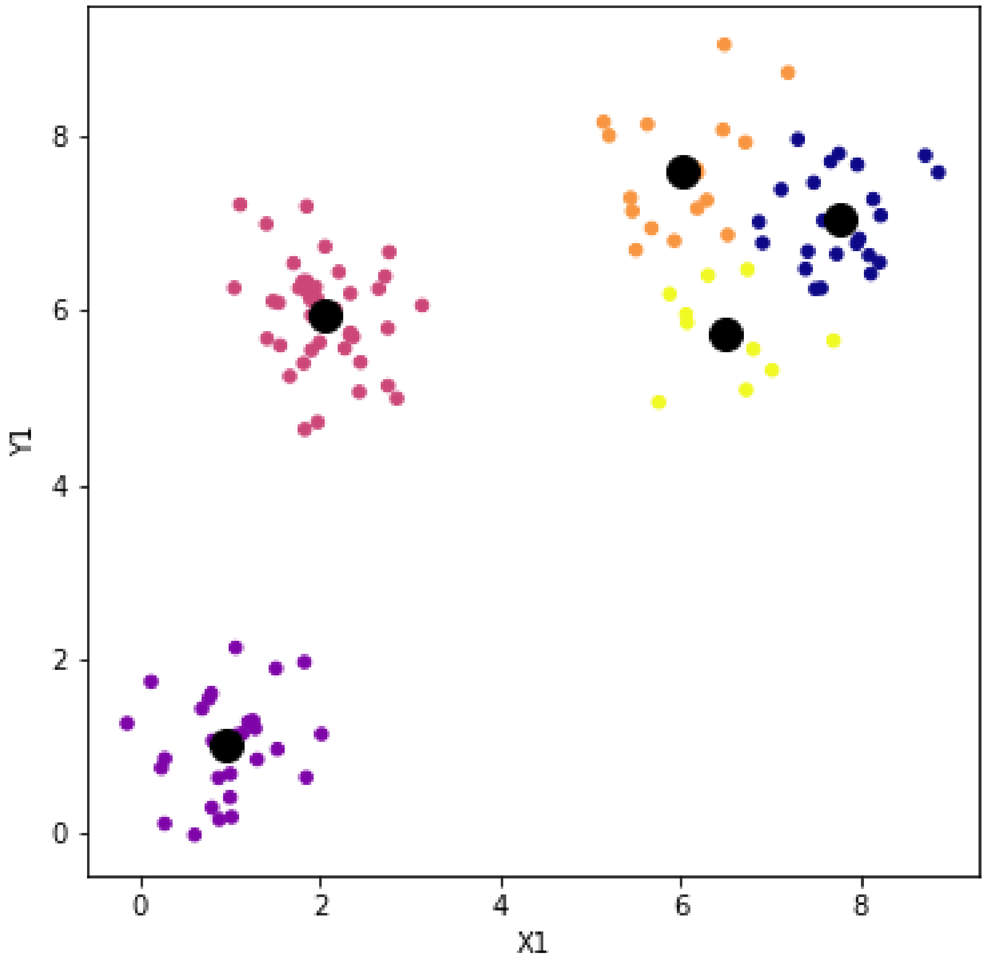
```
In [16]: K = 5 # guess what is going to happen?
```

execute k-means with a maximum of 100 iterations

```
In [17]: kmeans_5 = KMeans(n_clusters=K,max_iter=100)
         kmeans_5.fit(D.loc[:,['X1','Y1']]);
```

plot and paint the clusters (according to the computed assignments), plot the cluster centers

```
In [18]: D.plot.scatter(x='X1',
                        y='Y1',
                        c=kmeans_5.labels_,
                        colormap='plasma',
                        figsize=(6,6),
                        colorbar=False)
         plt.plot(kmeans_5.cluster_centers_[:,0],
                  kmeans_5.cluster_centers_[:,1],
                  'ko', markersize=12);
```



clustering quality as measured by the Calinski-Harabasz index

```
In [19]: CH_5 = calinski_harabaz_score(D.loc[:,['X1','Y1']],
                                       kmeans_5.labels_)
         CH_5
```

```
Out[19]: 653.0660770798015
```

