Mondragon Unibertsitatea

Escuela Politécnica Superior

Clustering

1

Introduction

Clustering

- Most frequent unsupervised method

Clustering

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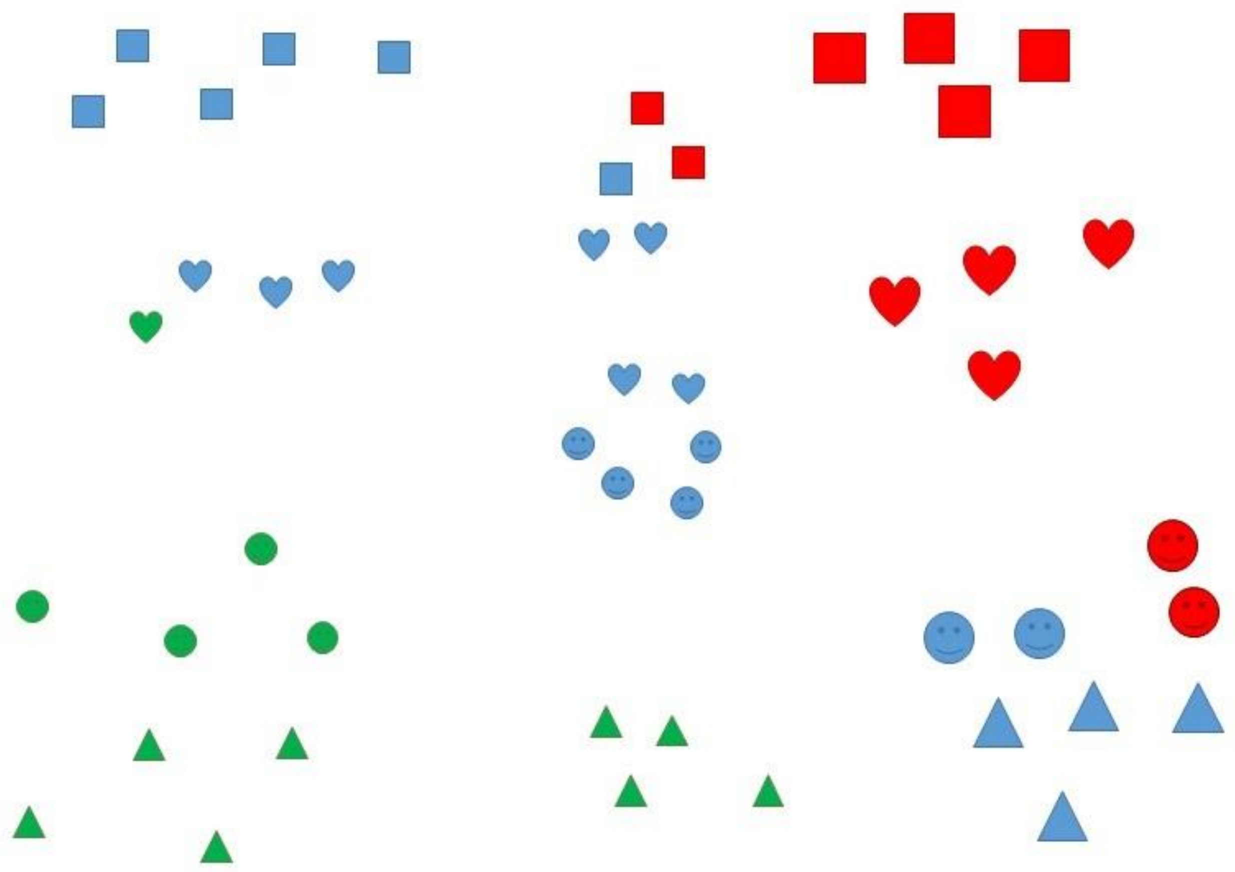

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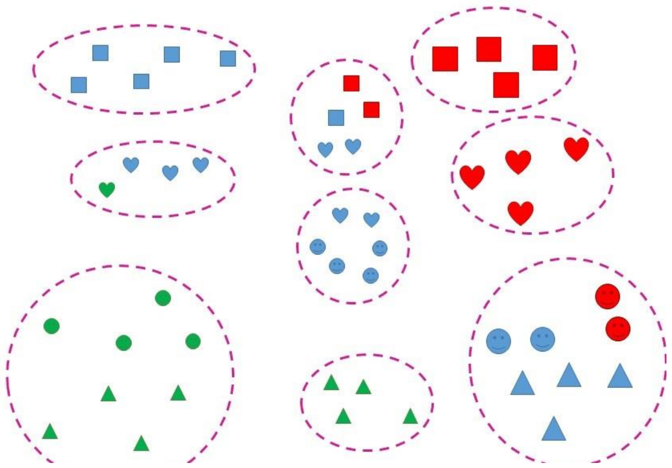

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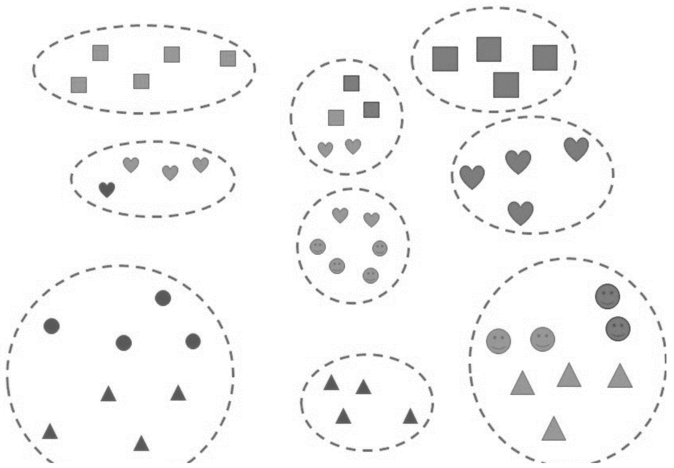

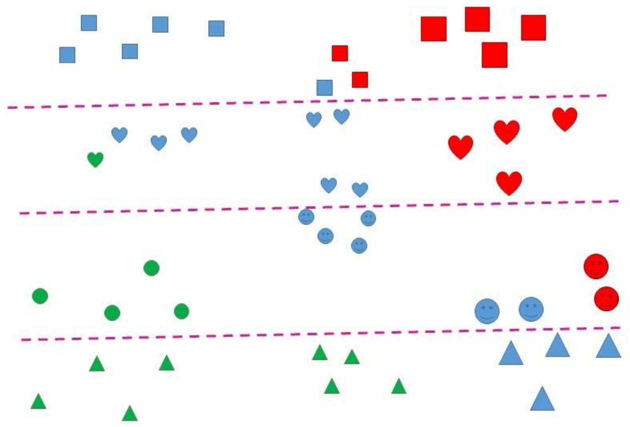

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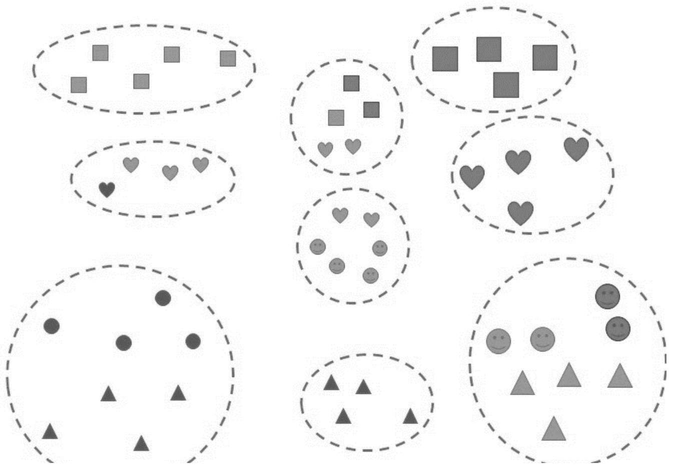

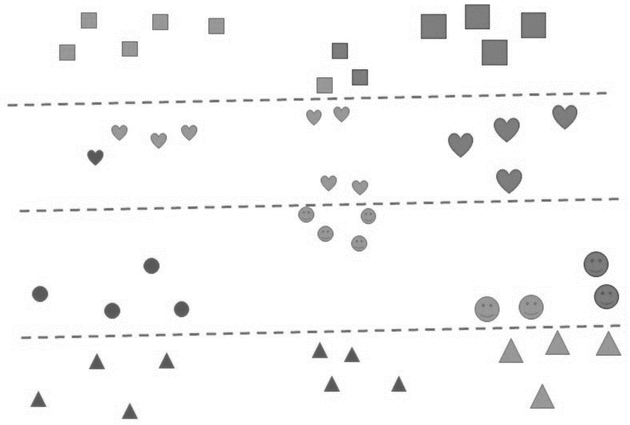

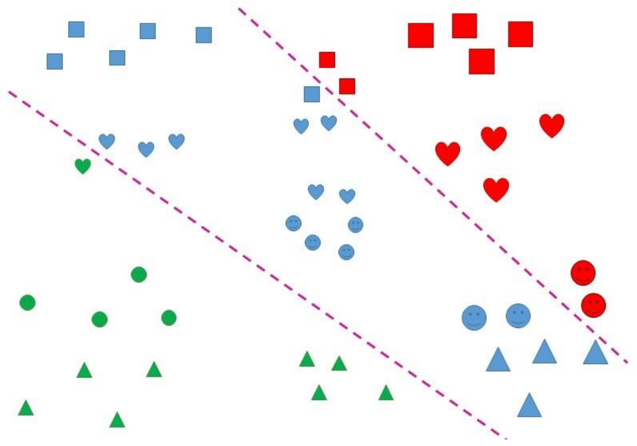

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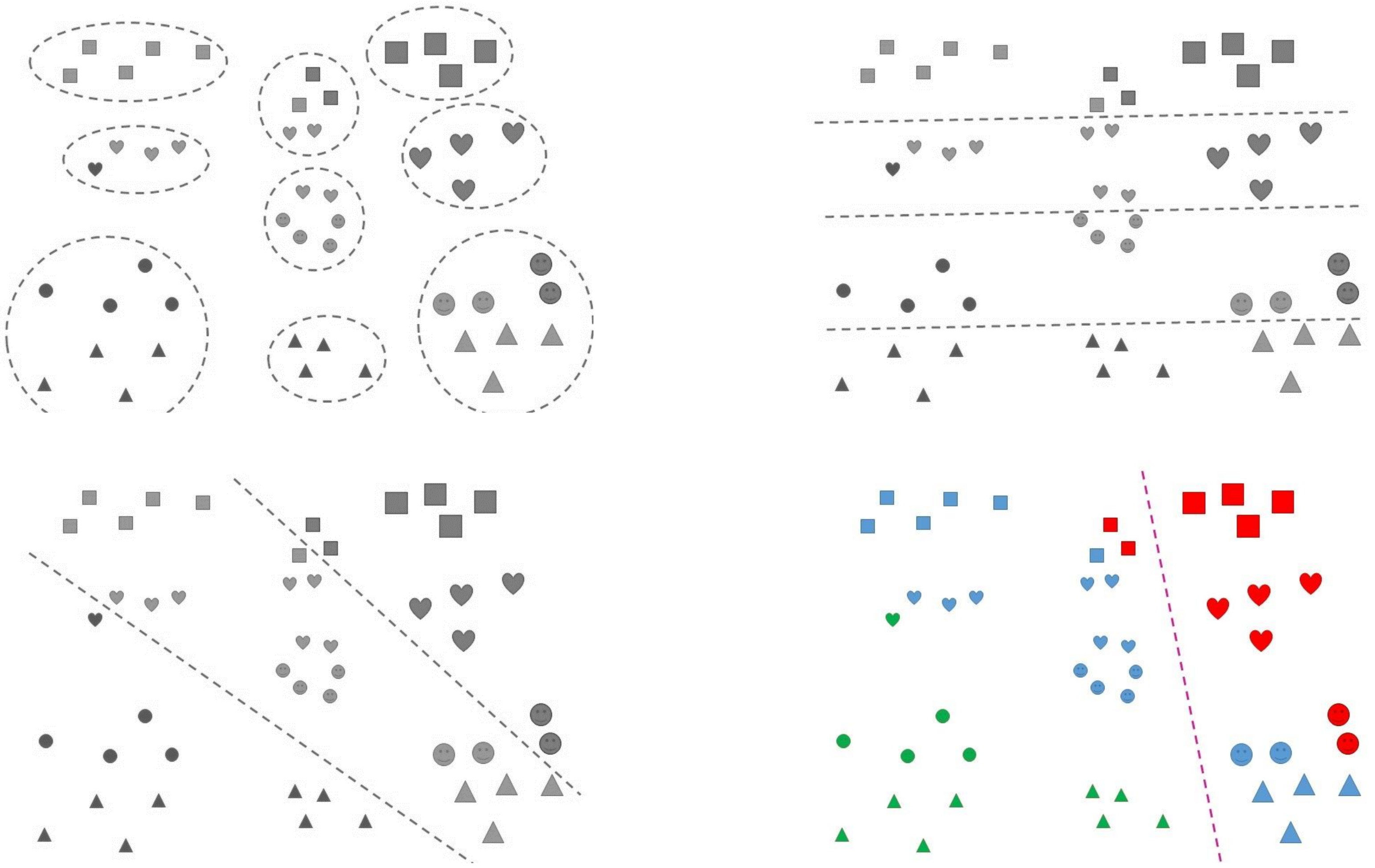
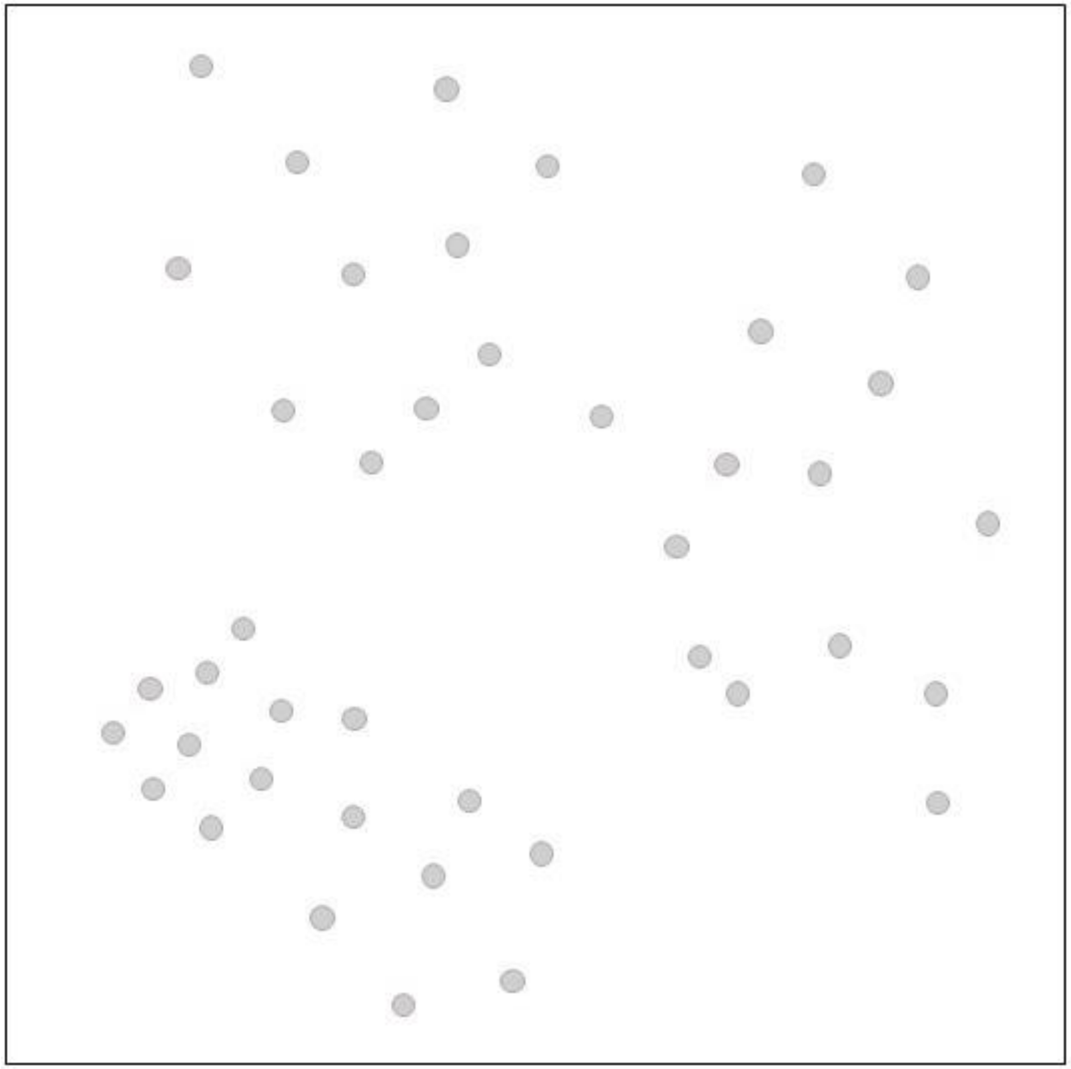


