Lecture 23 - Part 1: DBSCAN continued & Hierarchical Clustering

---

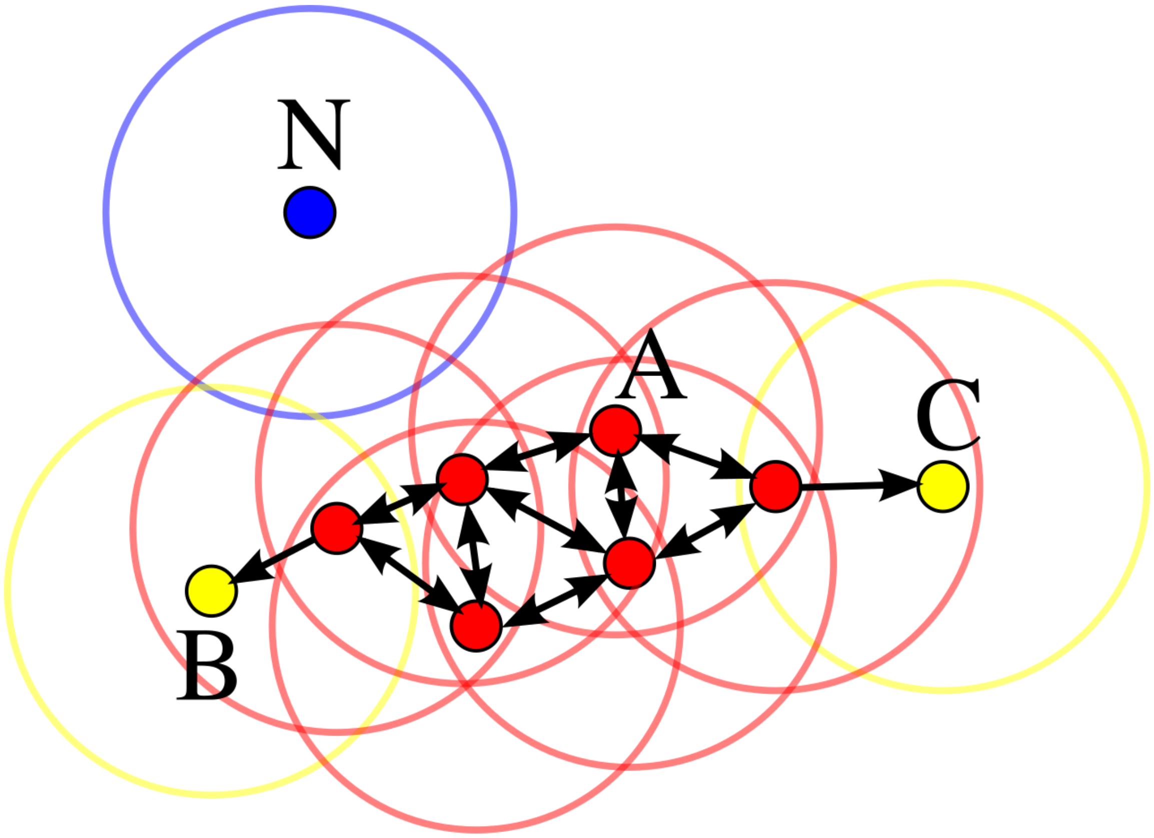
In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
plt.style.use('bmh')

from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
from sklearn.cluster import KMeans
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
```

Density-based Spatial Clustering of Applications with Noise (DBSCAN)

In density-based clustering, a cluster is formed if there is a *sufficient* amount of neighboring points (density). In DBSCAN, each point is marked as one of three categories:

- a **core point**, which is surrounded by a certain number of neighboring points in a given radius;
- a **border point**, which is not surrounded by the same amount of neighboring points but is within a radius of a core point; and
- a **noise point**, which is any other point that does not fall into the other two categories.

With these markings, the DBSCAN algorithm forms clusters for groups of core points and assigns the border points to the cluster with their respective core point. So **there will be as many clusters as there are core points**.



The parameters are:

1. *MinPts*: the value for the minimum number of neighboring points, this will determine the number of points a core point must have in order to be marked as a core point;
2. ϵ: the radius parameter determines a fixed radius region in which neighboring points must *live on* in order to be marked as a core point or border point.
3. Distance metric: the distance metric used to compute distances and neighbors.

Discussions

- DBSCAN has the advantage over both k-means and GMM in which it **finds clusters without needing to define the number of clusters a priori**.
- DBSCAN has the advantage over k-means as it is able to find groups with different number of points (different densities) and without making explicit assumptions about cluster shape.
- DBSCAN has the advantage over distribution-based clustering (with for example Gaussian Mixture Models or GMM) because it is of much lower computational complexity, in the order of $\mathrm{O}(\mathrm{N}\log(\mathrm{N}))$.

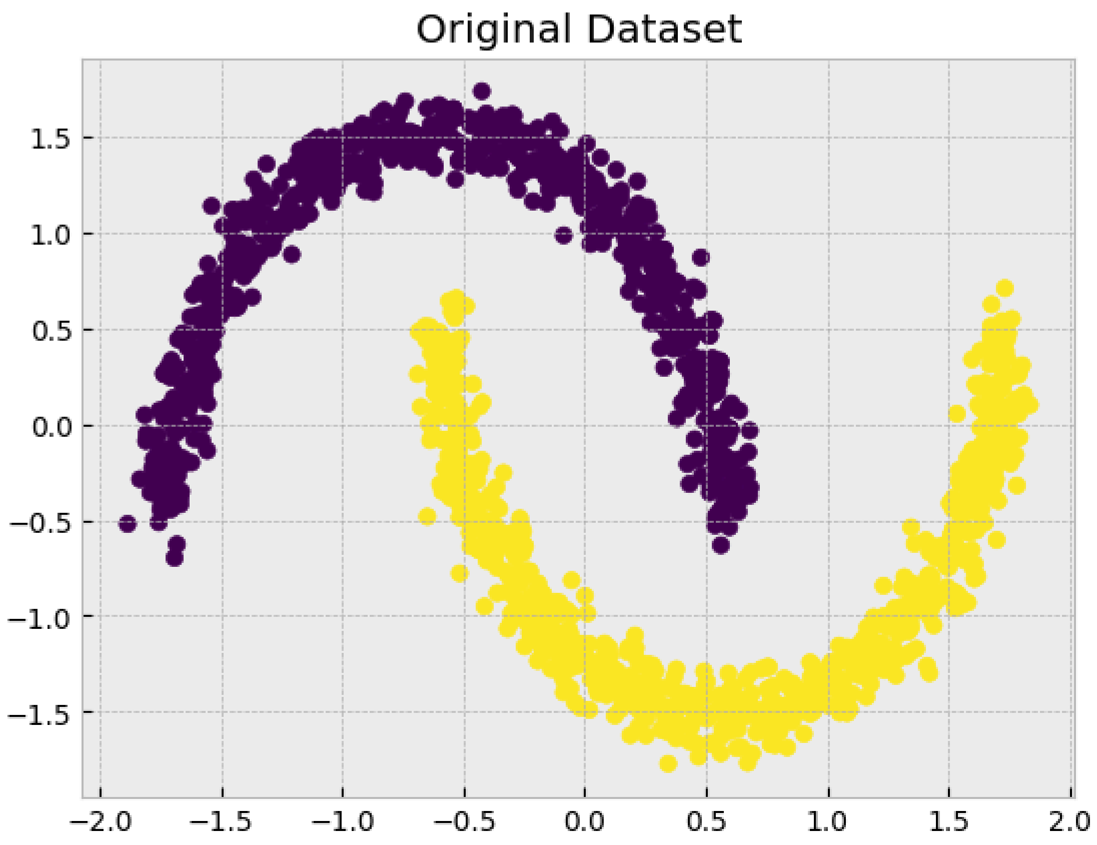
- Moreover, DBSCAN is able to mark points as noise points, making it robust against outliers for subsequent classification task.

- As with any algorithm that uses distances, DBSCAN will too be heavily affected by the curse of dimensionality. DBSCAN will also have trouble finding clusters with different densities (number of points).

In [3]:
```
from sklearn.cluster import DBSCAN
```

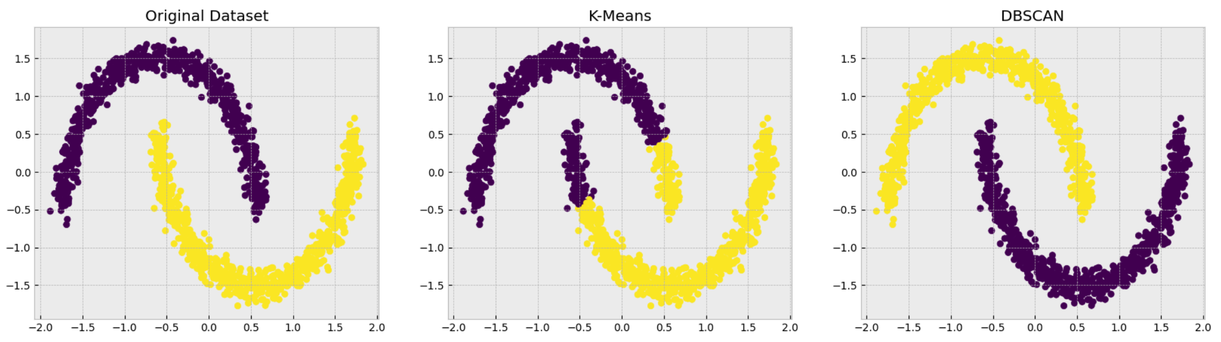
In [4]:
```
# DBSCAN?
```

In [5]:
```
from sklearn.datasets import make_moons