notice CH.3 > CH.5, so K=3 is better according to C-H

1.2 Example 2. Clustering not-so-easy artificial 2D data with k-means and E-M

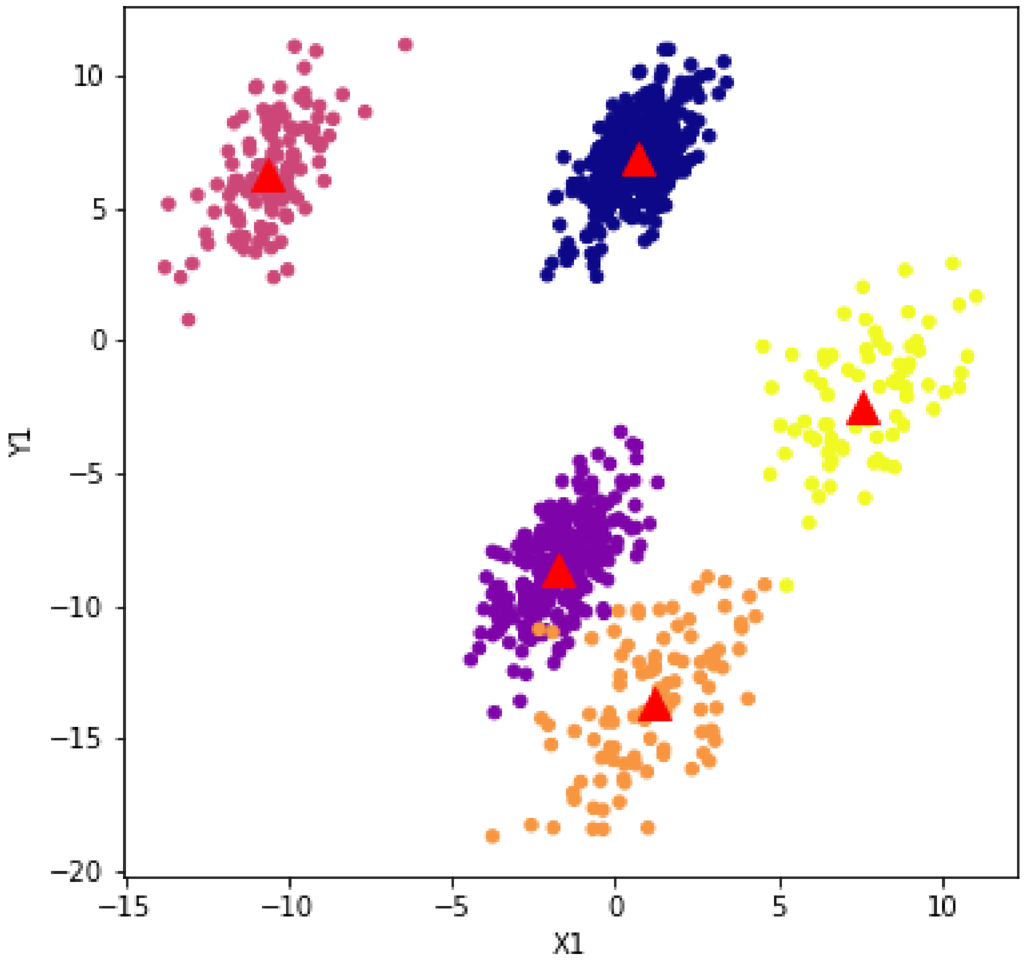
```
In [20]: np.random.seed(6)
         K =5
         N=2000
         center = np.array((0,0))
         dispersion = 30

         mu_k= multivariate_normal(center, np.eye(2)*dispersion,K)
         pi_k = uniform(0.2,1.5,size=K)
         data, labels = make_blobs(n_samples=N,
                                   n_features=2,
                                   centers=mu_k,
                                   cluster_std=pi_k)
         # Rotate and scale
         data = np.dot(data, np.array([[1,0.2],[0.6,1.8]]))
         # Rotate and scale
         mu_k = np.dot(mu_k, np.array([[1,0.2],[0.6,1.8]]))

         data = np.vstack((data[labels==0][:400],
                           data[labels==1][:300],
                           data[labels==2][:125],
                           data[labels==3][:100],
                           data[labels==4][:75]))
         labels=np.array([0]*400+[1]*300+[2]*125+[3]*100+[4]*75)
         d = pd.DataFrame({'X1': data[:,0],
                           'Y1':data[:,1],
                           'labels':labels})
```

generate 2D data as a mixture of 5 Gaussians, The rotation makes the two variable non independent with different variances the centers and coefficients of the mixture are chosen randomly

```
In [21]: d.plot.scatter(x='X1',
                        y='Y1',
                        c=labels,
                        colormap='plasma',
                        figsize=(6,6),
                        colorbar=False)
        plt.plot(mu_k[:,0], mu_k[:,1],
                 'r^', markersize=12);
```



may be we want to have a look at the unconditional density p(x)