2

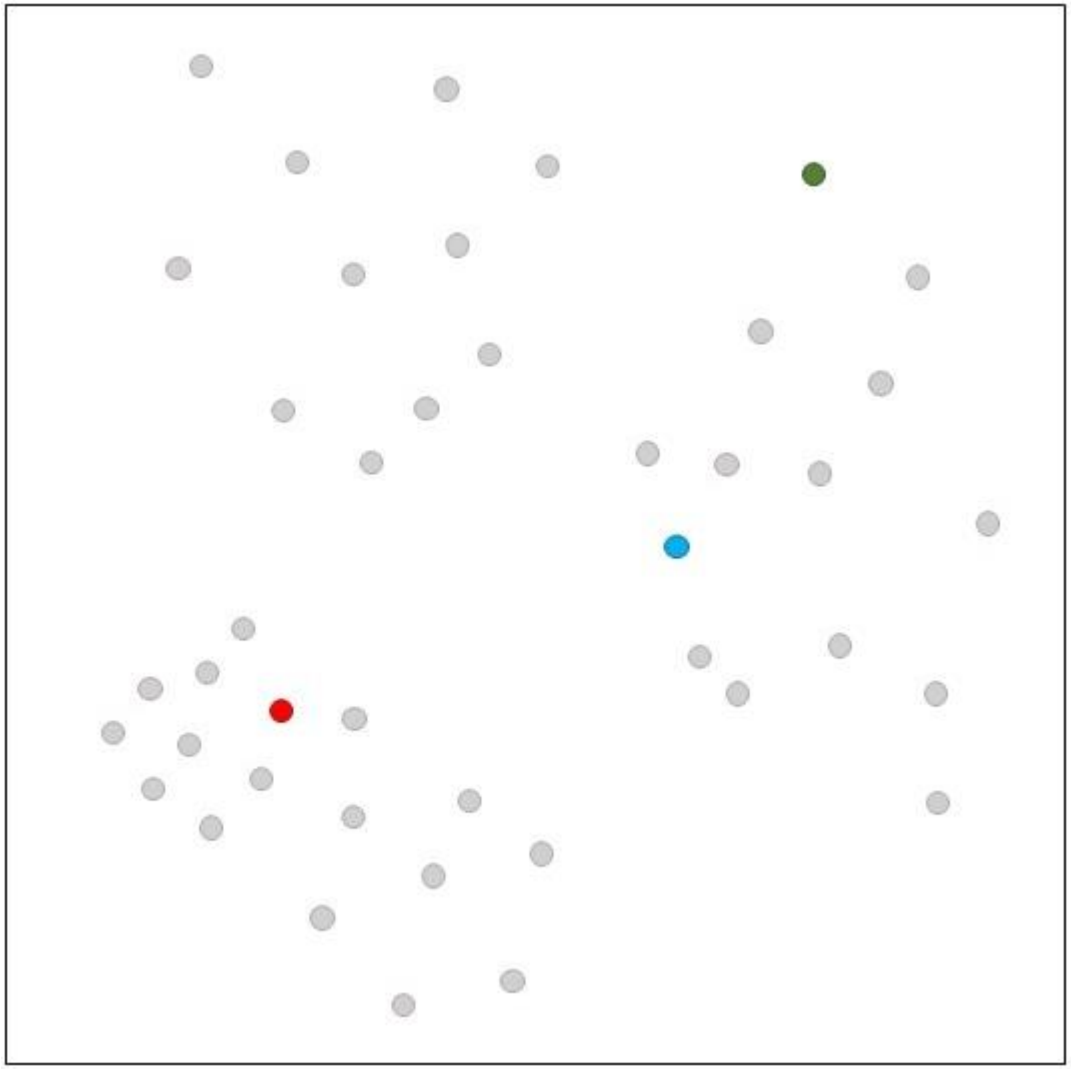
Algorithms

K-Means



We prefix K and begin from the original data

K-Means



K points are randomly chosen (here $K = 3$) as initial centroids

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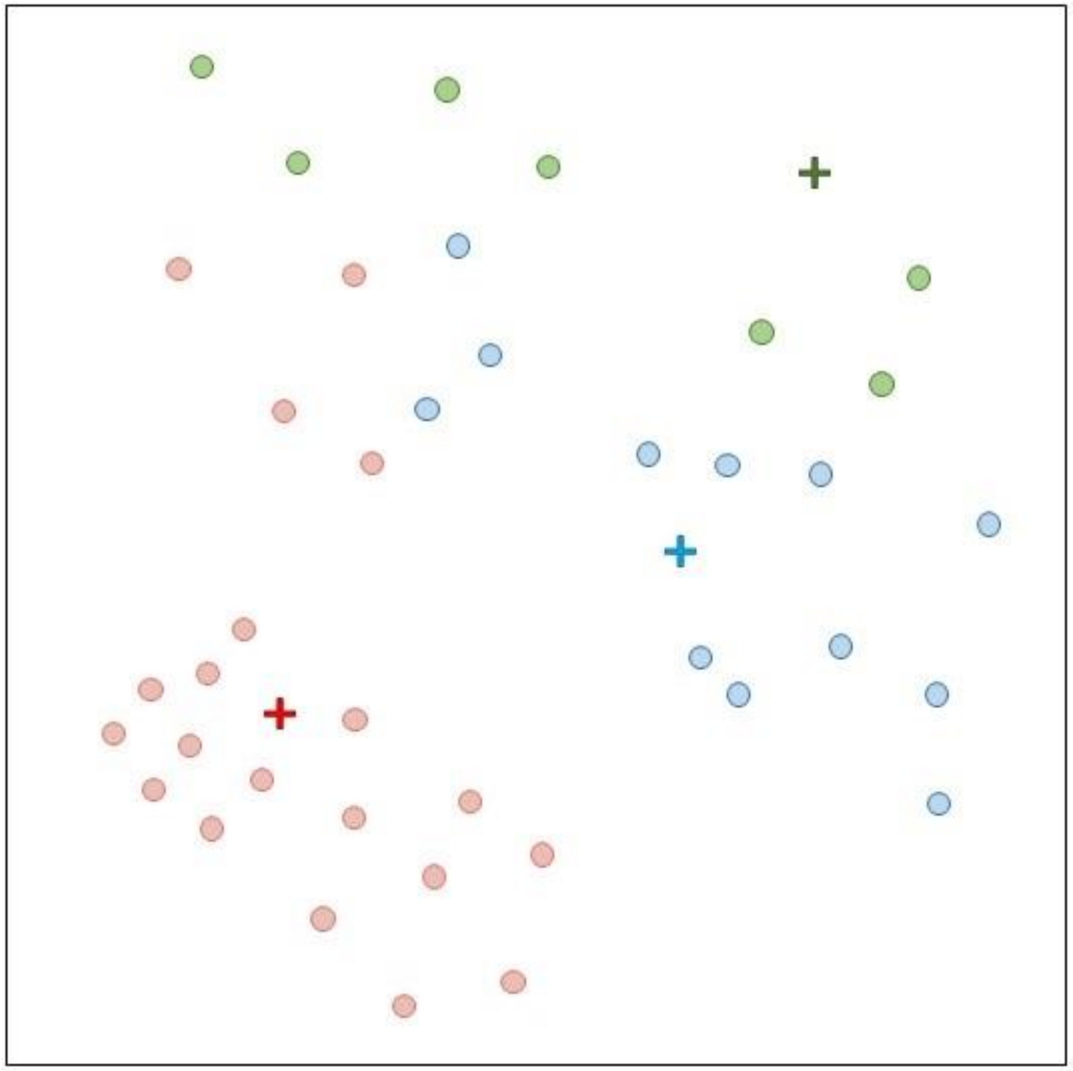

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K-Means

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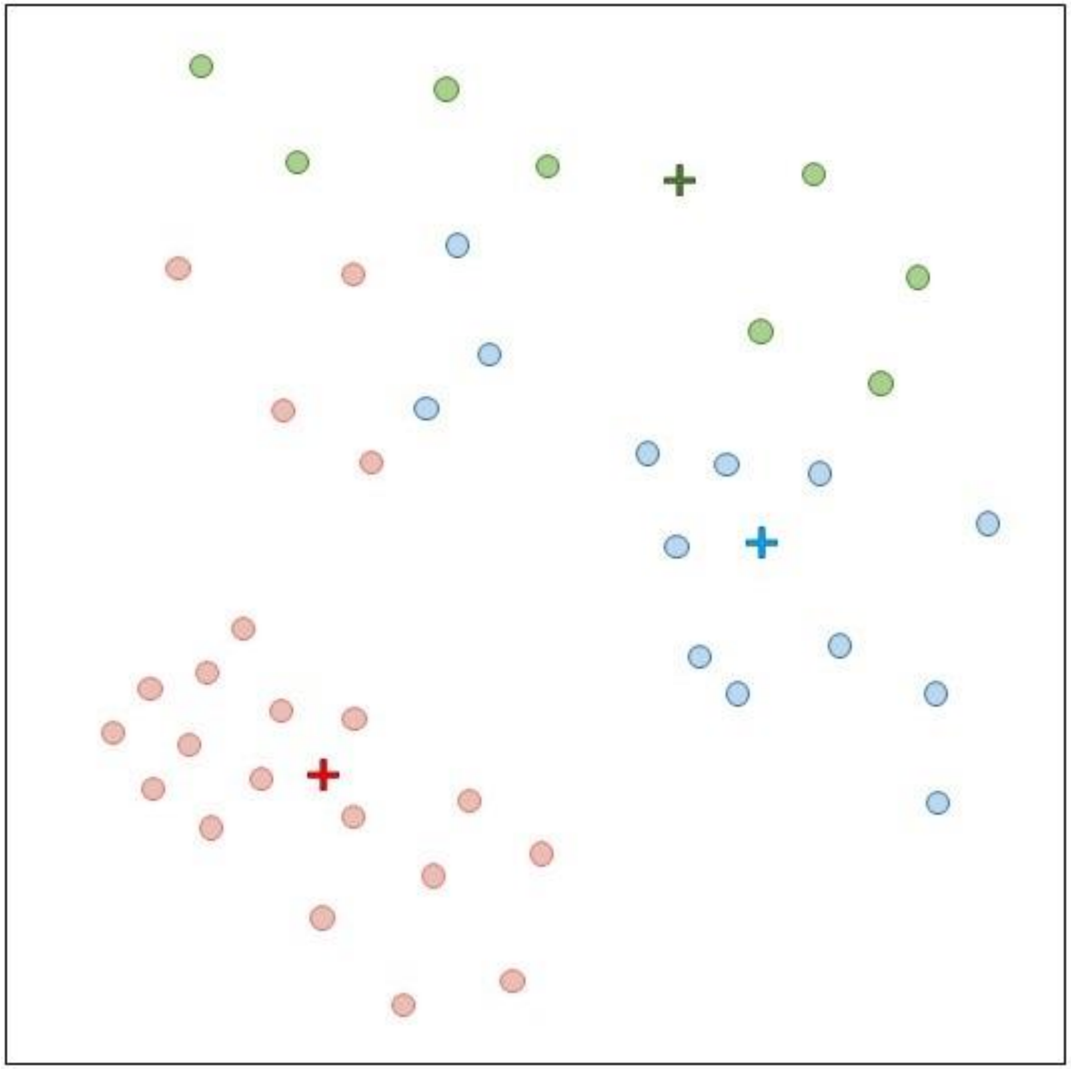

b) The centroid (mass center) of each cluster is obtained. It could be none of the points

