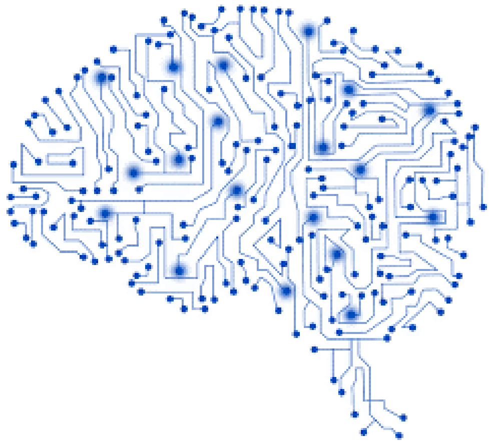
**University of Minho**
School of Engineering

Intelligent Systems Associate Laboratory



# Dados e Aprendizagem Automática

## Unsupervised Learning:
## K-means, K-medoids and DBSCAN

**DAA @ MEI-1º/MiEI-4º – 1º Semestre**

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*Part IX*

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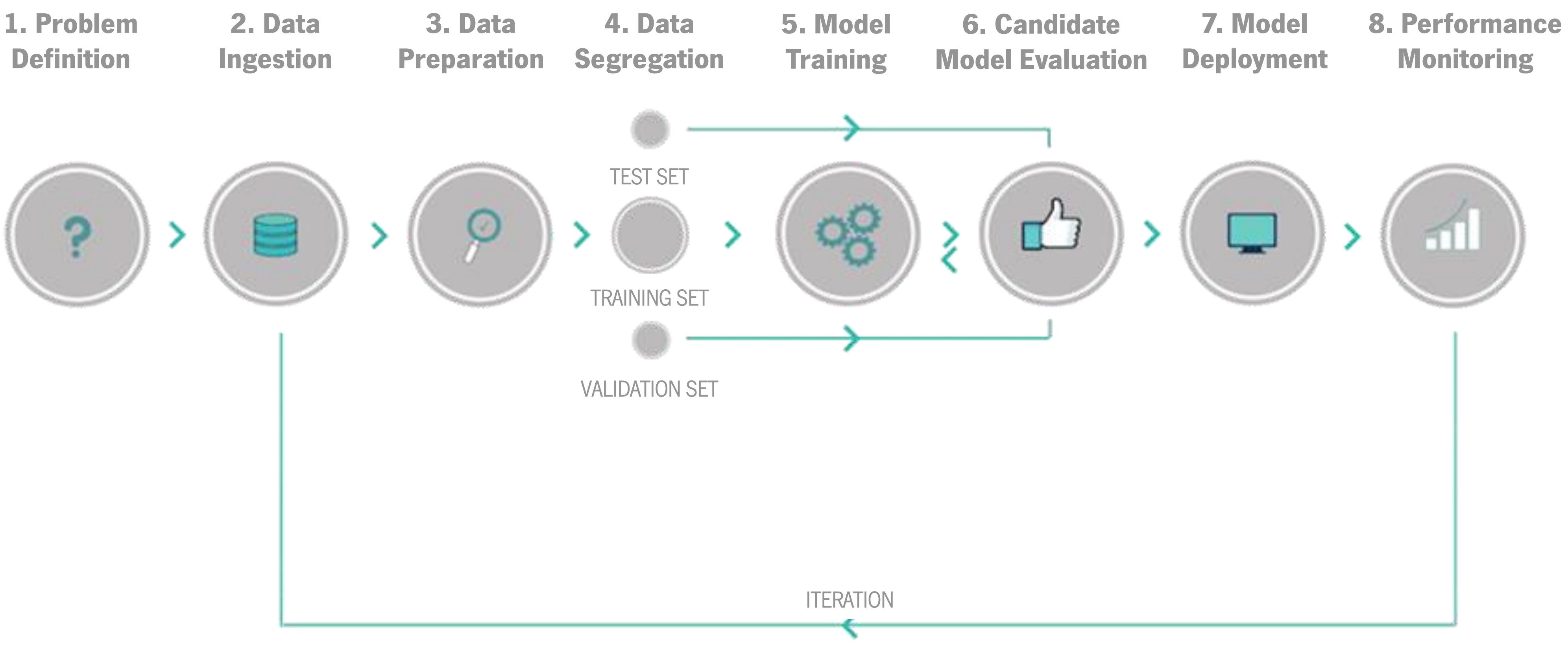
1. Problem Definition
2. Data Ingestion
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# Unsupervised Learning

# Unsupervised Learning



**Unsupervised learning** means that there is no outcome to be predicted, and the algorithm just tries to find patterns on the data. Using **clustering**, it tries to group (cluster) the data based on their similarity.

For this example, we create the data creating *isotropic Gaussian blobs* from `sklearn.datasets`.

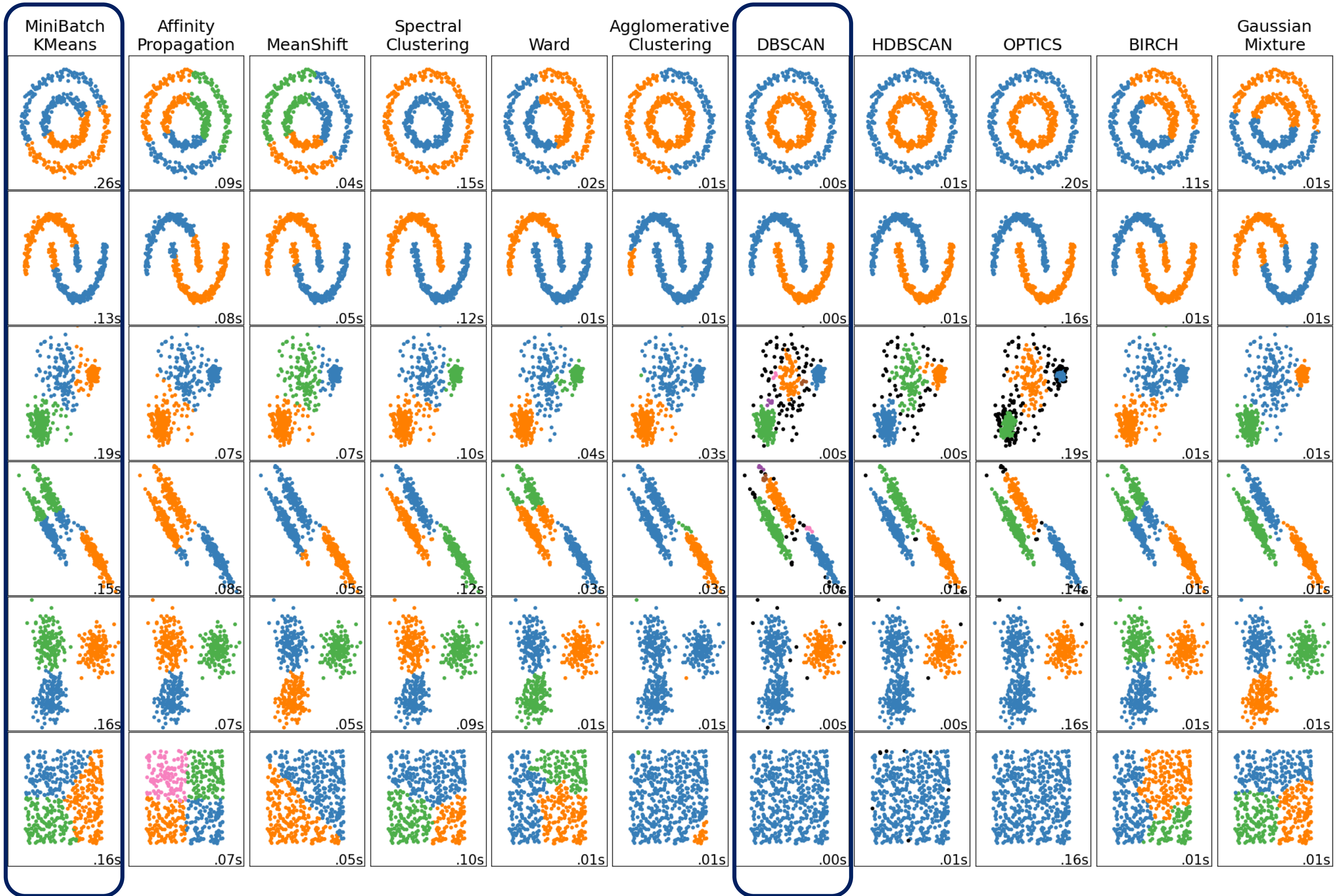
Note: all clustering algorithms require data preprocessing(e.g. dimensionality reduction) and standardization.

You may need to install `scikit-learn-extra`.

```
pip install https://github.com/scikit-learn-contrib/scikit-learn-extra/archive/master.zip
```

# Unsupervised Learning - Clustering

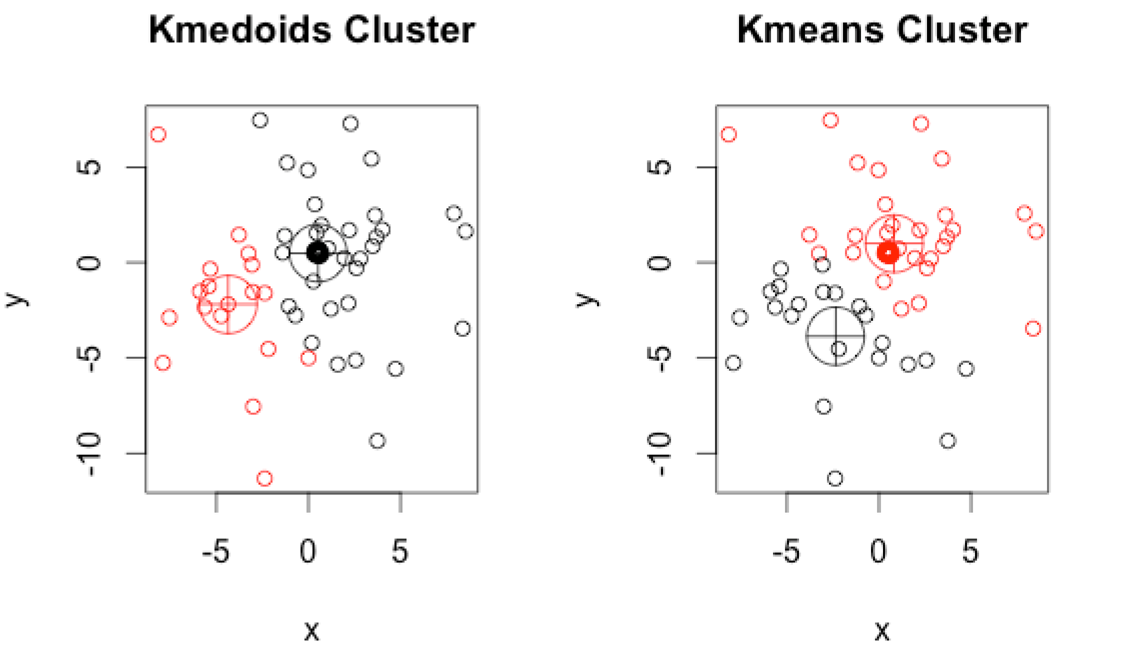




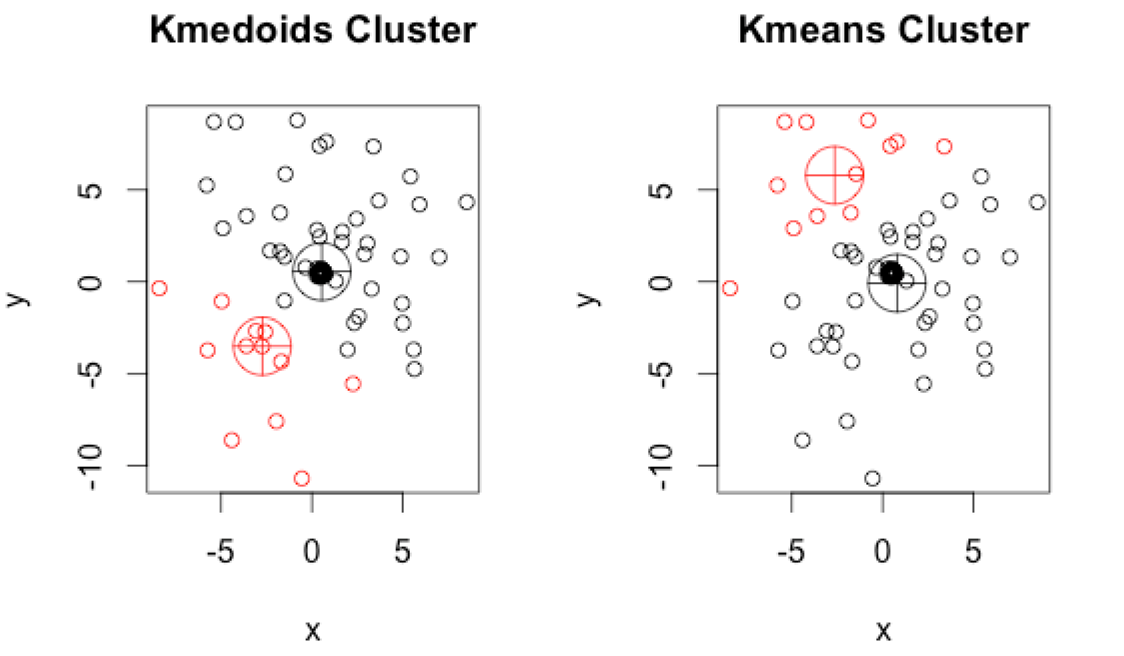
# Unsupervised Learning – K-Means and K-Medoids



1st iteration




2nd iteration




https://stats.stackexchange.com/questions/156210/an-example-where-the-output-of-the-k-medoid-algorithm-is-different-than-the-outp

# Unsupervised Learning – K-Means and K-Medoids



Both **K-Means** and **K-Medoids** algorithms follow the **partitioning method**. So they are:

- breaking the dataset up into *k* groups;
- trying to minimize the distance between points of the same cluster and a particular point which is the center of that cluster.