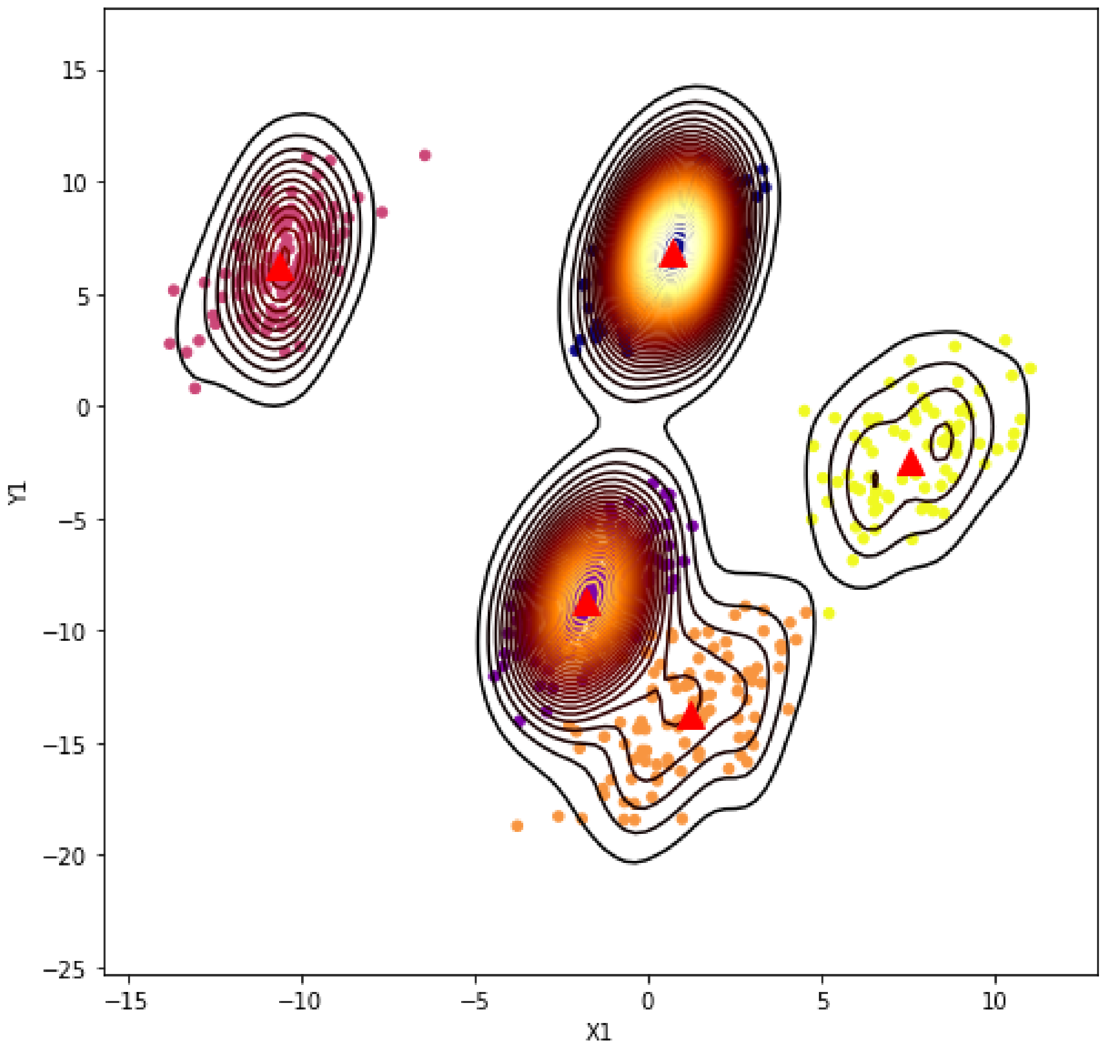
compute 2D kernel density

this is the raw data (what the clustering method sees) and a contour plot of the unconditional density

```
In [22]: d.plot.scatter(x='X1',
                        y='Y1',
                        c=labels,
                        colormap='plasma',
                        figsize=(8,8),colorbar=False)
         plt.plot(mu_k[:,0], mu_k[:,1],
                  'r^', markersize=12);
```

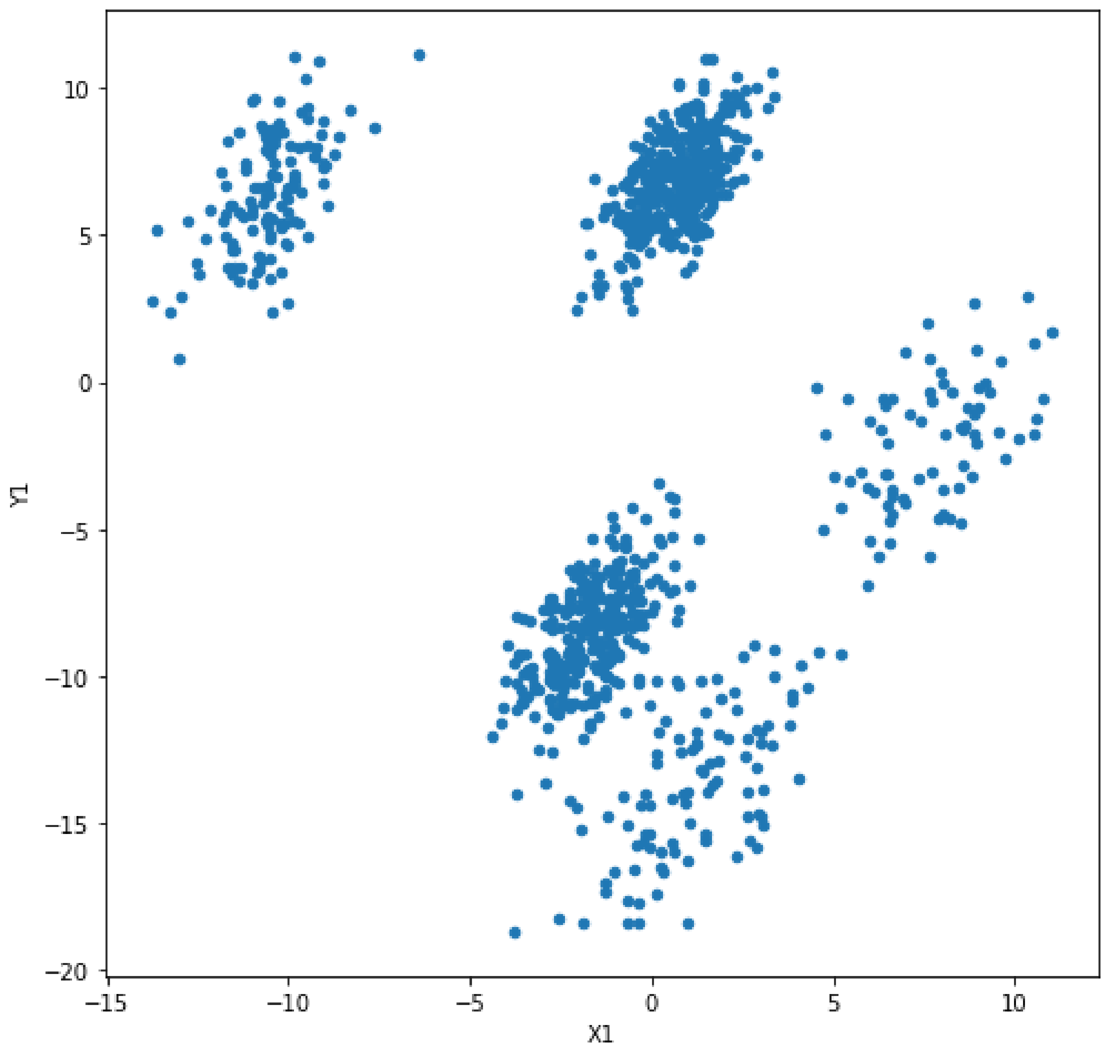
```
        sns.kdeplot(d.X1,d.Y1,
                    n_levels=50,cmap='afmhot');
```

```
/usr/lib64/python3.6/site-packages/scipy/stats/stats.py:1706: FutureWarning: Using a non-tuple s
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
```



