Unsupervised Learning: clustering

AAA-Python Edition

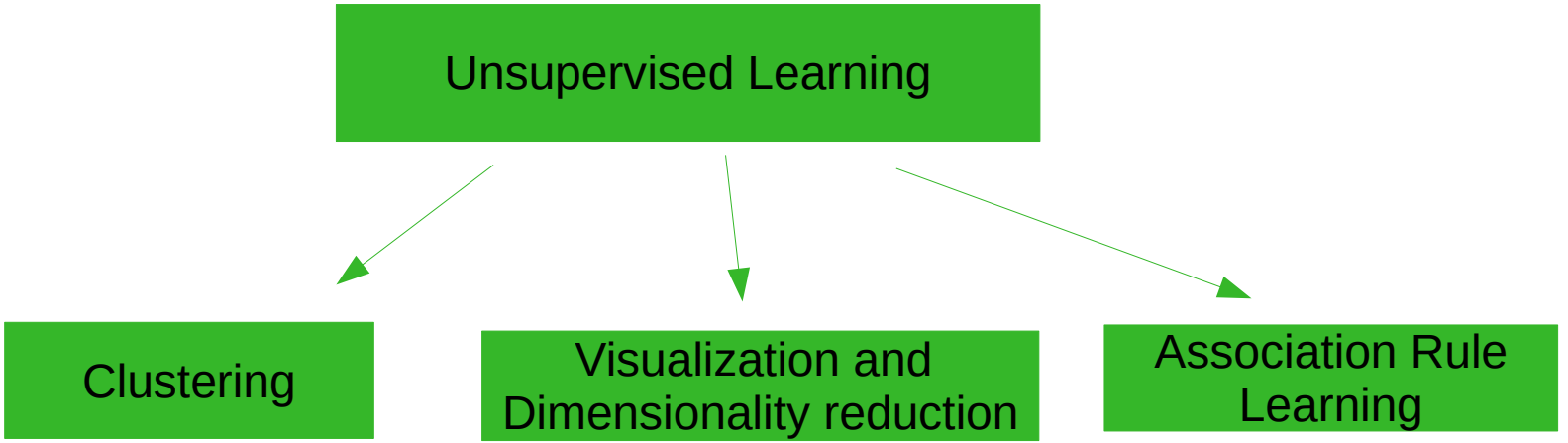
Plan

- 1- Clustering
- 2- K-mean example
- 3- Silhouette score
- 4- Mean Shift
- 5- Gaussian Mixture Model
- 6- Affinity Propagation Model

1- Clustering

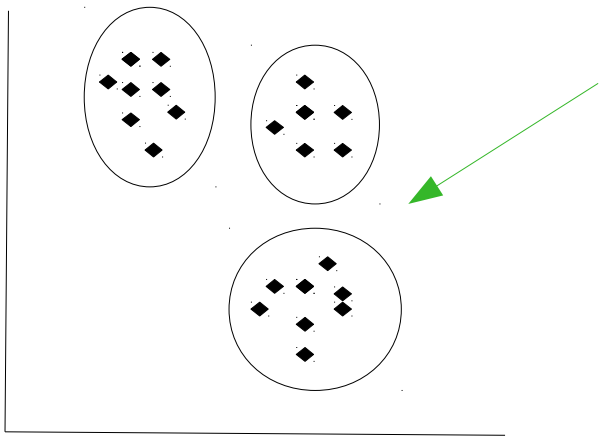
Unsupervised Learning

- Unsupervised learning is about Machine Learning using Unlabeled Data.
- It concerns several kind of tasks, that can be grouped into **3 categories:**



Clustering

- **Clustering** means finding the **clusters** within a given **data**.
- A **cluster** can be defined as a **group** of **similar points** (samples) of data.
- One way to identify similar points, is to use **similarity metrics**. **Euclidean Distance** in one of these similarity metrics.