The **K-Means** algorithm chooses *centroids*, the geometric center of a cluster using the mean to all cluster points.

On the other hand, the **K-Medoids** algorithm chooses *medoids*, points as centers that belong to the dataset and computes dissimilarities between data points.

The most common implementation of the K-Medoids clustering algorithm is the **Partitioning Around Medoids (PAM)** algorithm. The PAM algorithm uses a *greedy search*, which may not find the global optimum solution.

# Unsupervised Learning – K-Means and K-Medoids



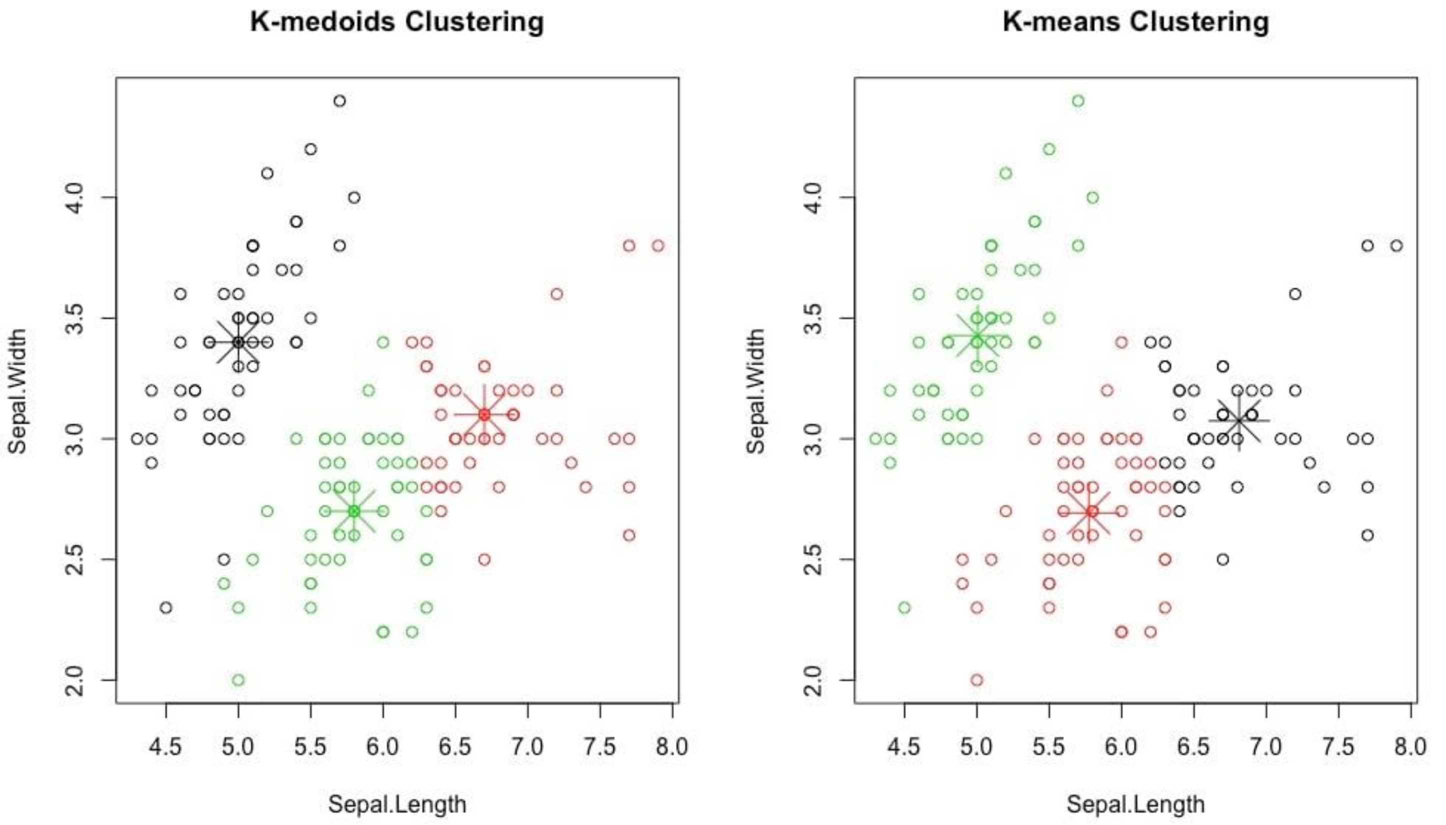
*Medoids* are more robust to outliers than *centroids*, but they need more computation for high dimensional data.

Strengths:
- simple and intuitive;
- scales to large datasets;
- as a result, we also have centroids that can be used as standard cluster representatives

Weaknesses:
- knowledge about the number of clusters is necessary and must be specified as a parameter;
- does not cope well with a very large number of features;
- separates only convex and homogeneous clusters well;
- can result in poor local solutions, so it needs to be run several times.

# Unsupervised Learning – K-Means and K-Medoids

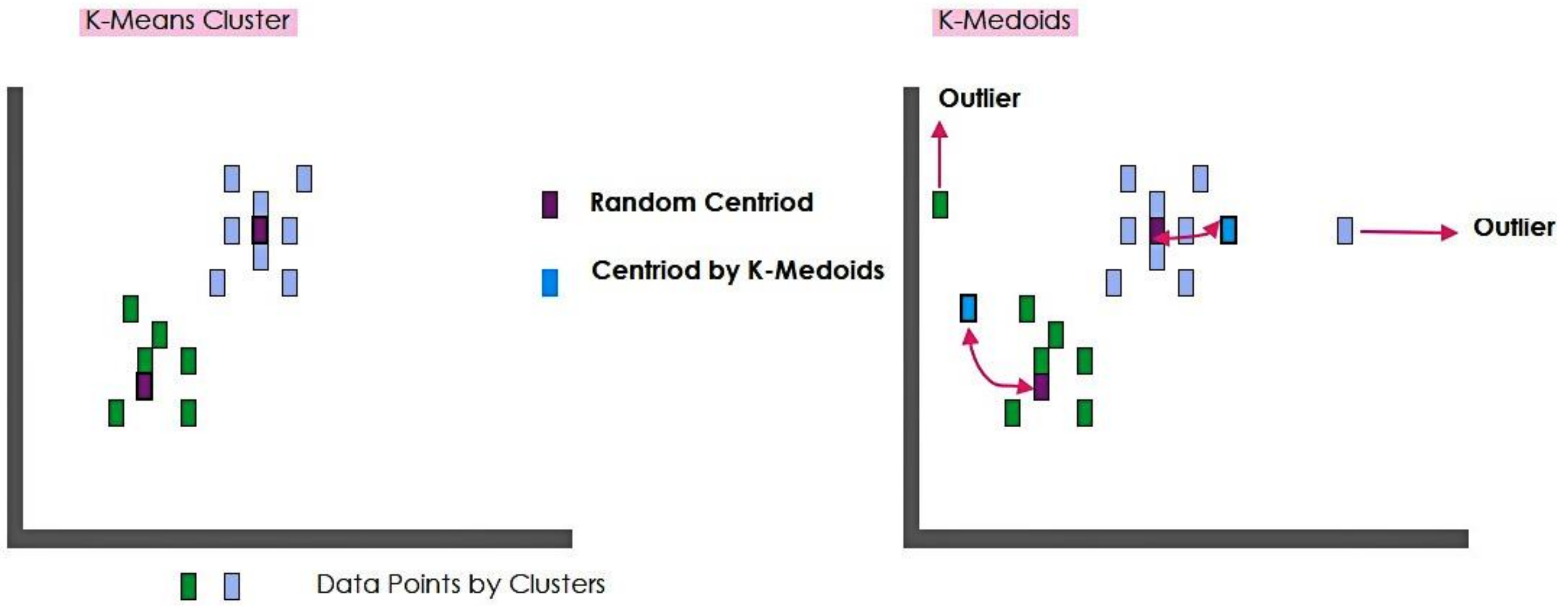





https://subscription.packtpub.com/book/big-data-and-business-intelligence/9781789956399/1/ch01lvl1sec08/introduction-to-k-medoids-clustering

# Unsupervised Learning – K-Means and K-Medoids





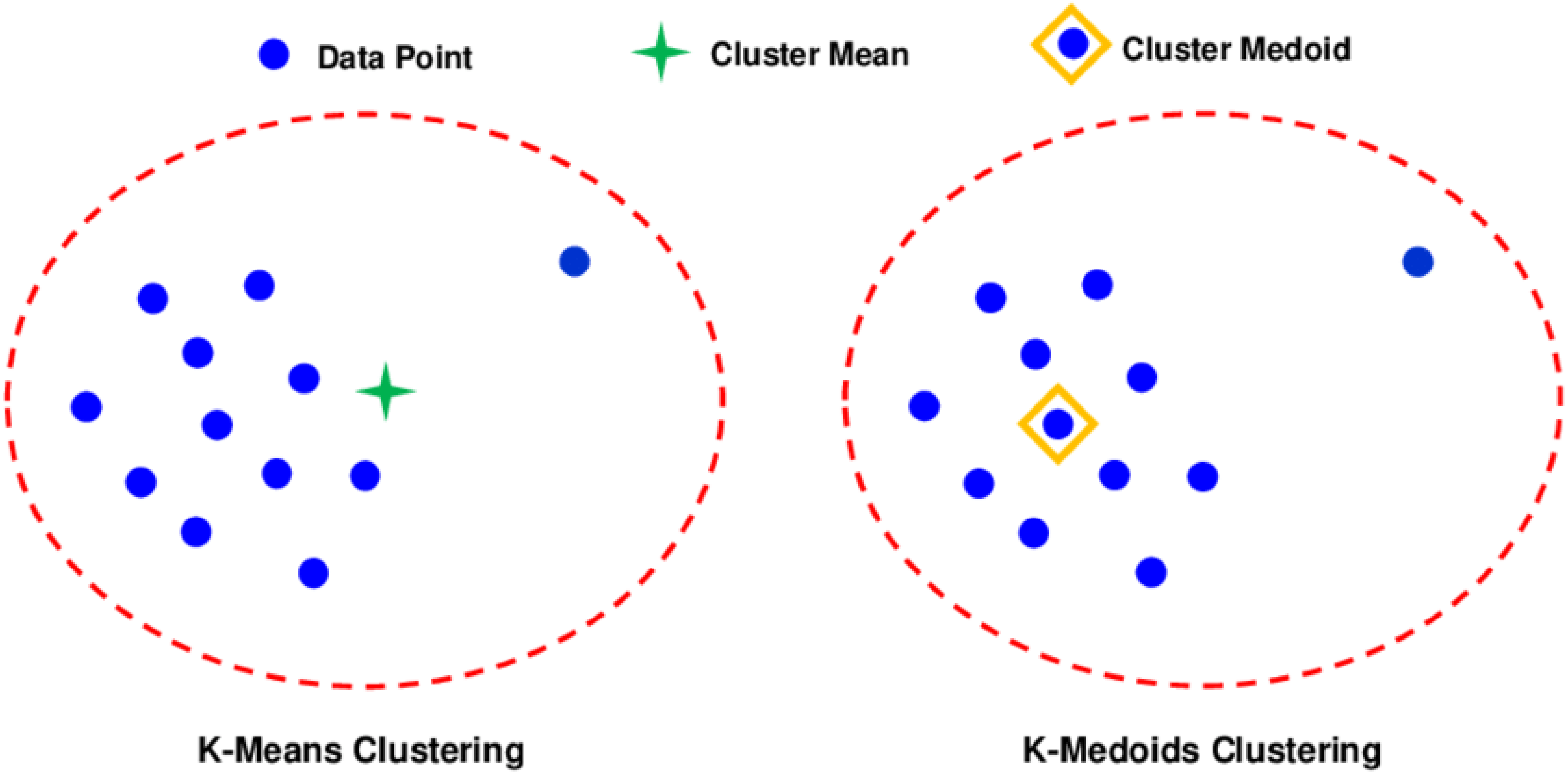

The Choice of Centriod in K-Means is random and what if there is presence of Outlier?