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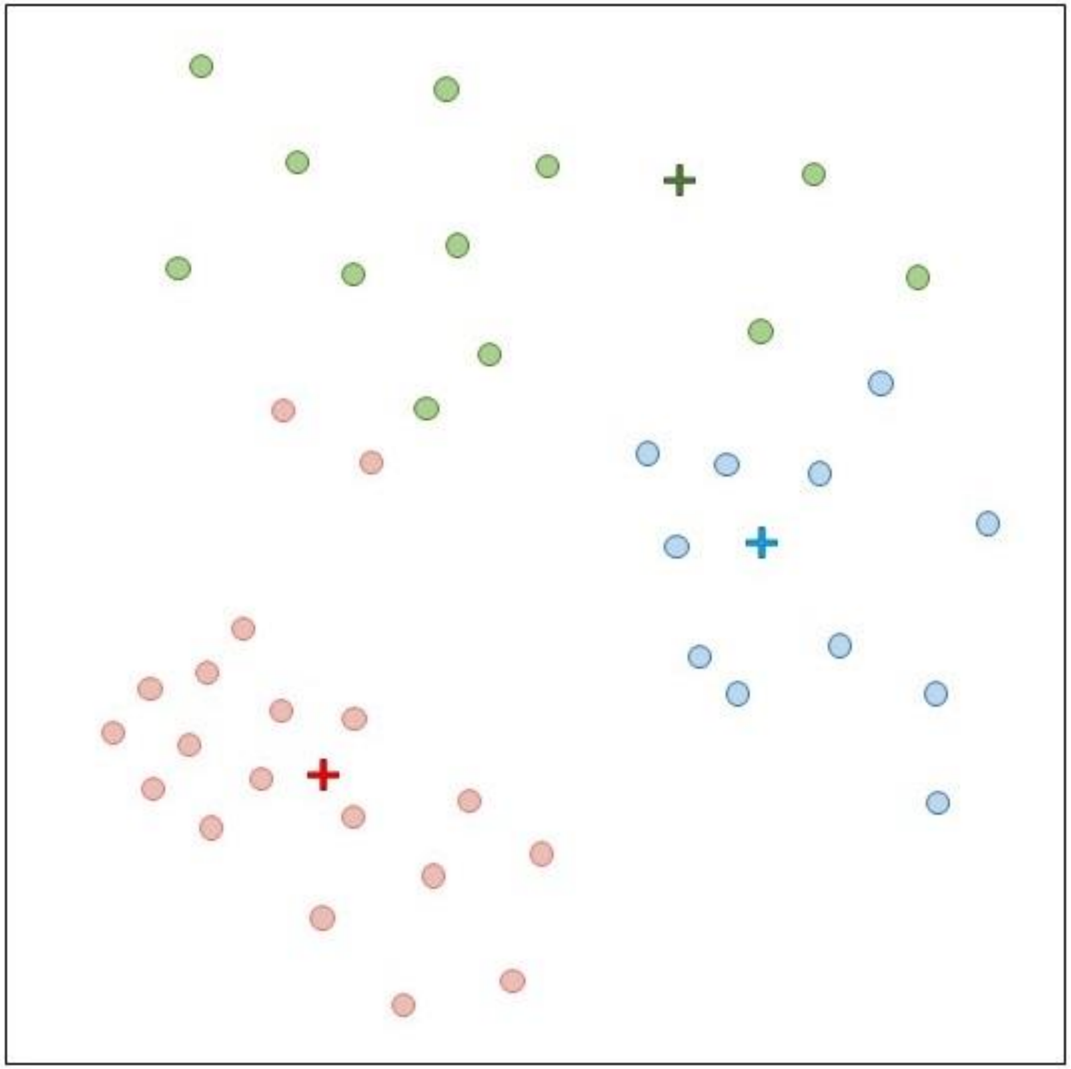

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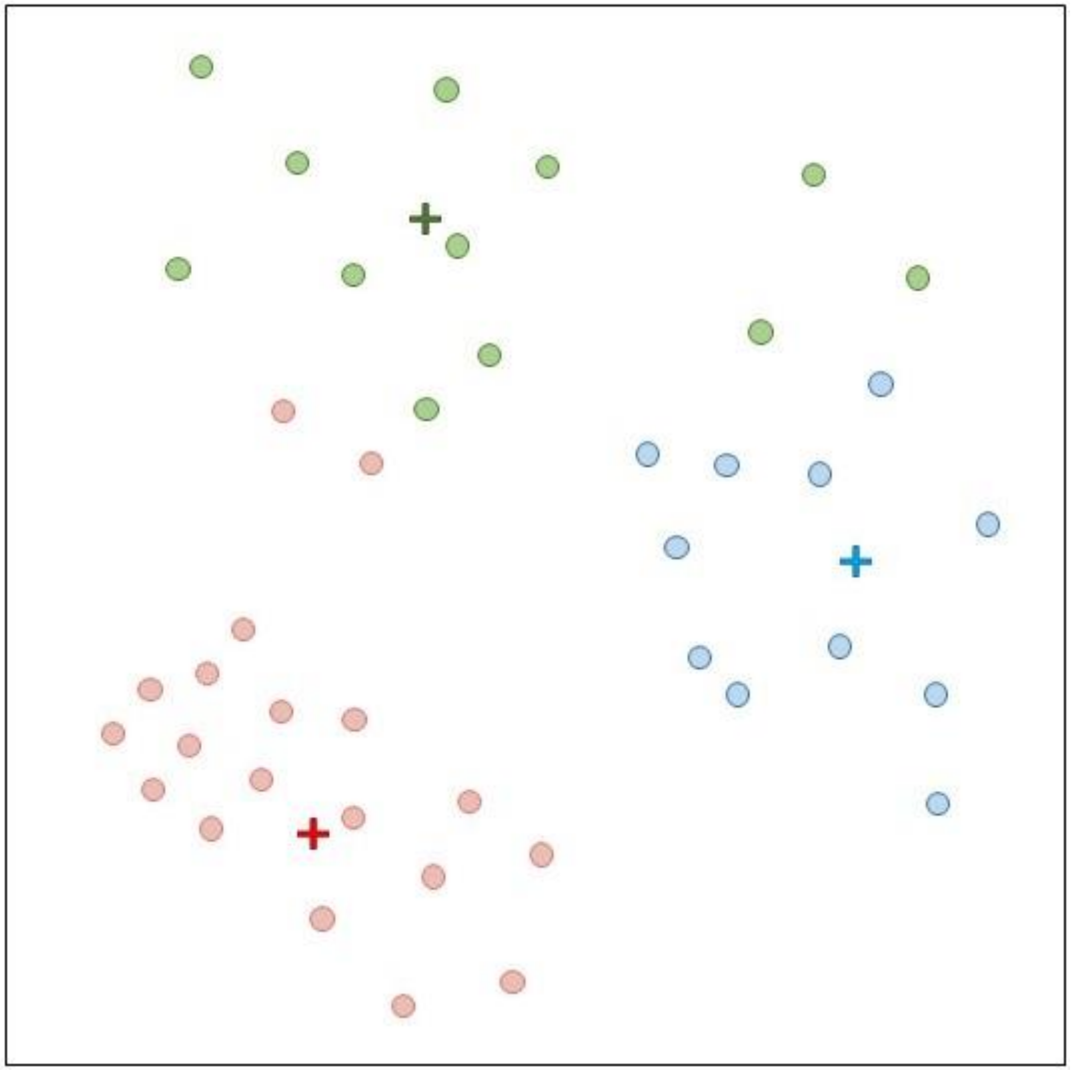
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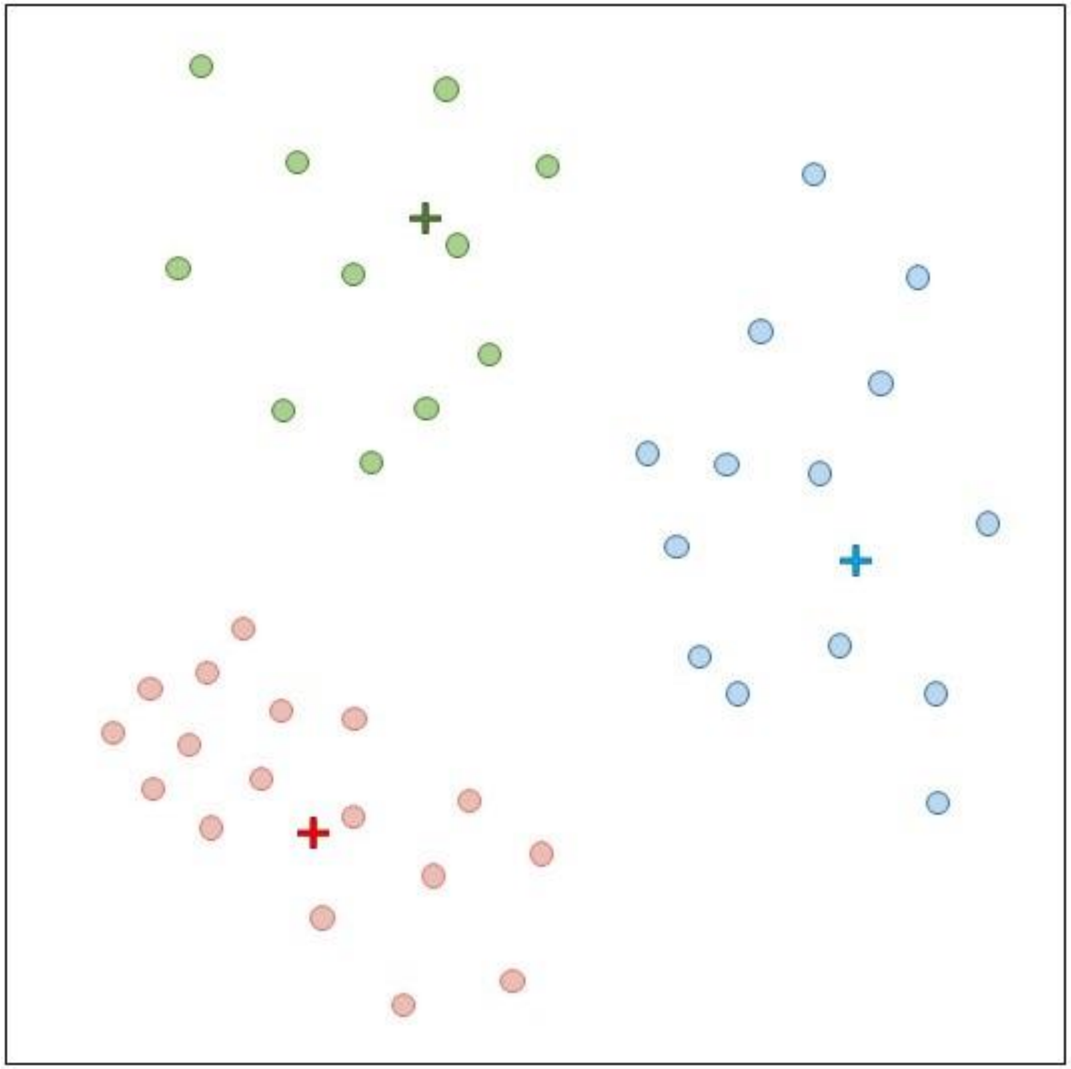

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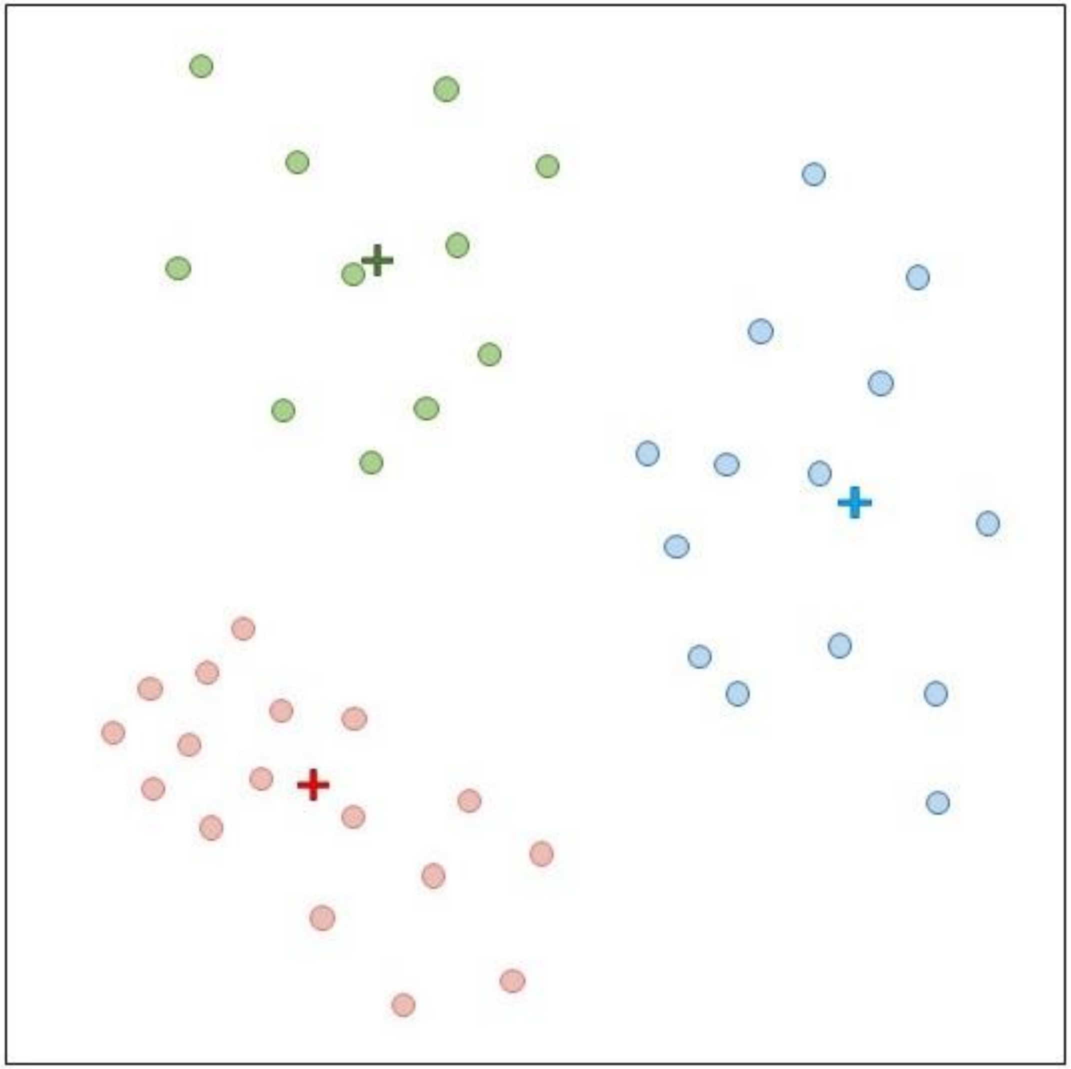