a simpler way of plotting the data

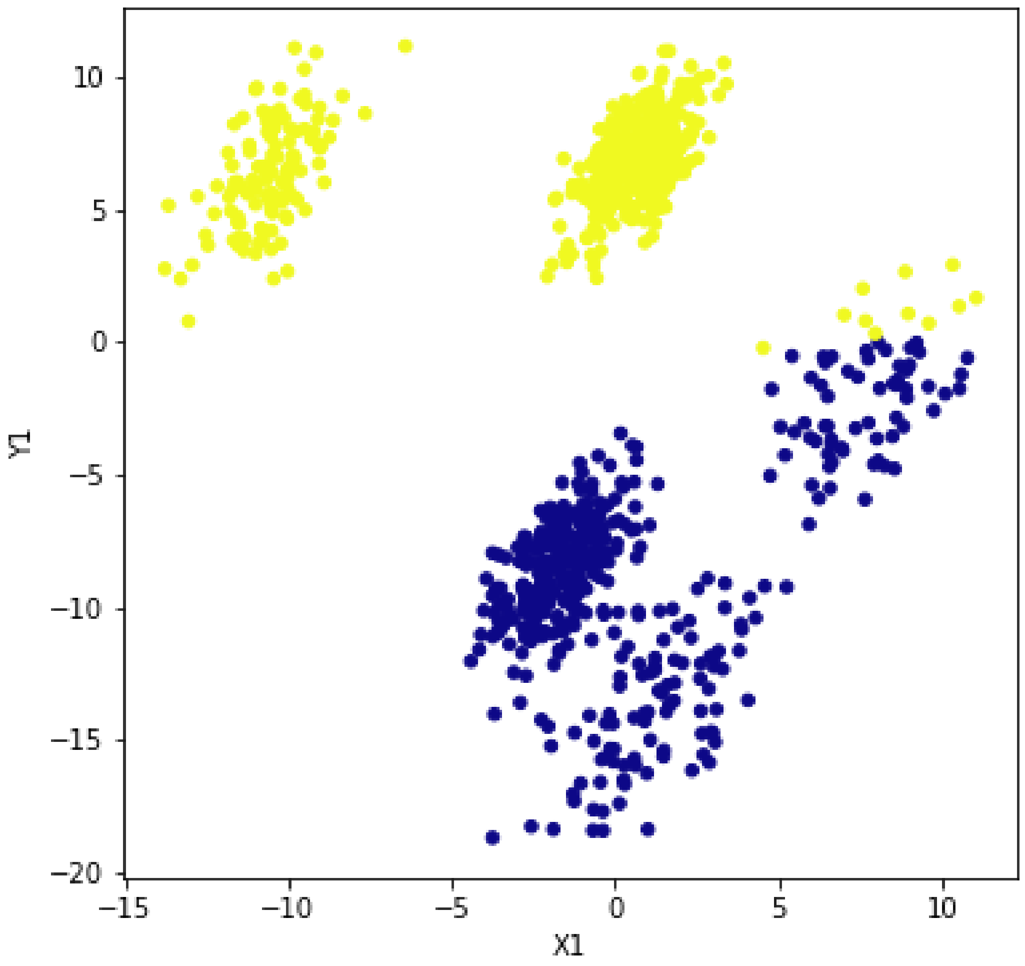
```
In [23]: d.plot.scatter(x='X1', y='Y1', figsize=(8,8));
```



let us try first with k-means (K=2)

```
In [24]: K=2

         kmeans_2 = KMeans(n_clusters=K,max_iter=100)
         kmeans_2.fit(d.loc[:,['X1','Y1']]);
         d.plot.scatter(x='X1', y='Y1',
                        c=kmeans_2.labels_,
                        colormap='plasma',
                        figsize=(6,6),colorbar=False);
```