Data distributed into 3 distinct clusters

K-mean algorithm

- It is one of the methods used in clustering. It uses the euclidean distance as a similarity metric.
- The steps are as follow:
  - 1- Set the number of clusters to be find: K
  - 2- Select randomly : k samples from the data ,or use an algorithm to select generally distant k points. The k samples are the initial centroids of the clusters.
  - 3- Divide the samples into these K clusters: for each sample:
    - Compute the distances from each centroid
    - Select the least one.
  - 4- Compute the new centroids of clusters u_j: the mean of the samples belonging to each cluster
  - 5- Compute the inertia, for **n** samples, using this formula: $\sum_{i=0}^{n} \left(\|x_i - u_j\|\right)^2$
  - 6- Repeat from step 3, until the inertia is minimized, or the clusters assignment do not change or a maximum number of iterations is reached.

The data

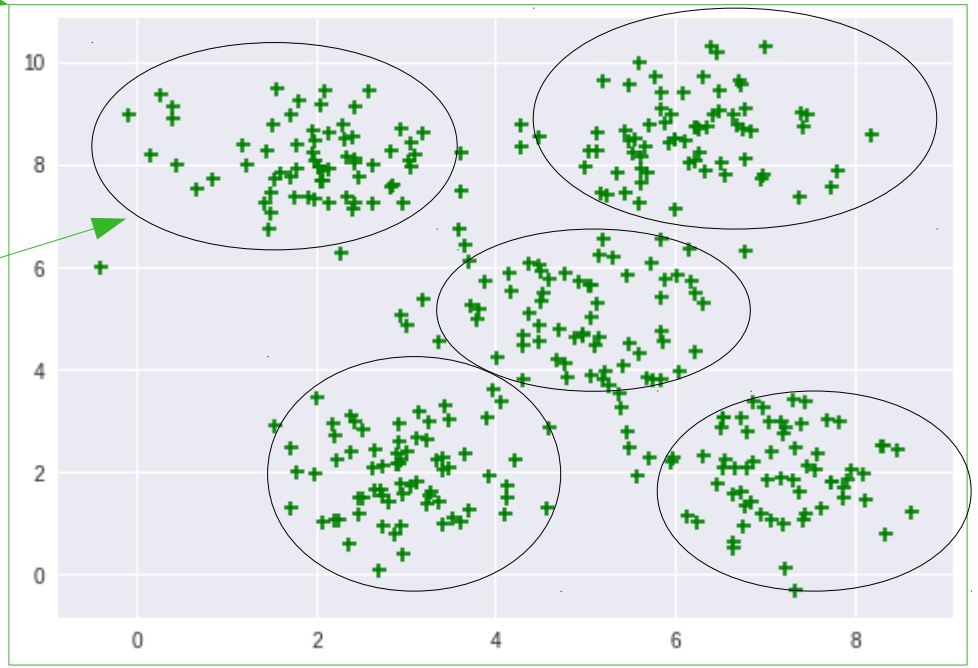
- The data: 2 features

```
X= dataF.values
print (X.shape)
```

```
(350, 2)
```

```
dataF = pd.read_csv('data_clustering.txt',header=-1)
dataF.head(5)
```

	0	1
0	2.08	1.05
1	2.05	7.70
2	4.53	5.49
3	6.23	1.02
4	5.35	7.86



We can clearly see the 5 clusters

2- K-mean example

Training

```
from sklearn.cluster import KMeans
```

```
# initialize the number of the clusters
num_clusters = 5
# Create KMeans object using random centroid initalization
kmeans = KMeans(init='random', n_clusters=num_clusters,verbose=1, n_init=1)
```

The algorithm will run **n_init** times with different random centroid initialization at each time. Then select the best result (the best final inertia value)

```
# Train the KMeans clustering model
kmeans.fit(X)
```

```
Initialization complete
start iteration
done sorting
end inner loop
Iteration 0, inertia 873.3646029796687
start iteration
done sorting
end inner loop
Iteration 1, inertia 762.7499327404964
```

```
Iteration 7, inertia 433.80300829447276
center shift 0.000000e+00 within tolerance 6.415290e-04
```

```
# the final centroids are
final_Centroids=kmeans.cluster_centers_
```

```
array([[2.97253521, 1.97267606],
       [6.10842857, 8.58428571],
       [7.09588235, 2.01735294],
       [1.98385714, 8.04942857],
       [4.92605634, 5.0184507 ]])
```

Those are the means of the samples belonging to each cluster.