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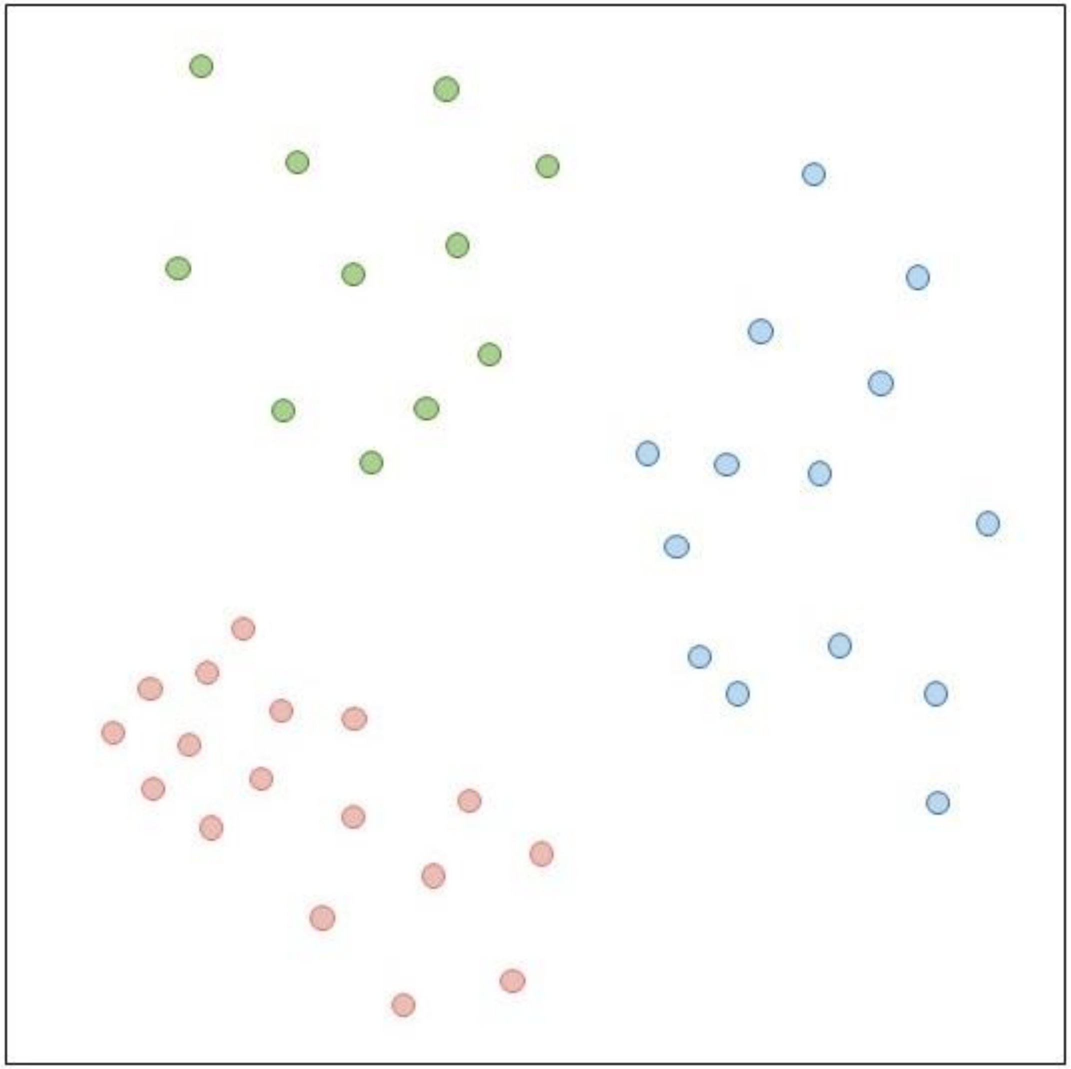

We stop when no more changes in the centroids occur
(or if a prefixed limit number of iterations a-b is reached)

Affinity propagation

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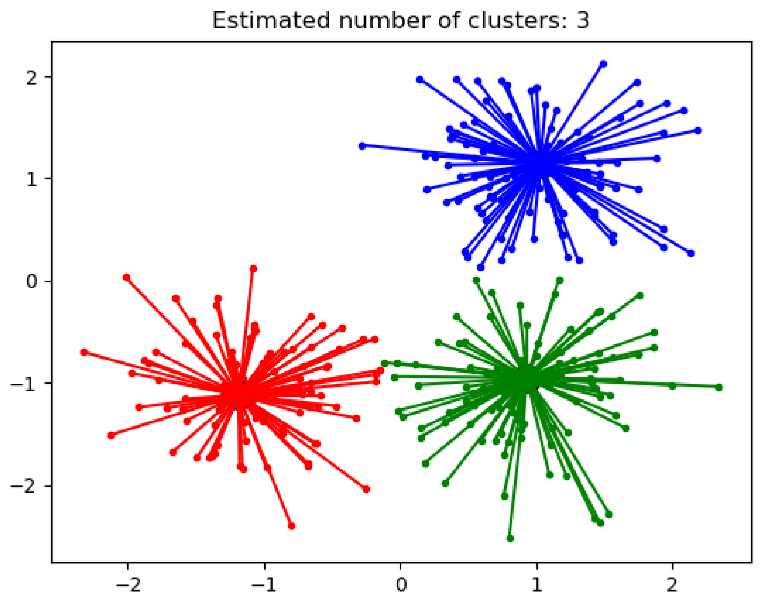

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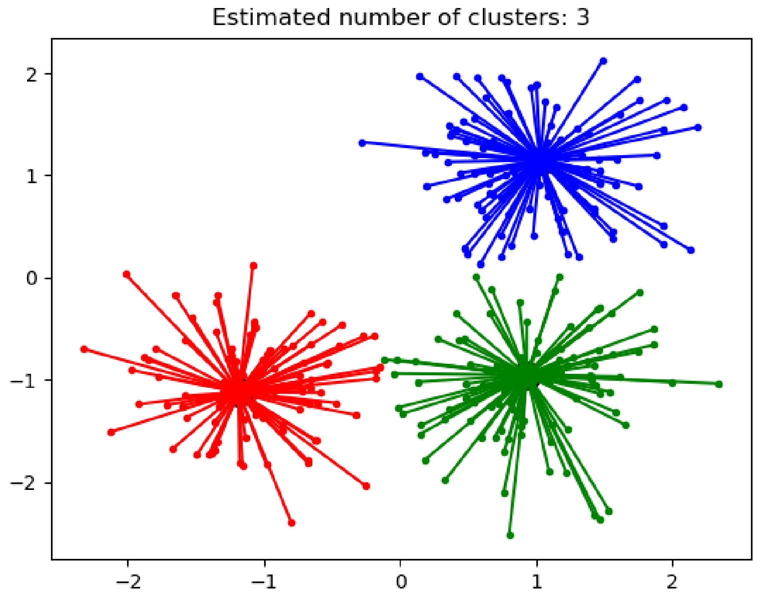

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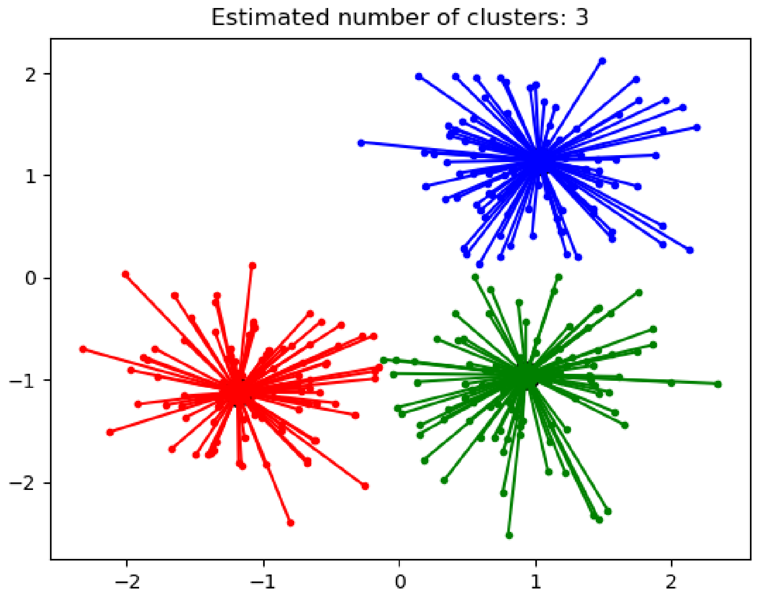

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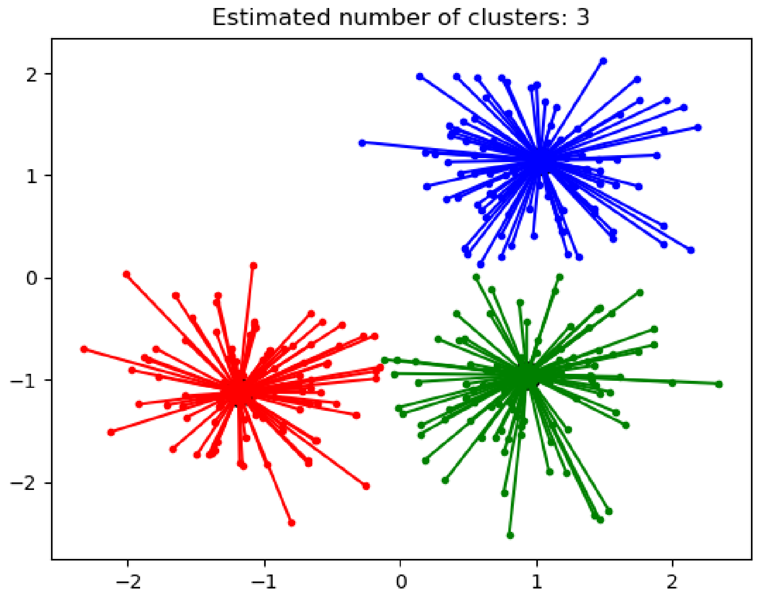

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- Its usage is recommended to be restricted to small or medium datasets.

Mean shift

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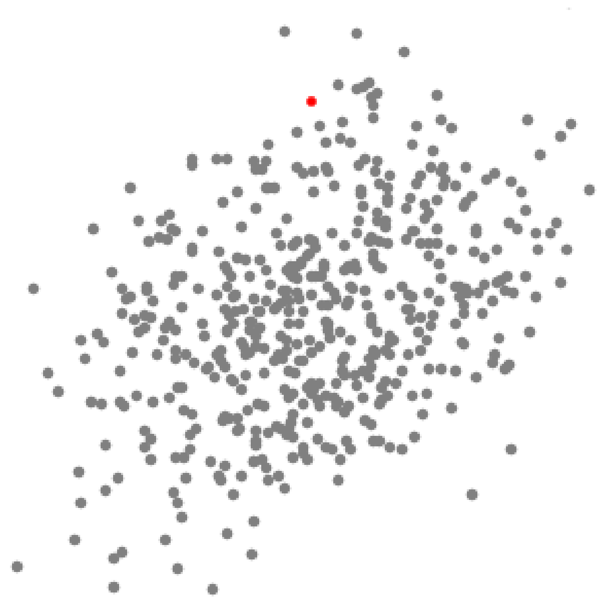

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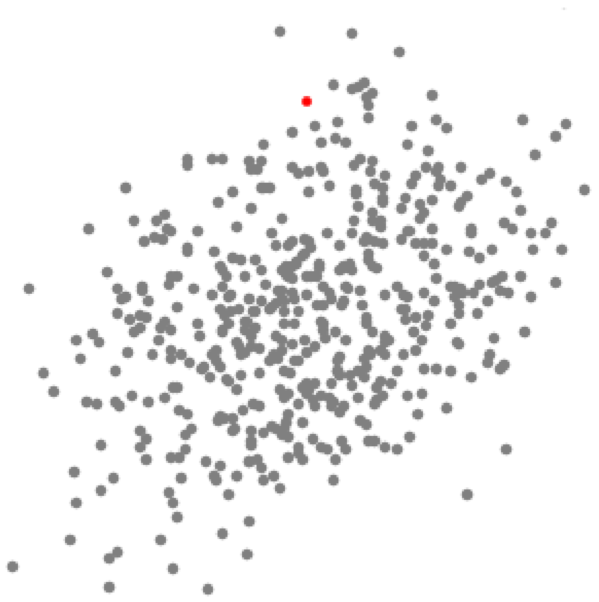

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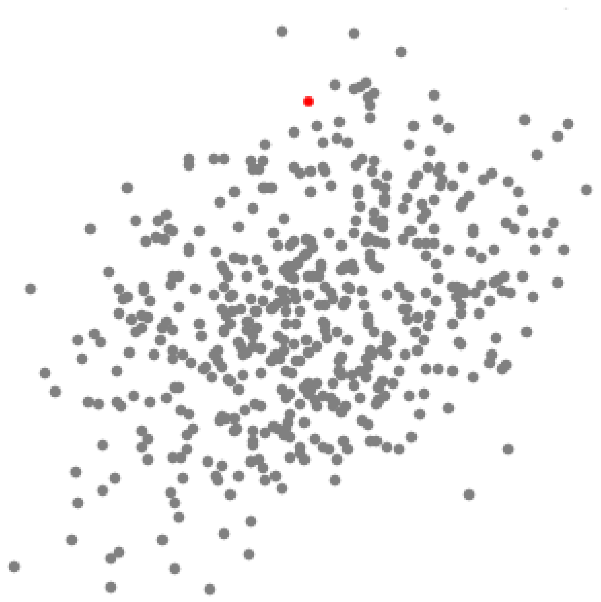

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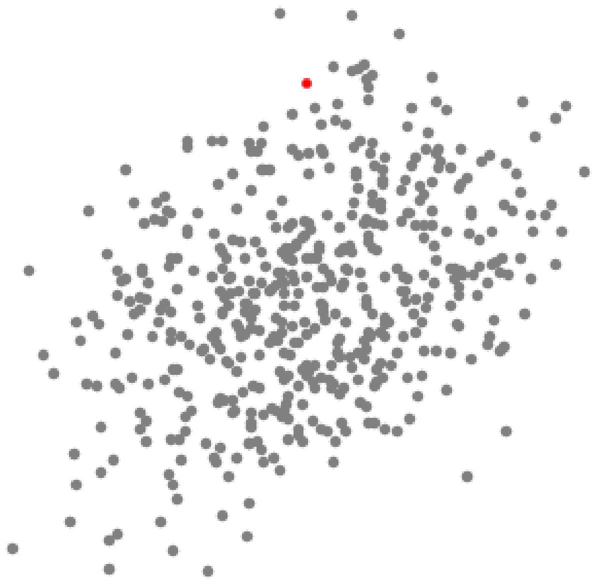

