Unsupervised Learning – Part 4

ESM3081 Programming for Data Science

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Learning algorithms covered in this course

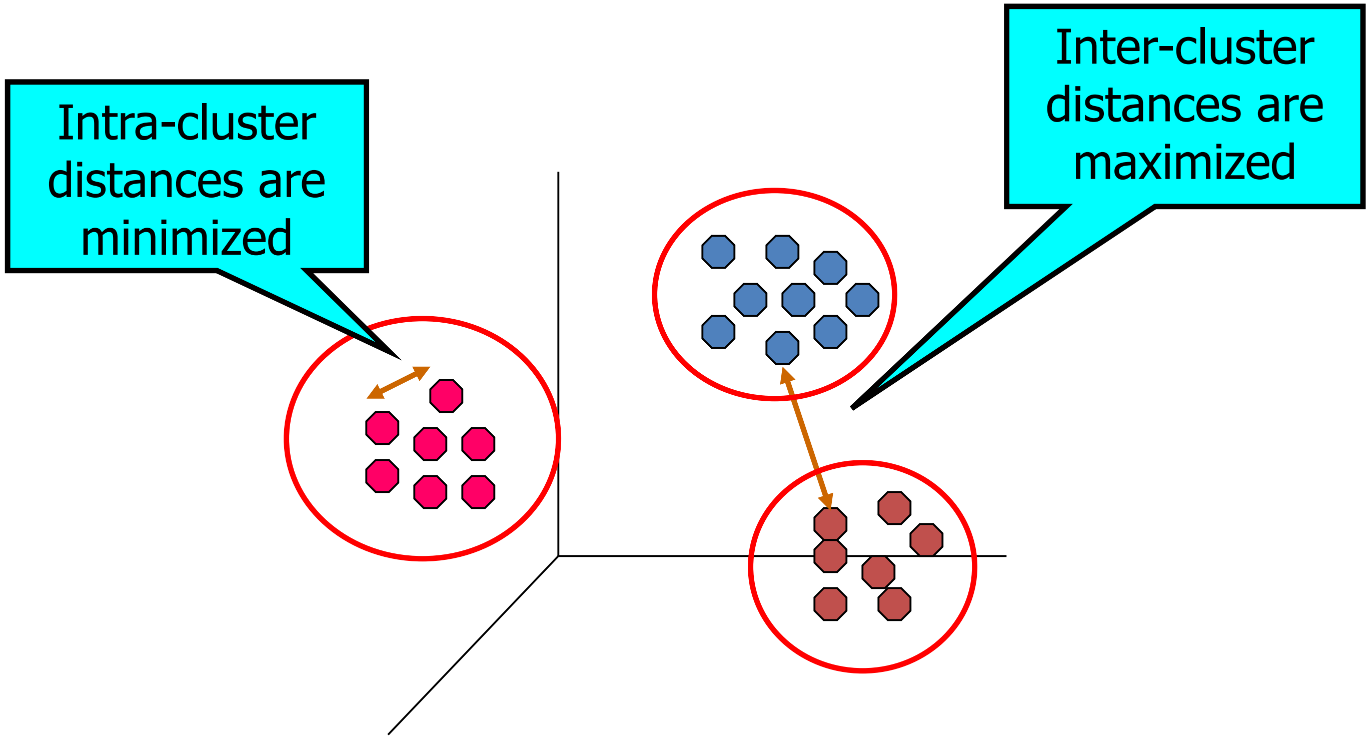
- **Data Preprocessing and Scaling**

- **Unsupervised Learning**
  - **Dimensionality Reduction & Visualization**
    - (Projection) Principal Component Analysis (PCA)
    - (Manifold Learning) t-distributed Stochastic Neighbor Embedding (t-SNE)
    - …
  - **Clustering**
    - **K-Means**
    - **Hierarchical Clustering**
    - DBSCAN
    - …

K-Means Clustering

Clustering

- ***Clustering*** **is the task of partitioning the dataset into groups, called clusters.**
  - The goal is to split up the data in such a way that points within a single cluster are very similar and points in different clusters are different.
  - Clustering is an exploratory tool, and is useful only when it produces meaningful clusters.
  - Data may not have definitive “real” clusters, so we need to be wary of chance results.
  - **Applications of Clustering:** *Data Understanding and Summarization (Compression)*


Intra-cluster distances are minimized
Inter-cluster distances are maximized

K-Means Clustering

- ***k*-means clustering finds *k cluster centers* that are representative of certain regions of the data based on an expectation-maximization procedure.**

  Given a (training) dataset $D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\}$ such that $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{id}) \in \mathbb{R}^d$ is the *i*-th input vector of *d* features

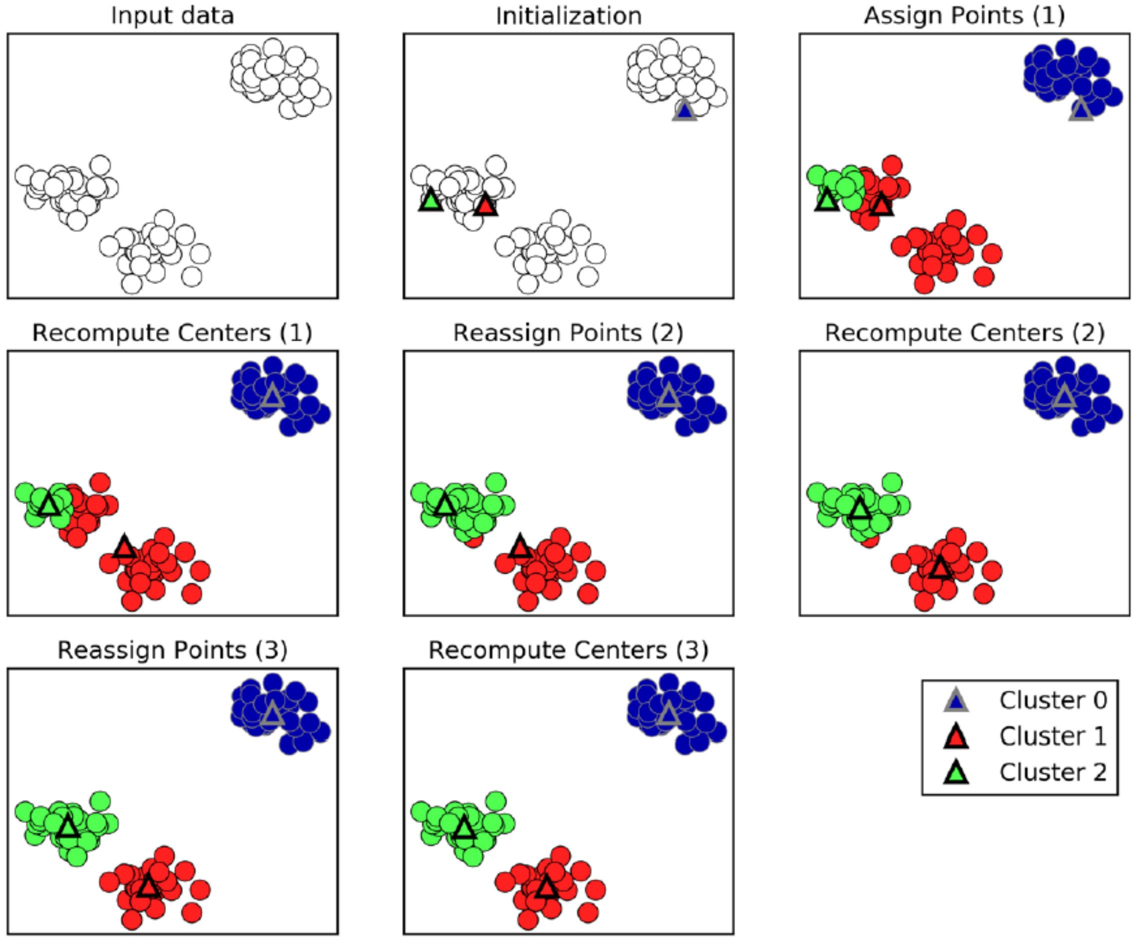
  1. The algorithm starts by selecting *k* points as the initial cluster centers.
  2. Then, alternates between two steps. It is finished when the assignment of data points to clusters no longer changes.
     - **(Expectation)** Assigning each data point to the closest cluster centers
     - **(Maximization)** Setting each cluster center as the mean of the data points that are assigned to it

       * Euclidean distance is used by default.

K-Means Clustering

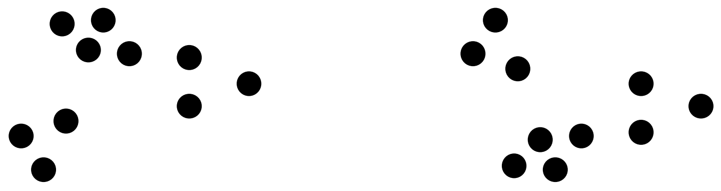
- **Example of *k*-means clustering**

  Example: Cluster centers are shown as triangles, while data points are shown as circles, Colors indicate cluster membership, We are looking for three clusters (k=3).

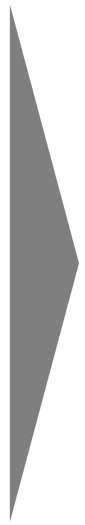


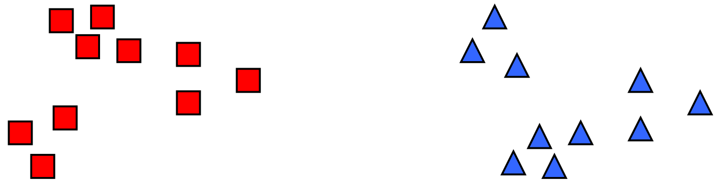
K-Means Clustering

- **Main hyperparameter**: the number of clusters *k*
  - Notion of a cluster can be ambiguous

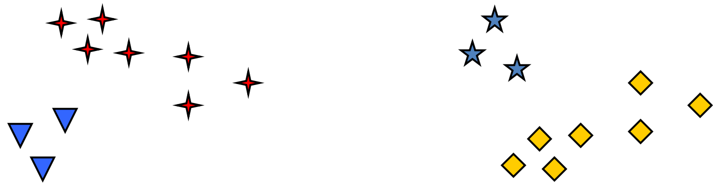


How many clusters?

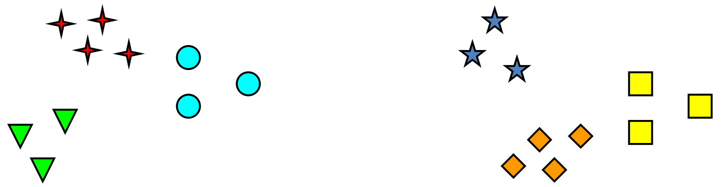




Two Clusters



Four Clusters

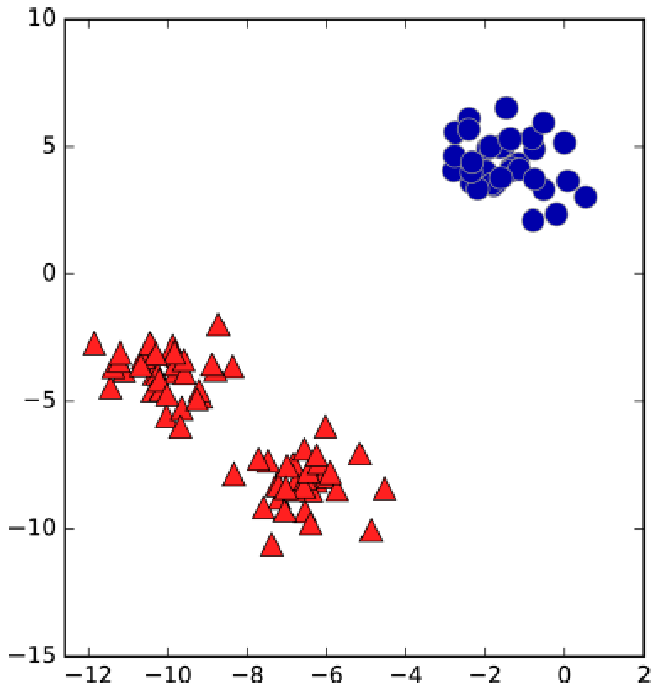


Six Clusters

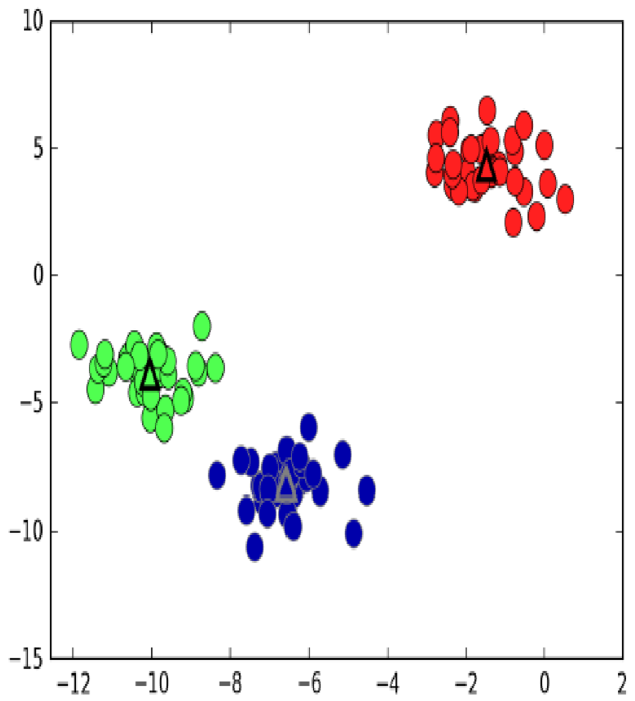
K-Means Clustering

- **Main hyperparameter**: the number of clusters *k*
  - The effect of the hyperparameter *k* (n_clusters)