K-Medoids solves the issue as it K-Medoids selected the precise centroid among all data points of the corresponding clusters

https://www.kaggle.com/getting-started/172928

# Unsupervised Learning – K-Means and K-Medoids

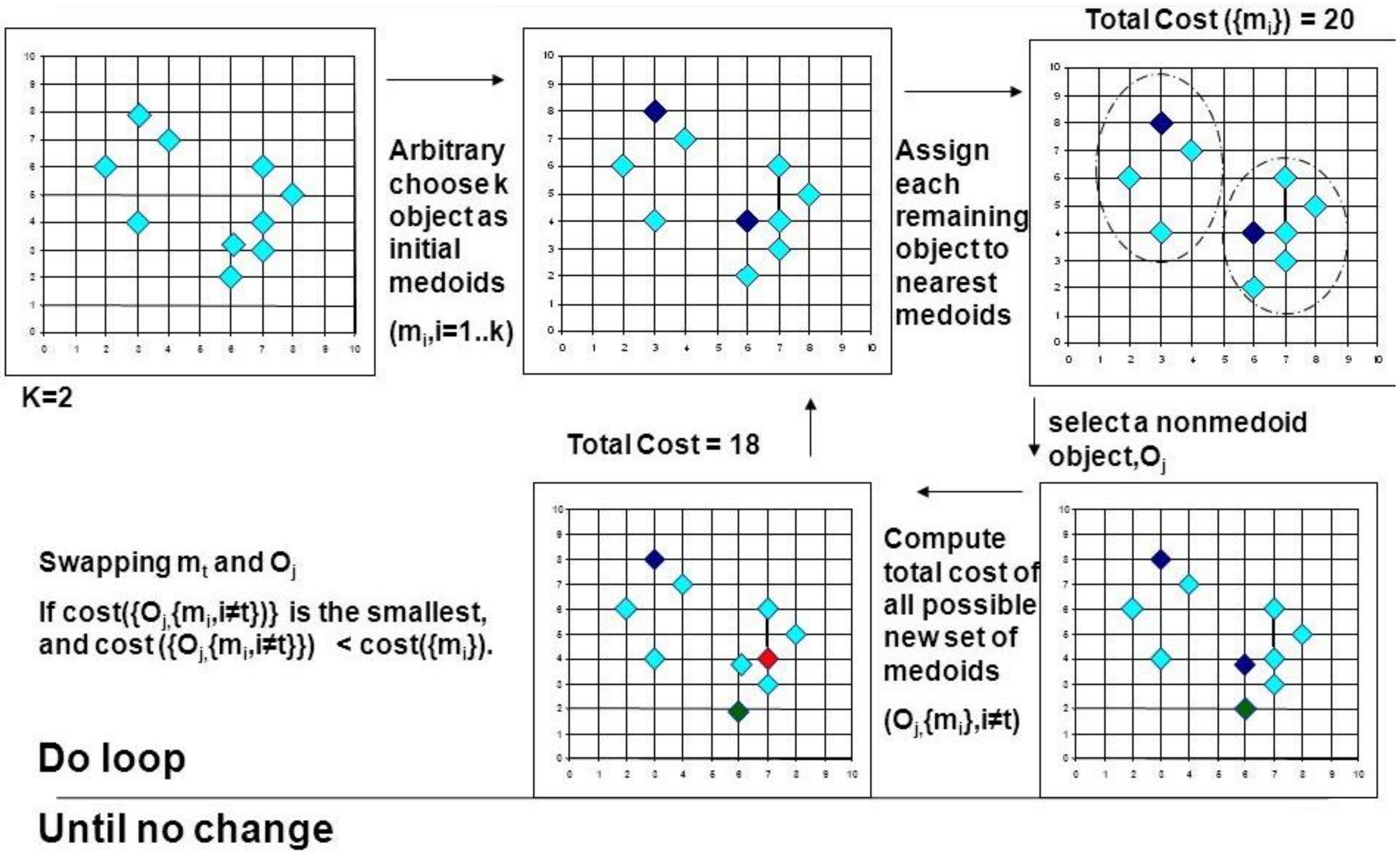





https://www.researchgate.net/figure/The-graphical-representation-of-the-difference-between-the-k-means-and-k-medoids_fig1_342871651

# Unsupervised Learning – K-Means and K-Medoids






https://alfredo-reyes-montero.gitbook.io/soft-computing/applications/matlab/kmeans-kmenoids

# Implementing K-Means



## Creating the dataset

```
from sklearn.datasets import make_blobs
```

```
data = make_blobs(n_samples = 200, n_features = 2, centers = 4, cluster_std = 1.8, random_state = 2022)
```

4 groups

## Defining X and y

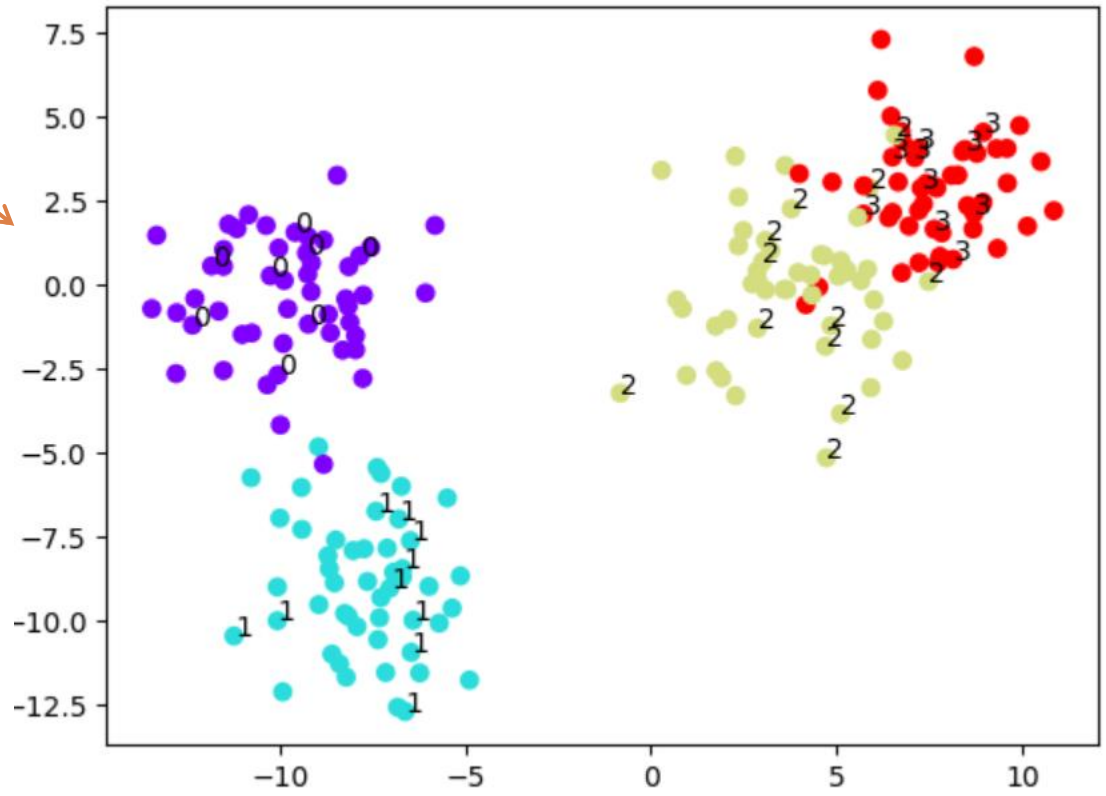
```
X = data[0]
y = data[1]
```

## Visualizing the data (first 5 instances)

```
print('X:', X[0:5, :])
print('Y:', y[0:5])
```

```
X: [[  5.88508997   2.9021639 ]
 [ -8.20429992 -11.68670283]
 [  1.9125188   -2.76746603]
 [ -9.39601207  -7.2830252 ]
 [  6.1986976    7.32152342]]
Y: [2 1 2 1 3]
```

```
plt.scatter(X[:, 0], X[:, 1], c = y, cmap = 'rainbow')
for i, txt in enumerate(y):
    if i%5 == 0:
        plt.annotate(txt, (X[i, 0], X[i, 1]))
```



# Implementing K-Means



sklearn.cluster.KMeans(n_clusters=8, *, init='k-means++', n_init='auto', max_iter=300, tol=0.0001, verbose=0, random_state=None, copy_x=True, algorithm='lloyd')

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

Creating the clusters

```
kmeans = KMeans(n_clusters = 4, n_init = 10, random_state = 2022)
```

```
kmeans.fit(X)
```

```
KMeans
KMeans(n_clusters=4, n_init=10, random_state=2022)
```

Vector with center of the clusters

```
kmeans.cluster_centers_
```

```
array([[-7.68797564, -8.88054369],
       [ 7.70499062,  2.96975295],
       [-9.78544862, -0.2509739 ],
       [ 3.60428123, -0.21752545]])
```

```
kmeans.labels_
```

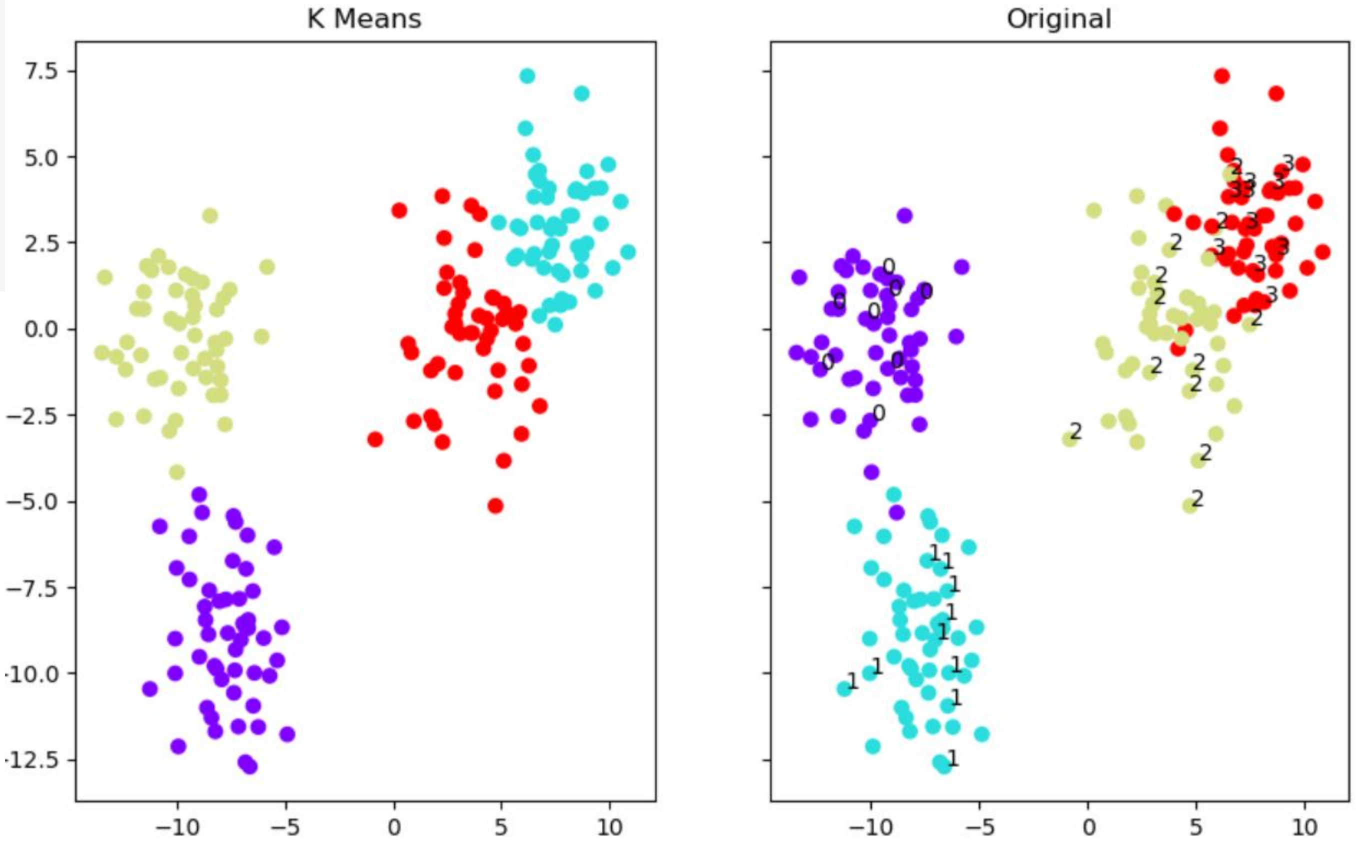
```
array([1, 0, 3, 0, 1, 2, 0, 2, 3, 3, 1, 1, 3, 1, 2, 1, 1, 1, 1, 2, 0, 3,
       1, 1, 0, 0, 3, 0, 3, 3, 1, 0, 1, 3, 1, 3, 0, 1, 0, 2, 1, 2, 1, 3,
       3, 3, 0, 0, 3, 0, 0, 3, 1, 1, 0, 3, 1, 3, 1, 2, 2, 2, 3, 3, 1, 2,
       0, 2, 2, 2, 3, 2, 3, 0, 0, 2, 2, 0, 0, 2, 1, 1, 2, 3, 0, 0, 1, 3,
       2, 0, 3, 1, 2, 3, 3, 1, 3, 2, 3, 3, 0, 1, 2, 0, 2, 3, 2, 3, 2, 2,
       1, 2, 2, 2, 3, 2, 3, 3, 0, 3, 1, 1, 1, 3, 0, 0, 1, 3, 2, 1, 0, 2,
       2, 0, 0, 0, 2, 2, 1, 0, 0, 0, 1, 3, 0, 1, 0, 2, 3, 2, 3, 3, 1, 1,
       1, 1, 1, 1, 0, 0, 0, 0, 0, 3, 1, 2, 0, 0, 1, 2, 3, 1, 1, 0, 3, 1,
       3, 0, 0, 2, 3, 0, 2, 2, 0, 2, 1, 1, 2, 3, 2, 3, 3, 0, 2, 1, 2, 0,
       2, 2])
```