Can we be indulgent with the result? we know the truth is there are 5 clusters,
Is this is a reasonable result if we ask for 2?
clustering quality as measured by the Calinski-Harabasz index

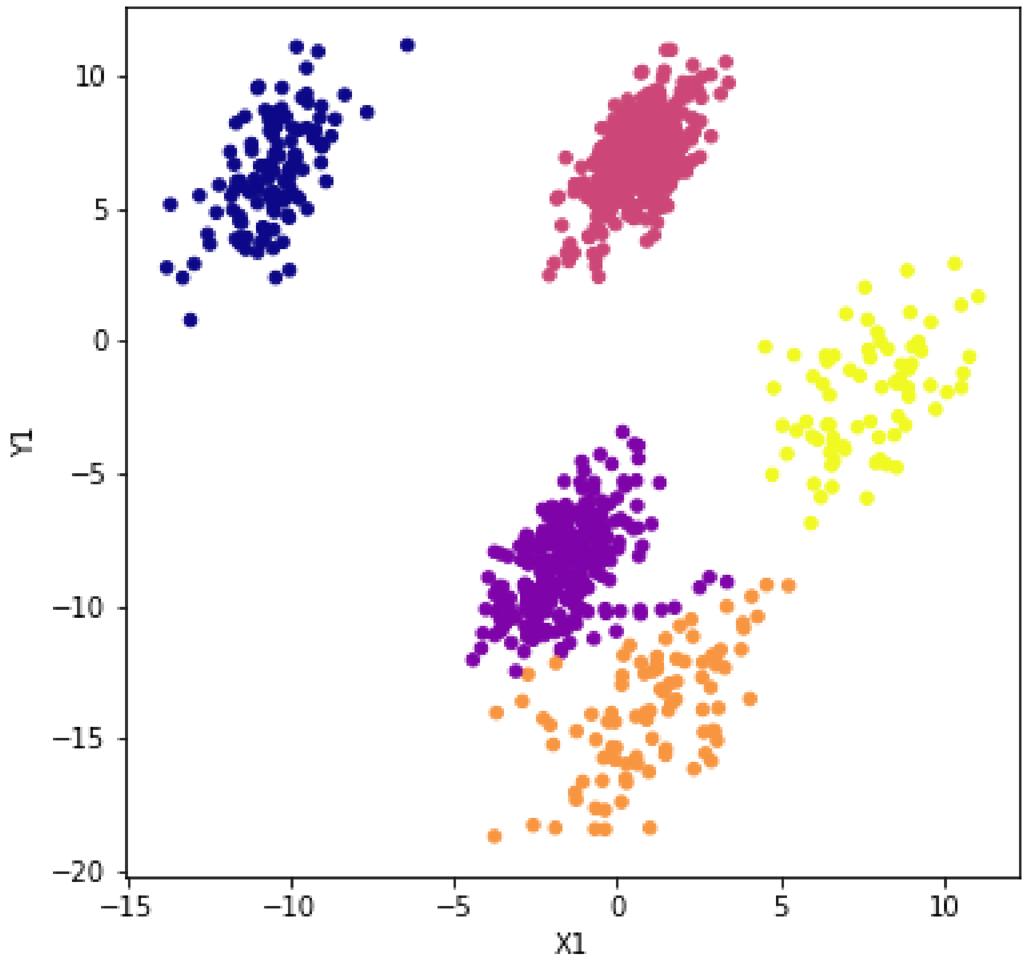
```
In [25]: CH_2 = calinski_harabaz_score(d.loc[:,['X1','Y1']],
                                        kmeans_2.labels_)
         CH_2

Out[25]: 2210.1921650543345
```

let us try now with k-means (K=5)

```
In [26]: K=5

         kmeans2_5 = KMeans(n_clusters=K,max_iter=100)
         kmeans2_5.fit(d.loc[:,['X1','Y1']]);
         d.plot.scatter(x='X1', y='Y1',
                        c=kmeans2_5.labels_,
                        colormap='plasma',
                        figsize=(6,6),colorbar=False);
```



This time the result has even more chances of being largely incorrect because there are more ways of getting a wrong solution
clustering quality as measured by the Calinski-Harabasz index

```
In [27]: CH2_5 = calinski_harabaz_score(d.loc[:,['X1','Y1']],
                                        kmeans2_5.labels_)
         CH2_5

Out[27]: 4511.6033865718355
```

at least CH2.5 >> CH2.2 ... so C-H does a good job
In class we saw that k-means is usually re-run several times

```
In [28]: kmeans2_5 = KMeans(n_clusters=K,max_iter=100,n_init=100)
         kmeans2_5.fit(d.loc[:,['X1','Y1']])
```