# Dataset
dataset, true_labels = make_moons(n_samples=1500, noise=.05)

# Feature scaling
scaler = StandardScaler()
dataset = scaler.fit_transform(dataset)

plt.scatter(dataset[:,0],dataset[:,1], c=true_labels); plt.title('Original Dataset'
```



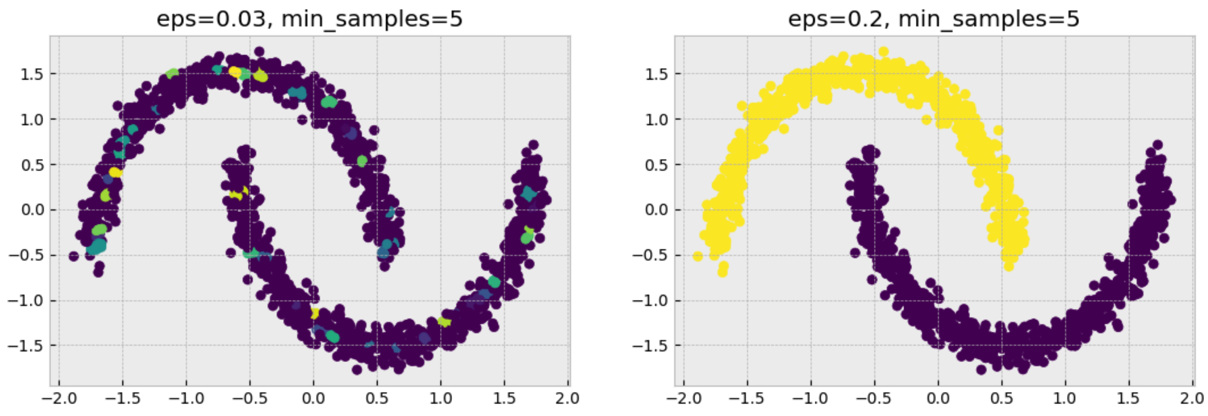
In [6]:
```
# K-Means
kmeans = KMeans(n_clusters=2, n_init='auto')
labels_kmeans = kmeans.fit_predict(dataset)

#DBSCAN
```

```
dbscan = DBSCAN(eps=0.2, min_samples=5)
labels_dbscan = dbscan.fit_predict(dataset)

plt.figure(figsize=(20,5))
plt.subplot(1,3,1)
plt.scatter(dataset[:,0],dataset[:,1], c=true_labels); plt.title('Original Dataset'
plt.subplot(1,3,2)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_kmeans); plt.title('K-Means')
plt.subplot(1,3,3)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_dbscan); plt.title('DBSCAN');
```



```
In [7]: dbscan.core_sample_indices_

Out[7]: array([   0,    1,    2, ..., 1497, 1498, 1499], dtype=int64)

In [8]: len(dbscan.core_sample_indices_)

Out[8]: 1498

In [9]: dbscan.components_.shape

Out[9]: (1498, 2)

In [10]: dbscan.components_

Out[10]: array([[ 0.83562416, -1.36484374],
               [ 1.77722173,  0.13061185],
               [-0.22264556, -1.00797752],
               ...,
               [ 0.57941694, -0.38642044],
               [-1.2720508 ,  1.01723268],
               [ 0.59397726,  0.08503041]])

In [11]: plt.figure(figsize=(13,4))
         plt.subplot(1,2,1)
         dbscan = DBSCAN(eps=0.03, min_samples=5)
         labels_dbscan = dbscan.fit_predict(dataset)
         plt.scatter(dataset[:,0],dataset[:,1], c=labels_dbscan);
         plt.title('eps=0.03, min_samples=5')

         plt.subplot(1,2,2)
         dbscan = DBSCAN(eps=0.2, min_samples=5)
         labels_dbscan = dbscan.fit_predict(dataset)
```