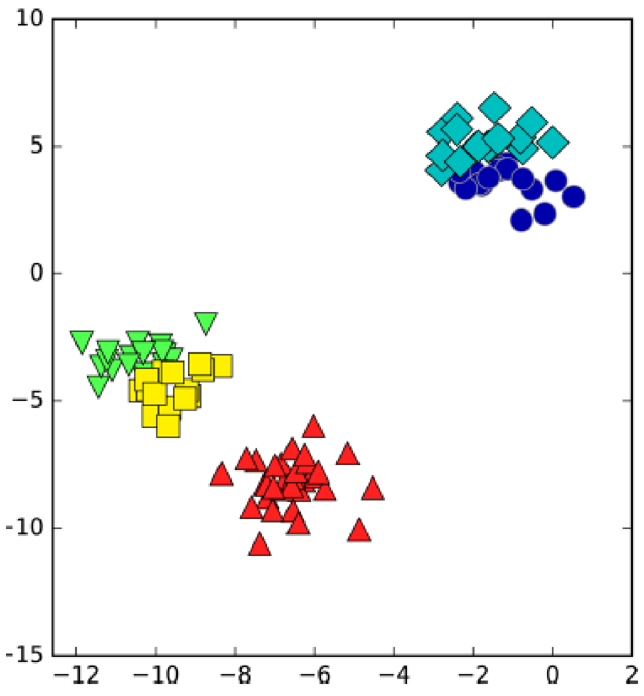
    Example: Cluster assignments and cluster centers found by k-means with different numbers of clusters



k = 2



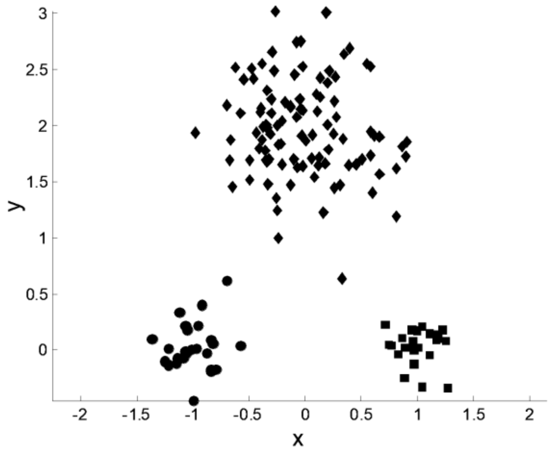
k = 3



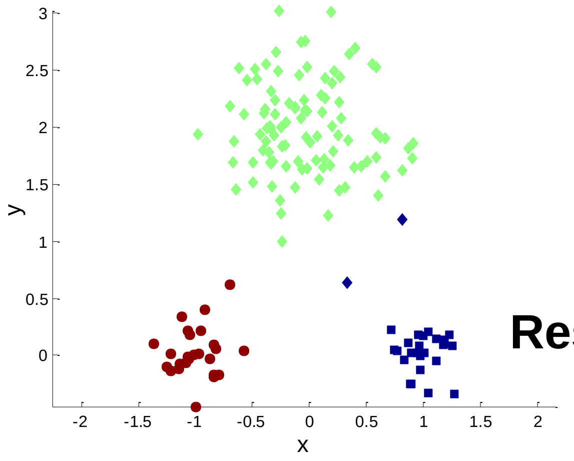
k = 5

K-Means Clustering

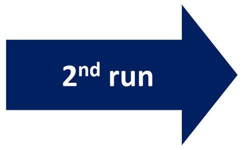
- **The effect of random initialization**
  - It is recommended to run the algorithm multiple times with different random initializations, and returns the best result.

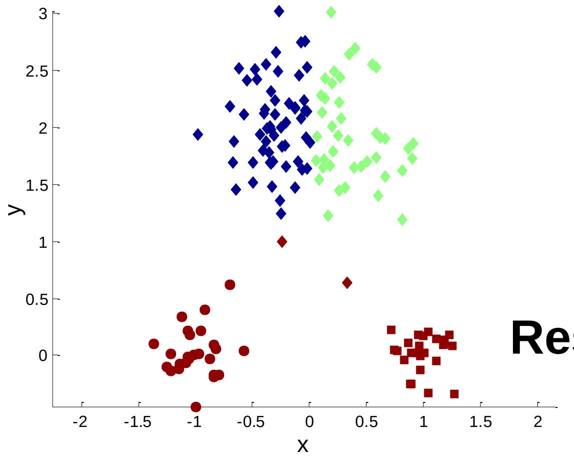


Original Points



Result 1

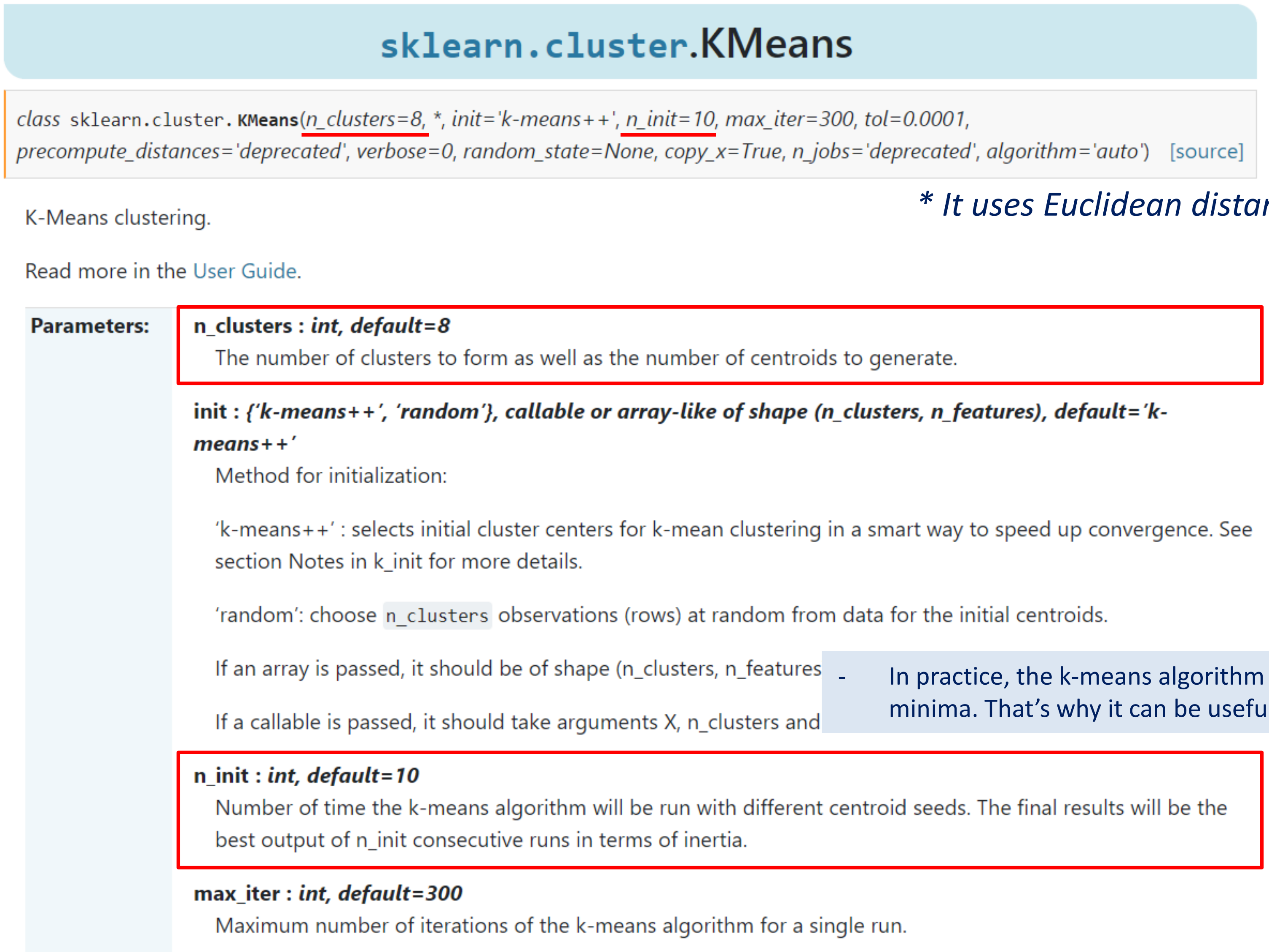




Result 2

scikit-learn Practice: *KMeans*

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html



sklearn.cluster.KMeans

class `sklearn.cluster.KMeans`(*n_clusters=8, *, init='k-means++', n_init=10, max_iter=300, tol=0.0001, precompute_distances='deprecated', verbose=0, random_state=None, copy_x=True, n_jobs='deprecated', algorithm='auto'*) [source]

K-Means clustering.

Read more in the User Guide.

Parameters:

n_clusters : *int, default=8*
The number of clusters to form as well as the number of centroids to generate.

init : *{'k-means++', 'random'}, callable or array-like of shape (n_clusters, n_features), default='k-means++'*
Method for initialization:

'k-means++' : selects initial cluster centers for k-mean clustering in a smart way to speed up convergence. See section Notes in k_init for more details.

'random': choose `n_clusters` observations (rows) at random from data for the initial centroids.

If an array is passed, it should be of shape (n_clusters, n_features

If a callable is passed, it should take arguments X, n_clusters and

n_init : *int, default=10*
Number of time the k-means algorithm will be run with different centroid seeds. The final results will be the best output of n_init consecutive runs in terms of inertia.

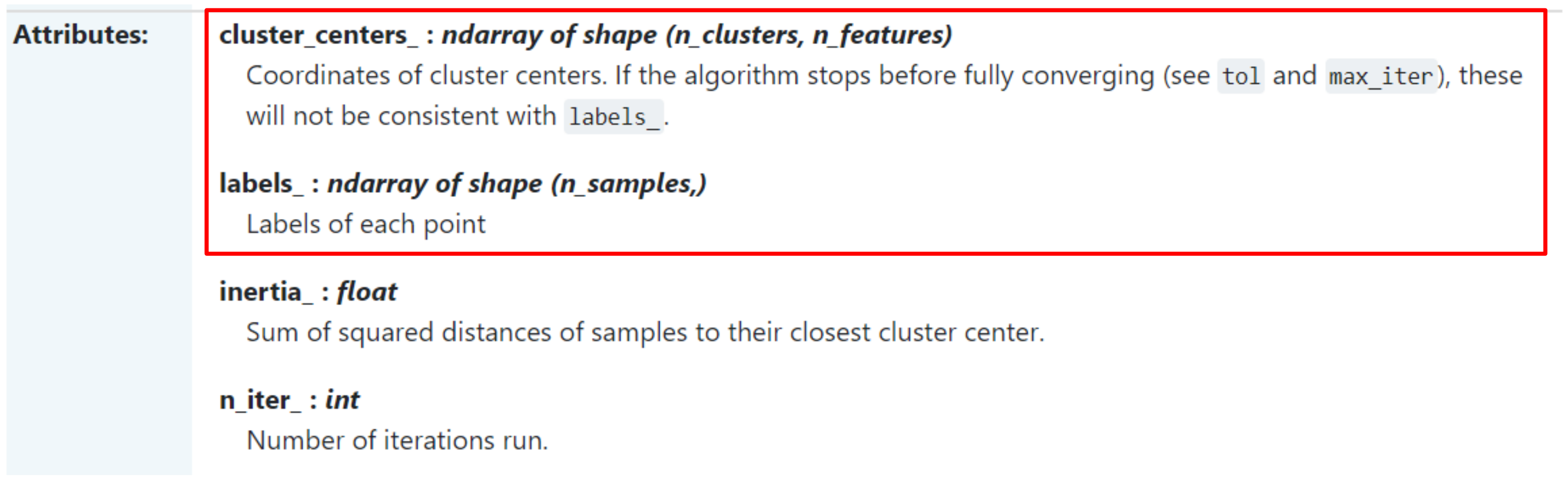
max_iter : *int, default=300*
Maximum number of iterations of the k-means algorithm for a single run.