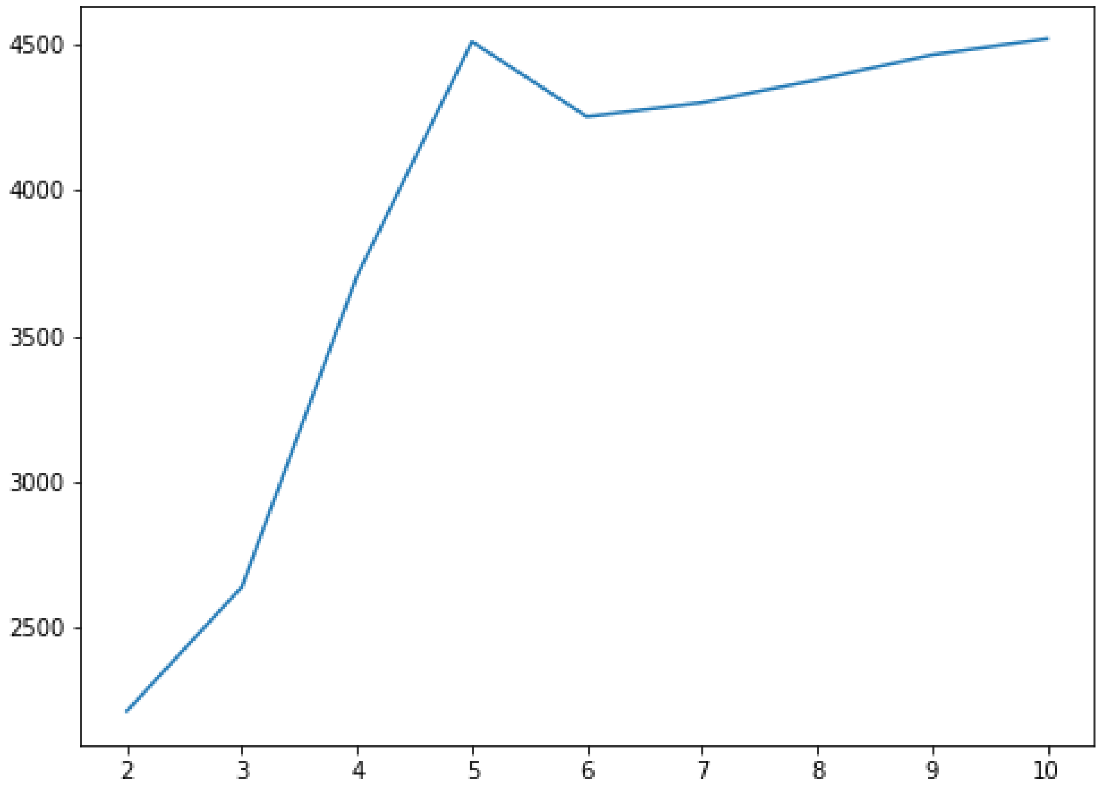
```
        CH2_5 = calinski_harabaz_score(d.loc[:,['X1','Y1']],
                                       kmeans2_5.labels_ )
        CH2_5
```

```
Out[28]: KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=100,
             n_clusters=5, n_init=100, n_jobs=1, precompute_distances='auto',
             random_state=None, tol=0.0001, verbose=0)
```

```
Out[28]: 4511.6033865718355
```

so it is not a matter of wrong initialization this is really the best k-means can do here this may take a while

```
In [29]: r = []
         for i in range(2,11):
             km = KMeans(n_clusters=i,
                         max_iter=100,
                         n_init=100).fit(d.loc[:,['X1','Y1']])
             r.append(calinski_harabaz_score(d.loc[:,['X1','Y1']],
                                             km.labels_ ))
         fig, ax = plt.subplots(figsize=(8,6))
         plt.plot(range(2,11),r);
```



the conclusion is that k-means + C-H bet for 5 clusters ... not bad, not bad ...

but the real *shape* of the clusters cannot be captured, because k-means only "sees" spherical clusters and these are ellipsoidal

let us try now E-M

This method performs E-M for mixture densities, including mixtures of Gaussians we can specify which family of gaussians we intend to fit:

- "full" each component has full covariance matrix, "diagonal" covariances are diagonal (just variance),
- "spherical" each component has his own diagonal univariance and "tied" all components share variance

  WARNING: default is "full".

suppose first that we know the truth and specify axis-aligned densities (i.e., independent variables)

```
In [30]: gm =GaussianMixture(n_components=5,
                             covariance_type='diag').fit(d.loc[:,['X1','Y1']])
         print('BIC=', gm.bic(d.loc[:,['X1','Y1']]))
         print('\nLOG Likelihood=', gm.lower_bound_)
         print('\nWEIGHTS=')
         pd.DataFrame(gm.weights_)
         print('\nMEANS=')
         pd.DataFrame(gm.means_)
         print('\nCOV=')
         pd.DataFrame(gm.covariances_)
```

```
BIC= 9962.697463368639

LOG Likelihood= -4.898688994806308

WEIGHTS=


Out[30]:        0
         0  0.400
         1  0.295
         2  0.125
         3  0.074
         4  0.106


MEANS=


Out[30]:         0       1
         0   0.692   6.890
         1  -1.659  -8.483
```