[By Amina Delali]

2- K-mean example

Visualization

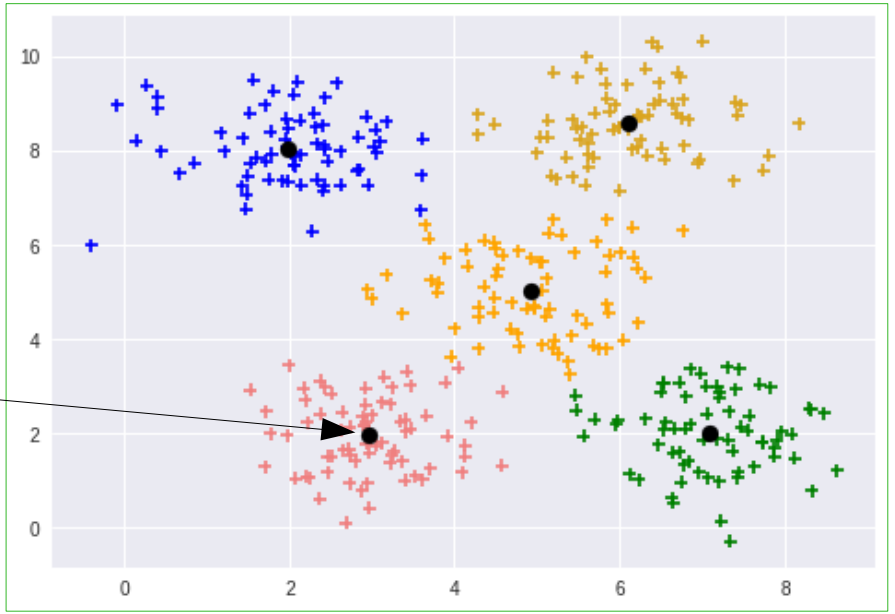
```
1 kmeans.labels_
```

```
array([3, 4, 1, 2, 0, 3, 4, 1, 1, 0, 3, 4,
       1, 3, 1, 3, 4, 1, 2, 0, 3, 4, 1, 2,
```

```
clus_colors=[ "goldenrod" if y ==1 else "green" if y == 2 else "blue" if y==3 else "orange" if y== 4
             else "lightcoral" for y in kmeans.labels_]

plt.figure()
plt.scatter(X[:,0], X[:,1], marker='+',c=clus_colors)
plt.scatter(final_Centroids[:,0],final_Centroids[:,1],marker="o",facecolor="black",
             s =80)
```

The centroids



[By Amina Delali]

3- Silhouette score

Definition

- **Silhouette score** is a measure that is used to indicate the quality of the clustering: it shows at which degree the data samples are similar to the others samples belonging to the same cluster.

- For one sample, it is computed as follow: $$s=\frac{b-a}{max(a,b)}$$
  - Where:
    - **a**: the mean distance between a sample and all other samples in the same cluster.
    - **b**: the mean distance between a sample and all other samples in the next nearest cluster.
    - The **distance** is computed by considering the samples as points and the features as coordinates. The distance between two samples, is computed as the euclidean distance between 2 points.
      For example: the distance between $c(x_1,y_1)$ and $d(x_2,y_2)$ is computed as follow: $$\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}$$

3- Silhouette score

Use

- For one sample, the silhouette value score ranges from 1 to -1. Many values close to 1 indicates **good** clustering. And in the other hand, many values close to -1, indicates **bad** clustering (too many or too few clusters).

- We can compute the overall silhouette score by computing the **mean** of all the samples silhouette scores.
  A value close to zero indicates cluster overlapping.