** It uses Euclidean distance by default*

- In practice, the k-means algorithm is very fast, but it falls in local minima. That's why it can be useful to restart it several times.

scikit-learn Practice: *KMeans*

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html



Attributes:

cluster_centers_ : *ndarray of shape (n_clusters, n_features)*

Coordinates of cluster centers. If the algorithm stops before fully converging (see `tol` and `max_iter`), these will not be consistent with `labels_`.

labels_ : *ndarray of shape (n_samples,)*

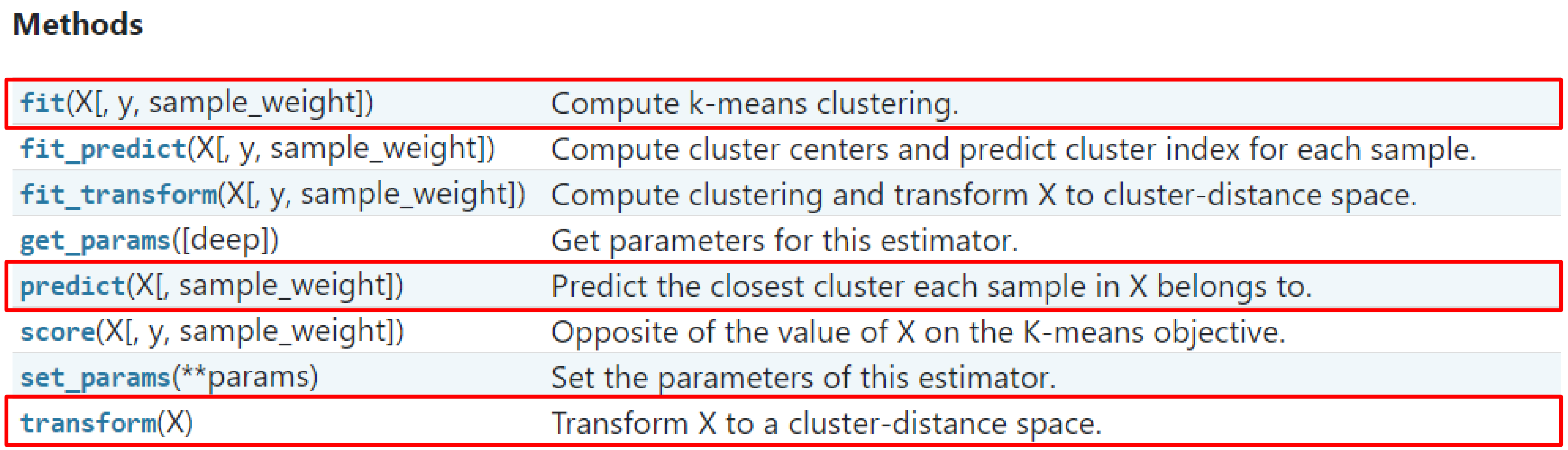
Labels of each point

inertia_ : *float*

Sum of squared distances of samples to their closest cluster center.

n_iter_ : *int*

Number of iterations run.



Methods

`fit`(X[, y, sample_weight])	Compute k-means clustering.
`fit_predict`(X[, y, sample_weight])	Compute cluster centers and predict cluster index for each sample.
`fit_transform`(X[, y, sample_weight])	Compute clustering and transform X to cluster-distance space.
`get_params`([deep])	Get parameters for this estimator.
`predict`(X[, sample_weight])	Predict the closest cluster each sample in X belongs to.
`score`(X[, y, sample_weight])	Opposite of the value of X on the K-means objective.
`set_params`(**params)	Set the parameters of this estimator.
`transform`(X)	Transform X to a cluster-distance space.

scikit-learn Practice: *KMeans*

- **Example (*blobs* dataset)**

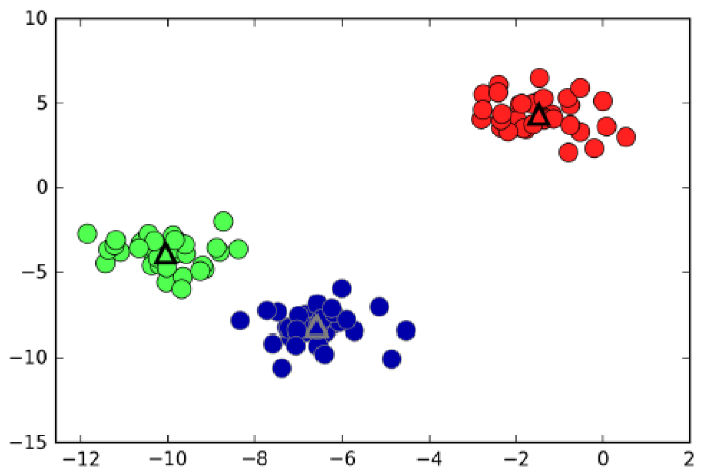
```
In [2]: from sklearn.datasets import make_blobs
        from sklearn.cluster import KMeans

        X_train, _ = make_blobs(random_state=1)
        print('X_train.shape:', X_train.shape)

        X_train.shape: (100, 2)
```

```
In [3]: kmeans = KMeans(n_clusters=3)
        kmeans.fit(X_train)

Out[3]: ▾        KMeans
        KMeans(n_clusters=3)
```

```
In [4]: print(kmeans.cluster_centers_)

        [[ -6.58197   -8.17239]
         [ -1.47108    4.33722]
         [-10.04935   -3.85954]]
```

```
In [5]: assignments_X_train = kmeans.labels_
        print(assignments_X_train)

        [1 2 2 2 0 0 0 2 1 1 2 2 0 1 0 0 0 1 2 2 0 2 0 1 2 0 0 1 1 0 1 1 0 1 2 0 2
         2 2 0 0 2 1 2 2 0 1 1 1 1 2 0 0 0 1 0 2 2 1 1 2 0 0 2 2 0 1 0 1 2 2 2 0 1
         1 2 0 0 1 2 1 2 2 0 1 1 1 1 2 1 0 1 1 2 2 0 0 1 0 1]
```

```
In [6]: X_new, _ = make_blobs()

        assignments_X_new = kmeans.predict(X_new)
        print(assignments_X_new)

        [1 0 0 1 0 1 0 0 1 2 0 2 0 1 0 0 1 0 1 1 0 0 0 0 1 0 0 1 0 0 1 0 0 0 0 1 2
         0 1 0 1 0 1 1 0 1 0 1 0 0 1 1 0 0 0 1 1 0 1 0 1 1 1 0 0 1 1 0 0 0 0 0 0 0
         0 0 0 0 1 0 1 0 2 2 2 0 1 0 1 0 0 0 0 2 0 0 1 0 0 2]
```



scikit-learn Practice: *KMeans*

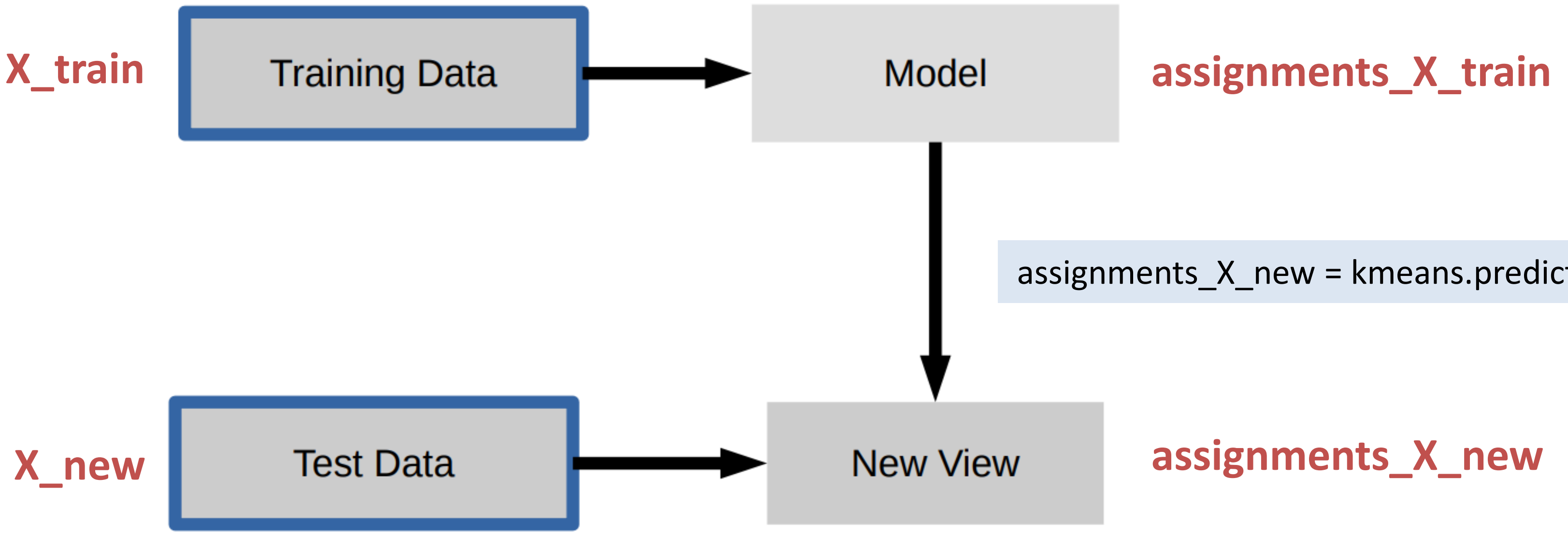
- **Example (*blobs* dataset)**

```
X_train, _ = make_blobs(random_state=1)
```

```
kmeans = KMeans(n_clusters=3)
kmeans.fit(X_train)
```

```
assignments_X_train = kmeans.labels_
```

```
assignments_X_new = kmeans.predict(X_new)
```

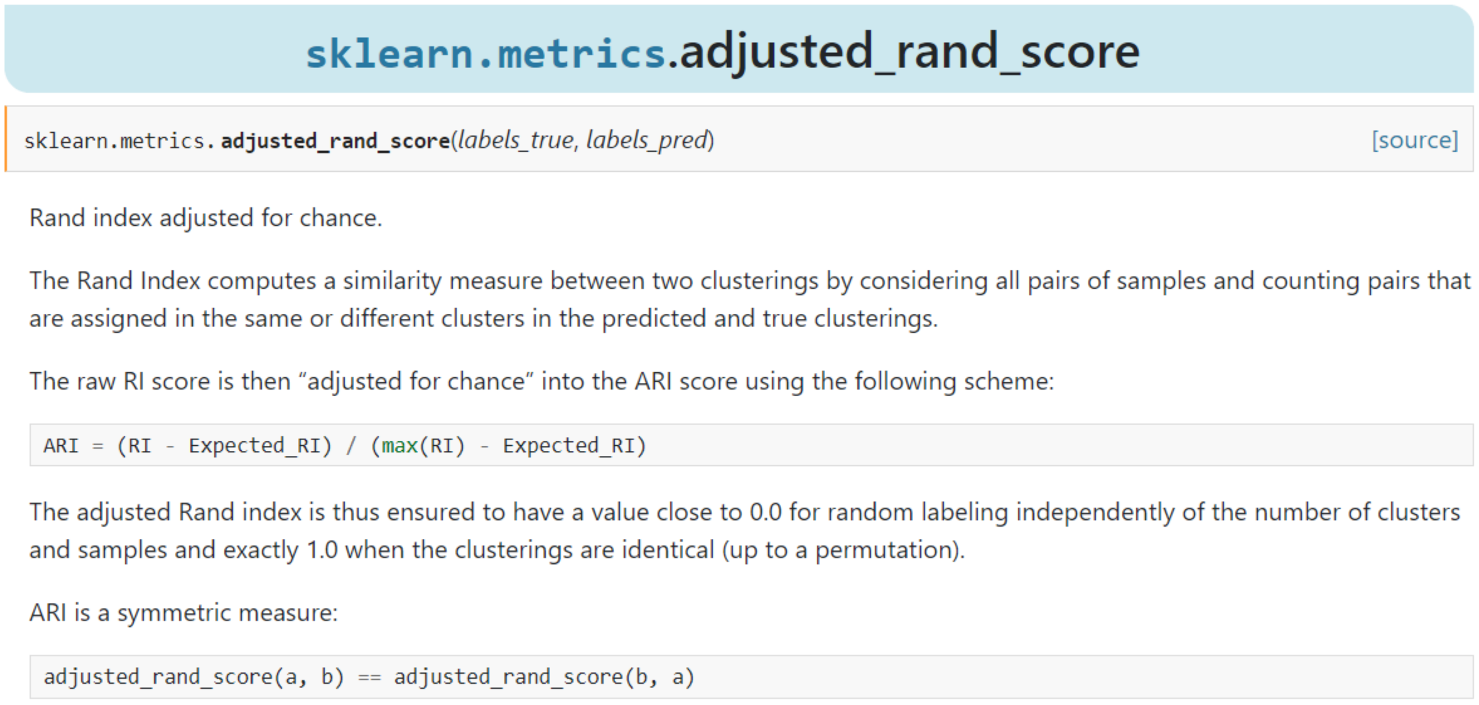


scikit-learn Practice: *KMeans*

https://scikit-learn.org/stable/modules/generated/sklearn.metrics.adjusted_rand_score.html

Given the knowledge of the ground truth class assignments **labels_true** and our clustering algorithm assignments of the same data points **labels_pred**, the **adjusted Rand index** is a function that measures the **similarity** of the two assignments

- Score between -1.0 and 1.0.
- Random labelings have an ARI close to 0.0.
- 1.0 stands for perfect match.



sklearn.metrics.adjusted_rand_score

`sklearn.metrics.adjusted_rand_score(labels_true, labels_pred)` [source]

Rand index adjusted for chance.

The Rand Index computes a similarity measure between two clusterings by considering all pairs of samples and counting pairs that are assigned in the same or different clusters in the predicted and true clusterings.