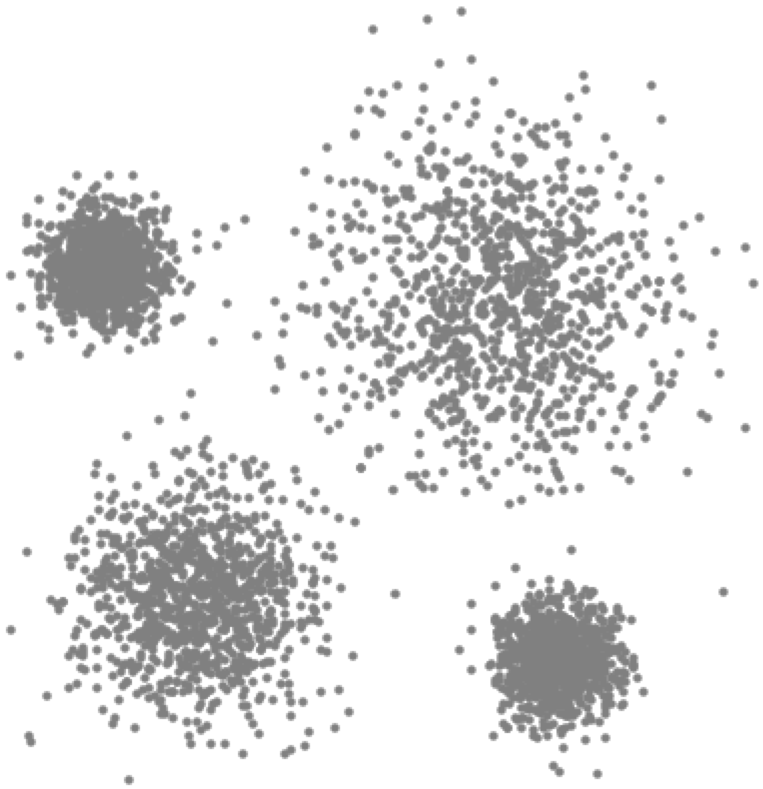

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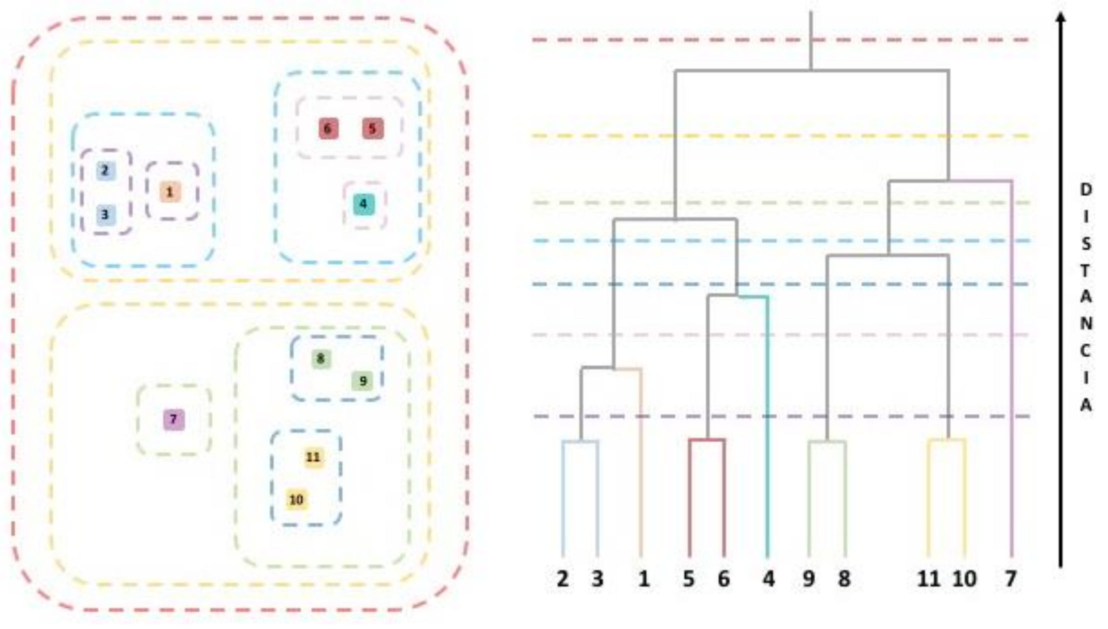

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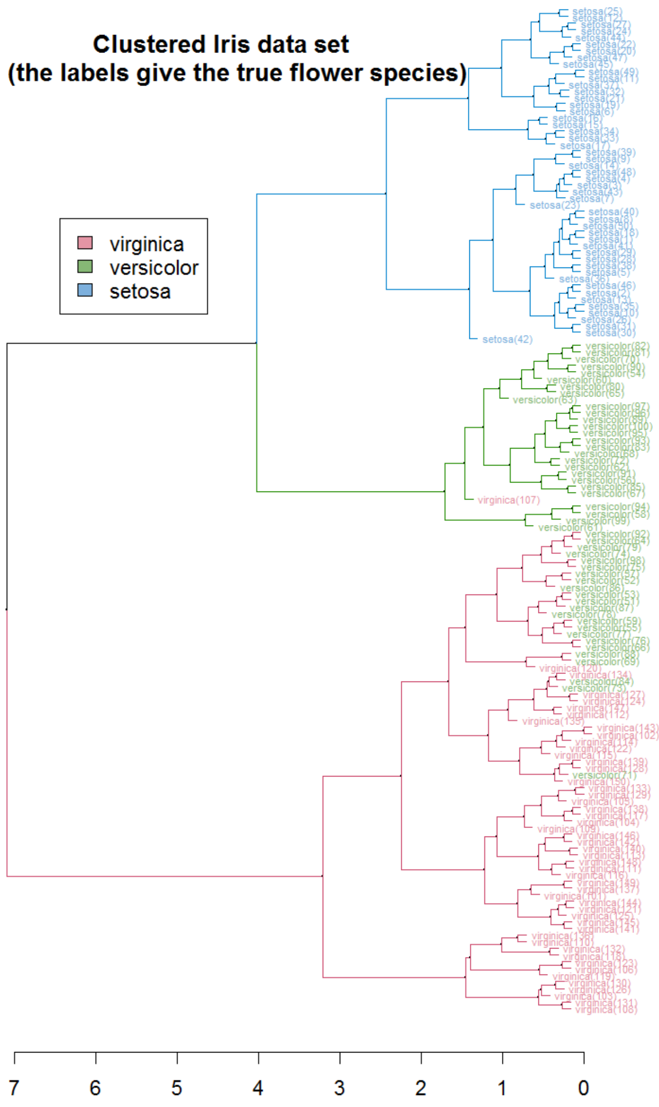

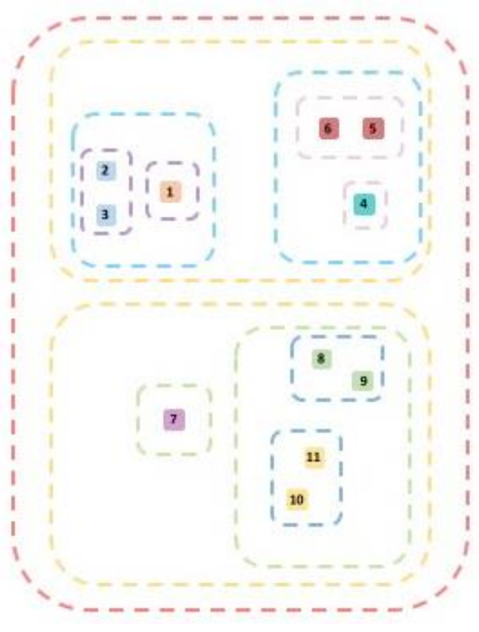

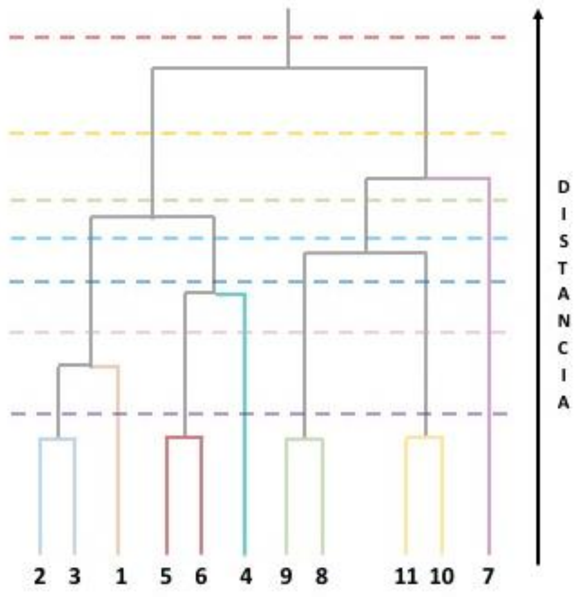

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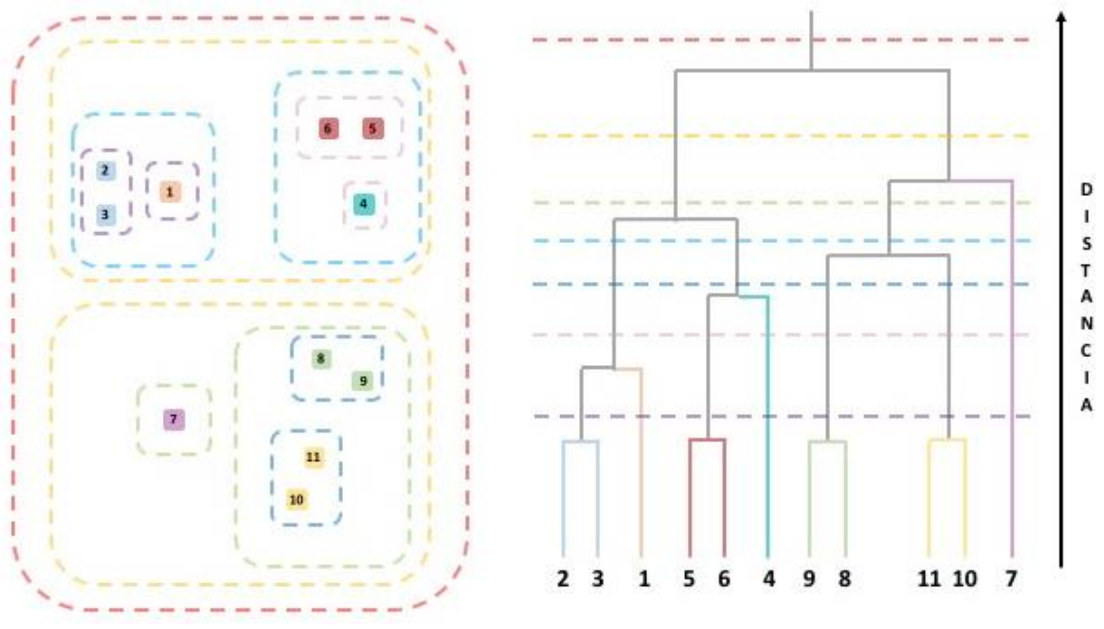
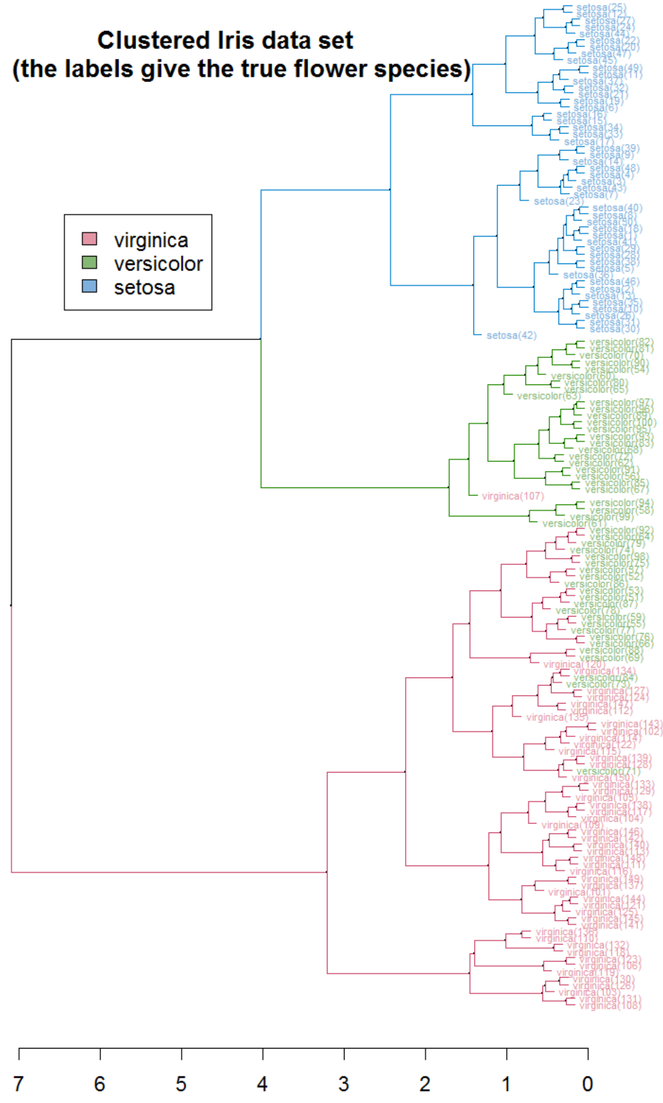
- In order to be able to perform an early-stopping operation in the process, top to bottom approach is usually preferred





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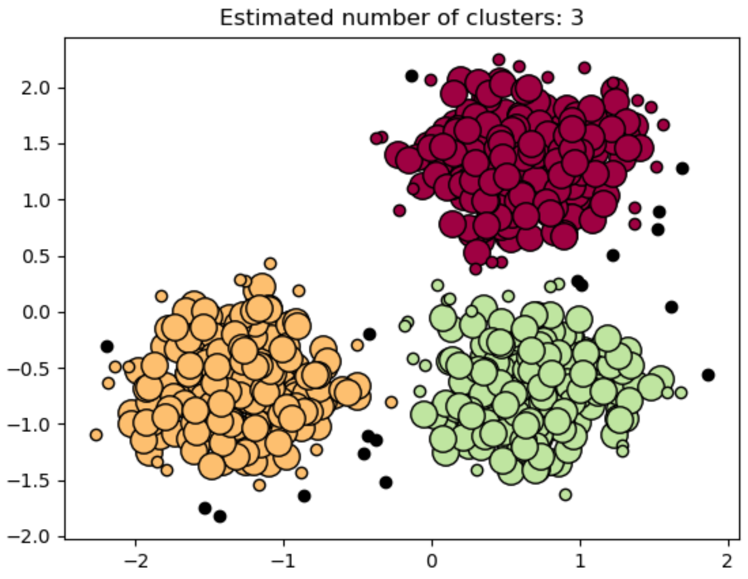

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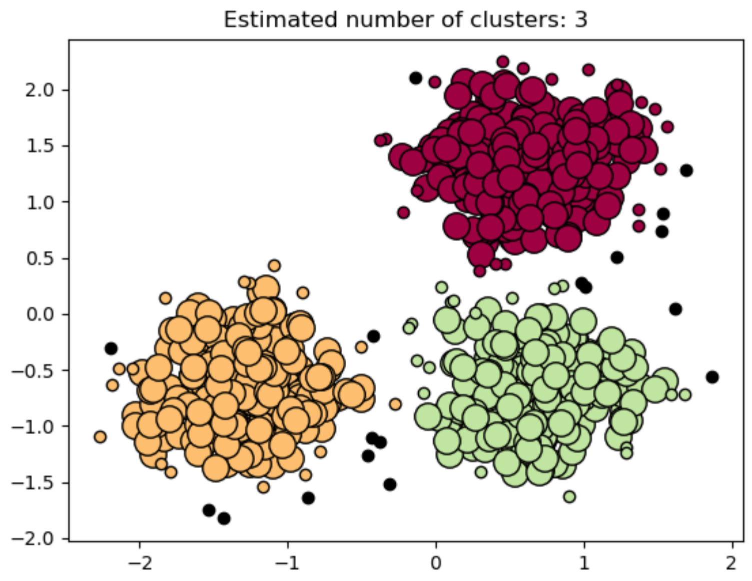