# Implementing K-Means



Visualizing the clusters

```
f, (ax1, ax2) = plt.subplots(1, 2, sharey = True, figsize = (10, 6))
ax1.set_title('K Means')
ax1.scatter(X[:, 0], X[:, 1], c = kmeans.labels_, cmap = 'rainbow')
ax2.set_title("Original")
ax2.scatter(X[:, 0], X[:, 1], c = y, cmap = 'rainbow')
for i, txt in enumerate(y):
    if i%5 == 0:
        plt.annotate(txt, (X[i, 0], X[i, 1]))
```




Note that the colors are meaningless when in reference to the two plots.

# Implementing K-Means



## Align K-Means prediction class with real values

```
y_pred = kmeans.predict(X)
```

```
y_pred
```

```
array([1, 0, 3, 0, 1, 2, 0, 2, 3, 3, 1, 1, 3, 1, 2, 1, 1, 1, 1, 2, 0, 3,
       1, 1, 0, 0, 3, 0, 3, 3, 1, 0, 1, 3, 1, 3, 0, 1, 0, 2, 1, 2, 1, 3,
       3, 3, 0, 0, 3, 0, 0, 3, 1, 1, 0, 3, 1, 3, 1, 2, 2, 2, 3, 3, 1, 2,
       0, 2, 2, 2, 3, 2, 3, 0, 0, 2, 2, 0, 0, 2, 1, 1, 2, 3, 0, 0, 1, 3,
       2, 0, 3, 1, 2, 3, 3, 1, 3, 2, 3, 3, 0, 1, 2, 0, 2, 3, 2, 3, 2, 2,
       1, 2, 2, 2, 3, 2, 3, 3, 0, 3, 1, 1, 1, 3, 0, 0, 1, 3, 2, 1, 0, 2,
       2, 0, 0, 0, 2, 2, 1, 0, 0, 0, 1, 3, 0, 1, 0, 2, 3, 2, 3, 3, 1, 1,
       1, 1, 1, 1, 0, 0, 0, 0, 0, 3, 1, 2, 0, 0, 1, 2, 3, 1, 1, 0, 3, 1,
       3, 0, 0, 2, 3, 0, 2, 2, 0, 2, 1, 1, 2, 3, 2, 3, 3, 0, 2, 1, 2, 0,
       2, 2])
```

```
y
```

```
array([2, 1, 2, 1, 3, 0, 1, 0, 2, 2, 3, 3, 2, 3, 0, 3, 3, 3, 3, 0, 1, 2,
       3, 3, 1, 1, 3, 1, 2, 2, 3, 1, 3, 3, 3, 2, 1, 3, 1, 0, 3, 0, 3, 2,
       2, 2, 1, 1, 2, 1, 1, 2, 3, 3, 1, 2, 3, 2, 3, 0, 0, 0, 2, 2, 3, 0,
       1, 0, 0, 0, 2, 0, 2, 1, 1, 0, 0, 1, 1, 0, 2, 3, 0, 2, 1, 1, 3, 2,
       0, 1, 2, 3, 0, 2, 2, 3, 2, 0, 2, 2, 1, 3, 0, 1, 0, 2, 0, 2, 0, 0,
       3, 0, 0, 0, 2, 0, 2, 2, 1, 2, 3, 3, 3, 2, 1, 1, 3, 2, 0, 3, 1, 0,
       0, 1, 1, 1, 0, 0, 3, 1, 1, 1, 3, 2, 1, 3, 1, 0, 2, 0, 2, 2, 3, 3,
       2, 3, 3, 3, 0, 1, 1, 1, 1, 2, 3, 0, 1, 1, 3, 0, 2, 3, 3, 1, 2, 3,
       2, 1, 1, 0, 2, 1, 0, 0, 1, 0, 3, 3, 0, 2, 0, 3, 2, 1, 0, 2, 0, 1,
       0, 0])
```

```
y_pred = np.where(y_pred==0, 10, y_pred)
y_pred = np.where(y_pred==2, 0, y_pred)
y_pred = np.where(y_pred==3, 2, y_pred)
y_pred = np.where(y_pred==1, 3, y_pred)
y_pred = np.where(y_pred==10, 1, y_pred)
```

```
y_pred
```

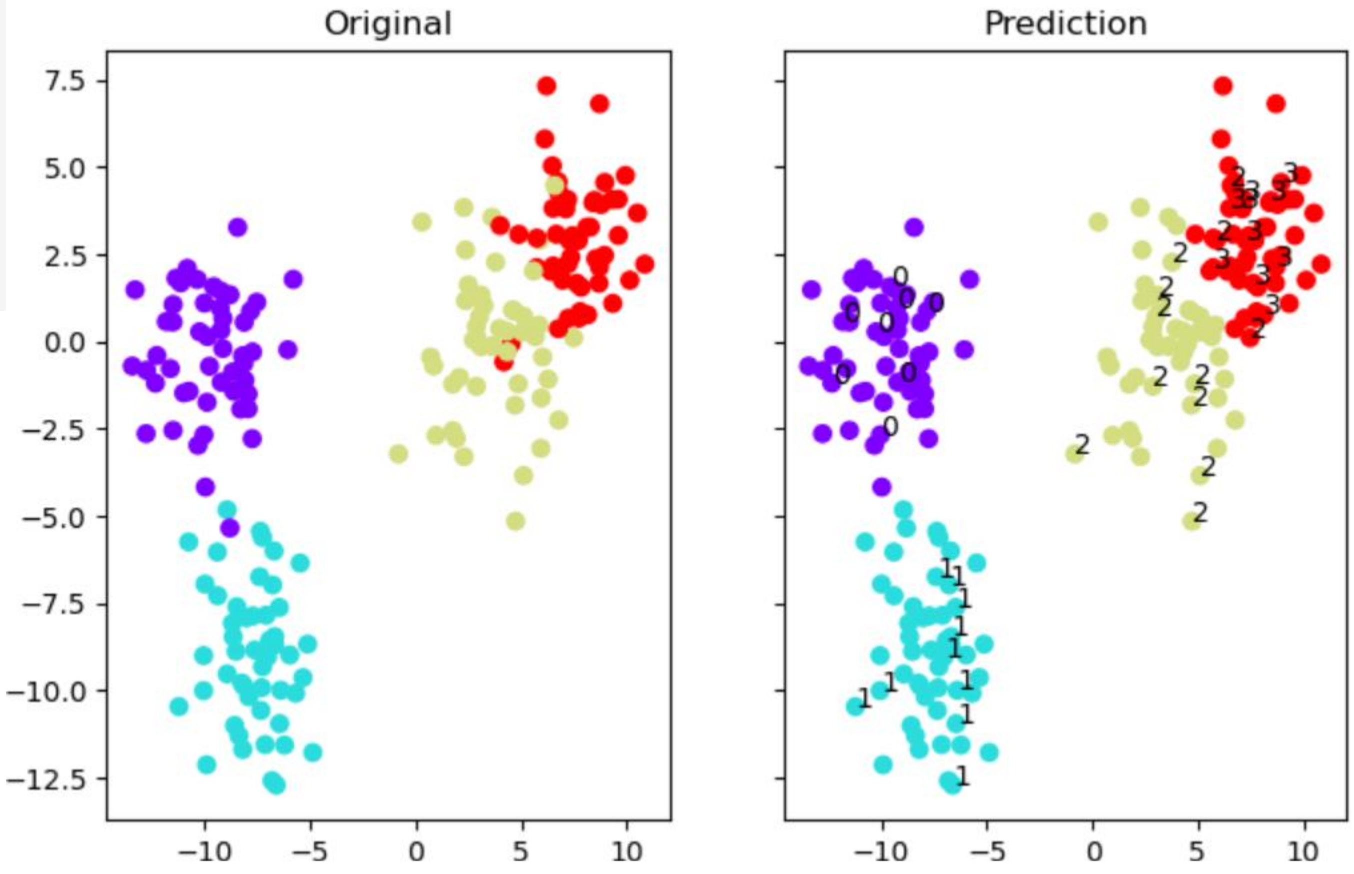
```
array([3, 1, 2, 1, 3, 0, 1, 0, 2, 2, 3, 3, 2, 3, 0, 3, 3, 3, 3, 0, 1, 2,
       3, 3, 1, 1, 2, 1, 2, 2, 3, 1, 3, 2, 3, 2, 1, 3, 1, 0, 3, 0, 3, 2,
       2, 2, 1, 1, 2, 1, 1, 2, 3, 3, 1, 2, 3, 2, 3, 0, 0, 0, 2, 2, 3, 0,
       1, 0, 0, 0, 2, 0, 2, 1, 1, 0, 0, 1, 1, 0, 3, 3, 0, 2, 1, 1, 3, 2,
       0, 1, 2, 3, 0, 2, 2, 3, 2, 0, 2, 2, 1, 3, 0, 1, 0, 2, 0, 2, 0, 0,
       3, 0, 0, 0, 2, 0, 2, 2, 1, 2, 3, 3, 3, 2, 1, 1, 3, 2, 0, 3, 1, 0,
       0, 1, 1, 1, 0, 0, 3, 1, 1, 1, 3, 2, 1, 3, 1, 0, 2, 0, 2, 2, 3, 3,
       3, 3, 3, 3, 1, 1, 1, 1, 1, 2, 3, 0, 1, 1, 3, 0, 2, 3, 3, 1, 2, 3,
       2, 1, 1, 0, 2, 1, 0, 0, 1, 0, 3, 3, 0, 2, 0, 2, 2, 1, 0, 3, 0, 1,
       0, 0])
```

# Implementing K-Means



Redo the visualizations

```
f, (ax1, ax2) = plt.subplots(1, 2, sharey = True, figsize = (8, 5))
ax1.set_title('Original')
ax1.scatter(X[:,0], X[:,1], c=y, cmap='rainbow')
ax2.set_title("Prediction")
ax2.scatter(X[:,0], X[:,1], c=y_pred, cmap='rainbow')
for i, txt in enumerate(y):
    if i%5 == 0:
        plt.annotate(txt, (X[i,0], X[i,1]))
plt.savefig("KMeans_pred.png")
```



# Implementing K-Means



Evaluate the model

```
print(confusion_matrix(y, y_pred))
```

```
[[49  1  0  0]
 [ 0 50  0  0]
 [ 0  0 46  4]
 [ 0  0  3 47]]
```

```
print(classification_report(y, y_pred))
```

```
              precision    recall  f1-score   support

           0       1.00      0.98      0.99        50
           1       0.98      1.00      0.99        50
           2       0.94      0.92      0.93        50
           3       0.92      0.94      0.93        50

    accuracy                           0.96       200
   macro avg       0.96      0.96      0.96       200
weighted avg       0.96      0.96      0.96       200
```

If you want to classify new points, it is best to train a classifier on your clustering result.

# Implementing K-Medoids



Let's use the dataset created earlier.