The raw RI score is then "adjusted for chance" into the ARI score using the following scheme:

```
ARI = (RI - Expected_RI) / (max(RI) - Expected_RI)
```

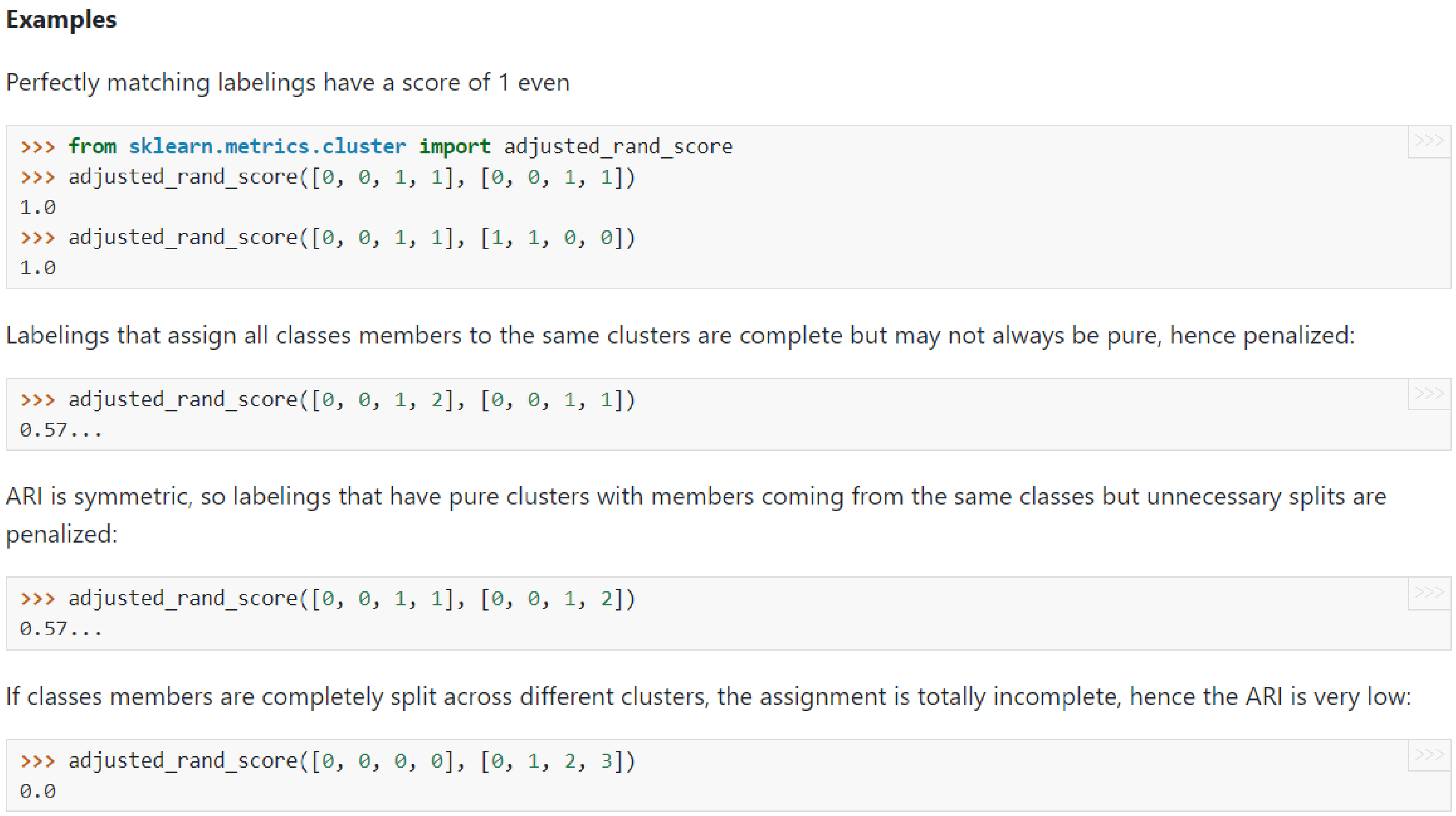
The adjusted Rand index is thus ensured to have a value close to 0.0 for random labeling independently of the number of clusters and samples and exactly 1.0 when the clusterings are identical (up to a permutation).

ARI is a symmetric measure:

```
adjusted_rand_score(a, b) == adjusted_rand_score(b, a)
```

scikit-learn Practice: *KMeans*

https://scikit-learn.org/stable/modules/generated/sklearn.metrics.adjusted_rand_score.html



Examples

Perfectly matching labelings have a score of 1 even

```
>>> from sklearn.metrics.cluster import adjusted_rand_score
>>> adjusted_rand_score([0, 0, 1, 1], [0, 0, 1, 1])
1.0
>>> adjusted_rand_score([0, 0, 1, 1], [1, 1, 0, 0])
1.0
```

Labelings that assign all classes members to the same clusters are complete but may not always be pure, hence penalized:

```
>>> adjusted_rand_score([0, 0, 1, 2], [0, 0, 1, 1])
0.57...
```

ARI is symmetric, so labelings that have pure clusters with members coming from the same classes but unnecessary splits are penalized:

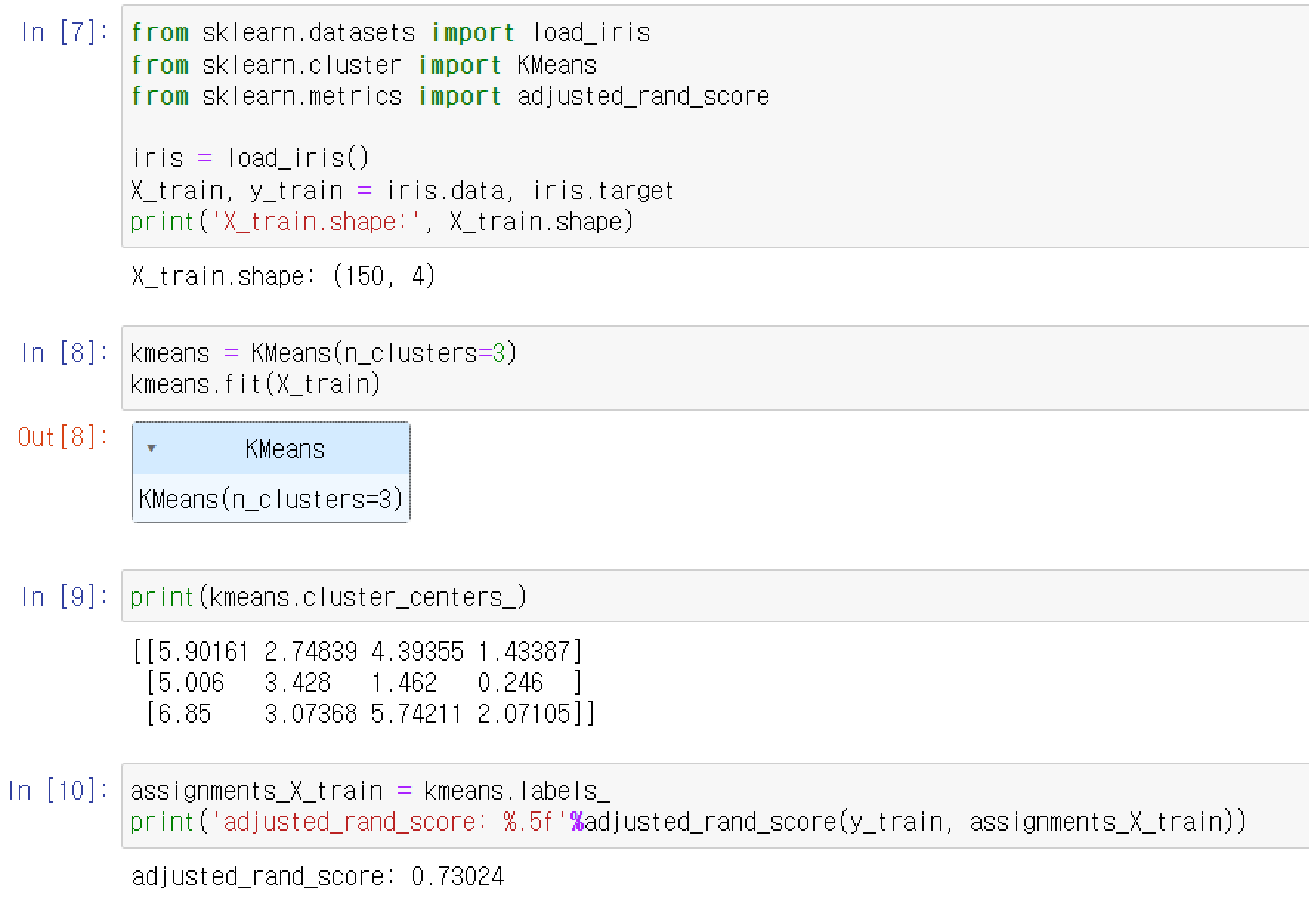
```
>>> adjusted_rand_score([0, 0, 1, 1], [0, 0, 1, 2])
0.57...
```

If classes members are completely split across different clusters, the assignment is totally incomplete, hence the ARI is very low:

```
>>> adjusted_rand_score([0, 0, 0, 0], [0, 1, 2, 3])
0.0
```

scikit-learn Practice: *KMeans*

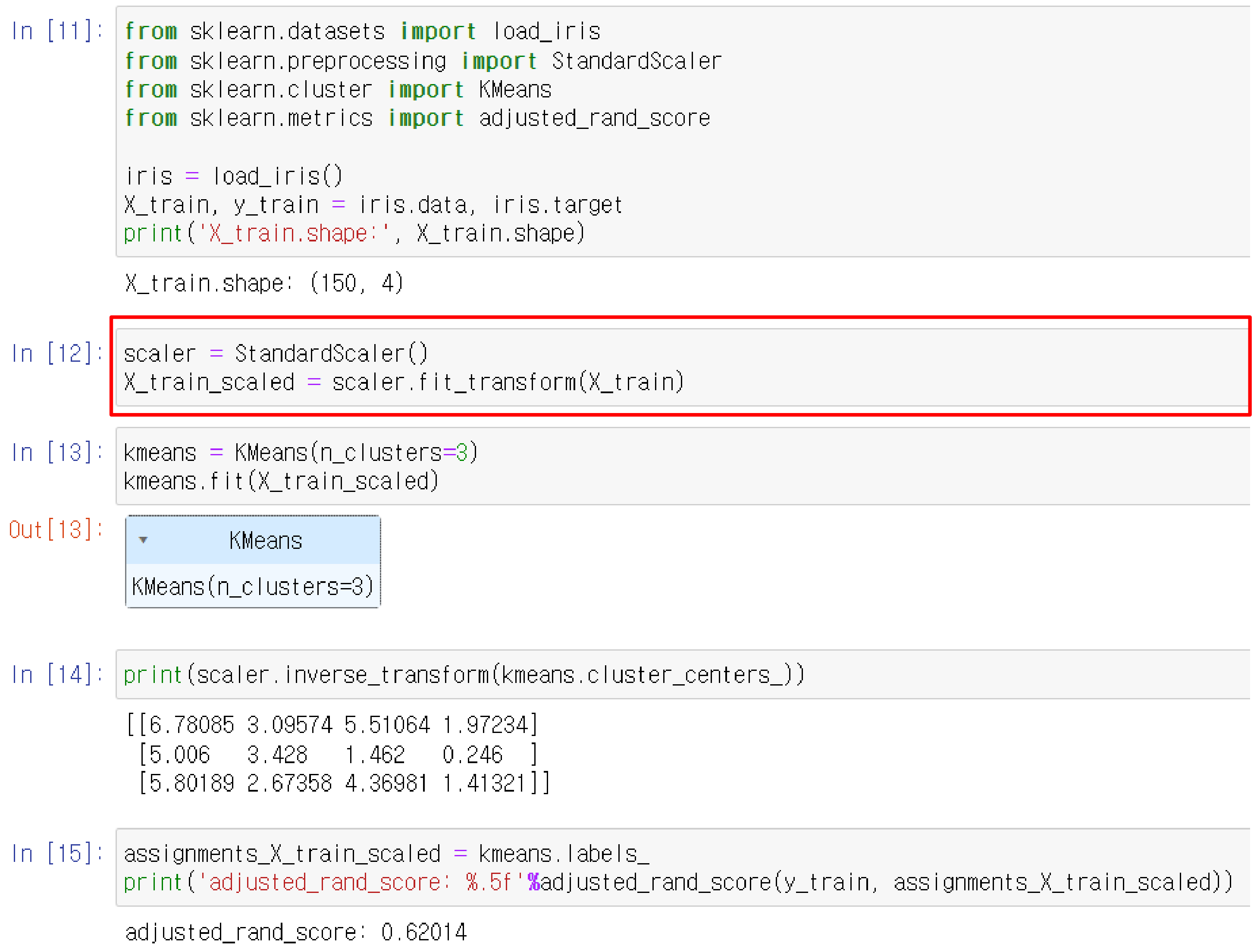
- **Example (*iris* dataset)**



```
In [7]: from sklearn.datasets import load_iris
        from sklearn.cluster import KMeans
        from sklearn.metrics import adjusted_rand_score

        iris = load_iris()
        X_train, y_train = iris.data, iris.target
        print('X_train.shape:', X_train.shape)

        X_train.shape: (150, 4)

In [8]: kmeans = KMeans(n_clusters=3)
        kmeans.fit(X_train)

Out[8]: ▾ KMeans
        KMeans(n_clusters=3)

In [9]: print(kmeans.cluster_centers_)

        [[5.90161 2.74839 4.39355 1.43387]
         [5.006   3.428   1.462   0.246  ]
         [6.85    3.07368 5.74211 2.07105]]

In [10]: assignments_X_train = kmeans.labels_
         print('adjusted_rand_score: %.5f'%adjusted_rand_score(y_train, assignments_X_train))

         adjusted_rand_score: 0.73024
```

scikit-learn Practice: *KMeans*

- **Example (*iris* dataset)**



```
In [11]: from sklearn.datasets import load_iris
         from sklearn.preprocessing import StandardScaler
         from sklearn.cluster import KMeans
         from sklearn.metrics import adjusted_rand_score

         iris = load_iris()
         X_train, y_train = iris.data, iris.target
         print('X_train.shape:', X_train.shape)

         X_train.shape: (150, 4)
```

```
In [12]: scaler = StandardScaler()
         X_train_scaled = scaler.fit_transform(X_train)
```

```
In [13]: kmeans = KMeans(n_clusters=3)
         kmeans.fit(X_train_scaled)

Out[13]: ▾ KMeans
         KMeans(n_clusters=3)
```

```
In [14]: print(scaler.inverse_transform(kmeans.cluster_centers_))

         [[6.78085 3.09574 5.51064 1.97234]
          [5.006   3.428   1.462   0.246  ]
          [5.80189 2.67358 4.36981 1.41321]]
```

```
In [15]: assignments_X_train_scaled = kmeans.labels_
         print('adjusted_rand_score: %.5f'%adjusted_rand_score(y_train, assignments_X_train_scaled))

         adjusted_rand_score: 0.62014
```