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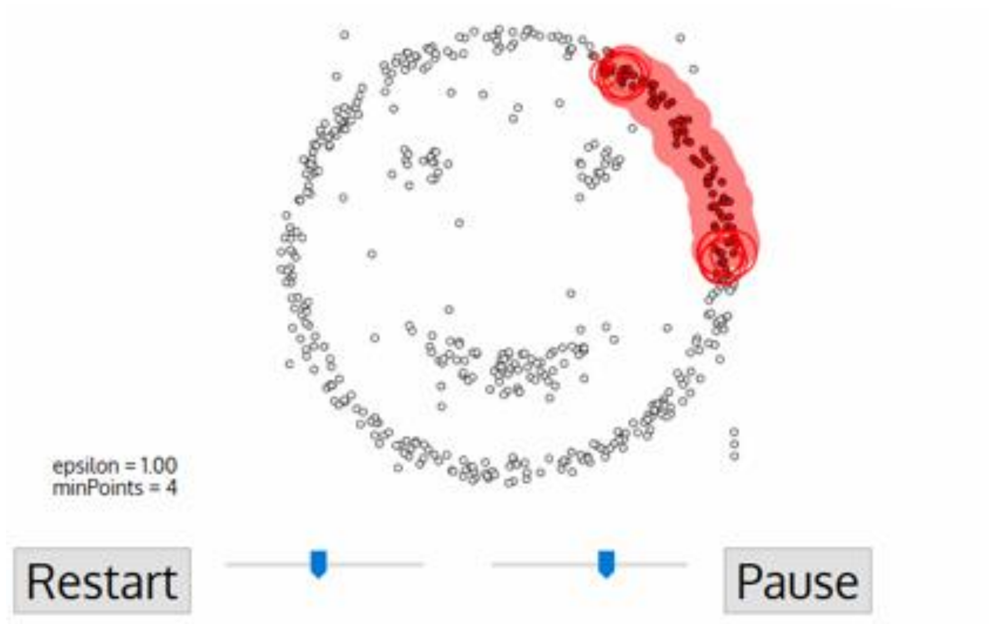

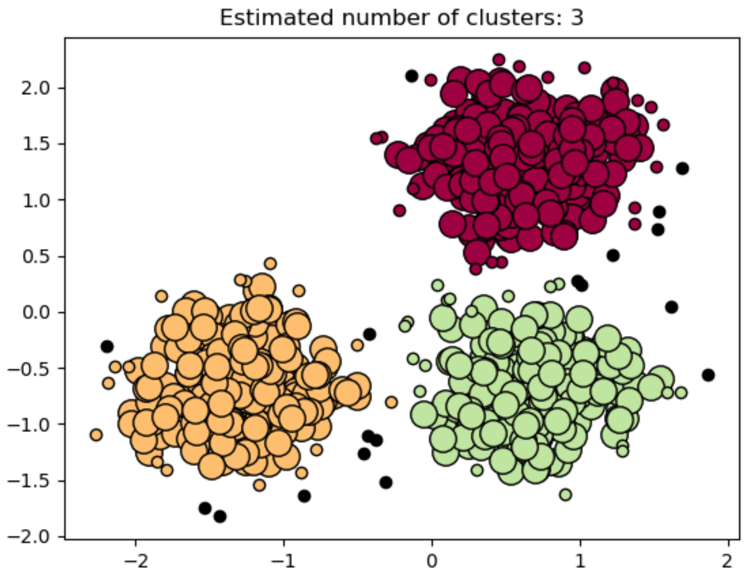

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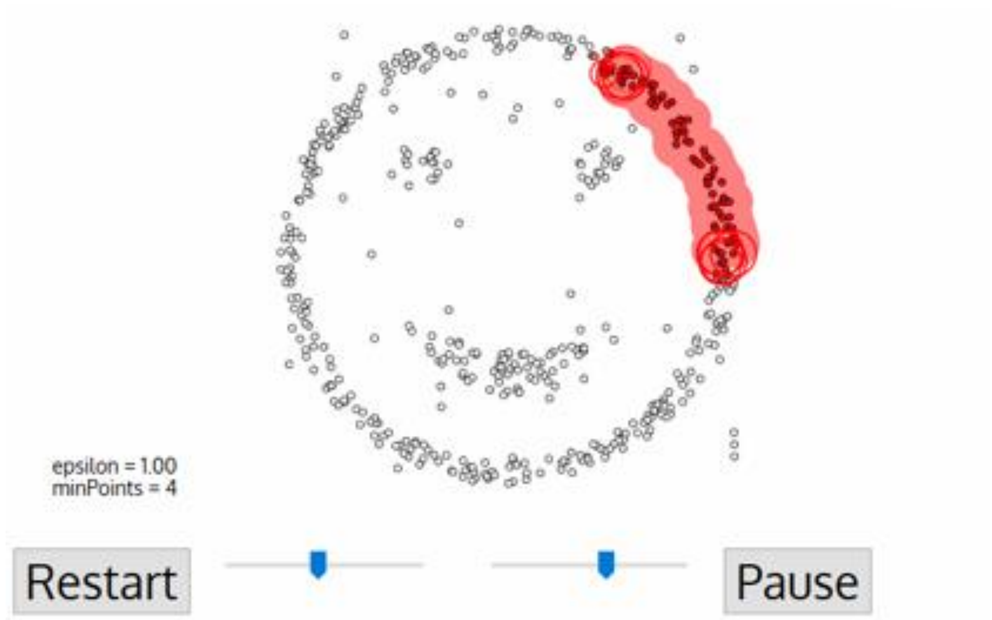

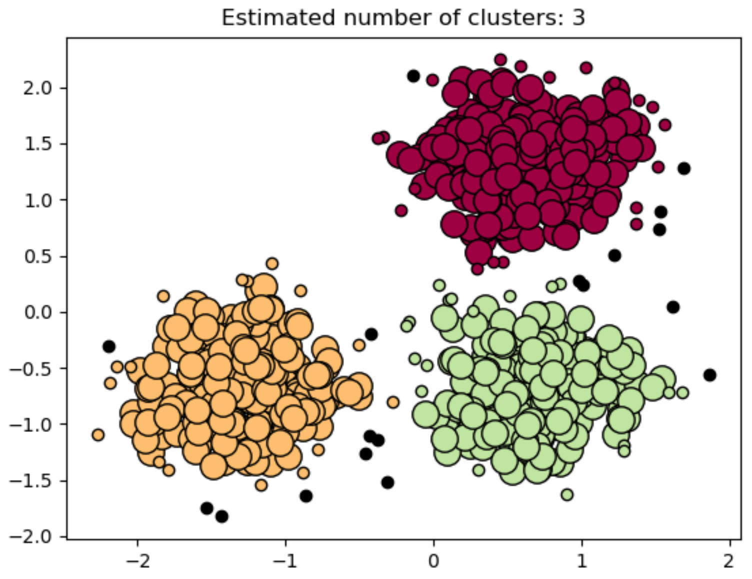

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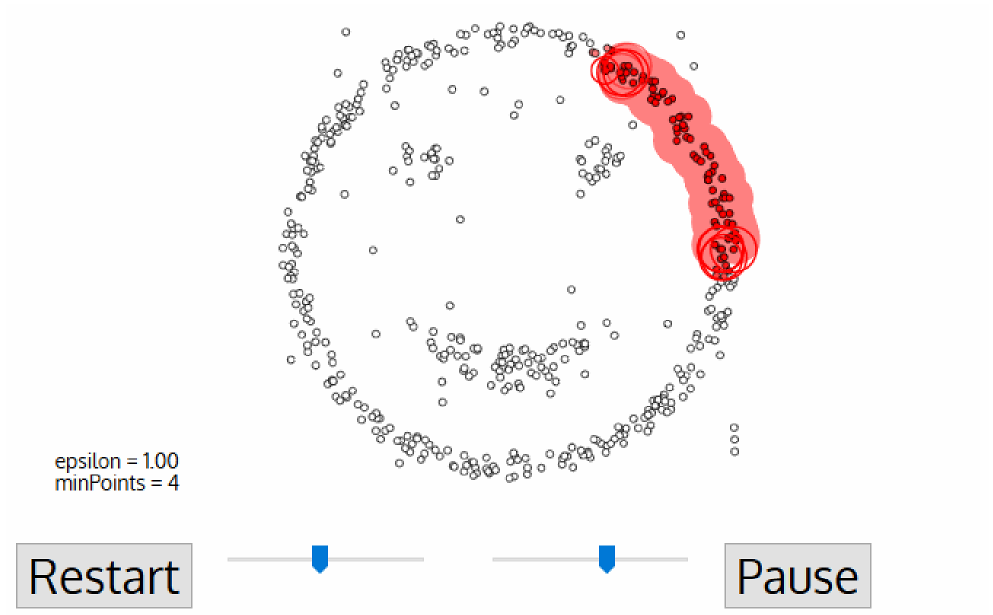

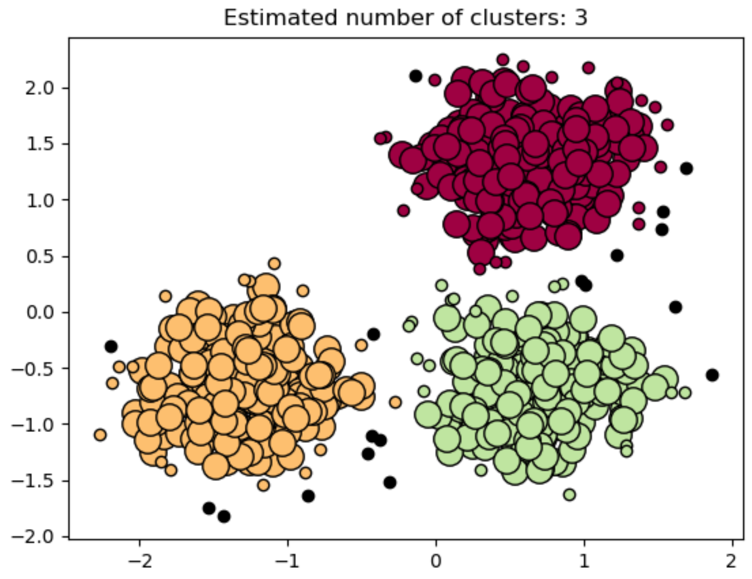

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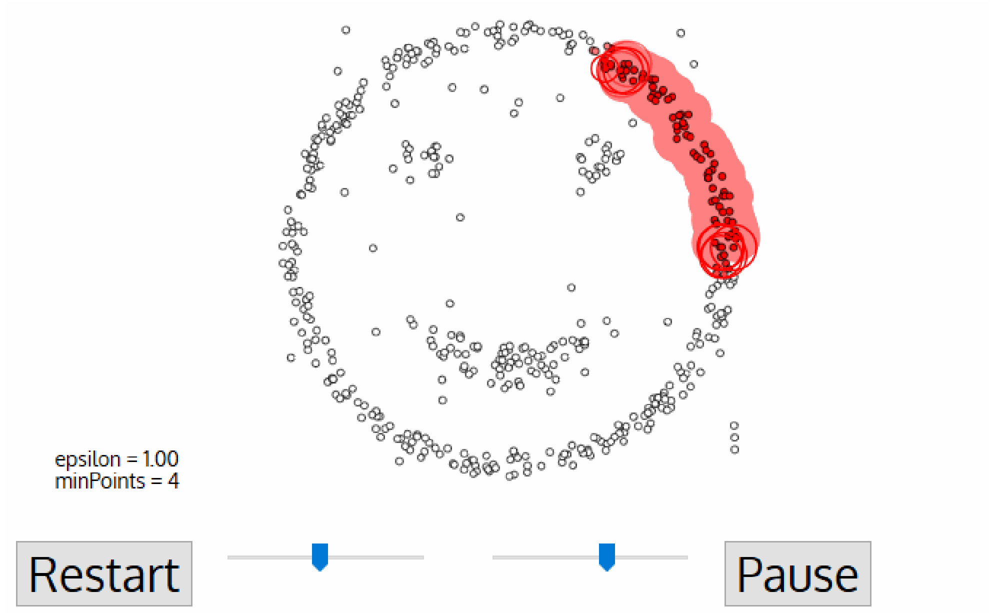
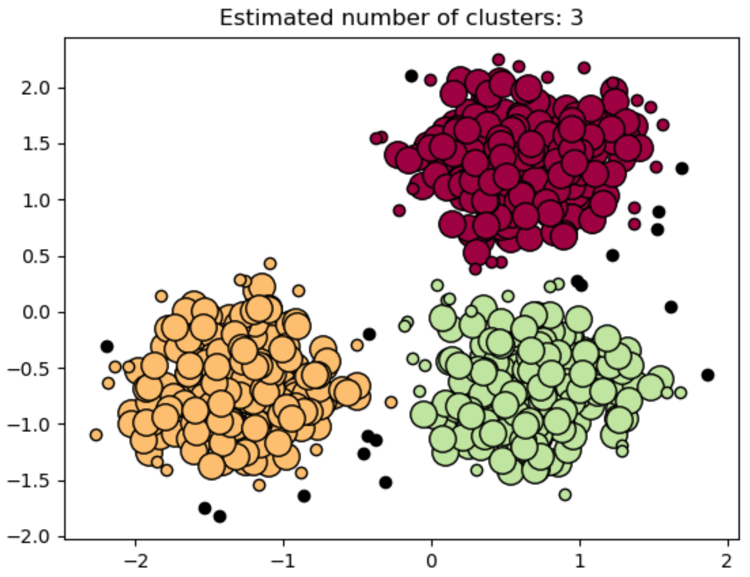
- It is **computationally expensive**, but there are variants in the form of **speed-up versions**





Gaussian Mixture Models

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- It is a **probabilistic model**. It assumes that all the points have been generated by the **mixture of a finite number of Gaussian distributions** with unknown parameters, which will be approximated by means of the ***expectation maximization* (EM)** algorithm.