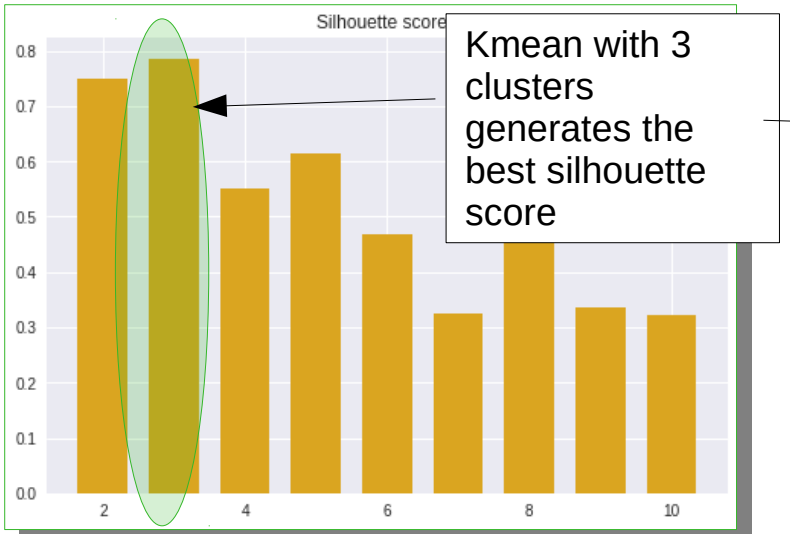
- The overall silhouette score can be used to find the best **k** number of clusters.

- Sklearn implements the silhouette score calculation: the overall (mean) and the singular coefficient (for one sample).
  - sklearn.metrics.silhouette_score: the mean
  - klearn.metrics.silhouette_samples: for each sample

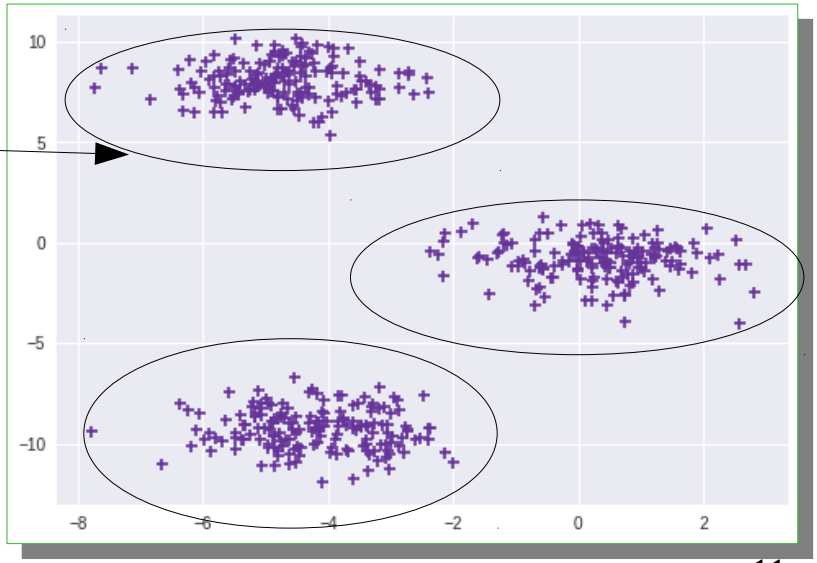
3- Silhouette score

Example

```
# testing cluster numbers: from 2 to 10
k_values = range(2,11)
scores =[]
for n_clusters in k_values:
  # initialise a kmean clusterer with the actual tested
  # cluster number
  myKmean = KMeans (init='random', n_clusters=n_clusters, n_init=1)
  # train it
  myKmean.fit(X)
  # compute the ovreall silhouette score
  overall_score=  silhouette_score(X, myKmean.labels_,metric='euclidean', sample_size=len(X))
  # add it to list of previously computed scores
  scores.append(overall_score)
```



Kmean with 3 clusters generates the best silhouette score



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4- Mean Shift

Concept & Steps

- **Mean shift** clustering is an other method used to identify clusters in a dataset. Is supposes that the data distribution may tend to be dense around certain points: the centers of the clusters (centroids).
- To identify these points, it defines the following steps:
  - Make a copy of your data
  - For each sample in the copy, repeat these steps:
    - Compute the mean of samples contained in a window (fixed size) around the sample. The mean is computed as follow:

$$m(x) = \frac{\sum_{x_i \in N(x)} K(x_i - x)\, x}{\sum_{x_i \in N(x)} K(x_i - x)}$$

Where: K is a function that will affect weights to the neighbors of x, regarding their distance from x (bigger distance, small weight). N(x) represents the points near x(neighbors of x).