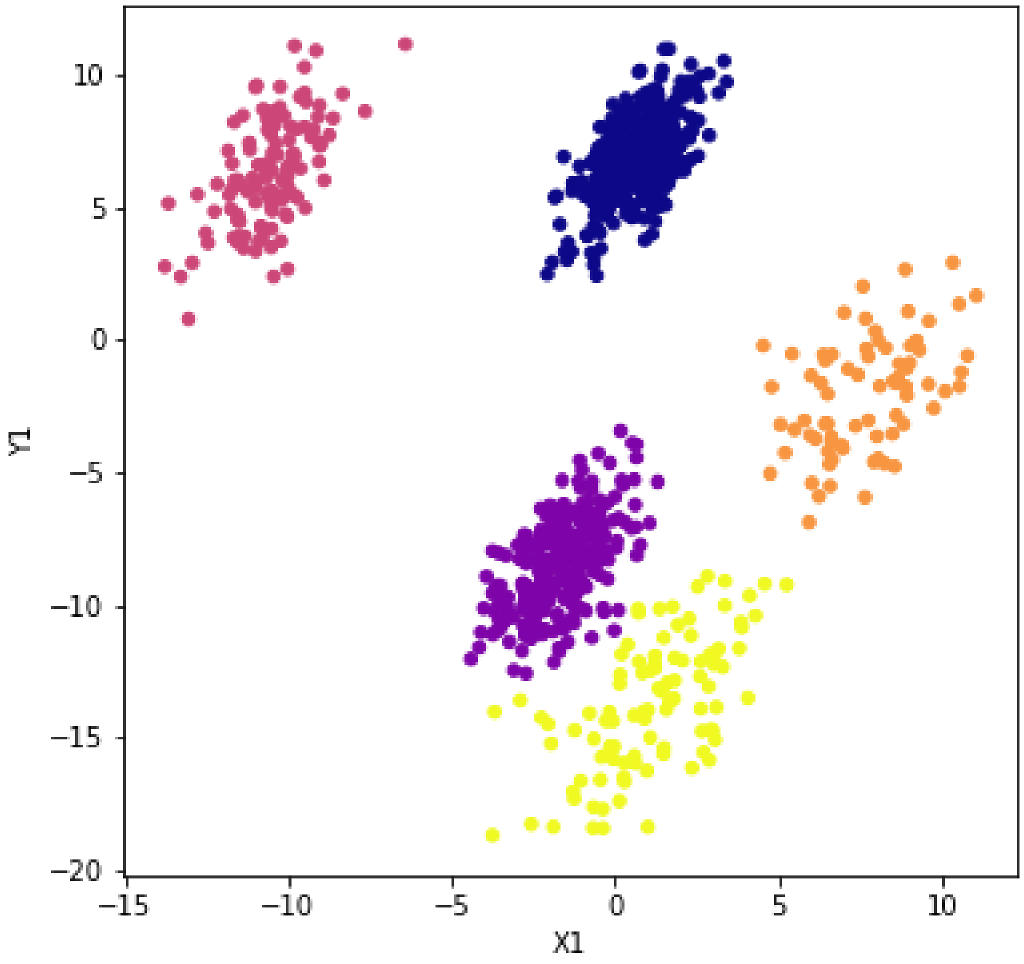
```
        2 -10.535   6.444
        3   7.664  -2.046
        4   0.854 -13.396
```

```
COV=
```

```
Out[30]:        0      1
        0  0.898  2.310
        1  1.126  2.819
        2  1.249  4.071
        3  2.490  4.672
        4  4.031  7.404
```

This is a graphical summary of the clustering

```
In [31]: d.plot.scatter(x='X1', y='Y1',
                        c=gm.predict(d.loc[:,['X1','Y1']]),
                        colormap='plasma',
                        figsize=(6,6),colorbar=False);
```



it was very likely that E-M performed extremely well why? because we knew the truth (cluster form and number)

suppose now we do not the know the truth but we still wish to fit general gaussians

```
In [32]: gm =GaussianMixture(n_components=5,
                             covariance_type='full').fit(d.loc[:,['X1','Y1']])
         print('BIC=', gm.bic(d.loc[:,['X1','Y1']]))
         print('\nLOG Likelihood=', gm.lower_bound_)
         print('\nWEIGHTS=')
         pd.DataFrame(gm.weights_)
         print('\nMEANS=')
         pd.DataFrame(gm.means_)
         print('\nCOV=')
         gm.covariances_
```

```
BIC= 9609.070993641648

LOG Likelihood= -4.704401604690396

WEIGHTS=
```

```
Out[32]:        0
         0  0.125
         1  0.303
         2  0.400
         3  0.098
         4  0.074
```

```
MEANS=
```

```
Out[32]:          0       1
         0 -10.535   6.444
         1  -1.692  -8.528
         2   0.692   6.890
         3   1.186 -13.669
         4   7.667  -2.039
```

```
COV=
```