Discussion

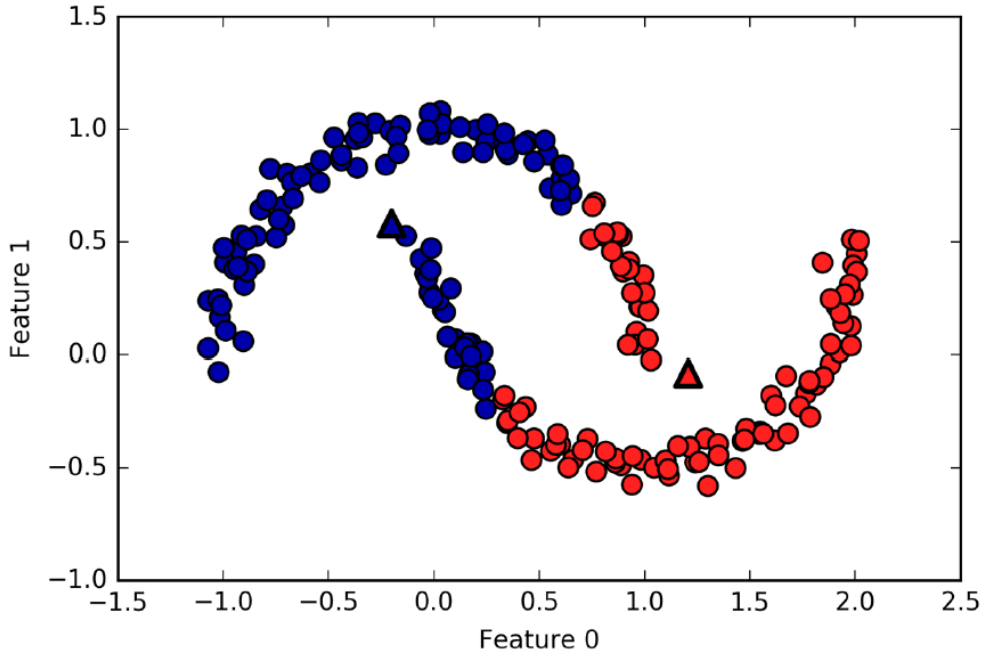
- **The main hyperparameters of K-Means**
  - *n_clusters (the number of clusters k), distance metric*

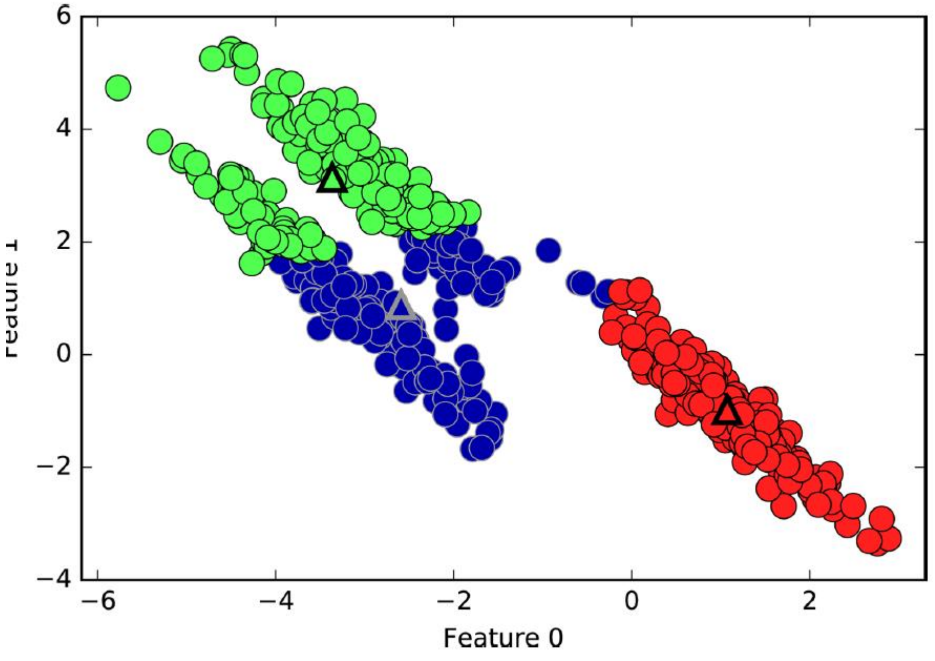
  * In scikit-learn, Euclidean distance is used by default.

  * It's important to preprocess your data (including *feature scaling* and *one-hot encoding*)
- **Strengths**
  - K-Means is relatively easy to understand and implement
  - It runs relatively quickly, and scales easily to large datasets
- **Weaknesses**
  - It relies on a random initialization, which means the outcome of the algorithm depends on a random seed.
  - It requires to specify the number of clusters you are looking for (which might not be known in a real-world application).
  - The performance depends highly on scaling of features.
  - The relatively restrictive assumptions are made on the shape of clusters.

Failure Cases of K-Means

- K-Means can only capture relatively simple (convex) shapes, as each cluster is defined solely by its center.
- K-Means fails to identify non-spherical or complex shaped clusters.
- Even if you know the “right” number of clusters for a given dataset, K-Means might not always be able to recover them.

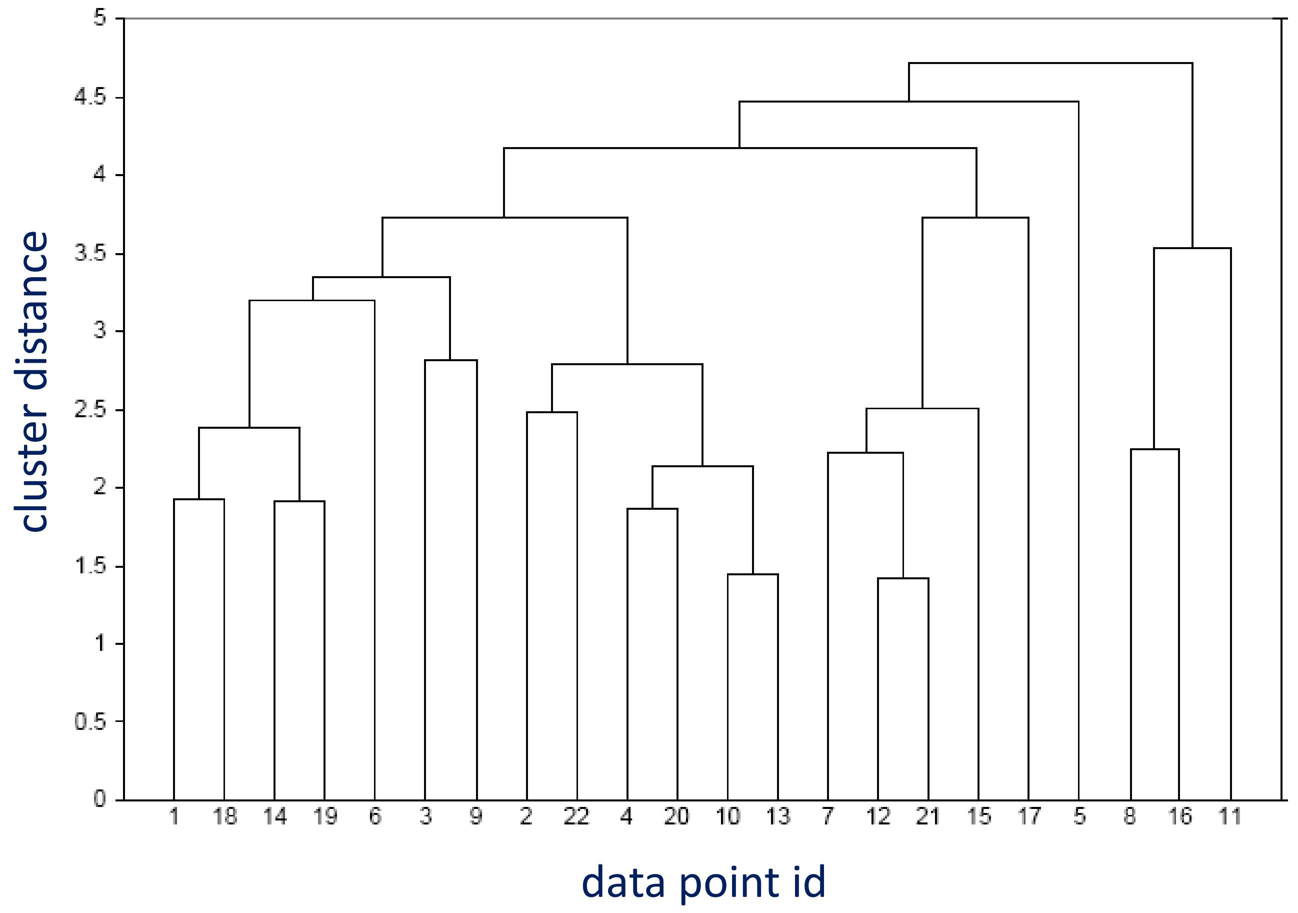




Hierarchical Clustering

Hierarchical Clustering

- **Hierarchical clustering produces a set of nested clusters organized as a hierarchical tree, which can be visualized as a dendrogram**
  - Dendrogram is a tree like diagram that records the sequences of merges or splits



Hierarchical Clustering

- **Two main types of hierarchical clustering**
  - **Agglomerative clustering (most popular)**
    - Start with the data points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - **Divisive clustering**
    - Start with one all-inclusive cluster (the entire dataset as a cluster)
    - At each step, split a cluster until each cluster contains an individual point (or there are k clusters)

Agglomerative Clustering

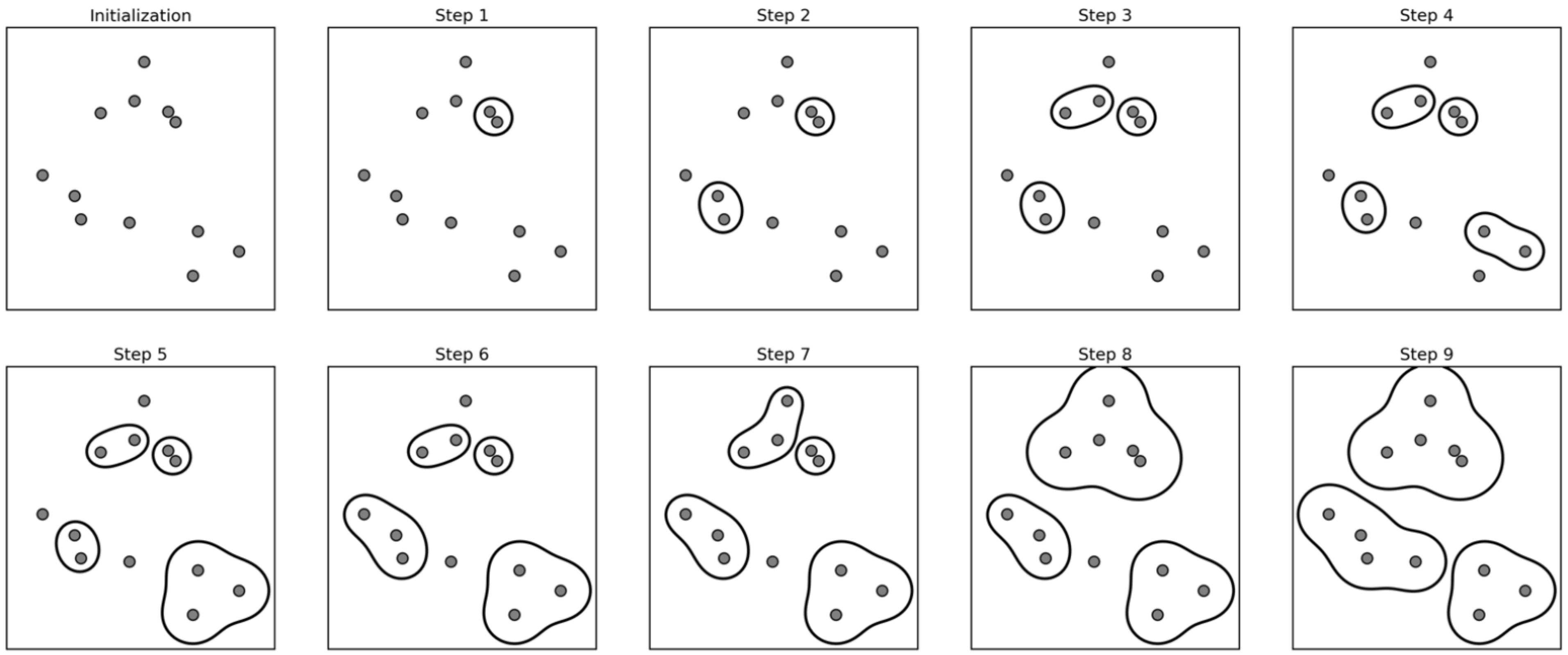
- ***Agglomerative clustering*** **refers to a collection of clustering algorithms that all build upon the following principles**

  Given a (training) dataset $D = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_n\}$ such that $\boldsymbol{x}_i = (x_{i1}, \dots, x_{id}) \in \mathbb{R}^d$ is the *i*-th input vector of *d* features

  1. The algorithm starts by declaring each point its own cluster.
  2. Then, merges the two most similar clusters until some stopping criterion is satisfied.