    - Update the sample's location to that new mean.
  - Stop the process when the samples doesn't move, or the shift is not significant. Then, Filter out near-similar points to keep the final centroids.

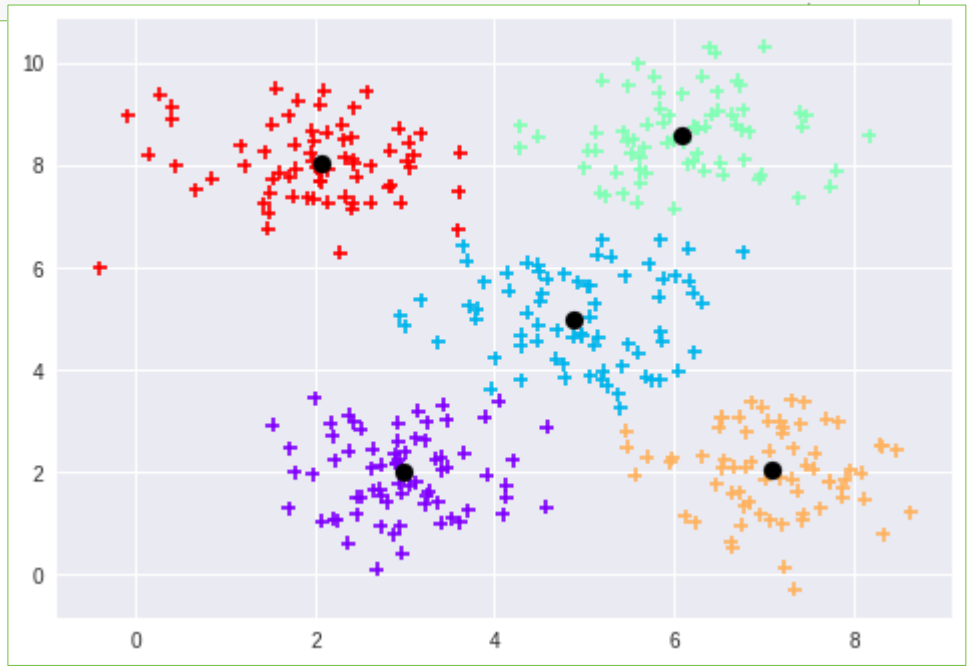
[By Amina Delali]

Example

```
# Cluster data with MeanShift
myMeanShift = MeanShift(bandwidth=2)
myMeanShift.fit(X)
```

```
labels = myMeanShift.labels_
final_Centroids2 = myMeanShift.cluster_centers_
plt.figure()
plt.scatter(X[:,0], X[:,1], marker='+',c=labels, cmap ="rainbow")
plt.scatter(final_Centroids2[:,0],final_Centroids2[:,1],marker="o",facecolor="black",
            s =80)
```

We don't know the number of clusters in advance. We have to plot according to labels values.