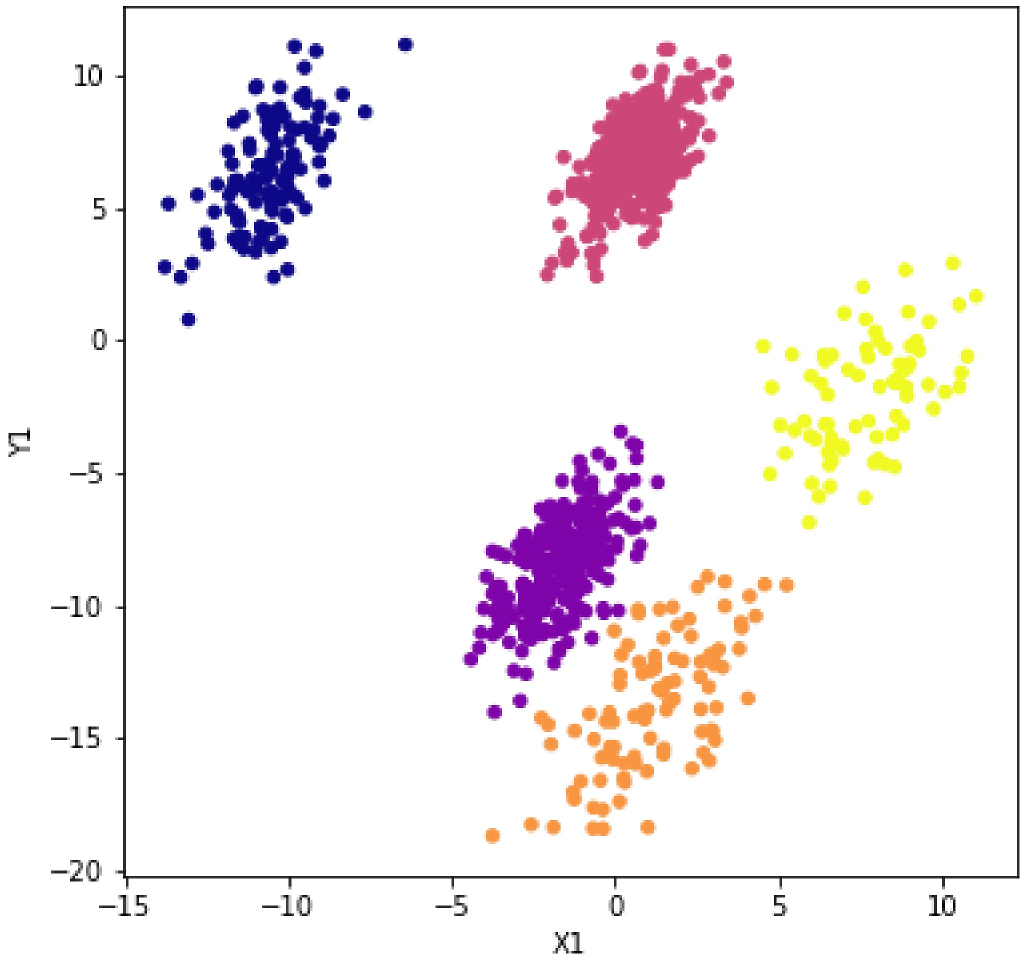
```
Out[32]: array([[[1.24862465, 1.29165545],
                 [1.29165545, 4.07145078]],
                [[1.13364653, 1.07469376],
                 [1.07469376, 3.01171371]],

                [[0.8979744 , 0.84783988],
                 [0.84783988, 2.30951699]],

                [[3.11324278, 2.83240408],
                 [2.83240408, 6.49679973]],

                [[2.49337285, 1.55130335],
                 [1.55130335, 4.66268719]]])
```

```
In [33]: d.plot.scatter(x='X1', y='Y1',
                        c=gm.predict(d.loc[:,['X1','Y1']]),
                        colormap='plasma',
                        figsize=(6,6),colorbar=False);
```



the method works also very smoothly why? because the data *is* gaussian
compare the estimated centers

```
In [34]: pd.DataFrame(gm.means_)
```

```
Out[34]:         0       1
         0 -10.535   6.444
         1  -1.692  -8.528
         2   0.692   6.890
         3   1.186 -13.669
         4   7.667  -2.039
```

with the truth (note the clusters may appear in a different order)

```
In [35]: pd.DataFrame(mu_k)
```

```
Out[35]:         0       1
         0   0.688   6.846
         1  -1.762  -8.626
         2 -10.619   6.280
         3   1.197 -13.693
         4   7.566  -2.443
```

or the estimated coefficients

```
In [36]: pd.DataFrame(gm.weights_)
```

```
Out[36]:       0
         0  0.125
         1  0.303
         2  0.400
         3  0.098
         4  0.074
```

with the truth

```
In [37]: c= Counter(labels)
         pd.DataFrame(np.array([c[v] for v in c])/1000.0)
```

```
Out[37]:       0
         0  0.400
         1  0.300
         2  0.125
         3  0.100
         4  0.075
```