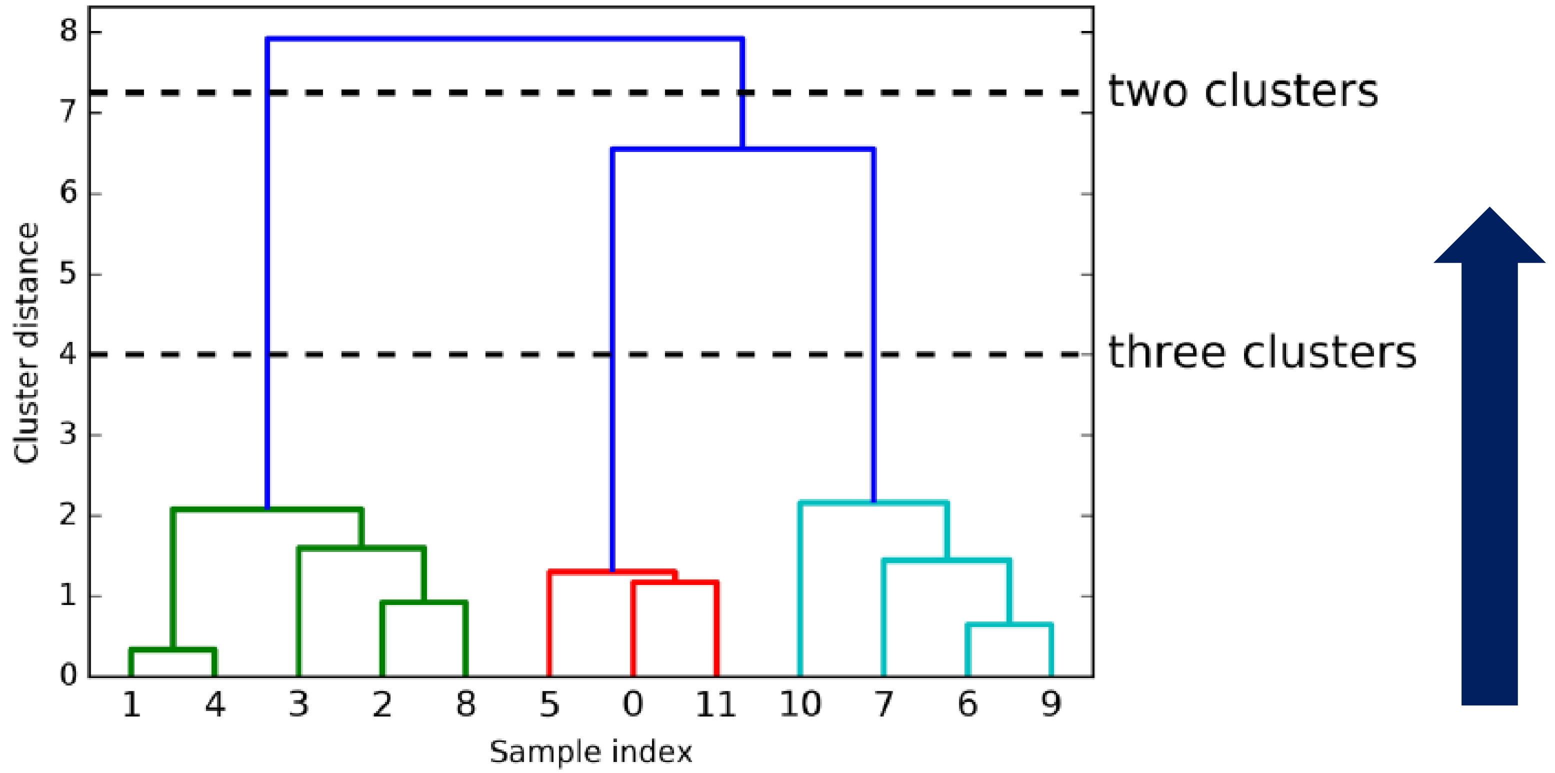
Agglomerative Clustering

- **Example of agglomerative clustering**
  - Initially, each point is its own cluster.
  - Then, in each step, the two clusters that are closest are merged.



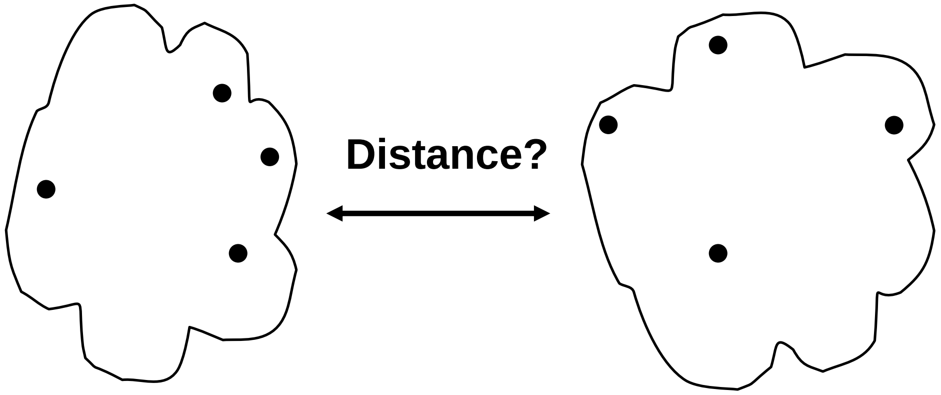
Agglomerative Clustering

- **Determining the number of clusters**
  - **Dendrogram** is helpful to look at all possible clusterings jointly
  - Each intermediate step provides a clustering of the data (with a different number of clusters).
  - A horizontal line intersects the clusters that are that far apart, to create clusters



Agglomerative Clustering

- There are several ***linkage*** criteria to evaluate the distance between two clusters.
  - This specifies how exactly the "most similar cluster" is selected.
  - Single (Minimum), Complete (Maximum), Average, Ward

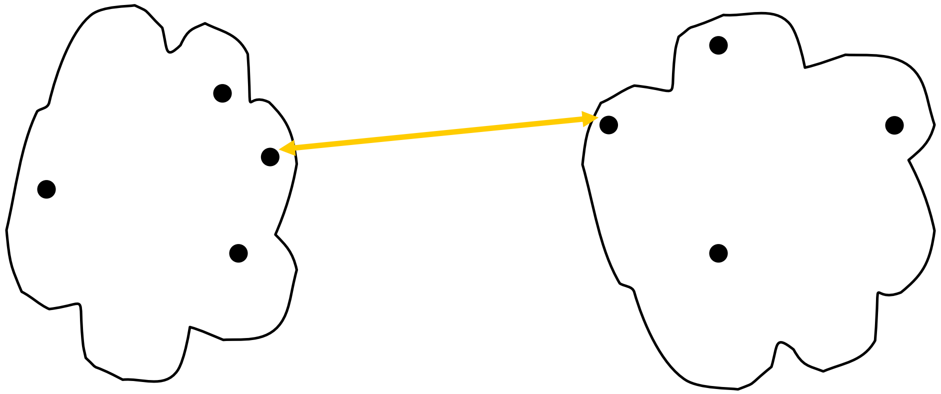


* Ward works on most datasets

* If the clusters have very dissimilar numbers of members (e.g., one is much bigger than all the others), average or complete might work better.

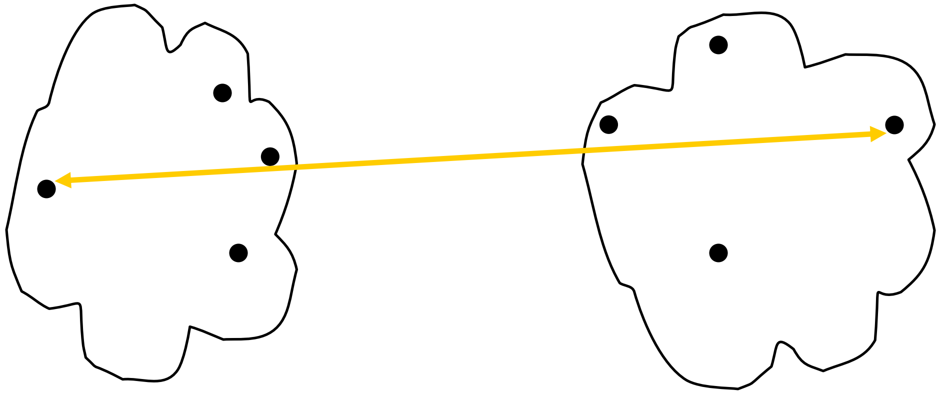
Agglomerative Clustering

- **Single (Minimum) Linkage**: the minimum of the distances between all data points of the two clusters.
  - Can handle non-globular shapes
  - Sensitive to noise and outliers



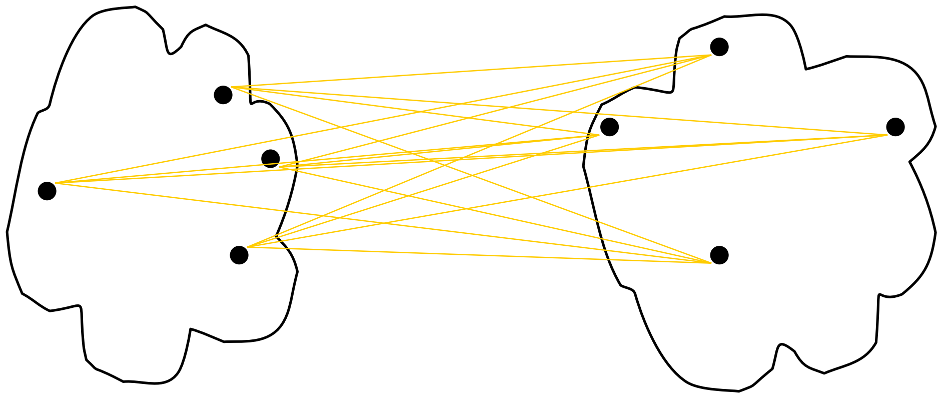
Agglomerative Clustering

- **Complete (Maximum) Linkage**: the maximum of the distances between all data points of the two clusters.
  - Less susceptible to noise and outliers
  - Tends to break large clusters
  - Biased towards globular clusters



Agglomerative Clustering

- **Average Linkage**: the average of the distances between all data points of the two clusters.
  - Compromise between Single and Complete Linkage
  - Less susceptible to noise and outliers
  - Biased towards globular clusters

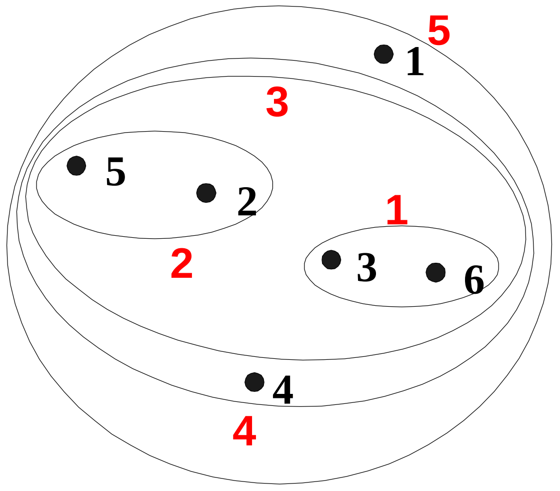


Agglomerative Clustering

- **Ward Linkage**: the minimum increase in variance when the two clusters are merged.
  - Less susceptible to noise and outliers
  - Biased towards globular clusters
  - Often leads to clusters that are relatively equally sized
  - Hierarchical analogue of K-means
  - The default choice in scikit-learn

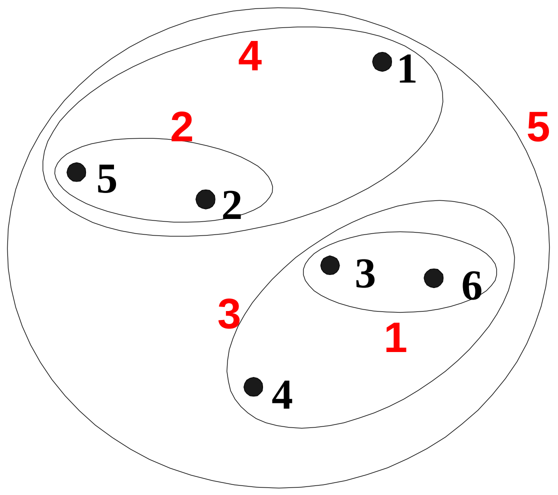
Agglomerative Clustering

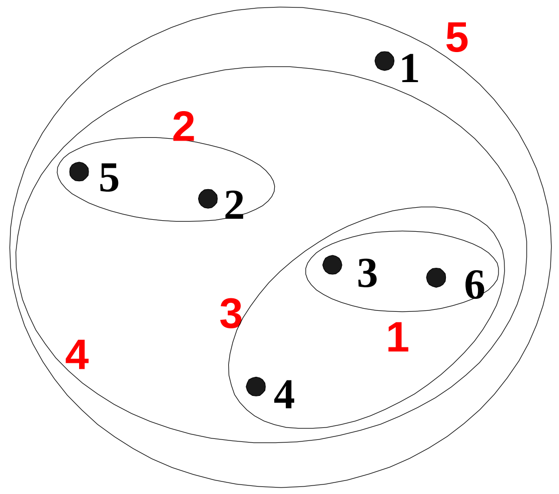
- **Example of Agglomerative Clustering with Different Linkages**