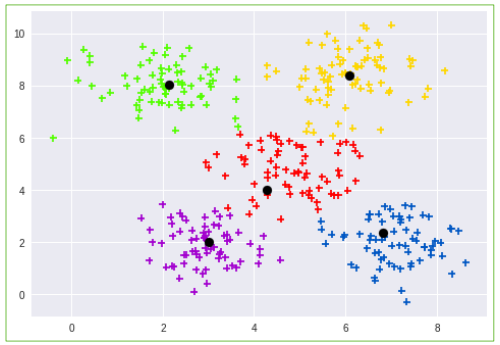


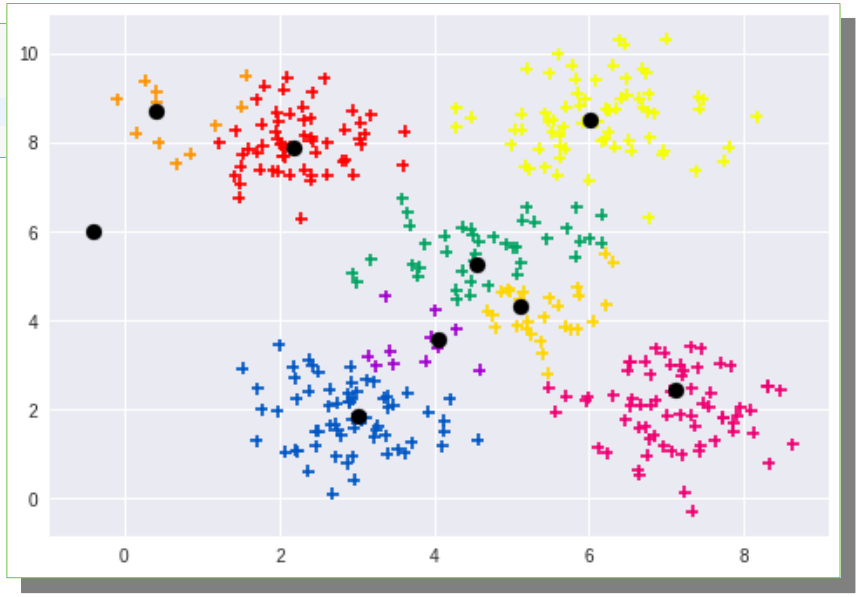
Bandwidth

- If you change the bandwidth value, you will have different clustering:

```
1 from sklearn.cluster import estimate_bandwidth
2
3 myBW = estimate_bandwidth(X,quantile=0.2);
4 print("The estimated bandwidth is:\n",myBW)
```

```
The estimated bandwidth is:  2.35
```





Bandwidth == **1**

5- Gaussian Mixture Model

Concept

- The **Gaussian Mixture Model** is simply a **mixture** of **Gaussian models.**
- A **Gaussian Model,** is a model that makes the hypothesis that the data is drawn following the Gaussian distribution, or more exactly, the function:

$$f(x)=\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

The parameters of that model are μ : the mean, and σ : the standard deviation

- Gaussian Mixture clustering consist of identifying to which distribution each point belongs.

- This identification is done using algorithms like: **Expectation-Maximization (EM)** algortihm.

[By Amina Delali]

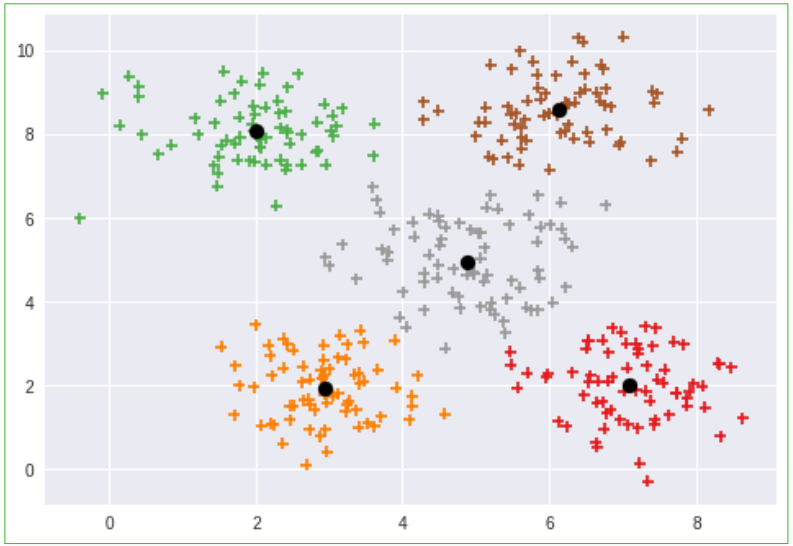
Example with scikit-learn

- Scikit-learn will use the expectation maximization algorithm to determine the different Gaussian distributions.

```
myGMM = GaussianMixture(n_components= 5,)
myGMM.fit(X)
```

There is no cluster centers but mean of each identified distribution.