```
plt.scatter(dataset[:,0],dataset[:,1], c=labels_dbscan);
plt.title('eps=0.2, min_samples=5');
```



Hierarchical Clustering

We will now take a look at an alternative approach of **prototype-based clustering**: **hierarchical clustering**. One advantage of the hierarchical clustering algorithm is that it allows us to plot **dendrograms** (visualizations of a binary hierarchical clustering), which can help with the interpretation of the results by creating meaningful taxonomies. Another advantage of this hierarchical approach is that we do not need to specify the number of clusters upfront.

The two main approaches to hierarchical clustering are **agglomerative** and **divisive** hierarchical clustering.

- In **divisive hierarchical clustering**, we start with one cluster that encompasses the complete dataset, and we iteratively split the cluster into smaller clusters until each cluster only contains one example.

- In **agglomerative hierarchical clustering**, we start with each example as an individual cluster and merge the closest pairs of clusters until only one cluster remains.

Agglomerative Hierarchical Clustering

The two standard algorithms for agglomerative hierarchical clustering are **single linkage** and **complete linkage**.

- Using single linkage, we compute the distances between the most similar members for each pair of clusters and merge the two clusters for which the distance between the most similar members is the smallest.

- The complete linkage approach is similar to single linkage but, instead of comparing the most similar members in each pair of clusters, we compare the most dissimilar members to perform the merge.

Let's illustrate it with an example:

In [12]:
```
import pandas as pd
np.random.seed(123)

variables = ['X', 'Y', 'Z']
labels = ['ID_0', 'ID_1', 'ID_2', 'ID_3', 'ID_4']

X = np.random.random_sample([5, 3])*10

df = pd.DataFrame(X, columns=variables, index=labels)
df
```

Out[12]:

	X	Y	Z
ID_0	6.964692	2.861393	2.268515
ID_1	5.513148	7.194690	4.231065
ID_2	9.807642	6.848297	4.809319
ID_3	3.921175	3.431780	7.290497
ID_4	4.385722	0.596779	3.980443

Performing Hierarchical Clustering on a Distance Matrix

In [14]:
```
from scipy.spatial.distance import pdist, squareform

dist_matrix = pdist(df, metric='euclidean')

row_dist = pd.DataFrame(squareform(dist_matrix),
                        columns=labels, index=labels)

row_dist
```

Out[14]:

	ID_0	ID_1	ID_2	ID_3	ID_4
ID_0	0.000000	4.973534	5.516653	5.899885	3.835396
ID_1	4.973534	0.000000	4.347073	5.104311	6.698233
ID_2	5.516653	4.347073	0.000000	7.244262	8.316594
ID_3	5.899885	5.104311	7.244262	0.000000	4.382864
ID_4	3.835396	6.698233	8.316594	4.382864	0.000000

In [15]:
```
from scipy.cluster.hierarchy import linkage

linkage?
```

```
Signature: linkage(y, method='single', metric='euclidean', optimal_ordering=False)
Docstring:
Perform hierarchical/agglomerative clustering.

The input y may be either a 1-D condensed distance matrix
or a 2-D array of observation vectors.

If y is a 1-D condensed distance matrix,
then y must be a :math:`\binom{n}{2}` sized
vector, where n is the number of original observations paired
in the distance matrix. The behavior of this function is very
similar to the MATLAB linkage function.

A :math:`(n-1)` by 4 matrix ``Z`` is returned. At the
:math:`i`-th iteration, clusters with indices ``Z[i, 0]`` and
``Z[i, 1]`` are combined to form cluster :math:`n + i`. A
cluster with an index less than :math:`n` corresponds to one of
the :math:`n` original observations. The distance between
clusters ``Z[i, 0]`` and ``Z[i, 1]`` is given by ``Z[i, 2]``. The
fourth value ``Z[i, 3]`` represents the number of original
observations in the newly formed cluster.

The following linkage methods are used to compute the distance
:math:`d(s, t)` between two clusters :math:`s` and
:math:`t`. The algorithm begins with a forest of clusters that
have yet to be used in the hierarchy being formed. When two
clusters :math:`s` and :math:`t` from this forest are combined
into a single cluster :math:`u`, :math:`s` and :math:`t` are
removed from the forest, and :math:`u` is added to the
forest. When only one cluster remains in the forest, the algorithm
stops, and this cluster becomes the root.

A distance matrix is maintained at each iteration. The ``d[i,j]``
entry corresponds to the distance between cluster :math:`i` and
:math:`j` in the original forest.

At each iteration, the algorithm must update the distance matrix
to reflect the distance of the newly formed cluster u with the
remaining clusters in the forest.

Suppose there are :math:`|u|` original observations
:math:`u[0], \ldots, u[|u|-1]` in cluster :math:`u` and
:math:`|v|` original objects :math:`v[0], \ldots, v[|v|-1]` in
cluster :math:`v`. Recall, :math:`s` and :math:`t` are
combined to form cluster :math:`u`. Let :math:`v` be any
remaining cluster in the forest that is not :math:`u`.

The following are methods for calculating the distance between the
newly formed cluster :math:`u` and each :math:`v`.

  * method='single' assigns

    .. math::
       d(u,v) = \min(dist(u[i],v[j]))

    for all points :math:`i` in cluster :math:`u` and
  :math:`j` in cluster :math:`v`. This is also known as the
  Nearest Point Algorithm.

* method='complete' assigns

  .. math::
     d(u, v) = \max(dist(u[i],v[j]))

  for all points :math:`i` in cluster u and :math:`j` in
  cluster :math:`v`. This is also known by the Farthest Point
  Algorithm or Voor Hees Algorithm.

* method='average' assigns

  .. math::
     d(u,v) = \sum_{ij} \frac{d(u[i], v[j])}
                             {(|u|*|v|)}

  for all points :math:`i` and :math:`j` where :math:`|u|`
  and :math:`|v|` are the cardinalities of clusters :math:`u`
  and :math:`v`, respectively. This is also called the UPGMA
  algorithm.

* method='weighted' assigns

  .. math::
     d(u,v) = (dist(s,v) + dist(t,v))/2

  where cluster u was formed with cluster s and t and v
  is a remaining cluster in the forest (also called WPGMA).

* method='centroid' assigns

  .. math::
     dist(s,t) = ||c_s-c_t||_2

  where :math:`c_s` and :math:`c_t` are the centroids of
  clusters :math:`s` and :math:`t`, respectively. When two
  clusters :math:`s` and :math:`t` are combined into a new
  cluster :math:`u`, the new centroid is computed over all the
  original objects in clusters :math:`s` and :math:`t`. The
  distance then becomes the Euclidean distance between the
  centroid of :math:`u` and the centroid of a remaining cluster
  :math:`v` in the forest. This is also known as the UPGMC
  algorithm.