[sklearn_extra.cluster.KMedoids(n_clusters=8, metric='euclidean', method='alternate', init='heuristic', max_iter=300, random_state=None)]

```
from sklearn_extra.cluster import KMedoids
```

Creating the clusters

```
kmedoids = KMedoids(n_clusters = 4, random_state = 2022)
kmedoids.fit(X)
```

```
KMedoids
KMedoids(n_clusters=4, random_state=2022)
```

Vector with center of the clusters

```
kmedoids.cluster_centers_
```

```
array([[-7.62795904, -8.8354951 ],
       [-9.87312876,  0.13931247],
       [ 3.65994783, -0.13260646],
       [ 7.66163195,  2.9333056 ]])
```

```
kmedoids.labels_
```

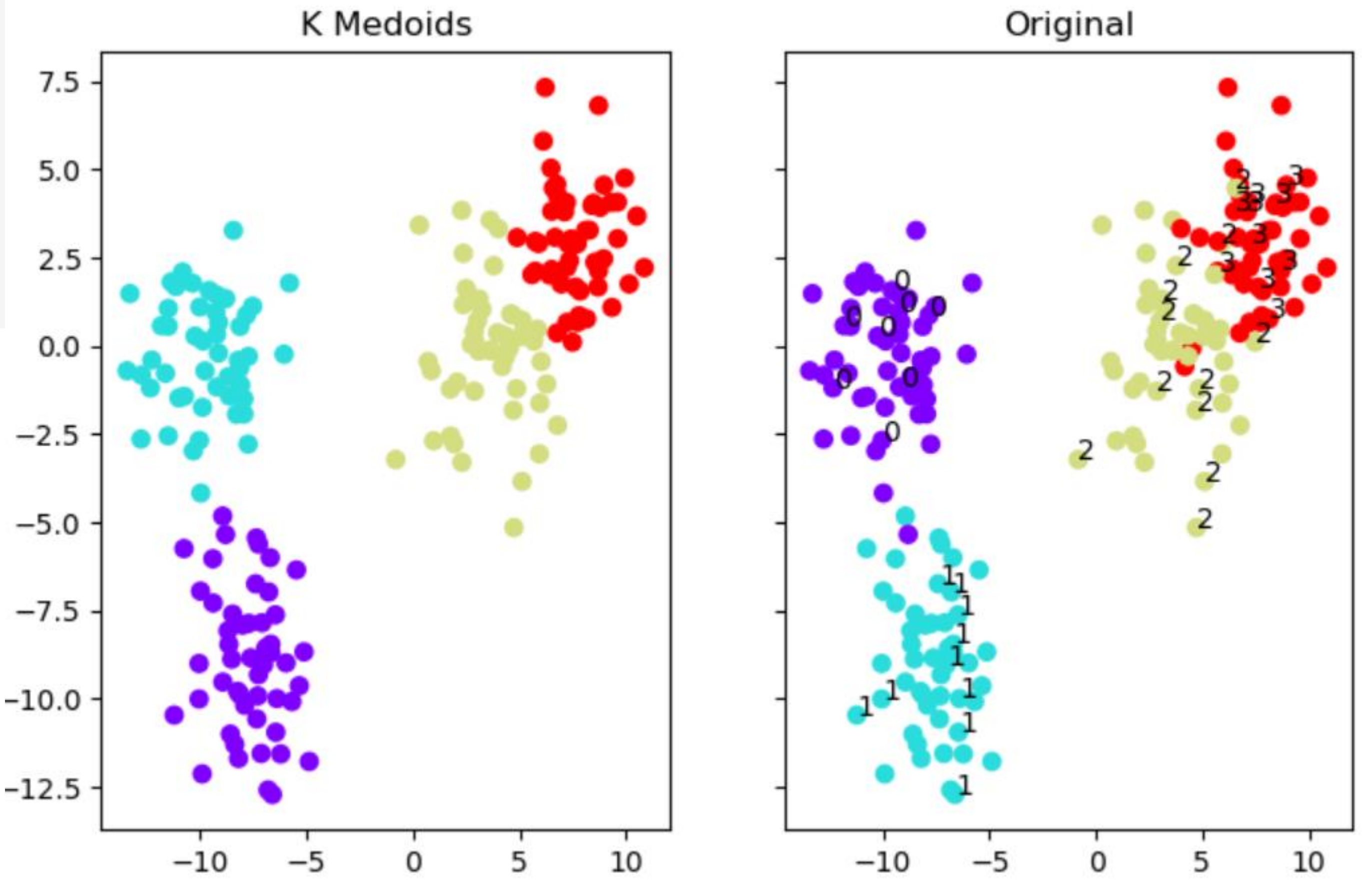
```
array([3, 0, 2, 0, 3, 1, 0, 1, 2, 2, 3, 3, 2, 3, 1, 3, 3, 3, 3, 1, 0, 2,
       3, 3, 0, 0, 2, 0, 2, 2, 3, 0, 3, 2, 3, 2, 0, 3, 0, 1, 3, 1, 3, 2,
       2, 2, 0, 0, 2, 0, 0, 2, 3, 3, 0, 2, 3, 2, 3, 1, 1, 1, 2, 2, 3, 1,
       0, 1, 1, 1, 2, 1, 2, 0, 0, 1, 1, 0, 0, 1, 3, 3, 1, 2, 0, 0, 3, 2,
       1, 0, 2, 3, 1, 2, 2, 3, 2, 1, 2, 2, 0, 3, 1, 0, 1, 2, 1, 2, 1, 1,
       3, 1, 1, 1, 2, 1, 2, 2, 0, 2, 3, 3, 3, 2, 0, 0, 3, 2, 1, 3, 0, 1,
       1, 0, 0, 0, 1, 1, 3, 0, 0, 0, 3, 2, 0, 3, 0, 1, 2, 1, 2, 2, 3, 3,
       3, 3, 3, 3, 0, 0, 0, 0, 0, 2, 3, 1, 0, 0, 3, 1, 2, 3, 3, 0, 2, 3,
       2, 0, 0, 1, 2, 0, 1, 1, 0, 1, 3, 3, 1, 2, 1, 2, 2, 0, 1, 3, 1, 0,
       1, 1], dtype=int64)
```

# Implementing K-Medoids



Visualizing the clusters

```
f, (ax1, ax2) = plt.subplots(1, 2, sharey=True,figsize=(8,5))
ax1.set_title('K Medoids')
ax1.scatter(X[:, 0], X[:, 1], c = kmedoids.labels_, cmap = 'rainbow')
ax2.set_title("Original")
ax2.scatter(X[:, 0], X[:, 1], c = y, cmap = 'rainbow')
for i, txt in enumerate(y):
    if i%5 == 0:
        plt.annotate(txt, (X[i, 0], X[i, 1]))
plt.savefig("KMedoids.png")
```



# Implementing K-Medoids



## Align K-Medoids prediction class with real values

```
y_pred = kmedoids.predict(X)
```

```
y_pred
```

```
array([3, 0, 2, 0, 3, 1, 0, 1, 2, 2, 3, 3, 2, 3, 1, 3, 3, 3, 3, 1, 0, 2,
       3, 3, 0, 0, 2, 0, 2, 2, 3, 0, 3, 2, 3, 2, 0, 3, 0, 1, 3, 1, 3, 2,
       2, 2, 0, 0, 2, 0, 0, 2, 3, 3, 0, 2, 3, 2, 3, 1, 1, 1, 2, 2, 3, 1,
       0, 1, 1, 1, 2, 1, 2, 0, 0, 1, 1, 0, 0, 1, 3, 3, 1, 2, 0, 0, 3, 2,
       1, 0, 2, 3, 1, 2, 2, 3, 2, 1, 2, 2, 0, 3, 1, 0, 1, 2, 1, 2, 1, 1,
       3, 1, 1, 1, 2, 1, 2, 2, 0, 2, 3, 3, 3, 2, 0, 0, 3, 2, 1, 3, 0, 1,
       1, 0, 0, 0, 1, 1, 3, 0, 0, 0, 3, 2, 0, 3, 0, 1, 2, 1, 2, 2, 3, 3,
       3, 3, 3, 3, 0, 0, 0, 0, 0, 2, 3, 1, 0, 0, 3, 1, 2, 3, 3, 0, 2, 3,
       2, 0, 0, 1, 2, 0, 1, 1, 0, 1, 3, 3, 1, 2, 1, 2, 2, 0, 1, 3, 1, 0,
       1, 1], dtype=int64)
```

```
y
```

```
array([2, 1, 2, 1, 3, 0, 1, 0, 2, 2, 3, 3, 2, 3, 0, 3, 3, 3, 3, 0, 1, 2,
       3, 3, 1, 1, 3, 1, 2, 2, 3, 1, 3, 3, 3, 2, 1, 3, 1, 0, 3, 0, 3, 2,
       2, 2, 1, 1, 2, 1, 1, 2, 3, 3, 1, 2, 3, 2, 3, 0, 0, 0, 2, 2, 3, 0,
       1, 0, 0, 0, 2, 0, 2, 1, 1, 0, 0, 1, 1, 0, 2, 3, 0, 2, 1, 1, 3, 2,
       0, 1, 2, 3, 0, 2, 2, 3, 2, 0, 2, 2, 1, 3, 0, 1, 0, 2, 0, 2, 0, 0,
       3, 0, 0, 0, 2, 0, 2, 2, 1, 2, 3, 3, 3, 2, 1, 1, 3, 2, 0, 3, 1, 0,
       0, 1, 1, 1, 0, 0, 3, 1, 1, 1, 3, 2, 1, 3, 1, 0, 2, 0, 2, 2, 3, 3,
       2, 3, 3, 3, 0, 1, 1, 1, 1, 2, 3, 0, 1, 1, 3, 0, 2, 3, 3, 1, 2, 3,
       2, 1, 1, 0, 2, 1, 0, 0, 1, 0, 3, 3, 0, 2, 0, 3, 2, 1, 0, 2, 0, 1,
       0, 0])
```

```
y_pred = np.where(y_pred==1, 10, y_pred)
y_pred = np.where(y_pred==0, 1, y_pred)
y_pred = np.where(y_pred==10, 0, y_pred)
```

```
y_pred
```

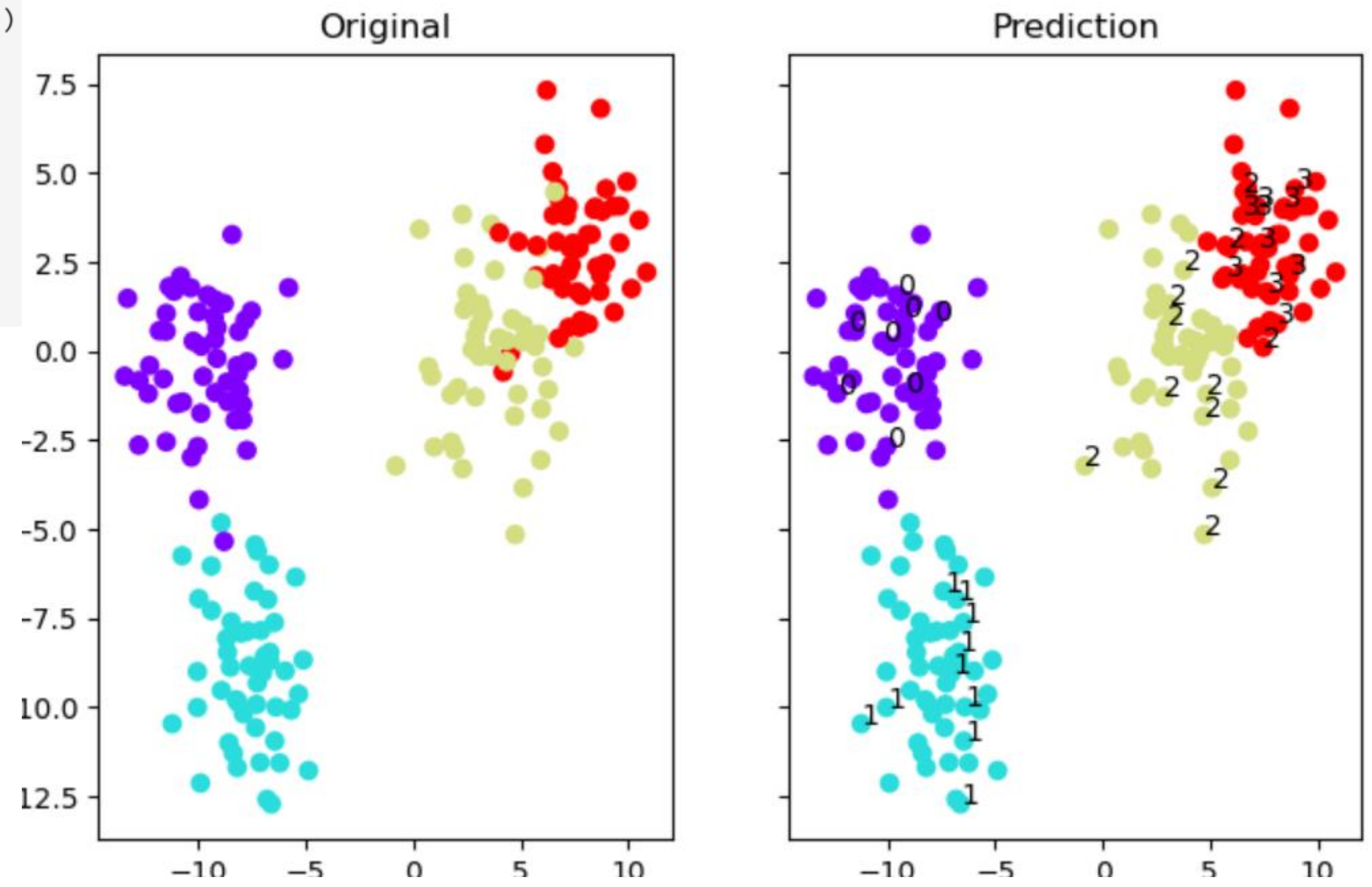
```
array([3, 1, 2, 1, 3, 0, 1, 0, 2, 2, 3, 3, 2, 3, 0, 3, 3, 3, 3, 0, 1, 2,
       3, 3, 1, 1, 2, 1, 2, 2, 3, 1, 3, 2, 3, 2, 1, 3, 1, 0, 3, 0, 3, 2,
       2, 2, 1, 1, 2, 1, 1, 2, 3, 3, 1, 2, 3, 2, 3, 0, 0, 0, 2, 2, 3, 0,
       1, 0, 0, 0, 2, 0, 2, 1, 1, 0, 0, 1, 1, 0, 3, 3, 0, 2, 1, 1, 3, 2,
       0, 1, 2, 3, 0, 2, 2, 3, 2, 0, 2, 2, 1, 3, 0, 1, 0, 2, 0, 2, 0, 0,
       3, 0, 0, 0, 2, 0, 2, 2, 1, 2, 3, 3, 3, 2, 1, 1, 3, 2, 0, 3, 1, 0,
       0, 1, 1, 1, 0, 0, 3, 1, 1, 1, 3, 2, 1, 3, 1, 0, 2, 0, 2, 2, 3, 3,
       3, 3, 3, 3, 1, 1, 1, 1, 1, 2, 3, 0, 1, 1, 3, 0, 2, 3, 3, 1, 2, 3,
       2, 1, 1, 0, 2, 1, 0, 0, 1, 0, 3, 3, 0, 2, 0, 2, 2, 1, 0, 3, 0, 1,
       0, 0], dtype=int64)
```