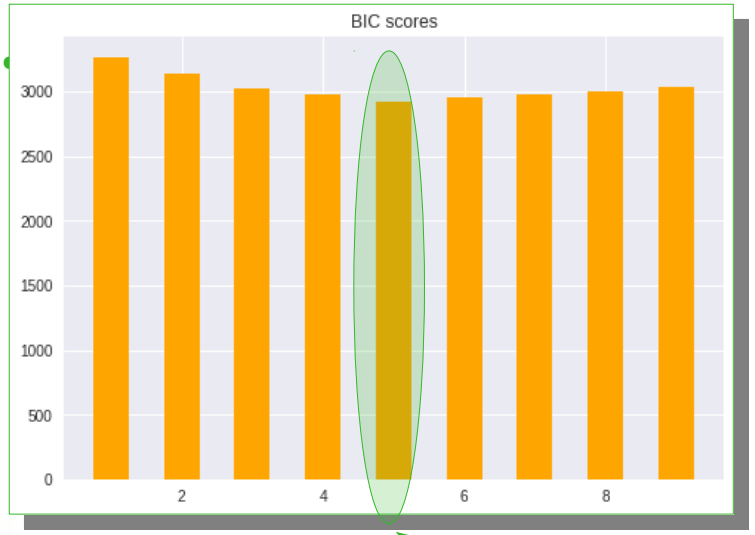
```
labels = myGMM.predict(X)
centroids= myGMM.means_
plt.figure()
plt.scatter(X[:,0], X[:,1], marker='+', c=labels,cmap ="Set1")
plt.scatter(centroids[:,0],centroids[:,1],marker="o",facecolor="black",
            s =80)
```



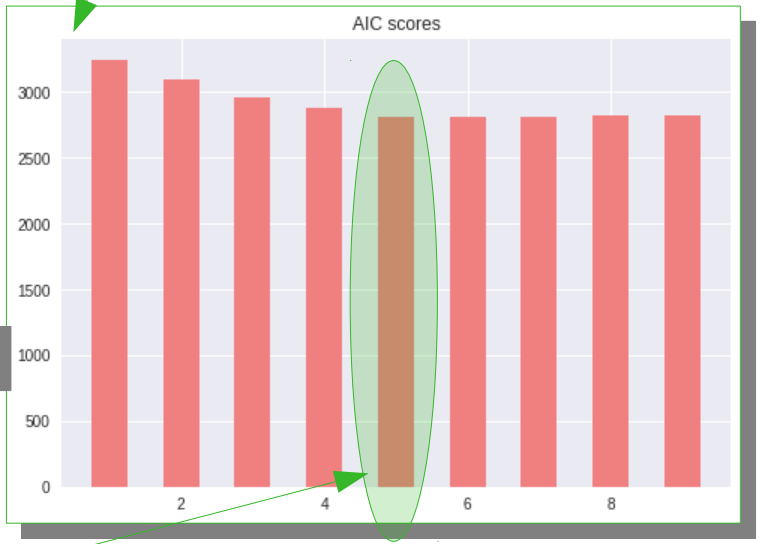
5- Gaussian Mixture Model

Selection of n_components

We compute the BIC score (or the AIC score) for each model corresponding to each number of components. Then, select the number of components corresponding to of lowest score




```
n_components = range(1,10)
bics=[]
aics=[]
for i in n_components:
  model = GaussianMixture(n_components=i)
  model.fit(X)
  bics.append(model.bic(X))
  aics.append(model.aic(X))
```




```
np.round(bics,2)
```

```
array([3263.51, 3139.39, 3028.19, 2973.55, 2920.83, 2954.91, 2983.97,
       3002.4 , 3034.91])
```

```
np.round(aics,2)
```

```
array([3244.22, 3096.95, 2962.61, 2884.81, 2808.95, 2819.88, 2825.8 ,
       2821.08, 2830.44])
```

[By Amina Delali]