* method='median' assigns :math:`d(s,t)` like the ``centroid``
  method. When two clusters :math:`s` and :math:`t` are combined
  into a new cluster :math:`u`, the average of centroids s and t
  give the new centroid :math:`u`. This is also known as the
  WPGMC algorithm.

* method='ward' uses the Ward variance minimization algorithm.
  The new entry :math:`d(u,v)` is computed as follows,

  .. math::
       d(u,v) = \sqrt{\frac{|v|+|s|}
                           {T}d(v,s)^2
                    + \frac{|v|+|t|}
                           {T}d(v,t)^2
                    - \frac{|v|}
                           {T}d(s,t)^2}

    where :math:`u` is the newly joined cluster consisting of
    clusters :math:`s` and :math:`t`, :math:`v` is an unused
    cluster in the forest, :math:`T=|v|+|s|+|t|`, and
    :math:`|*|` is the cardinality of its argument. This is also
    known as the incremental algorithm.

Warning: When the minimum distance pair in the forest is chosen, there
may be two or more pairs with the same minimum distance. This
implementation may choose a different minimum than the MATLAB
version.

Parameters
----------
y : ndarray
    A condensed distance matrix. A condensed distance matrix
    is a flat array containing the upper triangular of the distance matrix.
    This is the form that ``pdist`` returns. Alternatively, a collection of
    :math:`m` observation vectors in :math:`n` dimensions may be passed as
    an :math:`m` by :math:`n` array. All elements of the condensed distance
    matrix must be finite, i.e., no NaNs or infs.
method : str, optional
    The linkage algorithm to use. See the ``Linkage Methods`` section below
    for full descriptions.
metric : str or function, optional
    The distance metric to use in the case that y is a collection of
    observation vectors; ignored otherwise. See the ``pdist``
    function for a list of valid distance metrics. A custom distance
    function can also be used.
optimal_ordering : bool, optional
    If True, the linkage matrix will be reordered so that the distance
    between successive leaves is minimal. This results in a more intuitive
    tree structure when the data are visualized. defaults to False, because
    this algorithm can be slow, particularly on large datasets [2]_. See
    also the `optimal_leaf_ordering` function.

    .. versionadded:: 1.0.0

Returns
-------
Z : ndarray
    The hierarchical clustering encoded as a linkage matrix.

See Also
--------

:func:`scipy.spatial.distance.pdist`
    pairwise distance metrics
```

Notes

1. For method 'single', an optimized algorithm based on minimum spanning tree is implemented. It has time complexity :math:`O(n^2)`.
   For methods 'complete', 'average', 'weighted' and 'ward', an algorithm called nearest-neighbors chain is implemented. It also has time complexity :math:`O(n^2)`.
   For other methods, a naive algorithm is implemented with :math:`O(n^3)` time complexity.
   All algorithms use :math:`O(n^2)` memory.
   Refer to [1]_ for details about the algorithms.
2. Methods 'centroid', 'median', and 'ward' are correctly defined only if Euclidean pairwise metric is used. If `y` is passed as precomputed pairwise distances, then it is the user's responsibility to assure that these distances are in fact Euclidean, otherwise the produced result will be incorrect.

`linkage` has experimental support for Python Array API Standard compatible backends in addition to NumPy. Please consider testing these features by setting an environment variable ``SCIPY_ARRAY_API=1`` and providing CuPy, PyTorch, JAX, or Dask arrays as array arguments. The following combinations of backend and device (or other capability) are supported.

Library	CPU	GPU
NumPy	✅	n/a
CuPy	n/a	⛔
PyTorch	✅	⛔
JAX	✅	⛔
Dask	⚠️ merges chunks	n/a

See :ref:`dev-arrayapi` for more information.

References

.. [1] Daniel Mullner, "Modern hierarchical, agglomerative clustering algorithms", :arXiv:`1109.2378v1`.
.. [2] Ziv Bar-Joseph, David K. Gifford, Tommi S. Jaakkola, "Fast optimal leaf ordering for hierarchical clustering", 2001. Bioinformatics :doi:`10.1093/bioinformatics/17.suppl_1.S22`

Examples

```
>>> from scipy.cluster.hierarchy import dendrogram, linkage
>>> from matplotlib import pyplot as plt
>>> X = [[i] for i in [2, 8, 0, 4, 1, 9, 9, 0]]

>>> Z = linkage(X, 'ward')
>>> fig = plt.figure(figsize=(25, 10))
>>> dn = dendrogram(Z)

>>> Z = linkage(X, 'single')
>>> fig = plt.figure(figsize=(25, 10))
>>> dn = dendrogram(Z)
>>> plt.show()
File:      c:\users\hp\appdata\local\programs\python\python312\lib\site-packages\sci
py\cluster\hierarchy.py
Type:      function
```

In [16]:
```
row_clusters = linkage(dist_matrix, method='complete')