# Implementing K-Medoids



Redo the visualizations

```
f, (ax1, ax2) = plt.subplots(1, 2, sharey = True, figsize = (8, 5))
ax1.set_title('Original')
ax1.scatter(X[:, 0], X[:, 1], c = y, cmap = 'rainbow')
ax2.set_title("Prediction")
ax2.scatter(X[:, 0], X[:, 1], c = y_pred, cmap = 'rainbow')
for i, txt in enumerate(y):
    if i%5 == 0:
        plt.annotate(txt, (X[i, 0], X[i, 1]))
plt.savefig("KMedoid_pred.png")
```



# Implementing K-Medoids



## Evaluate the model

```
print(confusion_matrix(y, y_pred))
```

```
[[49  1  0  0]
 [ 0 50  0  0]
 [ 0  0 46  4]
 [ 0  0  3 47]]
```

```
print(classification_report(y, y_pred))
```

```
              precision    recall  f1-score   support

           0       1.00      0.98      0.99        50
           1       0.98      1.00      0.99        50
           2       0.94      0.92      0.93        50
           3       0.92      0.94      0.93        50

    accuracy                           0.96       200
   macro avg       0.96      0.96      0.96       200
weighted avg       0.96      0.96      0.96       200
```

# K-Means vs. K-Medoids



## K-Means

```
print(confusion_matrix(y, y_pred))
```

```
[[49  1  0  0]
 [ 0 50  0  0]
 [ 0  0 46  4]
 [ 0  0  3 47]]
```

```
print(classification_report(y, y_pred))
```

```
              precision    recall  f1-score   support

           0       1.00      0.98      0.99        50
           1       0.98      1.00      0.99        50
           2       0.94      0.92      0.93        50
           3       0.92      0.94      0.93        50

    accuracy                           0.96       200
   macro avg       0.96      0.96      0.96       200
weighted avg       0.96      0.96      0.96       200
```

## K-Medoids

```
print(confusion_matrix(y, y_pred))
```

```
[[49  1  0  0]
 [ 0 50  0  0]
 [ 0  0 46  4]
 [ 0  0  3 47]]
```

```
print(classification_report(y, y_pred))
```

```
              precision    recall  f1-score   support

           0       1.00      0.98      0.99        50
           1       0.98      1.00      0.99        50
           2       0.94      0.92      0.93        50
           3       0.92      0.94      0.93        50

    accuracy                           0.96       200
   macro avg       0.96      0.96      0.96       200
weighted avg       0.96      0.96      0.96       200
```

**Can we compare these two models?**

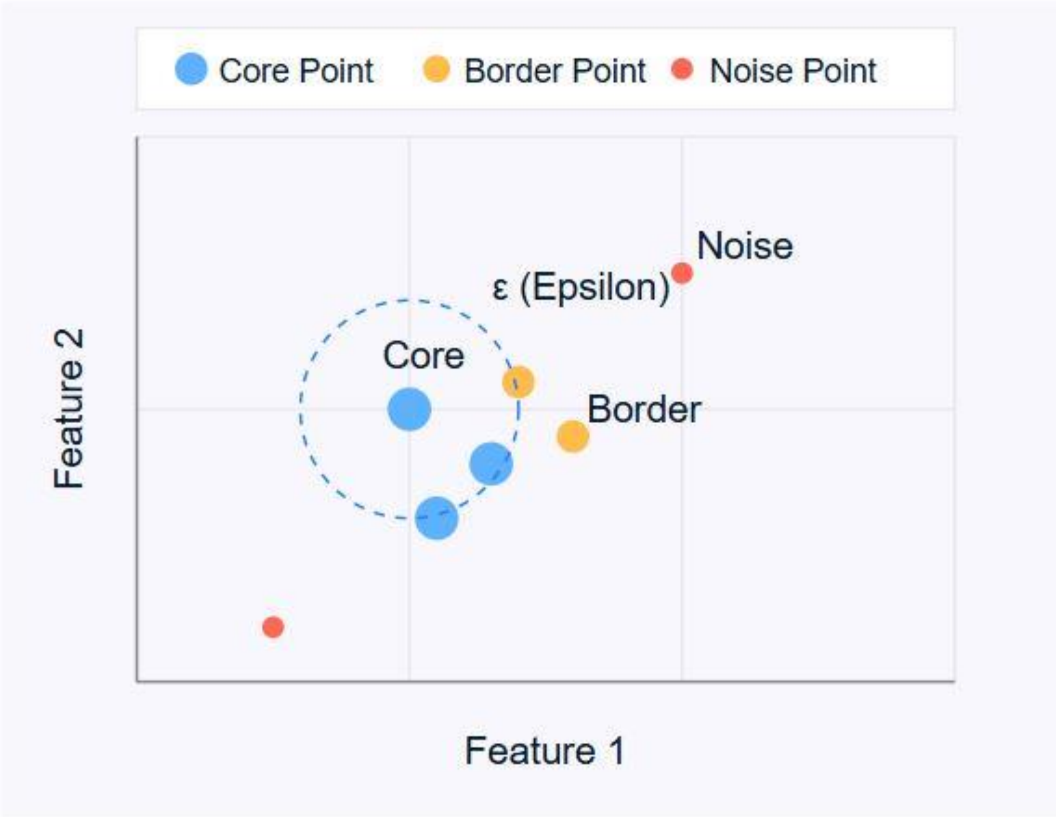
# Unsupervised Learning - DBSCAN



The **DBSCAN** (Density-Based Spatial Clustering of Applications with Noise) algorithm finds core samples in high-density regions and expands clusters for them.

**High-density regions**, where data points are located close to each other, are separated by **low-density regions**, where the data points are located far from each other.

The idea of **a core sample** means a sample located in an area of high-density. Data point A is considered a core sample if at least minimum number of points required to form a dense region (usually including A) are located within ε distance from A.

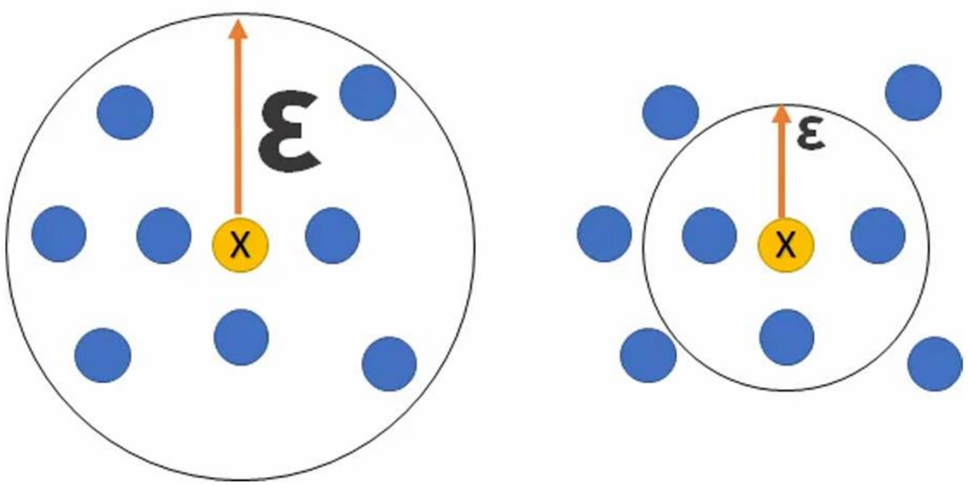



https://www.datacamp.com/tutorial/dbscan-clustering-algorithm

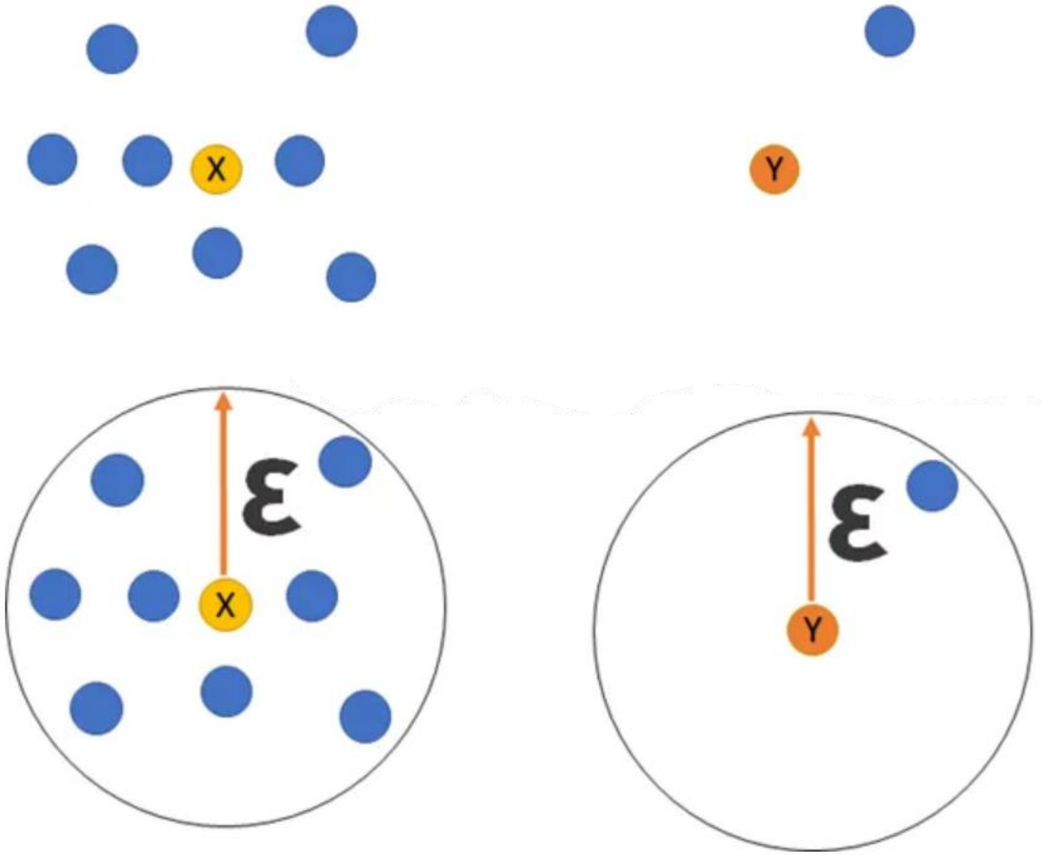
# Unsupervised Learning - DBSCAN



## Influence of the size of $\varepsilon$




## Influence of the density of the region




https://towardsdatascience.com/a-practical-guide-to-dbscan-method-d4ec5ab2bc99

# Unsupervised Learning - DBSCAN



Strengths:

- knowledge about the number of clusters is not necessary;
- also solves the anomaly detection task.

Weaknesses:

- need to select and tune the density parameter ($\varepsilon$);
- does not cope well with sparse data.