6-Affinity Propagation Model

Concept

- An other clustering method: **Affinity propagation model.** It is defined by these terms : **Exemplars, responsibility, availability,preference, damping factor** and **message passing.**

  - **Exemplars** are the clusters centers.
  - **Preference** influence the resulting number of clusters by affecting a preference value for a sample to be an exemplar (its similarity score between it and itself).
  - **Message:** responsibility or availability values.
  - **Message passing**: responsibility and availability calculation
  - **Responsibility r(i,k):** accumulated evidence that the sample **k** should be the **exemplar** of **i.**
  - **Availability a(i,k):** accumulated evidence that the sample **i** should select **k** to be its **exemplar.**
  - **Damping factor** λ **:** influence the resulting number of clusters by affecting a value for the relationship between new and current messages values. Must be >= 0.5 and < 1

6-Affinity Propagation Model

Process

- Select a similarity measure. For example, the **negative** of Euclidean Distance
- Select preferences and a damping factor values.
- Set **r** and **a matrices** to **0.** Fill **S** with the similarity scores between all points. Its diagonal is filled with the preferences values.
- **Repeat until convergence (**changes for exemplars values are too small or non-existent**) is reached**
  - Compute r using this formulas:
    - $r_{t+1}(i,k) = s(i,k) - max[a_t(i,k') + s(i,k') \forall k' \neq k]$
    - $r_{t+1}(i,k) = \lambda \cdot r_t(i,k) + (1-\lambda) \cdot r_{t+1}(i,k)$
  - Compute a using this formulas:
    - $a_{t+1}(i,k) = min[0, r_{t+1}(k,k) + \sum_{i',\ i' \notin \{i,k\}} r_{t+1}(i',k)]$
    - $a_{t+1}(i,k) = \lambda \cdot a_t(i,k) + (1-\lambda) \cdot a_{t+1}(i,k)$
- **Select** the **exemplars** from: r(i,i) + a(i,i) >0

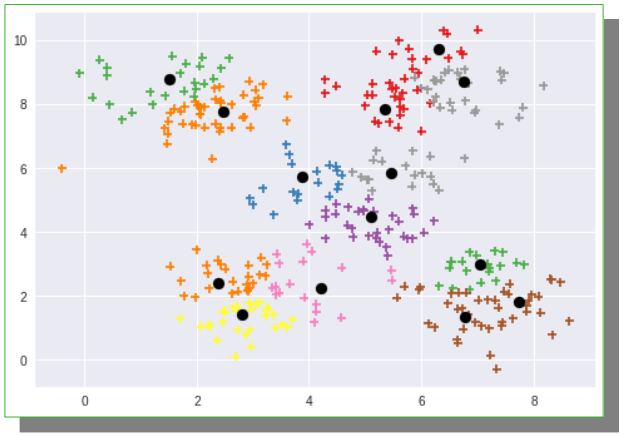
[By Amina Delali]

Example

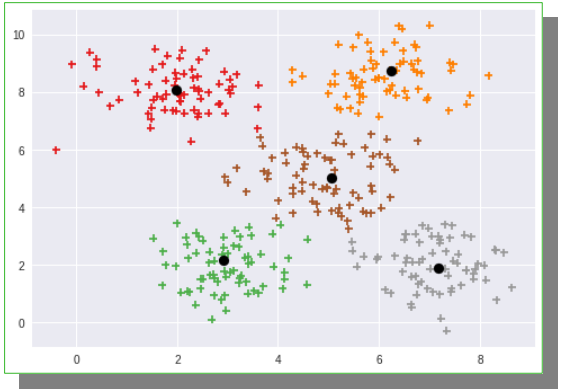
```
from sklearn.cluster import AffinityPropagation
# initialization of the model with default values
myModel= AffinityPropagation()
```

```
myModel.fit(X)
```

Default value for **preferences** is the **median** of all similarity scores (median = the value in the **middle** of ordered similarity scores)




```
myModel= AffinityPropagation(preference=-100)
myModel.fit(X)
```



[By Amina Delali]

References

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Thank you!

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