Single (Minimum)

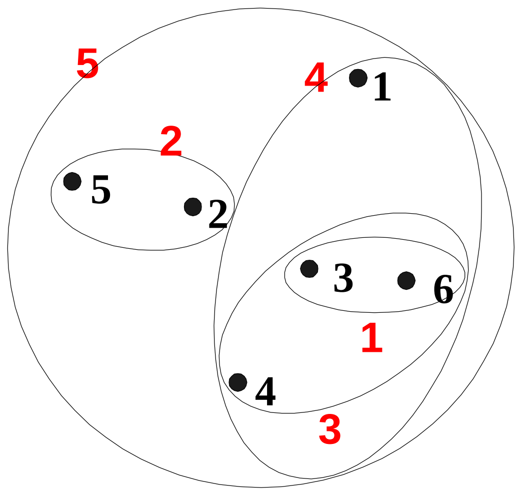
Complete (Maximum)





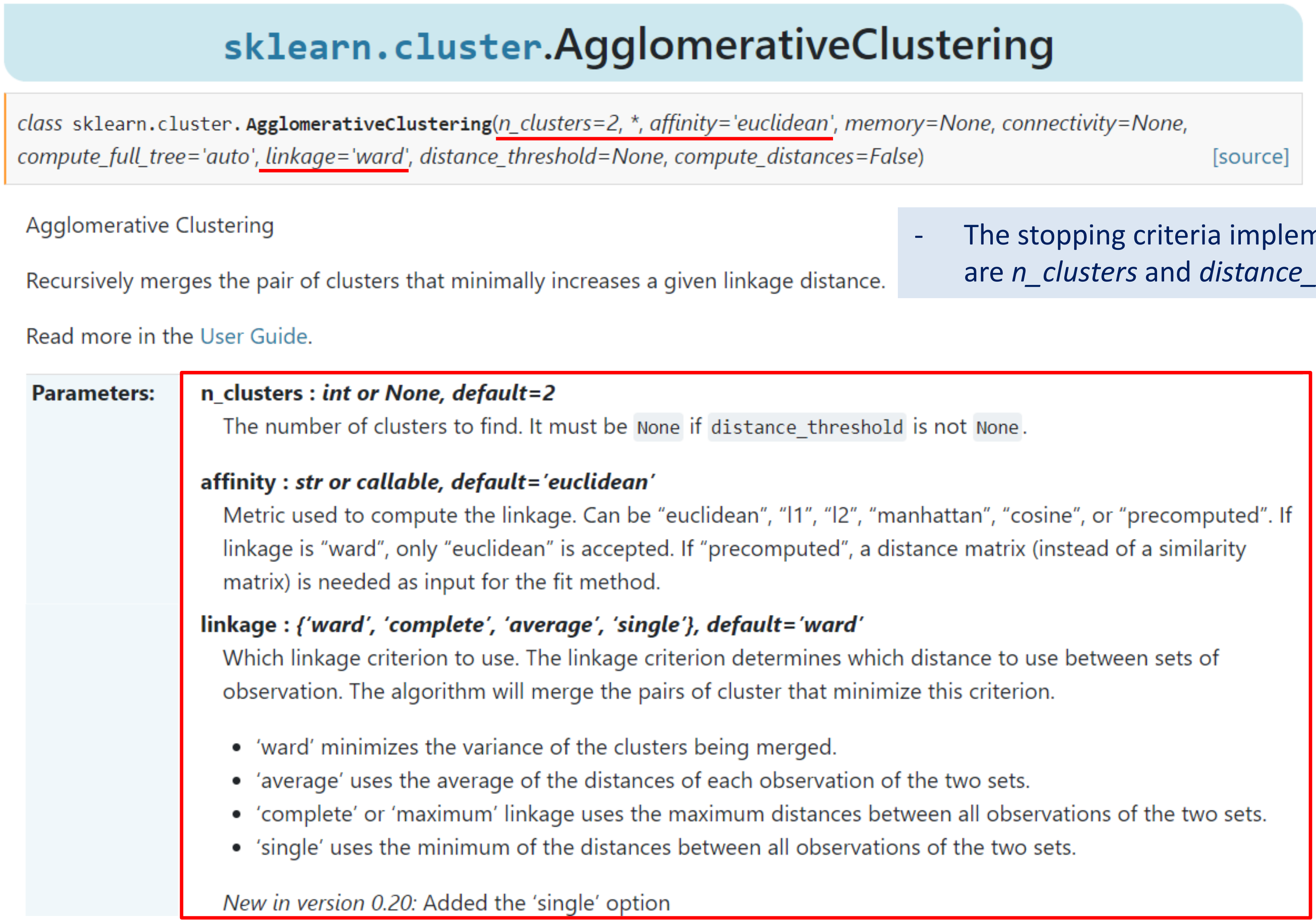
Average

Ward



scikit-learn Practice: *AgglomerativeClustering*

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.AgglomerativeClustering.html



sklearn.cluster.AgglomerativeClustering

class `sklearn.cluster.`**`AgglomerativeClustering`**(*n_clusters=2, *, affinity='euclidean', memory=None, connectivity=None, compute_full_tree='auto', linkage='ward', distance_threshold=None, compute_distances=False*) [source]

Agglomerative Clustering

Recursively merges the pair of clusters that minimally increases a given linkage distance.

Read more in the User Guide.

Parameters:

n_clusters : *int or None, default=2*
The number of clusters to find. It must be `None` if `distance_threshold` is not `None`.

affinity : *str or callable, default='euclidean'*
Metric used to compute the linkage. Can be "euclidean", "l1", "l2", "manhattan", "cosine", or "precomputed". If linkage is "ward", only "euclidean" is accepted. If "precomputed", a distance matrix (instead of a similarity matrix) is needed as input for the fit method.

linkage : *{'ward', 'complete', 'average', 'single'}, default='ward'*
Which linkage criterion to use. The linkage criterion determines which distance to use between sets of observation. The algorithm will merge the pairs of cluster that minimize this criterion.

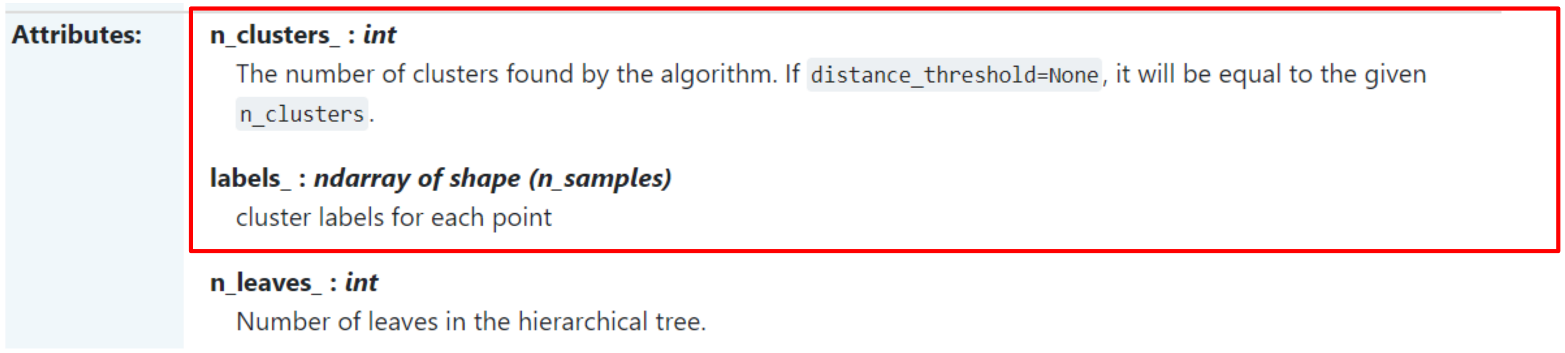
- 'ward' minimizes the variance of the clusters being merged.
- 'average' uses the average of the distances of each observation of the two sets.
- 'complete' or 'maximum' linkage uses the maximum distances between all observations of the two sets.
- 'single' uses the minimum of the distances between all observations of the two sets.

New in version 0.20: Added the 'single' option

- The stopping criteria implemented in scikit-learn are *n_clusters* and *distance_threshold*.

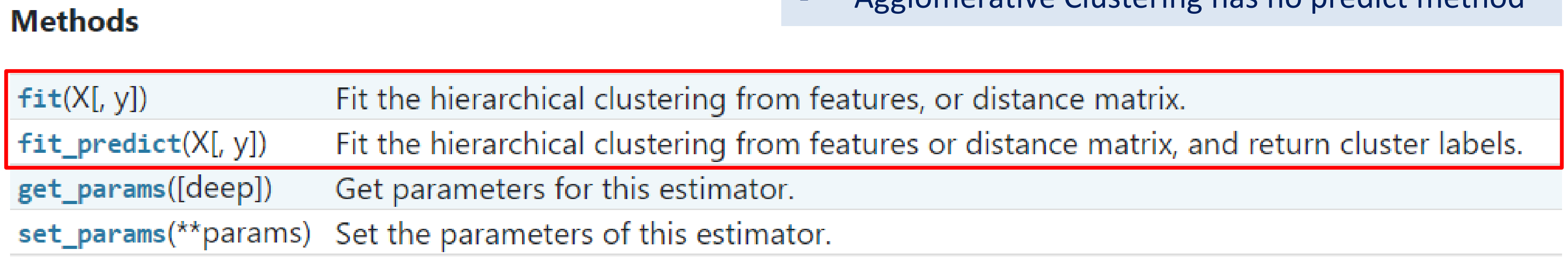
scikit-learn Practice: *AgglomerativeClustering*

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.AgglomerativeClustering.html



Attributes:	**n_clusters_ : *int*** The number of clusters found by the algorithm. If `distance_threshold=None`, it will be equal to the given `n_clusters`. **labels_ : *ndarray of shape (n_samples)*** cluster labels for each point **n_leaves_ : *int*** Number of leaves in the hierarchical tree.

- Agglomerative Clustering has no predict method

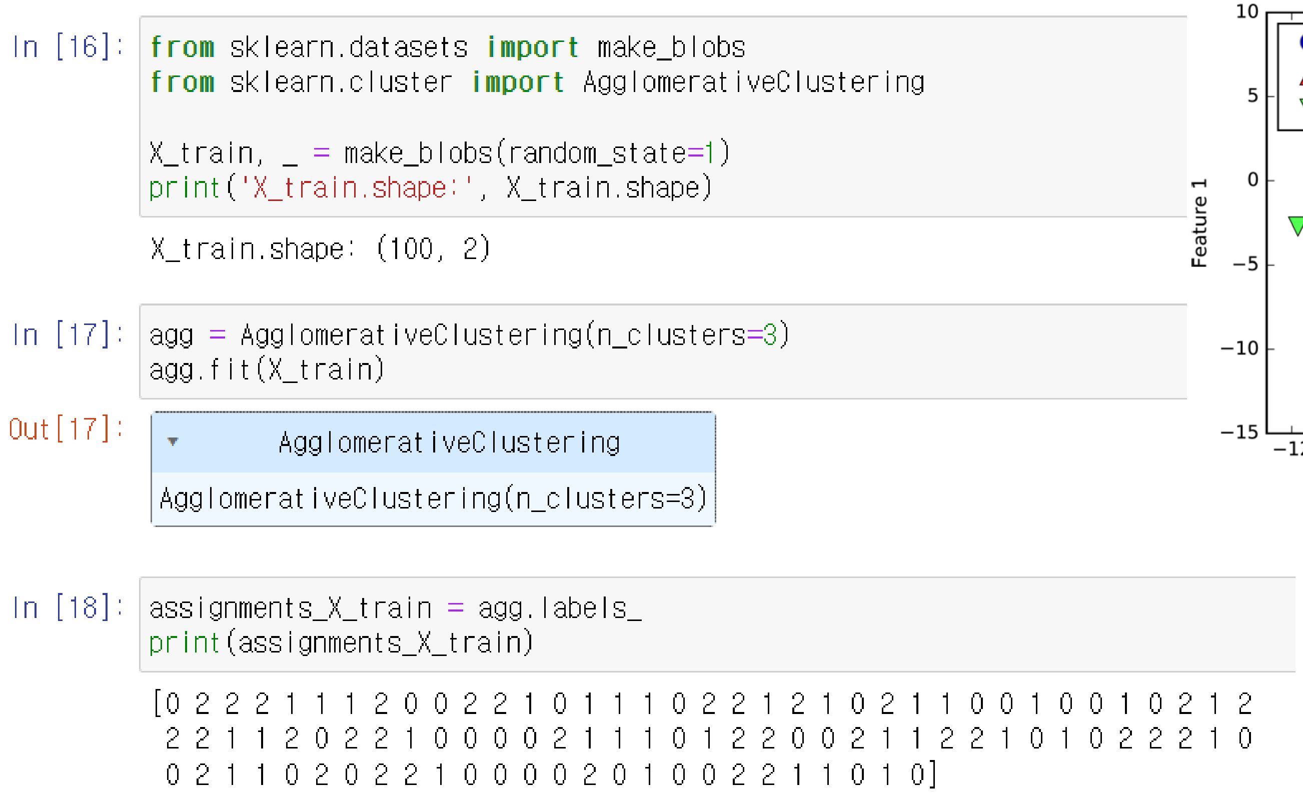


Methods

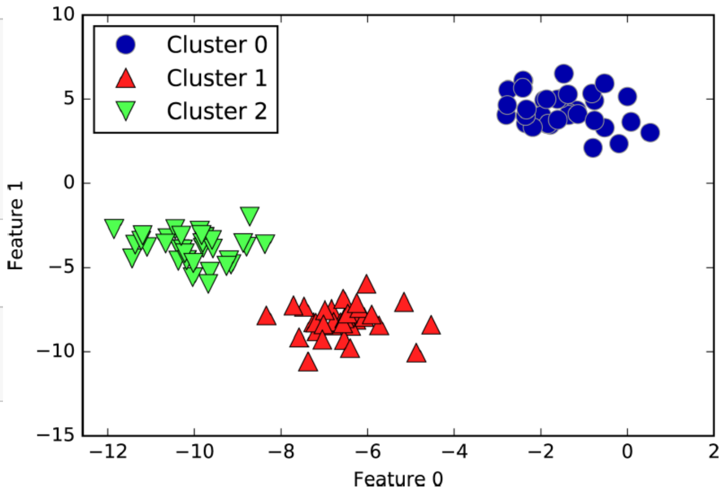
`fit`(X[, y])	Fit the hierarchical clustering from features, or distance matrix.
`fit_predict`(X[, y])	Fit the hierarchical clustering from features or distance matrix, and return cluster labels.
`get_params`([deep])	Get parameters for this estimator.
`set_params`(**params)	Set the parameters of this estimator.