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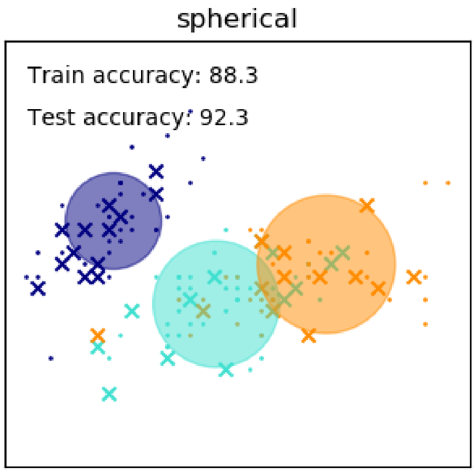
  - Spherical: Each component has its own individual variance



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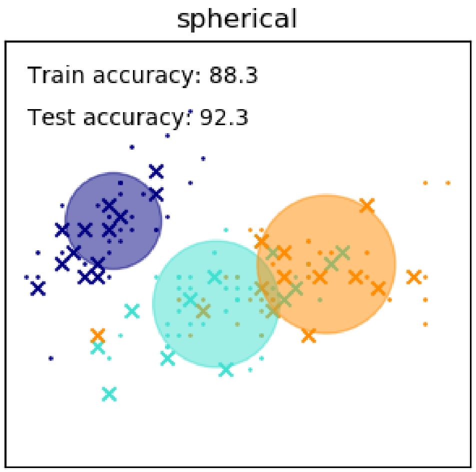

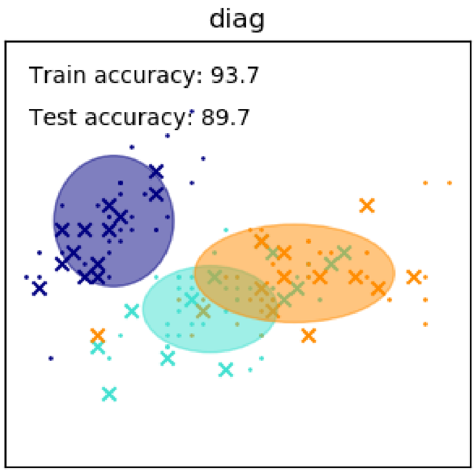

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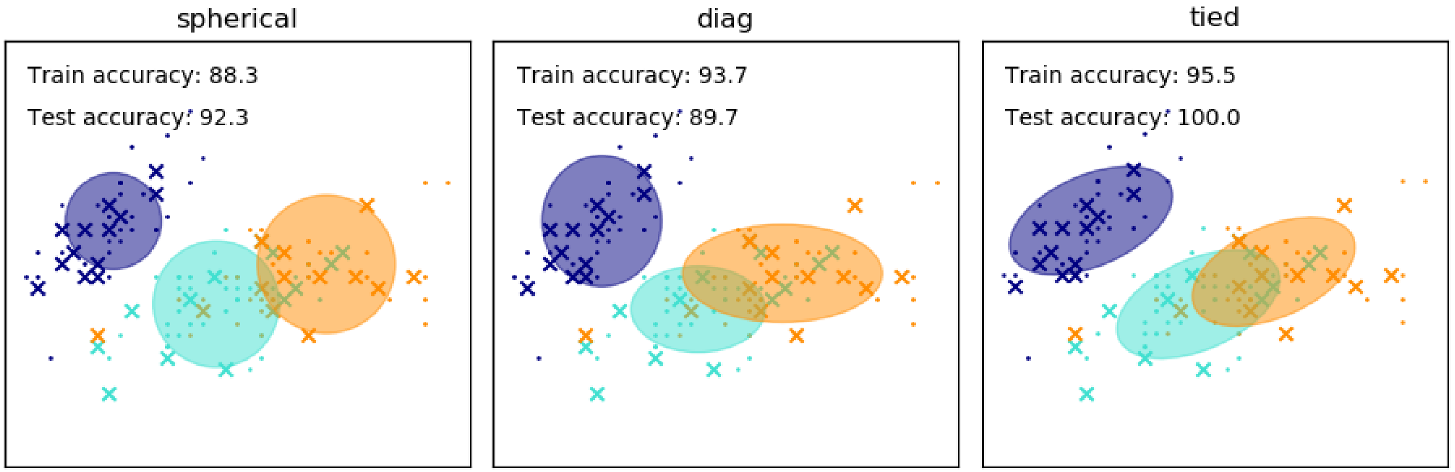

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- Depending on the type of covariance we consider, there are 4 variants:
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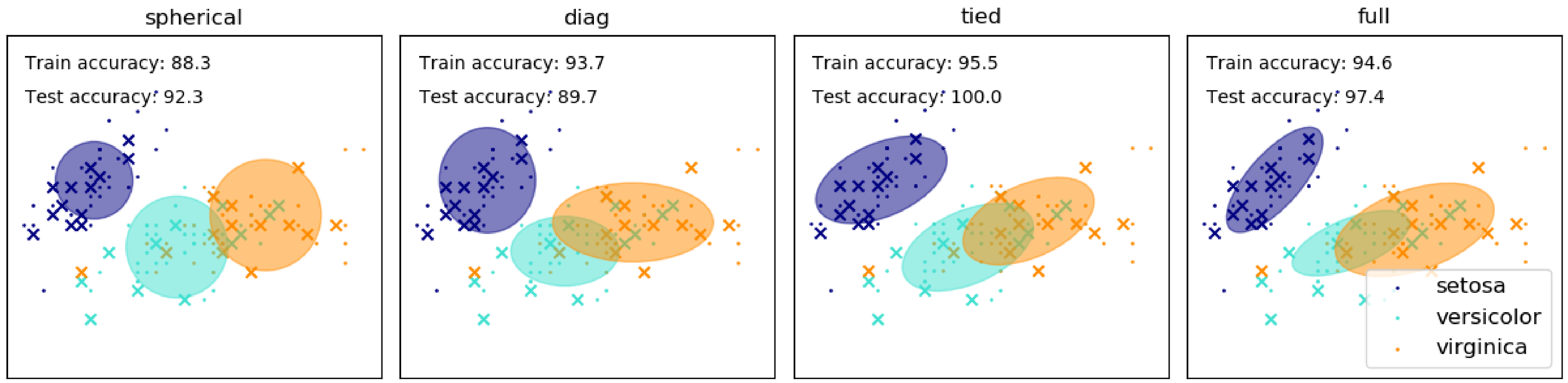
  - Tied: All components have the same covariance matrix
  - Full: Each component has its own covariance matrix



Python functions

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Algorithm	Function	Use / Parameters of interest

K-Means	KMeans
	MiniBatchKMeans
		sklearn.cluster.KMeans(n_clusters=8, init=‘k-means++’, max_iter=300, tol=0.0001, random_state=None, n_jobs=None)
		sklearn.cluster.MiniBatchKMeans(n_clusters=8, init=‘k-means++’, max_iter=100, batch_size=100, tol=0.0, random_state=None)

Affinity propagation	AffinityPropagation	sklearn.cluster.AffinityPropagation(damping=0.5, max_iter=200, convergence_iter=15, preference=None, affinity=’euclidean’)
Mean shift	MeanShift	sklearn.cluster.MeanShift(bandwidth=None, min_bin_freq=1, cluster_all=True, n_jobs=None)
Hierarchical	AgglomerativeClustering	sklearn.cluster.AgglomerativeClustering(n_clusters=2, affinity=’euclidean’, connectivity=None, linkage=’ward’)
DBSCAN	DBSCAN	sklearn.cluster.DBSCAN(eps=0.5, min_samples=5, metric=’euclidean’, algorithm=’auto’, n_jobs=None)
Gaussian Mixture Models	GaussianMixture	sklearn.mixture.GaussianMixture(n_components=1, covariance_type=’full’, tol=0.001, max_iter=100, init_params=’kmeans’, random_state=None)

3

Validation

Validation

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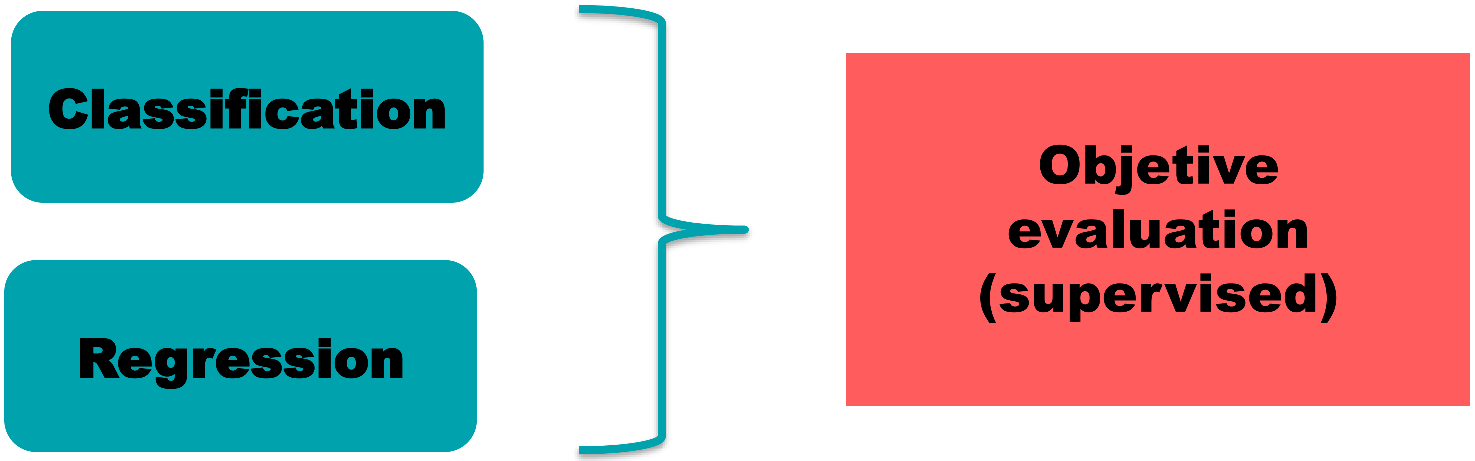
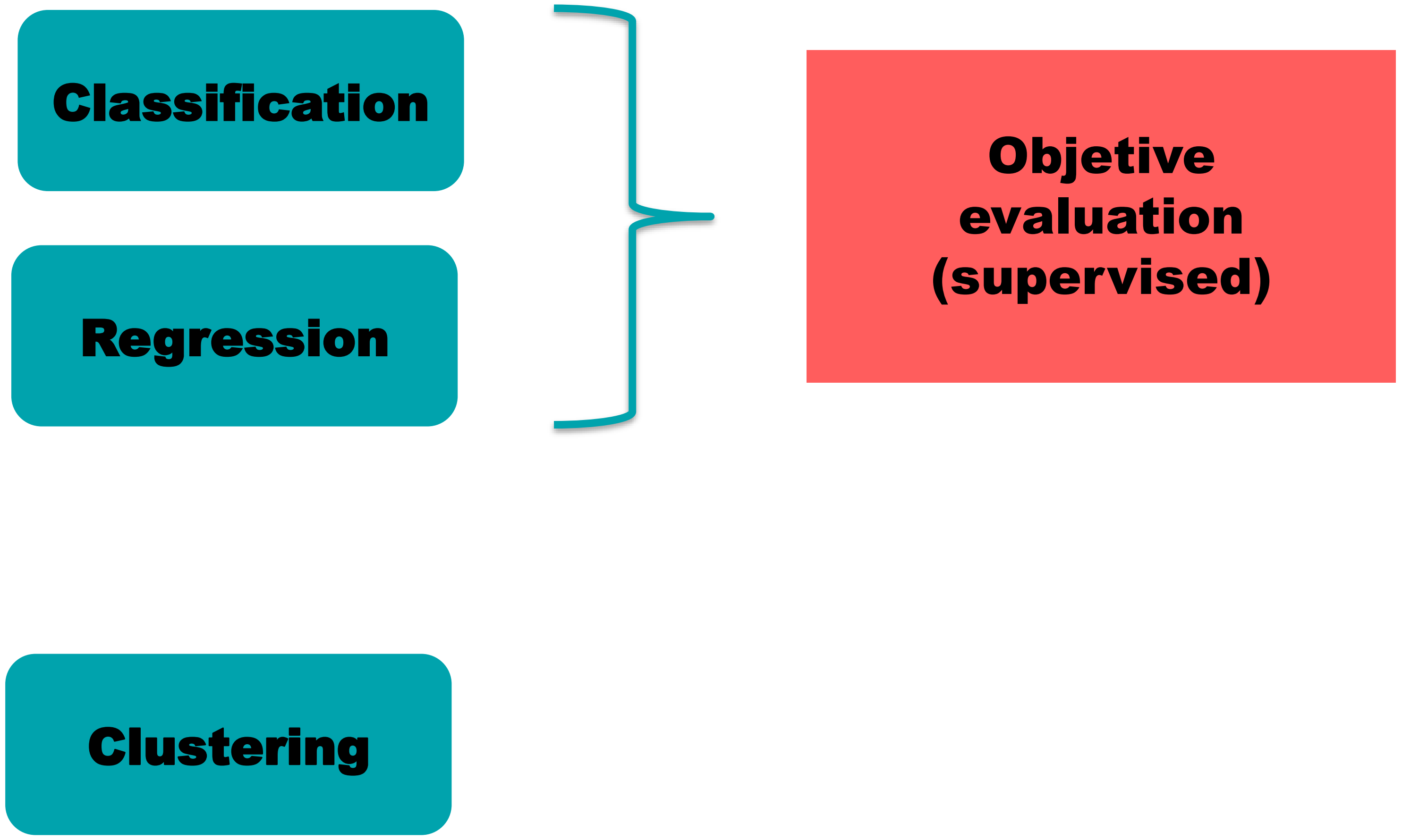
Classification

Regression

Validation


Classification
Regression
Objective evaluation (supervised)

Validation


Classification
Regression
Objetive evaluation (supervised)
Clustering

Validation

Classification

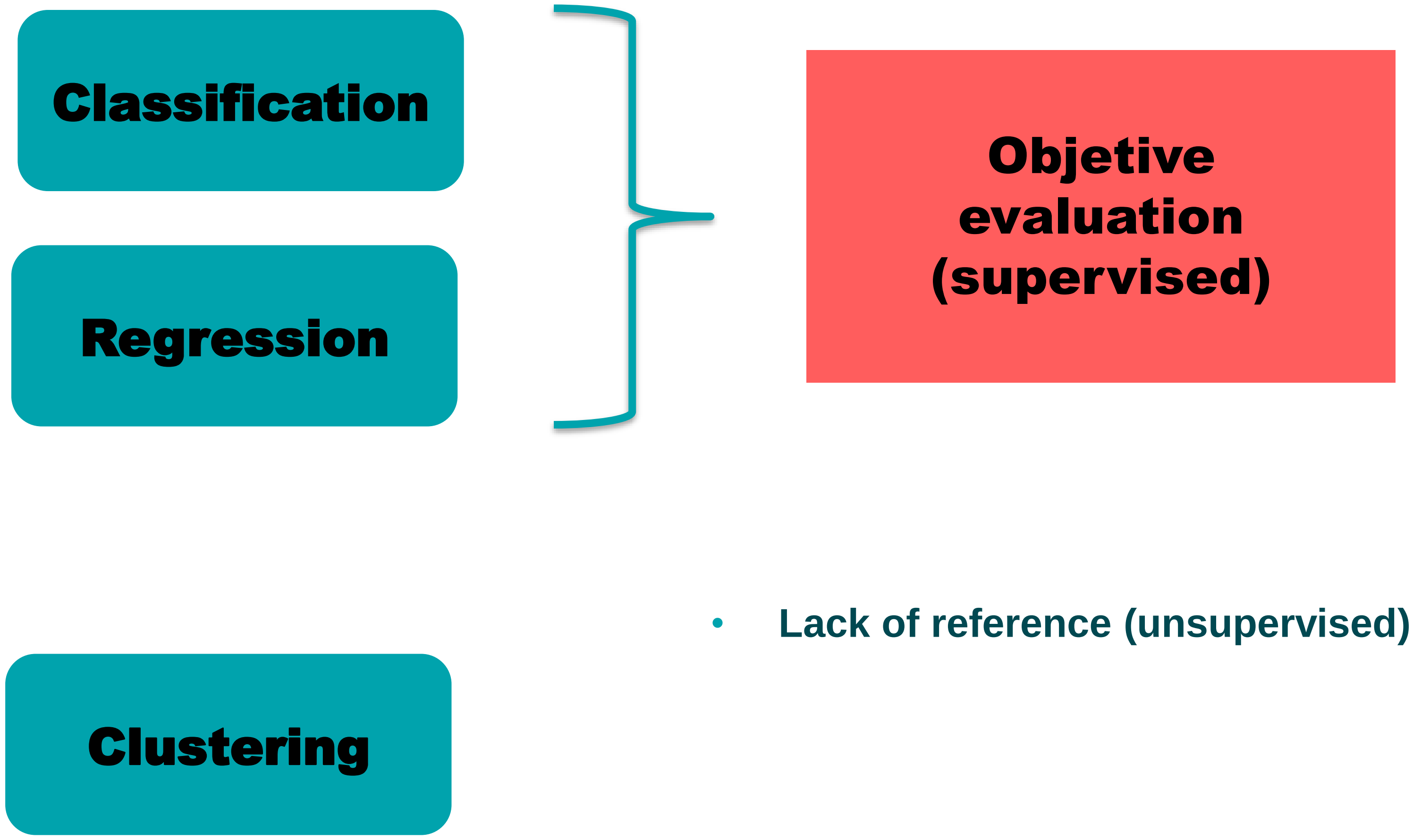
Regression

Objetive evaluation (supervised)

Clustering

?