row_clusters
```

Out[16]:
```
array([[0.        , 4.        , 3.83539555, 2.        ],
       [1.        , 2.        , 4.34707339, 2.        ],
       [3.        , 5.        , 5.89988504, 3.        ],
       [6.        , 7.        , 8.31659367, 5.        ]])
```

In [17]:
```
pd.DataFrame(row_clusters,
             columns=['row label 1', 'row label 2', 'distance', 'no. of items in cl
             index=['cluster %d' % (i + 1) for i in range(row_clusters.shape[0])])
```

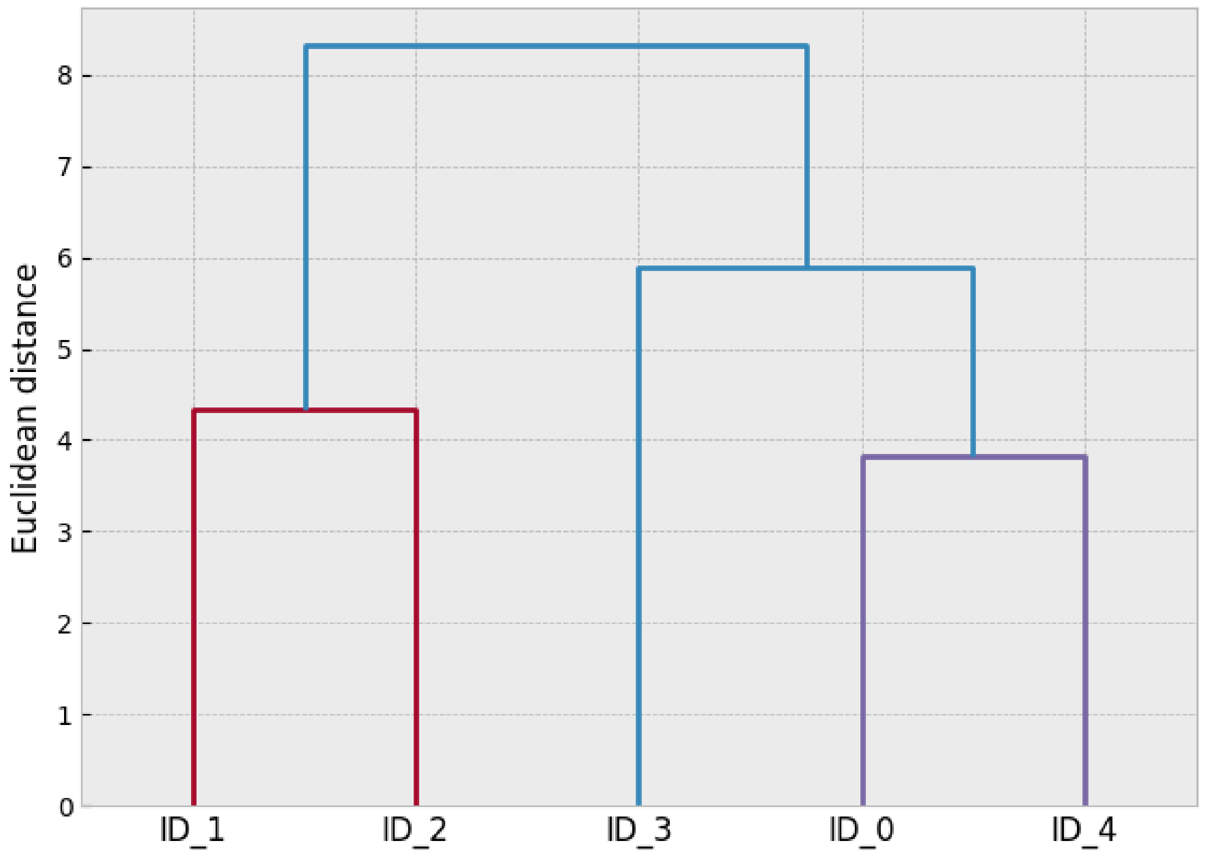
Out[17]:

	row label 1	row label 2	distance	no. of items in clust.
cluster 1	0.0	4.0	3.835396	2.0
cluster 2	1.0	2.0	4.347073	2.0
cluster 3	3.0	5.0	5.899885	3.0
cluster 4	6.0	7.0	8.316594	5.0

Now that we have computed the **linkage matrix**, we can visualize the results in the form of a **dendrogram**:

In [18]:
```
from scipy.cluster.hierarchy import dendrogram

# dendrogram?
```

In [19]:
```
row_dendr=dendrogram(row_clusters, labels=labels)
plt.tight_layout()
plt.ylabel('Euclidean distance');
```



Applying agglomerative clustering via `scikit-learn`

The `AgglomerativeClustering` implementation in `scikit-learn` allows us to choose the number of clusters that we want to return. This is useful if we want to prune the hierarchical cluster tree. By setting the `n_cluster` parameter to 3, we will now cluster the input examples into three groups using the same complete linkage approach based on the Euclidean distance metric, as before:

In [20]:
```
from sklearn.cluster import AgglomerativeClustering

# AgglomerativeClustering?
```

In [21]:
```
ac = AgglomerativeClustering(n_clusters=3,
                             metric='euclidean',
                             linkage='complete',
                             compute_distances=True)

labels = ac.fit_predict(X)
labels
```

Out[21]:
```
array([1, 0, 0, 2, 1], dtype=int64)
```

In [22]:
```
ac.children_
```

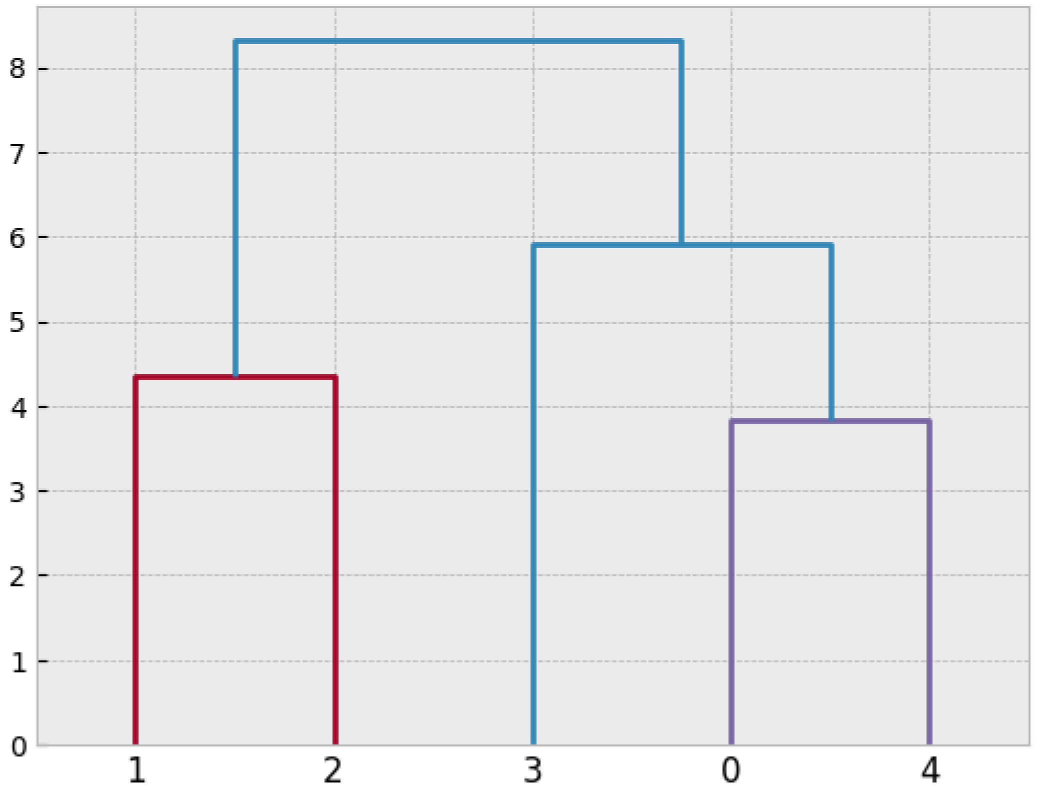
```
Out[22]: array([[0, 4],
                [1, 2],
                [3, 5],
                [6, 7]])
```

```
In [23]: ac.distances_
```

```
Out[23]: array([3.83539555, 4.34707339, 5.89988504, 8.31659367])
```

```
In [24]: def plot_dendrogram(model):
             # Create linkage matrix and then plot the dendrogram