scikit-learn Practice: *AgglomerativeClustering*

- **Example (*blobs* dataset)**



```
In [16]: from sklearn.datasets import make_blobs
         from sklearn.cluster import AgglomerativeClustering

         X_train, _ = make_blobs(random_state=1)
         print('X_train.shape:', X_train.shape)

         X_train.shape: (100, 2)

In [17]: agg = AgglomerativeClustering(n_clusters=3)
         agg.fit(X_train)

Out[17]: ▾       AgglomerativeClustering
          AgglomerativeClustering(n_clusters=3)

In [18]: assignments_X_train = agg.labels_
         print(assignments_X_train)

         [0 2 2 2 1 1 1 2 0 0 2 2 1 0 1 1 1 0 2 2 1 2 1 0 2 1 1 0 0 1 0 0 1 0 2 1 2
          2 2 1 1 2 0 2 2 1 0 0 0 0 2 1 1 1 0 1 2 2 0 0 2 1 1 2 2 1 0 1 0 2 2 2 1 0
          0 2 1 1 0 2 0 2 2 1 0 0 0 0 2 0 1 0 0 2 2 1 1 0 1 0]
```



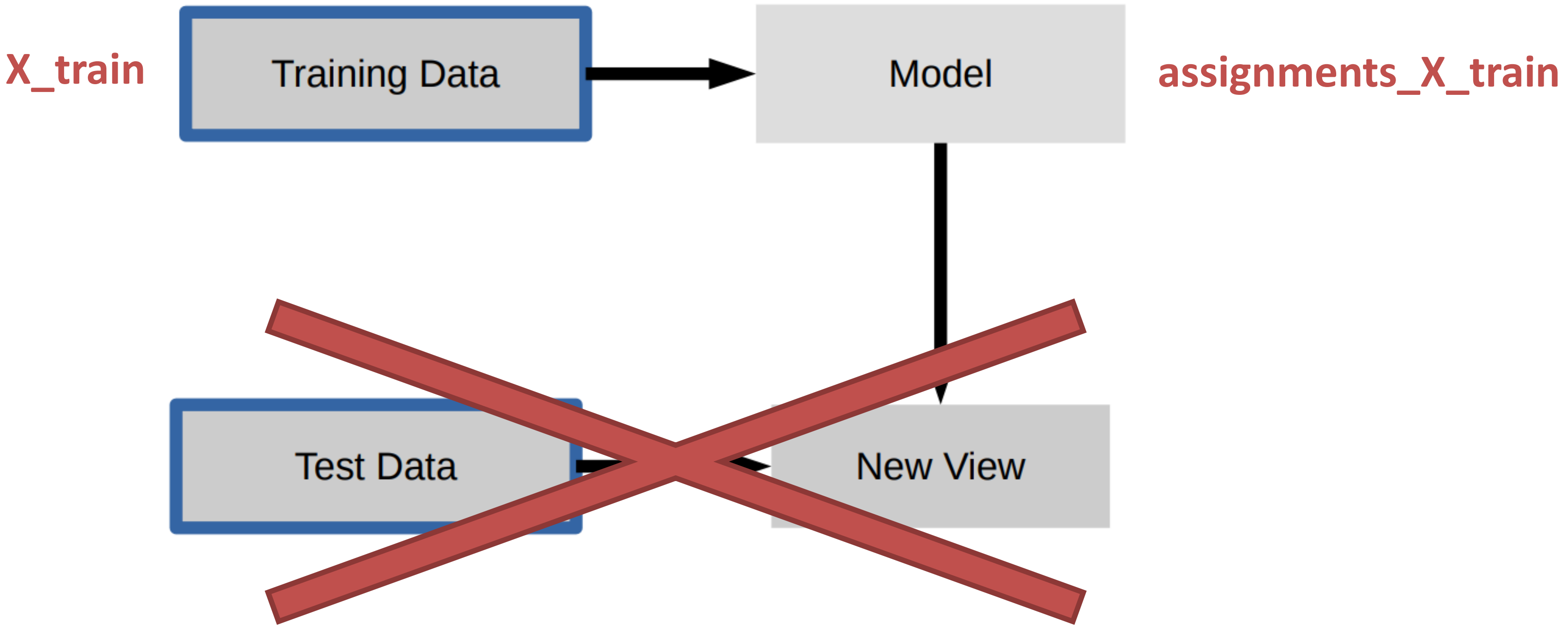
scikit-learn Practice: *AgglomerativeClustering*

- **Example (*blobs* dataset)**

```
X_train, _ = make_blobs(random_state=1)
```

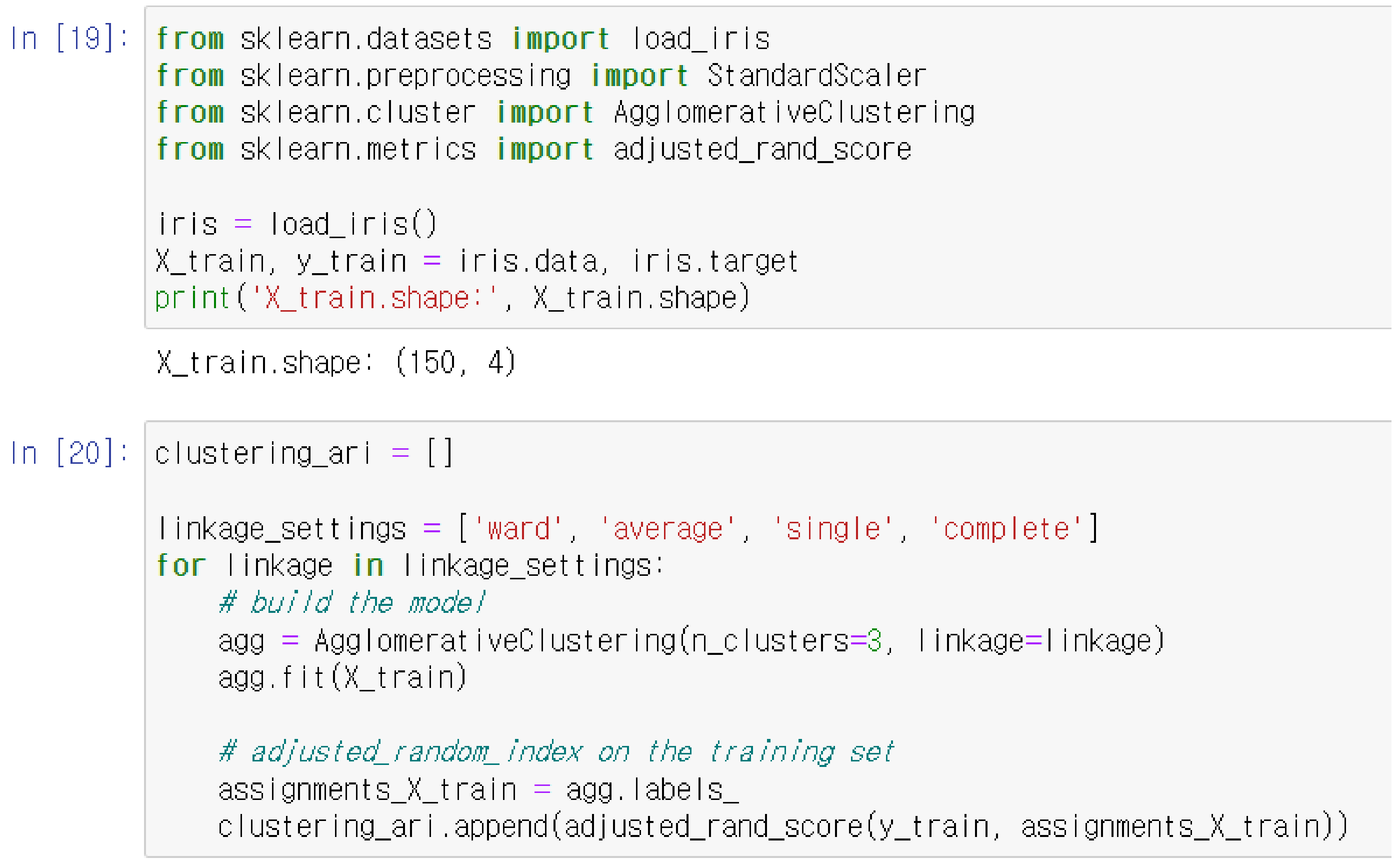
```
agg = AgglomerativeClustering(n_clusters=3)
agg.fit(X_train)
```

```
assignments_X_train =agg.labels_
```

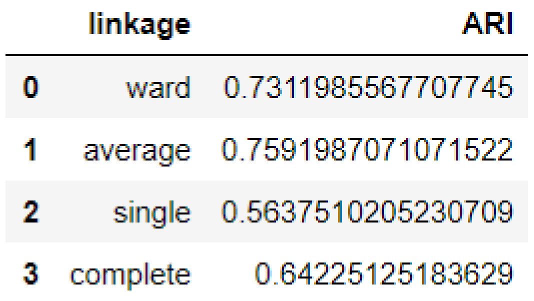


scikit-learn Practice: *AgglomerativeClustering*

- **Example (*iris* dataset) with different linkages**



```
In [19]: from sklearn.datasets import load_iris
         from sklearn.preprocessing import StandardScaler
         from sklearn.cluster import AgglomerativeClustering
         from sklearn.metrics import adjusted_rand_score

         iris = load_iris()
         X_train, y_train = iris.data, iris.target
         print('X_train.shape:', X_train.shape)

         X_train.shape: (150, 4)

In [20]: clustering_ari = []

         linkage_settings = ['ward', 'average', 'single', 'complete']
         for linkage in linkage_settings:
             # build the model
             agg = AgglomerativeClustering(n_clusters=3, linkage=linkage)
             agg.fit(X_train)

             # adjusted_random_index on the training set
             assignments_X_train = agg.labels_
             clustering_ari.append(adjusted_rand_score(y_train, assignments_X_train))
```



	linkage	ARI
0	ward	0.7311985567707745
1	average	0.7591987071071522
2	single	0.5637510205230709
3	complete	0.64225125183629

scikit-learn Practice: *AgglomerativeClustering*

- **Example (*iris* dataset) with different linkages (feature scaling)**

```
In [22]: from sklearn.datasets import load_iris
         from sklearn.preprocessing import StandardScaler
         from sklearn.cluster import AgglomerativeClustering
         from sklearn.metrics import adjusted_rand_score

         iris = load_iris()
         X_train, y_train = iris.data, iris.target
         print('X_train.shape:', X_train.shape)

         X_train.shape: (150, 4)
```

```
In [23]: scaler = StandardScaler()
         X_train_scaled = scaler.fit_transform(X_train)
```

```
In [24]: clustering_ari = []

         linkage_settings = ['ward','average','single','complete']
         for linkage in linkage_settings:
             # build the model
             agg = AgglomerativeClustering(n_clusters=3, linkage=linkage)
             agg.fit(X_train_scaled)

             # adjusted_random_index on the training set
             assignments_X_train = agg.labels_
             clustering_ari.append(adjusted_rand_score(y_train, assignments_X_train))
```

	linkage	ARI
0	ward	0.615322993214545
1	average	0.5621364251426576
2	single	0.5583714437541352
3	complete	0.5726305793711642

Discussion

- **The main hyperparameters of (agglomerative) hierarchical clustering**
  - *affinity, linkage* (measuring the distances between clusters)
  - *n_clusters* or *distance_threshold* (termination condition)

  * It's important to preprocess your data (including *feature scaling* and *one-hot encoding*)
- **Strengths**
  - Hierarchical clustering gives visual representation (dendrogram) of different levels of clustering, which may correspond to meaningful taxonomies.
  - It does not have to assume any particular number of clusters.
- **Weaknesses**
  - Once a decision is made to combine two clusters, it cannot be undone.
  - It is computationally expensive.
  - The performance depends highly on scaling of features.
  - It fails at separating complex shapes.