# Implementing DBSCAN



**Creating the dataset**

```
X, y = make_blobs(n_samples=750, cluster_std=0.4, random_state=0)
```

3 groups

Shape of X and y and visualizing the data

```
X.shape
```

```
(750, 2)
```

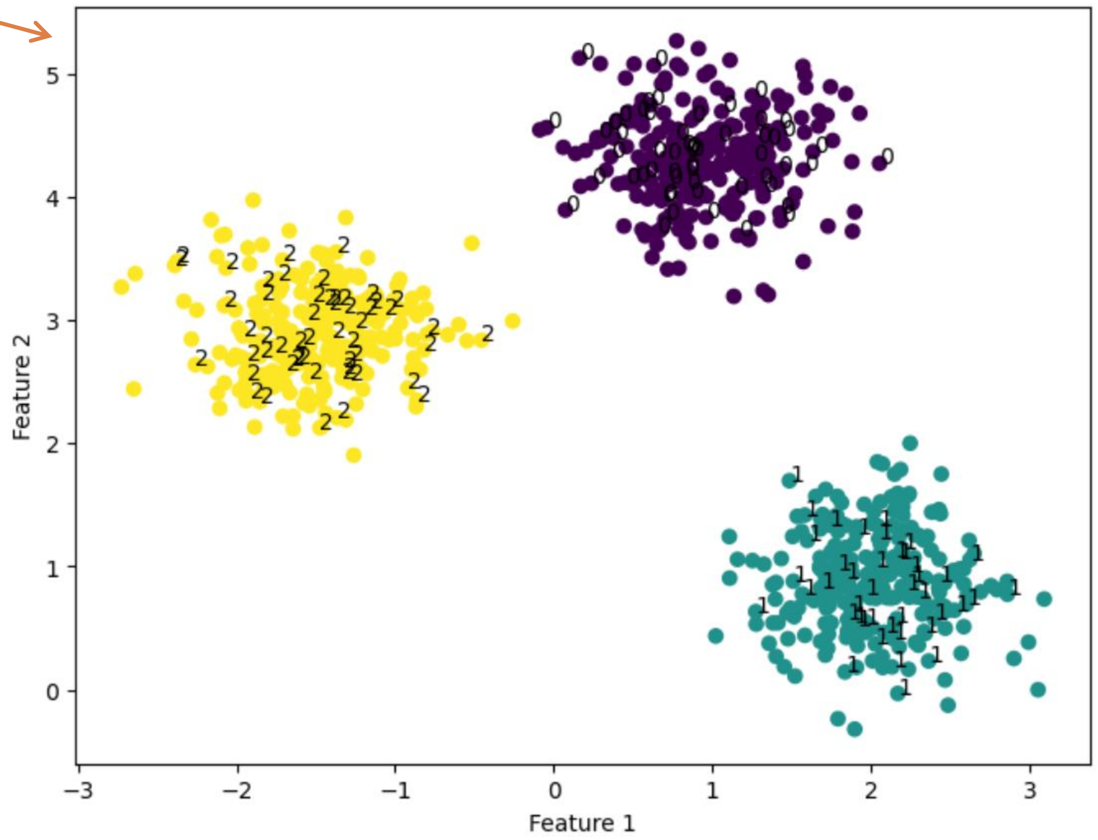
```
y.shape
```

```
(750,)
```

```
print('X:', X[0:5])
print('y:', y[0:5])
```

```
X: [[ 2.36434546  0.23302434]
 [ 0.92311785  4.18467098]
 [ 1.64221028  0.72296432]
 [ 1.97590796  0.93534058]
 [-1.68752703  2.73049184]]
y: [1 0 1 1 2]
```

```
plt.figure(figsize=(8, 6))
plt.scatter(X[:, 0], X[:, 1], c = y, cmap = 'viridis')
for i, txt in enumerate(y):
    if i%5 == 0:
        plt.annotate(txt, (X[i, 0], X[i, 1]))
plt.title('Blobs Dataset')
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.show()
```



# Implementing DBSCAN



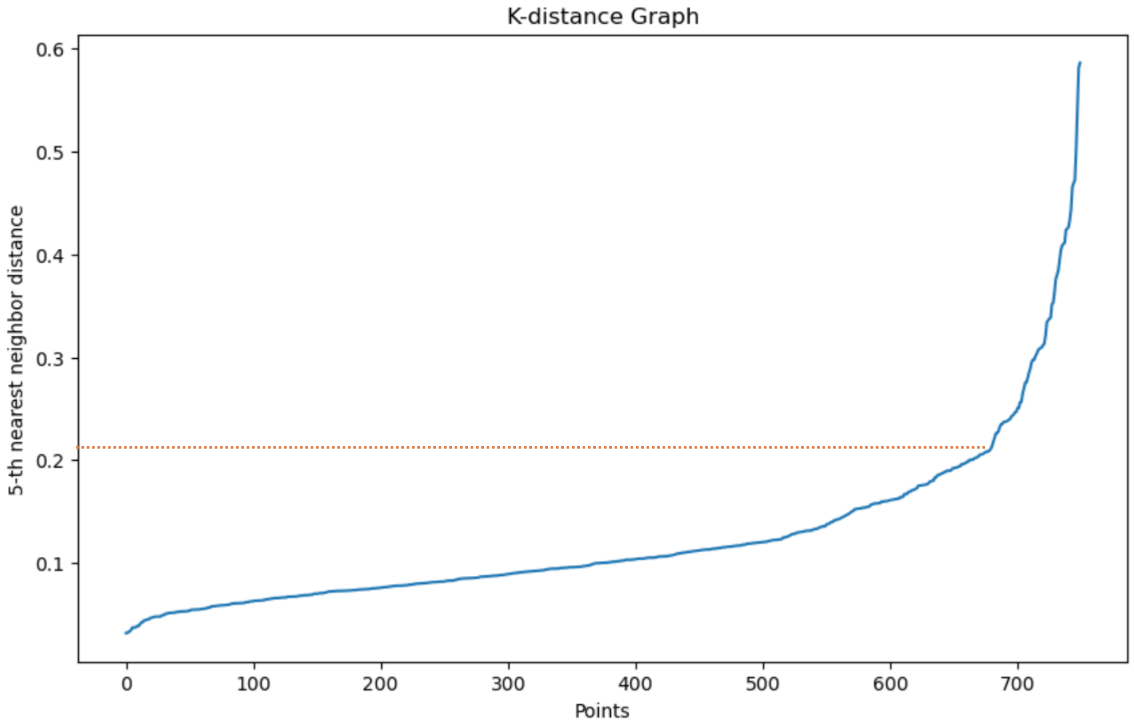
**Determining the epsilon parameter**

We use the *k*-distance graph method to help choose an appropriate $\varepsilon$ value:

1. We define a function `plot_k_distance_graph` that calculates the distance to the $k^{th}$ nearest neighbor for each point
2. The distances are sorted and plotted.
3. We look for an "elbow" in the resulting graph to choose $\varepsilon$.

```
from sklearn.neighbors import NearestNeighbors

def plot_k_distance_graph(X, k):
    neigh = NearestNeighbors(n_neighbors=k)
    neigh.fit(X)
    distances, _ = neigh.kneighbors(X)
    distances = np.sort(distances[:, k-1])
    plt.figure(figsize=(10, 6))
    plt.plot(distances)
    plt.xlabel('Points')
    plt.ylabel(f'{k}-th nearest neighbor distance')
    plt.title('K-distance Graph')
    plt.show()
plot_k_distance_graph(X, k=5)
```



# Implementing DBSCAN



sklearn.cluster.DBSCAN(eps=0.5, *, min_samples=5, metric='euclidean', metric_params=None, algorithm='auto', leaf_size=30, p=None, n_jobs=None)

```
from sklearn.cluster import DBSCAN
```

## Creating the clusters

```
db = DBSCAN(eps=0.2, min_samples=10)
```

```
db.fit(X)
```

```
DBSCAN
DBSCAN(eps=0.2, min_samples=10)
```

Confirm the labels shape

```
labels = db.labels_
labels.shape
```

```
(750,)
```

# Implementing DBSCAN



## Interpreting the results

Indices of core samples

```
db.core_sample_indices_
```

```
array([  1,    2,    3,    4,    6,    8,   10,   12,   14,   15,   16,   18,   20,
       ...,
       736, 738, 739, 740, 741, 742, 743, 745, 746, 748, 749], dtype=int64)
```

Components

```
db.components_
```

```
array([[0.92311785, 4.18467098],
       [1.64221028, 0.72296432],
       [1.97590796, 0.93534058],
       ...,
       [1.04724054, 4.14307495],
       [2.16897939, 1.59473117],
       [0.73774446, 4.28276041]])
```

Number of features

```
db.n_features_in_
```

```
2
```

Number of clusters and noise points in *labels*

```
n_clusters_ = len(set(labels)) - (1 if -1 in labels else 0)
n_noise_ = list(labels).count(-1)
```

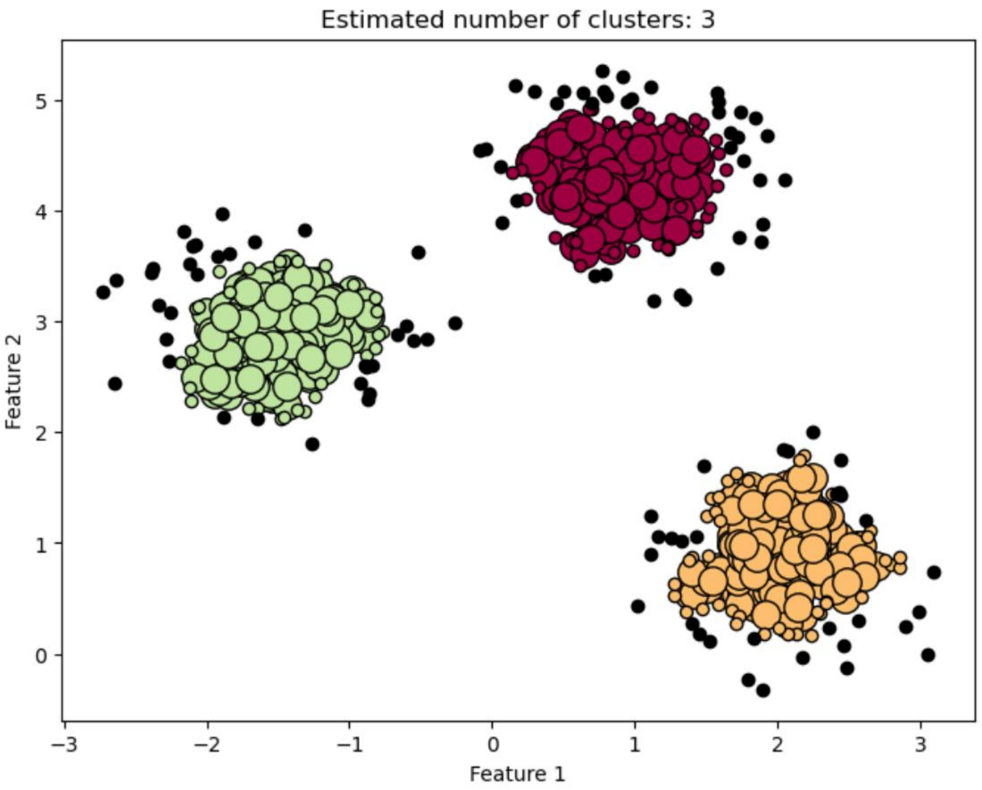
```
print("Estimated number of clusters: %d" % n_clusters_)
print("Estimated number of noise points: %d" % n_noise_)
```

```
Estimated number of clusters: 3
Estimated number of noise points: 104
```