             # create the counts of samples under each node
             counts = np.zeros(model.children_.shape[0])
             n_samples = len(model.labels_)
             for i, merge in enumerate(model.children_):
                 current_count = 0
                 for child_idx in merge:
                     if child_idx < n_samples:
                         current_count += 1  # leaf node
                     else:
                         current_count += counts[child_idx - n_samples]
                 counts[i] = current_count

             linkage_matrix = np.column_stack(
                 [model.children_, model.distances_, counts]
             ).astype(float)

             # Plot the corresponding dendrogram
             dendrogram(linkage_matrix)
```

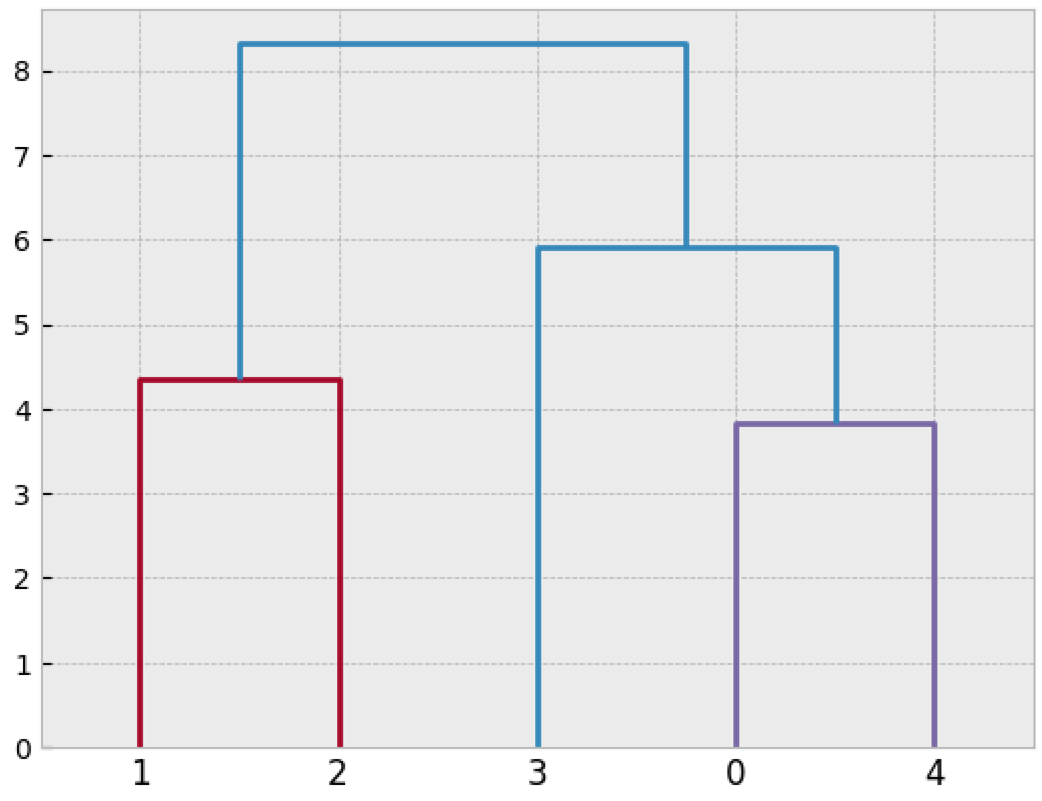
```
In [25]: plot_dendrogram(ac)
```



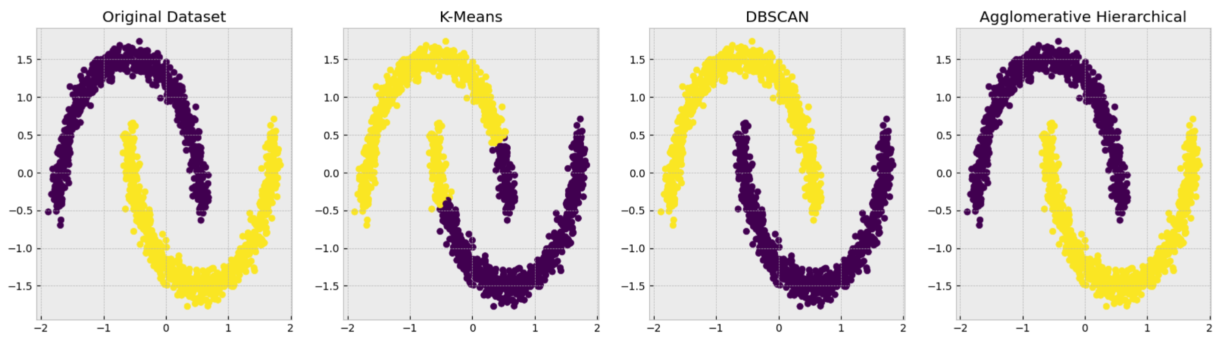
In [26]:
```
ac = AgglomerativeClustering(n_clusters=2,
                             metric='euclidean',
                             linkage='complete',
                             compute_distances=True)

labels = ac.fit_predict(X)
labels
```

Out[26]:
```
array([0, 1, 1, 0, 0], dtype=int64)
```

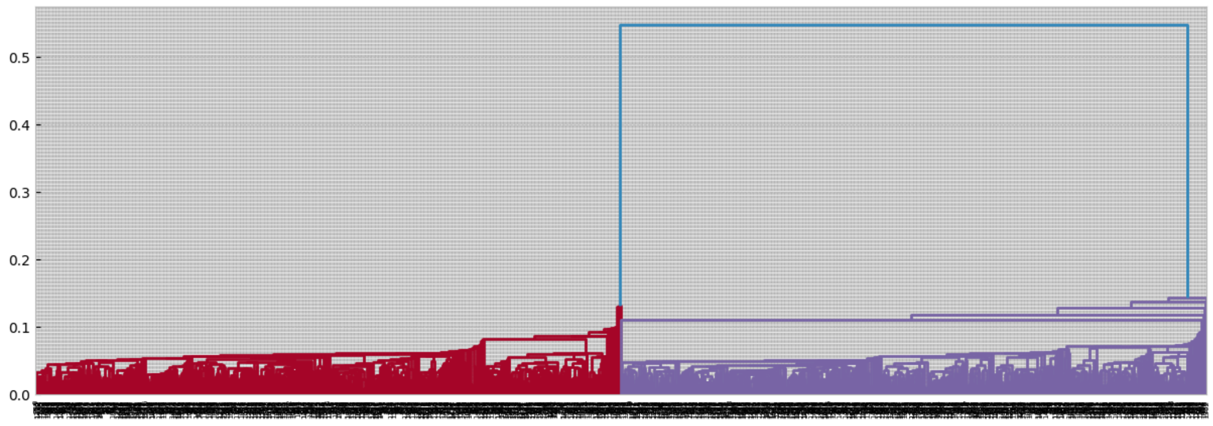
In [27]:
```
plot_dendrogram(ac)
```



In [28]:
```
# K-Means
kmeans = KMeans(n_clusters=2, n_init='auto')
labels_kmeans = kmeans.fit_predict(dataset)