Validation



- Lack of reference (unsupervised)

Validation

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Classification

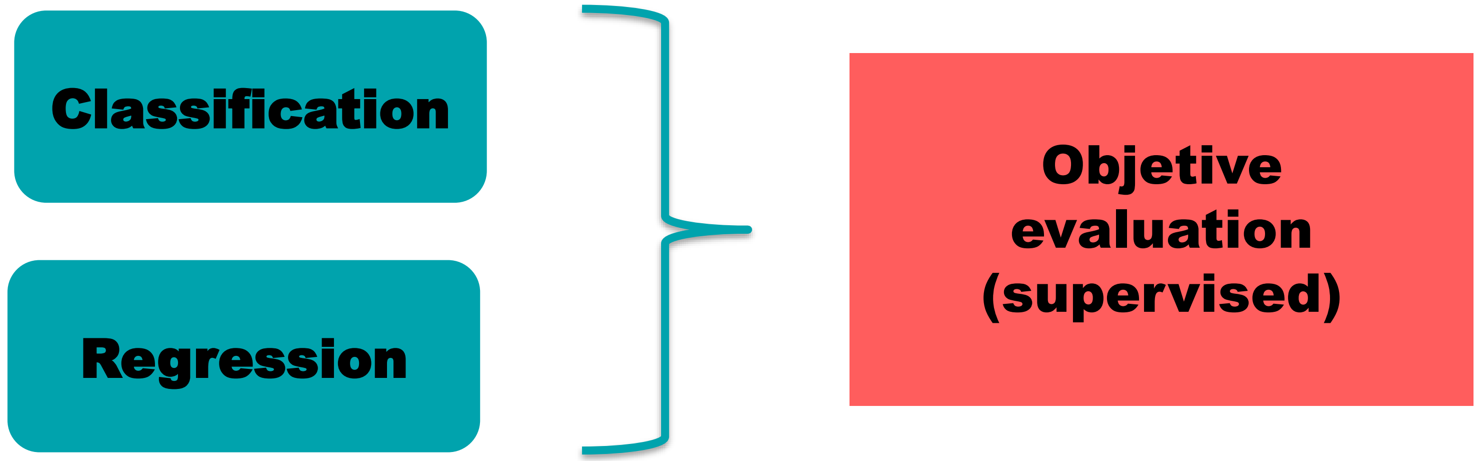
Regression

Objective evaluation (supervised)

Clustering

- Lack of reference (unsupervised)
- Subjetivity of goodness

Validation



Clustering

- Lack of reference (unsupervised)
- Subjetivity of goodness
- Dependency on the similarity measure

Validation

Key questions

Validation

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Key questions:

- Which is the most adequate **algorithm** for my problem?

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Key questions:

- Which is the most adequate **algorithm** for my problem?
- Which is the right **similarity measure**?
- If I have to do it by myself, how do I decide the **amount of clusters**?
- How do I evaluate the **quality of a solution** in a clustering problem?

Validation

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Key questions:

- Which is the most adequate **algorithm** for my problem?
- Which is the right **similarity measure**?
- If I have to do it by myself, how do I decide the **amount of clusters**?
- How do I evaluate the **quality of a solution** in a clustering problem?
- Which **data preprocessing scheme** would contribute to a better result?

Validation

Global answer:

“It depends…”

Validation

Global answer:

“It depends on the chosen way for evaluation.

Usually the right option is searched by a simple trial and error approach”.

Validation

Indices taxonomy

Validation

Indices taxonomy:

- **External indices**: Available external information is used. For instance, if information about classes is known, an (unsupervised) clustering algorithm can be evaluated checking how the underlying class distributions are represented by the clusters.

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Indices taxonomy:

- **External indices**: Available external information is used. For instance, if information about classes is known, an (unsupervised) clustering algorithm can be evaluated checking how the underlying class distributions are represented by the clusters.

- **Internal indices**: Only internal information is used. For instance, checking how homogeneous each of the clusters is (*intra-group homogeneity*), and how heterogeneous different clusters are (*inter-group heterogeneity*).

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- **External indices**: Available external information is used. For instance, if information about classes is known, an (unsupervised) clustering algorithm can be evaluated checking how the underlying class distributions are represented by the clusters.

- **Internal indices**: Only internal information is used. For instance, checking how homogeneous each of the clusters is (*intra-group homogeneity*), and how heterogeneous different clusters are (*inter-group heterogeneity*).

- **Relative indices**: They adapt the previous ones for comparing pairs of solutions for the same clustering problem. They are out of the scope of this lecture.

Adjusted Rand Index

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- **External** index, which needs to know the classes of the samples
- It is assumed that belonging to a cluster is equivalent to being in a class
- All "classifications" are compared
- It is a **symmetrical** score, thus it could be used for measuring **consensus**
- It takes values in [-1, 1]
- A **perfect consensus** gives a score 1, and the expectation in a **random clustering** would be 0. Negative or null values are considered bad scores

- Use in scikit-learn:

```
from sklearn.metrics import adjusted_rand_score
ars = adjusted_rand_score(labels_true, labels_pred)
```

Scores related with mutual information

- Three variants:
  - **Mutual Information Score**: Uses the original definition of mutual information. It suffers with high amounts of clusters.
  - **Normalized Mutual Information Score**: Normalizes using the average of both entropies. This normalization does not alleviate the multi-cluster problem.
  - **Adjusted Mutual Information Score**: Normalizes fixing the aforementioned problem.

- **External** index, which needs to know the classes of the samples
- It is assumed that belonging to a cluster is equivalent to being in a class
- All “classifications” are compared using mutual information, which is a simmetric measure
- It is a **symmetrical** score, thus it could be used for measuring **consensus**
- It takes values in (-∞, 1]
- A **perfect consensus** gives a score 1, and the expectation in a **random clustering** would be 0. Negative or null values are considered bad scores

- Uses in scikit-learn:

```
from sklearn import metrics
mis = metrics.mutual_info_score(labels_true, labels_pred)
nmis = metrics.normalized_mutual_info_score(labels_true, labels_pred)
amis = metrics.adjusted_mutual_info_score(labels_true, labels_pred)
```

Homogeneity, completeness and v-measure

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- Two properties, three scores:
  - **Homogeneity**: Each cluster contains members of one single class.
  - **Completeness**: All members of a class are in the same cluster.
  - **V-measure**: Armonic mean of both, which combines both in a balanced way.

- **External** index, which needs to know the classes of the samples
- It is assumed that belonging to a cluster is equivalent to being in a class
- Only v-measure is a **symmetrical** score, thus it is the only one to be used for measuring **consensus**
- Homogeneity and completeness take values in [0, 1], being the higher the better.
- A **perfect consensus** gives a v-score 1. The expectation in a **random clustering** can take different values.
- Obs: For low number of samples or many clusters, *adjusted* type is the right choice.

- Uses in scikit-learn:

```
from sklearn import metrics
hs = metrics.homogeneity_score(labels_true, labels_pred)
cs = metrics.completeness_score(labels_true, labels_pred)
vms = metrics.v_measure_score(labels_true, labels_pred)
hcvm = metrics.homogeneity_completeness_v_measure(labels_true, labels_pred)
```

Fowlkes-Mallows Index

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- **External** index, which needs to know the classes of the samples

- They are defined:
  - **True Positive(TP)**: Number of pairs of points belonging to the same clusters, both in the true and the predicted values
  - **False Positive (FP)**: Number of pairs of points belonging to the same clusters in the true values, but not in the predicted ones
  - **False Negative (FN)**: Number of pairs of points belonging to the same clusters in the predicted values, but not in the true ones

- The Fowlkes-Mallows Index is defined as the geometric mean of precision and recall:

$$FMI = \frac{TP}{\sqrt{(TP + FP)(TP + FN)}}$$

- It takes values in [0, 1], being the higher the better. In the case of **random clustering** the expectation would be close to 0. An exact 0 value would imply purely independent classifications, and 1 would be an indication of both classifications being the same (except permutations).

- Use in scikit-learn:

```
from sklearn.metrics import fowlkes_mallows_score
fms = fowlkes_mallows_score(labels_true, labels_pred)
```

Contingency matrix

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- It is an **external measure** (not an index) that precises to know the classes of the samples, which are considered as clusters by themselves
- It includes, for the pairs of clusters (predicted and true), an intersection level
- Example:

$$label\_true = [‘a’, ‘a’, ‘a’, ‘b’, ‘b’, ‘b’]$$
$$label\_pred = [’D’, ’D’, ’E’, ’E’, ’F’, ’F’]$$
$$cm = \begin{pmatrix} 2 & 1 & 0 \\ 0 & 1 & 2 \end{pmatrix}$$

- Use in scikit-learn:

```
from sklearn.metrics.cluster import contigency_matrix
cm = contigency_matrix(labels_true, labels_pred)
```

Contingency matrix

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Of the 3 true samples in ‘a’

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Of the 3 true samples in 'a',
2 have been predicted in 'D'

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Contingency matrix

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$$cm = \begin{pmatrix} \boxed{2} & \boxed{1} & 0 \\ 0 & 1 & 2 \end{pmatrix}$$

Of the 3 true samples in ‘a’,
2 have been predicted in ‘D’,
1 in ‘E’

- Use in scikit-learn:

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```

Contingency matrix

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Of the 3 true samples in ‘a’,
2 have been predicted in ‘D’,
1 in ‘E’ and 0 in ‘F’

- Use in scikit-learn:

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```

Contingency matrix

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- Example:

$$label\_true = [\text{‘a’}, \text{‘a’}, \text{‘a’}, \boxed{\text{‘b’}, \text{‘b’}, \text{‘b’}}]$$
$$label\_pred = [\text{’D’}, \text{’D’}, \text{’E’}, \text{’E’}, \text{’F’}, \text{’F’}]$$
$$cm = \begin{pmatrix} 2 & 1 & 0 \\ \boxed{0} & 1 & 2 \end{pmatrix}$$

Of the 3 true samples in ‘b’,
0 have been predicted in ‘D’

- Use in scikit-learn:

```
from sklearn.metrics.cluster import contigency_matrix
cm = contigency_matrix(labels_true, labels_pred)
```

Contingency matrix

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- It includes, for the pairs of clusters (predicted and true), an intersection level
- Example:

$$label\_true = [\text{'a'}, \text{'a'}, \text{'a'}, \boxed{\text{'b'}, \text{'b'}, \text{'b'}}]$$
$$label\_pred = [\text{'D'}, \text{'D'}, \text{'E'}, \text{'E'}, \text{'F'}, \text{'F'}]$$
$$cm = \begin{pmatrix} 2 & 1 & 0 \\ \boxed{0} & \boxed{1} & 2 \end{pmatrix}$$

Of the 3 true samples in 'b',
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1 in 'E'

- Use in scikit-learn:

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```

Contingency matrix

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Of the 3 true samples in ‘b’,
0 have been predicted in ‘D’,
1 in ‘E’ and 2 in ‘F’

- Use in scikit-learn:

```
from sklearn.metrics.cluster import contigency_matrix
cm = contigency_matrix(labels_true, labels_pred)
```

Silhouette Coefficient

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- It is an **internal index** that only needs the model itself
- They are defined:
  - **a**: Average distance between a sample and the rest of points of the same cluster
  - **b**: Average distance between a sample and the points of the closest cluster
- The Silhouette Coefficient (SC) is defined, for a single sample, as:

$$s = \frac{b - a}{\max(a, b)}$$

- For the whole set, the average SC for all samples is calculated.
- It takes values in [-1, 1], being the higher the better (i.e. clusters being more dense and better separated). Scores close to 0 indicate clusters overlapping
- Obs: If we use SC for comparing different clustering solutions provided by different clustering methods, we should take into account that SC is generally higher for convex clusters. Be careful when comparing clustering solutions coming from density-based methods with others, thus the latter tend to generate non-convex clusters.
- Use in scikit-learn:

```
from sklearn.metrics import silhouette_score
ss = silhouette_score(X, labels, metric='euclidean')      [X contains data (by default)]
ss = silhouette_score(X, labels, metric='precomputed')   [X contains pairwise distances]
```

Calinski-Harabaz Index

- It is an **internal index** that only needs the model itself
- It is also known as **Variance Ratio Criterion**, because it is defined as the ratio between the average variance between clusters and the internal dispersion inside them
- The higher it is, the more dense and disperse clusters are, thus better the clusters collection
- It is fast to calculate
- Obs: If we use it for comparing different clustering solutions provided by different clustering methods, we should take into account that it is generally higher for convex clusters. Be careful when comparing clustering solutions coming from density-based methods with others, thus the latter tend to generate non-convex clusters. Besides, the use of centroids forces us to use Euclidean distancies.
- Use in scikit-learn:

```
from sklearn.metrics import calinski_harabaz_score
dbs = calinski_harabaz_score(X, labels)
```

Davies-Bouldin Index

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- It is an **internal index** that only needs the model itself

- It is defined a similarity measure between clusters C_i and C_j, denoted by R_{ij}, which takes into account:
  - s_i: average distance between each point in cluster C_i and its centroid (diameter)
  - d_{ij}: the distance between the centroids of both clusters

- In the original paper, the similarity measure was defined as

$$R_{ij} = \frac{s_i + s_j}{d_{ij}}$$

- Then, the Davies-Bouldin Indexis defined as

$$DB = \frac{1}{k} \sum_{i=1}^{k} \max_{i \neq j} R_{ij}$$

- The lower the index, the better the clusters collection. The lower possible value is 0.

- It is faster to be calculated than Silhouette Coefficient

- Obs: If we use it for comparing different clustering solutions provided by different clustering methods, we should take into account that it is generally higher for convex clusters. Be careful when comparing clustering solutions coming from density-based methods with others, thus the latter tend to generate non-convex clusters. Besides, the use of centroids forces us to use Euclidean distancies.

- Use in scikit-learn:

```
from sklearn.metrics import davies_bouldin_score
dbs = davies_bouldin_score(X, labels)
```

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Eskerrik asko

Muchas gracias

Thank you

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