# Implementing DBSCAN



## Visualizing the resultant clusters



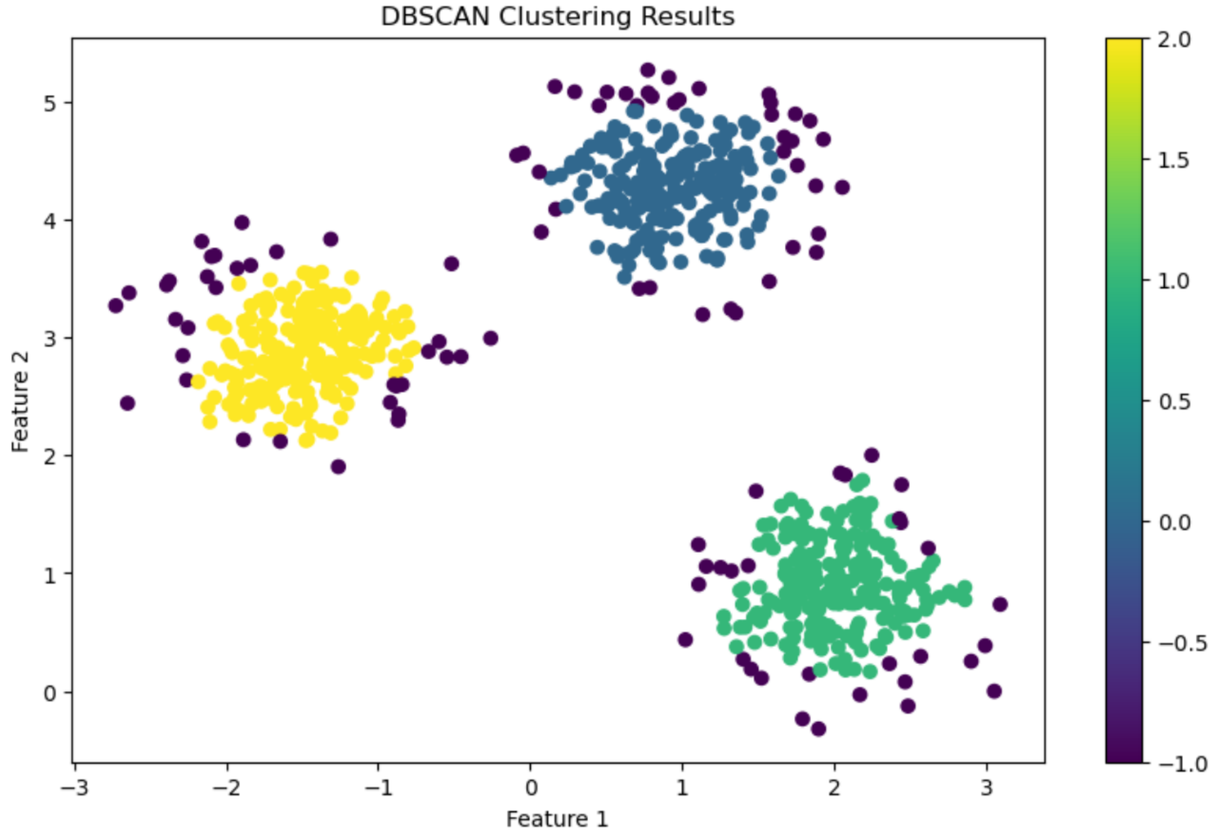

```python
unique_labels = set(labels)
core_samples_mask = np.zeros_like(labels, dtype=bool)
core_samples_mask[db.core_sample_indices_] = True

plt.figure(figsize=(8, 6))
colors = [plt.cm.Spectral(each) for each in np.linspace(0, 1, len(unique_labels))]
for k, col in zip(unique_labels, colors):
    if k == -1:
        col = [0, 0, 0, 1]
    class_member_mask = labels == k
    xy = X[class_member_mask & core_samples_mask]
    plt.plot(
        xy[:, 0],
        xy[:, 1],
        "o",
        markerfacecolor=tuple(col),
        markeredgecolor="k",
        markersize=14,)
    xy = X[class_member_mask & ~core_samples_mask]
    plt.plot(
        xy[:, 0],
        xy[:, 1],
        "o",
        markerfacecolor=tuple(col),
        markeredgecolor="k",
        markersize=6,)
plt.title(f"Estimated number of clusters: {n_clusters_}")
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.show()
```

# Implementing DBSCAN



```
plt.figure(figsize=(10, 6))
scatter = plt.scatter(X[:, 0], X[:, 1], c=pred, cmap='viridis')
plt.colorbar(scatter)
plt.title('DBSCAN Clustering Results')
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.show()
```



# Implementing DBSCAN



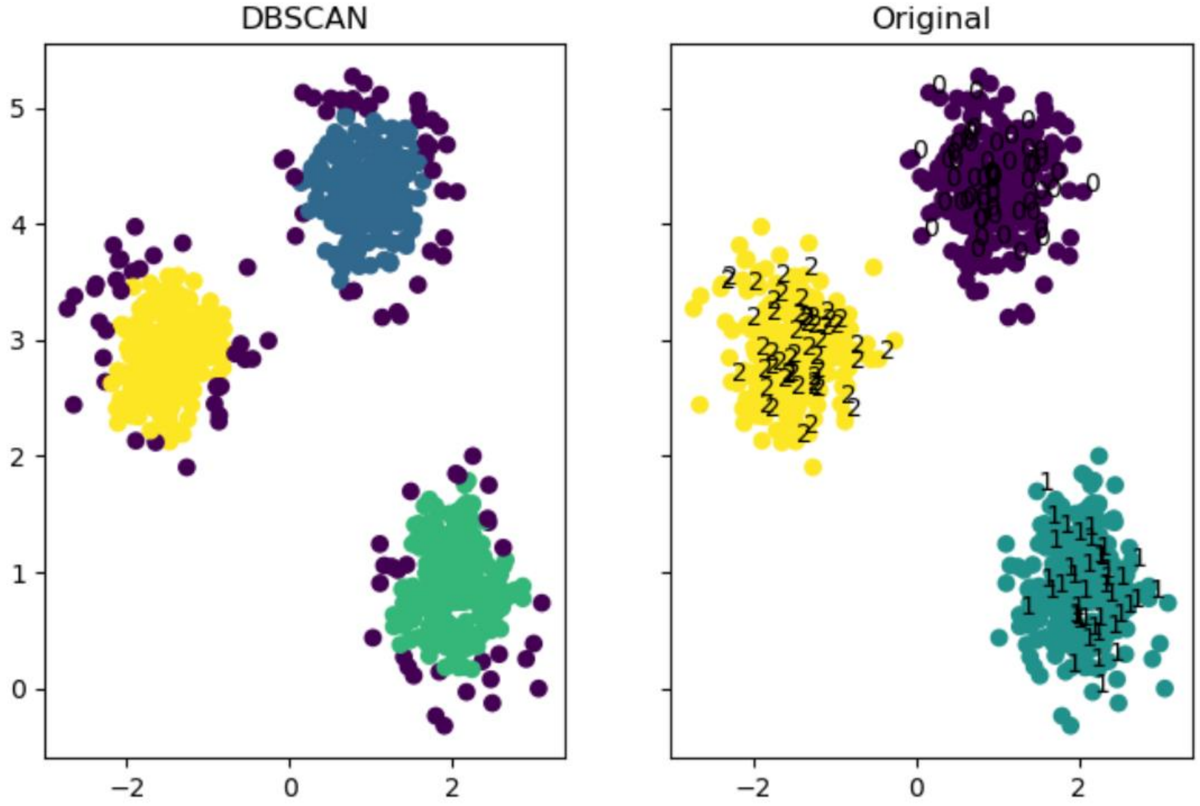
**Evaluating the model**

Obtain the predictions

```
pred = db.fit_predict(X)
```

Visualize the original vs. DBSCAN clusters

```
f, (ax1, ax2) = plt.subplots(1, 2, sharey=True,figsize=(8,5))
ax1.set_title('DBSCAN')
ax1.scatter(X[:, 0], X[:, 1], c = db.labels_, cmap = 'viridis')
ax2.set_title("Original")
ax2.scatter(X[:, 0], X[:, 1], c = y, cmap = 'viridis')
for i, txt in enumerate(y):
    if i%5 == 0:
        plt.annotate(txt, (X[i, 0], X[i, 1]))
plt.savefig("DBSCAN.png")
plt.show()
```



# Implementing DBSCAN



Because Blobs provides the true labels, we can analyze through the following metrics: homogeneity, completeness, V-measure, Adjusted Rand Index, Adjusted Mutual Information and Silhouette Coefficient

```python
print(f"Homogeneity: {metrics.homogeneity_score(y, labels):.3f}")
print(f"Completeness: {metrics.completeness_score(y, labels):.3f}")
print(f"V-measure: {metrics.v_measure_score(y, labels):.3f}")
print(f"Adjusted Rand Index: {metrics.adjusted_rand_score(y, labels):.3f}")
print(
    "Adjusted Mutual Information:"
    f" {metrics.adjusted_mutual_info_score(y, labels):.3f}"
)
print(f"Silhouette Coefficient: {metrics.silhouette_score(X, labels):.3f}")
```

```
Homogeneity: 0.862
Completeness: 0.702
V-measure: 0.774
Adjusted Rand Index: 0.781
Adjusted Mutual Information: 0.773
Silhouette Coefficient: 0.586
```

```python
print(confusion_matrix(y, pred))
```

```
[[  0   0   0   0]
 [ 39 211   0   0]
 [ 31   0 219   0]
 [ 34   0   0 216]]
```

```python
print(classification_report(y, pred))
```

```
              precision    recall  f1-score   support

          -1       0.00      0.00      0.00         0
           0       1.00      0.84      0.92       250
           1       1.00      0.88      0.93       250
           2       1.00      0.86      0.93       250

    accuracy                           0.86       750
   macro avg       0.75      0.65      0.69       750
weighted avg       1.00      0.86      0.93       750
```

What do these metrics mean?

# Implementing DBSCAN



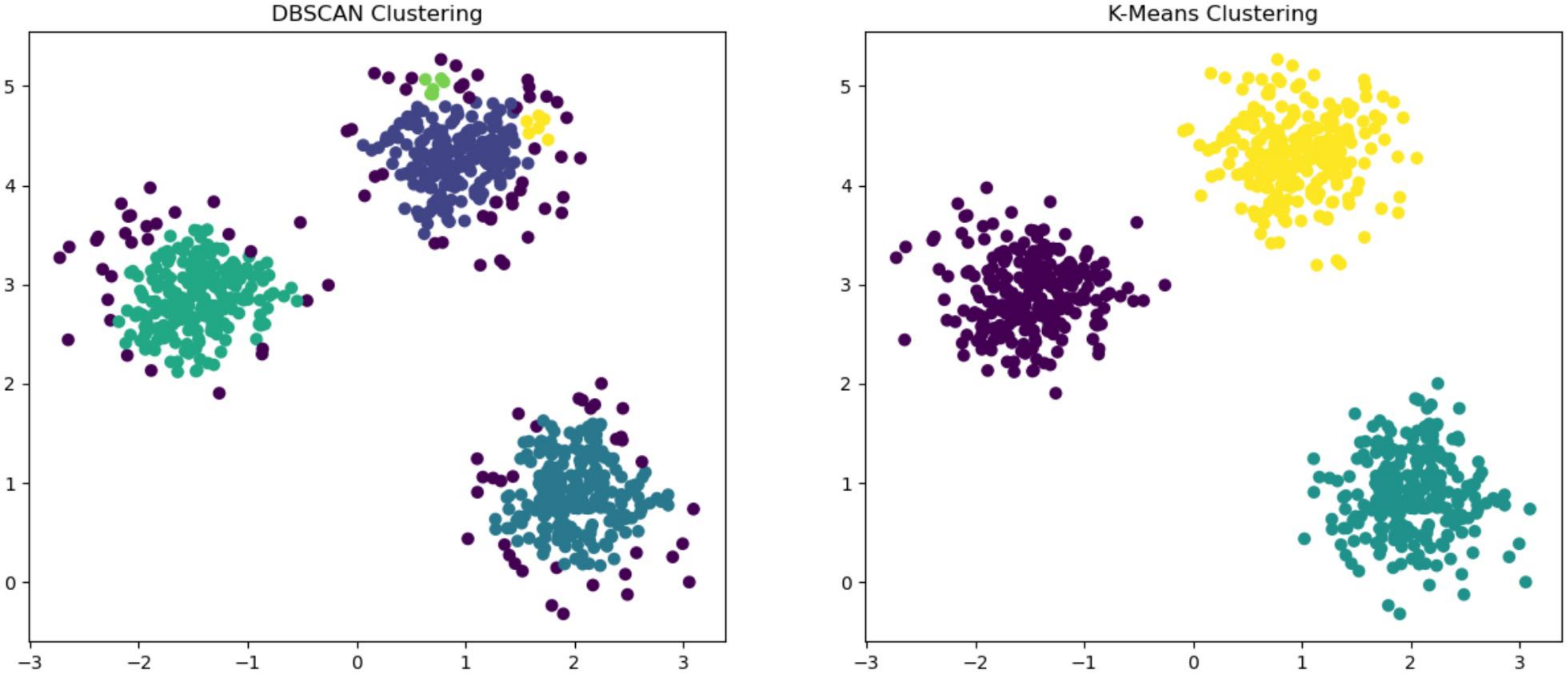
**Comparing DBSCAN and K-Means**

```
dbscan = DBSCAN(eps=0.15, min_samples=5)
dbscan_labels = dbscan.fit_predict(X)
kmeans = KMeans(n_clusters=3, random_state=42)
kmeans_labels = kmeans.fit_predict(X)
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(15, 6))
ax1.scatter(X[:, 0], X[:, 1], c=dbscan_labels, cmap='viridis')
ax1.set_title('DBSCAN Clustering')
ax2.scatter(X[:, 0], X[:, 1], c=kmeans_labels, cmap='viridis')
ax2.set_title('K-Means Clustering')
plt.show()
```

# Implementing DBSCAN



## Comparing DBSCAN and K-Means




What conclusions can be obtained?

# Hands On