# DBSCAN
dbscan = DBSCAN(eps=0.2, min_samples=5)
labels_dbscan = dbscan.fit_predict(dataset)

# Agglomerative Hierarchical Clustering
ac = AgglomerativeClustering(n_clusters=2, metric='euclidean',
                            linkage='single', compute_distances=True)
labels_ac = ac.fit_predict(dataset)

plt.figure(figsize=(20,5))
plt.subplot(1,4,1)
plt.scatter(dataset[:,0],dataset[:,1], c=true_labels); plt.title('Original Dataset'
plt.subplot(1,4,2)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_kmeans); plt.title('K-Means')
plt.subplot(1,4,3)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_dbscan); plt.title('DBSCAN')
plt.subplot(1,4,4)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_ac); plt.title('Agglomerative Hiera
```



```
In [29]: plt.figure(figsize=(15,5))
         plot_dendrogram(ac)
```



Nice, let's walk through the **whole code step-by-step** in baby language 😊 I'll group a few very related lines together so it doesn't become messy.

Setup & Imports

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
plt.style.use('bmh')

from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
from sklearn.cluster import KMeans
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
```

- `import numpy as np` → load NumPy and call it `np` (for arrays, math).
- `import matplotlib.pyplot as plt` → load plotting library as `plt`.
- `%matplotlib inline` → Jupyter magic: show plots **inside** the notebook.
- `plt.style.use('bmh')` → choose a nice plotting style.

The next imports are ML tools (even if not all are used later):

- `LogisticRegression` , `Pipeline` , `KMeans` , `train_test_split` , `GridSearchCV` , `StandardScaler` → models, pipelines, data split, and scaler from scikit-learn.

🌀 DBSCAN + K-Means on the moons data

```
from sklearn.cluster import DBSCAN
# DBSCAN?
from sklearn.datasets import make_moons
```

- `from sklearn.cluster import DBSCAN` → import DBSCAN algorithm.
- `from sklearn.datasets import make_moons` → function to create two-moon dataset.

---

1. Make the dataset

```
# Dataset
dataset, true_labels = make_moons(n_samples=1500, noise=.05)
```

- Comment for humans: `# Dataset` .
- `make_moons(...)` creates 1500 2D points shaped like two moons.
  - `noise=.05` adds a bit of randomness.
- `dataset` → the coordinates of all points (shape ~ (1500, 2)).
- `true_labels` → 0 or 1 for each point (which moon it belongs to).

---

2. Scale the features

```
# Feature scaling
scaler = StandardScaler()
dataset = scaler.fit_transform(dataset)
```

- `scaler = StandardScaler()` → create a scaler object.
- `scaler.fit_transform(dataset)` :
  - `fit` : compute mean and std of each column.
  - `transform` : subtract mean, divide by std → scaled data.
- Result replaces `dataset` .

---

3. Plot original data

```
plt.scatter(dataset[:,0],dataset[:,1], c=true_labels); plt.title('Original Dataset');
```

- `dataset[:,0]` → all rows, column 0 → x-axis.
- `dataset[:,1]` → all rows, column 1 → y-axis.
- `plt.scatter(...)` → scatter plot of points.
- `c=true_labels` → color by real moon labels.
- `plt.title('Original Dataset')` → add title.
- `;` just lets you put two commands on one line.

---

4. K-Means clustering

```
# K-Means
kmeans = KMeans(n_clusters=2, n_init='auto')
labels_kmeans = kmeans.fit_predict(dataset)
```

- Comment: `# K-Means`.
- `KMeans(n_clusters=2, n_init='auto')`:
  - ask K-Means to find **2 clusters**.
  - `n_init='auto'` → scikit decides how many initializations.
- `kmeans.fit_predict(dataset)`:
  - `fit`: learn cluster centers.
  - `predict`: assign each point to one center.
- `labels_kmeans` → cluster label (0/1) for each point from K-Means.

---

5. DBSCAN clustering

```
#DBSCAN
dbscan = DBSCAN(eps=0.2, min_samples=5)
labels_dbscan = dbscan.fit_predict(dataset)
```

- Comment: `#DBSCAN`.
- `DBSCAN(eps=0.2, min_samples=5)`:
  - `eps=0.2` → radius of neighborhood to look for neighbors.
  - `min_samples=5` → need ≥5 points in that radius to be a **core point**.
- `dbscan.fit_predict(dataset)`:
  - finds core, border, noise points.
  - assigns cluster labels.
- `labels_dbscan` → labels for each point (0,1,... or -1 for noise).

---

6. Compare all three visually

```
plt.figure(figsize=(20,5))
```

- Make a big figure canvas, width 20, height 5 (inches).

```
plt.subplot(1,3,1)
plt.scatter(dataset[:,0],dataset[:,1], c=true_labels); plt.title('Original Dataset')
```

- `subplot(1,3,1)` → grid of 1 row, 3 columns, pick position 1 (left).
- Plot original data colored by `true_labels`.

```
plt.subplot(1,3,2)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_kmeans); plt.title('K-Means')
```

- Middle panel, colored by K-Means labels.

```
plt.subplot(1,3,3)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_dbscan);
plt.title('DBSCAN');
```

- Right panel, colored by DBSCAN labels.

---

7. Look at DBSCAN internals

```
dbscan.core_sample_indices_
```

- Shows an array of indices of **core points**.

```
len(dbscan.core_sample_indices_)
```

- How many core points there are.

```
dbscan.components_.shape
```

- Shape of array containing coordinates of all core points (rows = number of core points, columns = 2).

```
dbscan.components_
```

- Print the actual coordinates of core points.

---

8. Effect of eps (small vs larger)

```
plt.figure(figsize=(13,4))
plt.subplot(1,2,1)
dbscan = DBSCAN(eps=0.03, min_samples=5)
labels_dbscan = dbscan.fit_predict(dataset)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_dbscan);
plt.title('eps=0.03, min_samples=5')
```

- New figure, 1 row, 2 columns.
- Left subplot.
- New DBSCAN with **tiny eps = 0.03**.
- Fit and plot: many points likely become noise.

```
plt.subplot(1,2,2)
dbscan = DBSCAN(eps=0.2, min_samples=5)
labels_dbscan = dbscan.fit_predict(dataset)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_dbscan);
plt.title('eps=0.2, min_samples=5');
```

- Right subplot.
- DBSCAN with **larger eps = 0.2**.
- Fit and plot: clusters are nicely formed.

🌲 Hierarchical Clustering Section

1. Make a small random dataset

```
import pandas as pd
np.random.seed(123)
```

- Import pandas as `pd` for tables.
- `np.random.seed(123)` → fix random numbers so results repeat.

```
variables = ['X', 'Y', 'Z']
labels = ['ID_0', 'ID_1', 'ID_2', 'ID_3', 'ID_4']
```

- Names for columns and row labels.

```
X = np.random.random_sample([5, 3])*10
```

- Create a 5×3 matrix of random numbers between 0 and 1, then `*10` → 0–10.

```
df = pd.DataFrame(X, columns=variables, index=labels)
df
```

- Put the data in a DataFrame with given row/column names.
- Last line prints it.

---

2. Distance matrix

```
from scipy.spatial.distance import pdist, squareform
```

- Import functions to compute pairwise distances.

```
dist_matrix = pdist(df, metric='euclidean')
```

- `pdist` → compute condensed distance vector (all pairwise distances) between rows of `df`.

```
row_dist = pd.DataFrame(squareform(dist_matrix),
                        columns=labels, index=labels)
```

```
row_dist
```

- `squareform(dist_matrix)` → turn 1D distance vector into full square matrix.
- Wrap in DataFrame for nice display.
- Print it.

---

3. Linkage (build cluster tree)

```
from scipy.cluster.hierarchy import linkage
```

```
linkage?
```

- Import `linkage` function for hierarchical clustering.
- `linkage?` in Jupyter shows documentation.

```
row_clusters = linkage(dist_matrix, method='complete')
```

- Build hierarchical clusters using:
  - the previously computed distances
  - `method='complete'` → use complete linkage (max distance between cluster points).

```
row_clusters
```

- Print the linkage matrix (each row: which clusters merged, at what distance).

```
pd.DataFrame(row_clusters,
             columns=['row label 1', 'row label 2', 'distance', 'no. of
items in clust.'],
             index=['cluster %d' % (i + 1) for i in
range(row_clusters.shape[0])])
```

- Wrap linkage matrix in a readable DataFrame:
  - columns explain what each number is.
  - index named like `cluster 1`, `cluster 2`, etc.

---

4. Dendrogram

```
from scipy.cluster.hierarchy import dendrogram
```

- Import function to draw dendrogram.

```
# dendrogram?
row_dendr=dendrogram(row_clusters, labels=labels)
plt.tight_layout()
plt.ylabel('Euclidean distance');
```

- `dendrogram(row_clusters, labels=labels)` → draw the tree using linkage matrix.
- Save handle in `row_dendr`.
- `plt.tight_layout()` → reduce overlaps.
- Label y-axis with "Euclidean distance".

🧬 AgglomerativeClustering with scikit-learn

```
from sklearn.cluster import AgglomerativeClustering
```

- Import the sklearn implementation.

```
# AgglomerativeClustering?
ac = AgglomerativeClustering(n_clusters=3,
                             metric='euclidean',
                             linkage='complete',
                             compute_distances=True)
```

- `AgglomerativeClustering?` → show docstring.
- Create model `ac`:
  - `n_clusters=3` → cut the hierarchy to get 3 clusters.
  - `metric='euclidean'` → distance type.
  - `linkage='complete'` → same logic as before.
  - `compute_distances=True` → store distances for dendrogram plotting.

```
labels = ac.fit_predict(X)
labels
```

- `fit_predict(X)` → group our 5 points into 3 clusters.
- Print cluster labels.

```
ac.children_
ac.distances_
```

- `children_` → which clusters got merged at each step.
- `distances_` → distance at each merge.

---

5. Helper to plot dendrogram from sklearn model

```
def plot_dendrogram(model):
    # Create linkage matrix and then plot the dendrogram
    # create the counts of samples under each node
    counts = np.zeros(model.children_.shape[0])
    n_samples = len(model.labels_)
    for i, merge in enumerate(model.children_):
        current_count = 0
        for child_idx in merge:
            if child_idx < n_samples:
                current_count += 1  # leaf node
            else:
                current_count += counts[child_idx - n_samples]
        counts[i] = current_count

    linkage_matrix = np.column_stack(
        [model.children_, model.distances_, counts]
    ).astype(float)

    # Plot the corresponding dendrogram
    dendrogram(linkage_matrix)
```

What this function does:

- Takes sklearn model (`AgglomerativeClustering`) and converts its attributes into a **linkage matrix** like SciPy's `linkage` output.
- `counts` array: number of original samples under each merge node.
- `for` loop:
  - goes through each merge (each internal node).
  - counts how many leaf samples are in the merged node.
- `linkage_matrix` = `children_` + `distances_` + `counts` stacked into columns.
- Finally calls `dendrogram(linkage_matrix)` to plot tree.

```
plot_dendrogram(ac)
```

- Draw dendrogram for current `ac` model (3 clusters).

---

6. Repeat with n_clusters = 2

```
ac = AgglomerativeClustering(n_clusters=2,
                             metric='euclidean',
                             linkage='complete',
                             compute_distances=True)

labels = ac.fit_predict(X)
labels

plot_dendrogram(ac)
```

- Create new model asking for 2 final clusters instead of 3.

- Fit on `X`, get labels, plot dendrogram again.

🌙 Compare methods on the moons dataset

Now we re-use the moon `dataset` again.

```
# K-Means
kmeans = KMeans(n_clusters=2, n_init='auto')
labels_kmeans = kmeans.fit_predict(dataset)
```

- K-Means, 2 clusters, auto init.

```
# DBSCAN
dbscan = DBSCAN(eps=0.2, min_samples=5)
labels_dbscan = dbscan.fit_predict(dataset)
```

- DBSCAN with earlier parameters.

```
# Agglomerative Hierarchical Clustering
ac = AgglomerativeClustering(n_clusters=2, metric='euclidean',
                             linkage='single', compute_distances=True)
labels_ac = ac.fit_predict(dataset)
```

- Agglomerative clustering on moon data:
  - 2 clusters.
  - `linkage='single'` (uses nearest point distance).
- `labels_ac` → cluster labels for each point.

---

7. Plot all 4 side-by-side

```
plt.figure(figsize=(20,5))
plt.subplot(1,4,1)
plt.scatter(dataset[:,0],dataset[:,1], c=true_labels); plt.title('Original
Dataset')
```

- New figure, 1×4 grid.
- First panel: true labels.

```
plt.subplot(1,4,2)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_kmeans); plt.title('K-
Means')
```

- Second panel: K-Means clustering.

```
plt.subplot(1,4,3)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_dbscan);
plt.title('DBSCAN')
```

- Third panel: DBSCAN clustering.

```
plt.subplot(1,4,4)
plt.scatter(dataset[:,0],dataset[:,1], c=labels_ac);
plt.title('Agglomerative Hierarchical');
```

- Fourth panel: Agglomerative clustering result.

```
plt.figure(figsize=(15,5))
plot_dendrogram(ac)
```

- New figure.
- Draw dendrogram for the `ac` model trained on the moons data.
