

There are several Machine Learning algorithms, one such important algorithm of machine learning is Clustering.

Clustering is an unsupervised learning method in machine learning. It means that it is a machine learning algorithm that can draw inferences from a given dataset on its own, without any kind of human intervention.

Types of clustering method

There are five types of clustering methods in machine learning, these are as follows:

- 1.Partitioning Clustering
- 2.Density-Based Clustering
- 3.Distribution Model-Based Clustering
- 4.Hierarchical Clustering
- 5.Fuzzy Clustering

About Hierarchical Clustering

Hierarchical clustering, also known as hierarchical cluster analysis or HCA, is another unsupervised machine learning approach for grouping unlabeled datasets into clusters.

The hierarchy of clusters is developed in the form of a tree in this technique, and this tree-shaped structure is known as the dendrogram.

Simply speaking, Separating data into groups based on some measure of similarity, finding a technique to quantify how they're alike and different, and limiting down the data is what hierarchical clustering is all about.

Hierarchical clustering method functions in two approaches-

1. Agglomerative

2. Divisive

▼ Approaches of Hierarchical Clustering

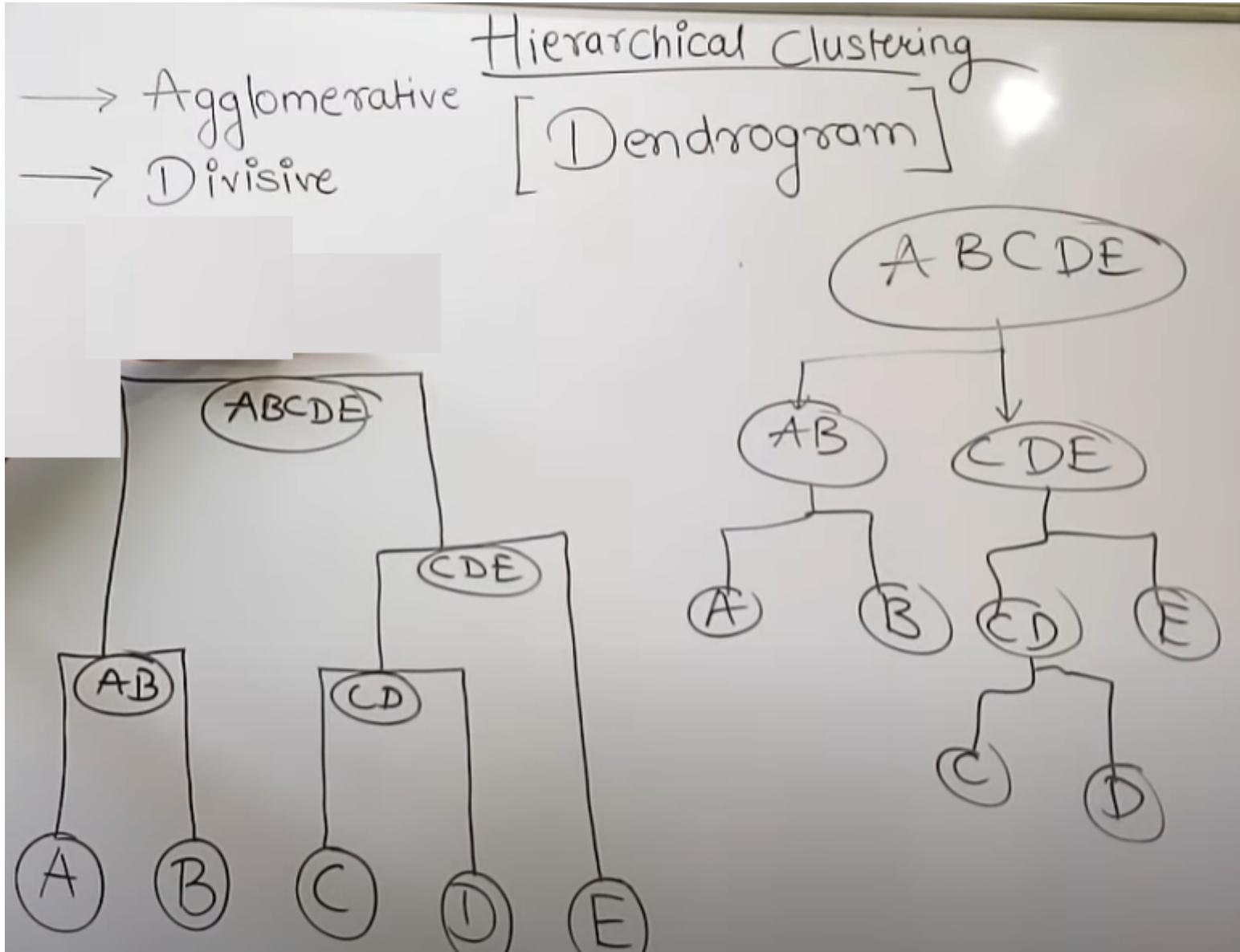
1. Agglomerative clustering:

Agglomerative Clustering is a bottom-up strategy in which each data point is originally a cluster of its own, and as one travels up the hierarchy, more pairs of clusters are combined. In it, two nearest clusters are taken and joined to form one single cluster.

2. Divisive clustering:

The divisive clustering algorithm is a top-down clustering strategy in which all points in the dataset are initially assigned to one cluster and then divided iteratively as one progresses down the hierarchy.

It partitions data points that are clustered together into one cluster based on the slightest difference. This process continues till the desired number of clusters is obtained.



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▼ How hierarchical clustering works

Hierarchical clustering starts by treating each observation as a separate cluster. Then, it repeatedly executes the following two steps:

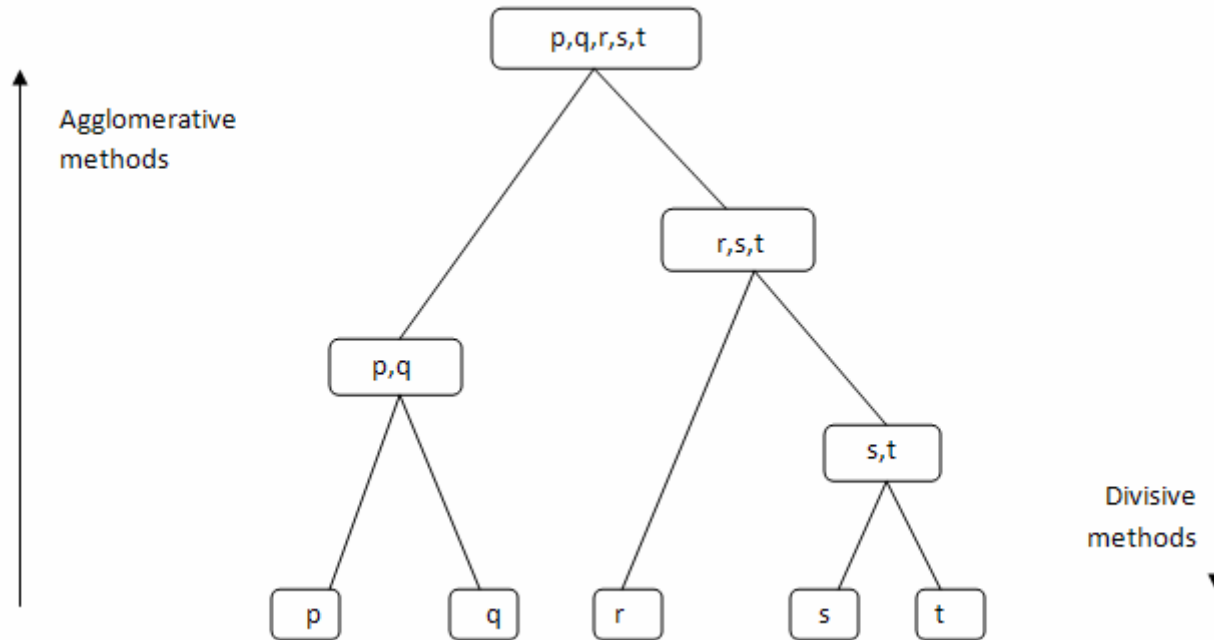
(1) identify the two clusters that are closest together,

and (2) merge the two most similar clusters. This iterative process continues until all the clusters are merged together. This is illustrated in the diagrams below

Hierarchical clustering algorithms group similar objects into groups called clusters. There are two types of hierarchical clustering algorithms:

Agglomerative — Bottom up approach. Start with many small clusters and merge them together to create bigger clusters.

Divisive — Top down approach. Start with a single cluster than break it up into smaller clusters.



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Some pros and cons of Hierarchical Clustering

Pros

No assumption of a particular number of clusters (i.e. k-means) May correspond to meaningful taxonomies

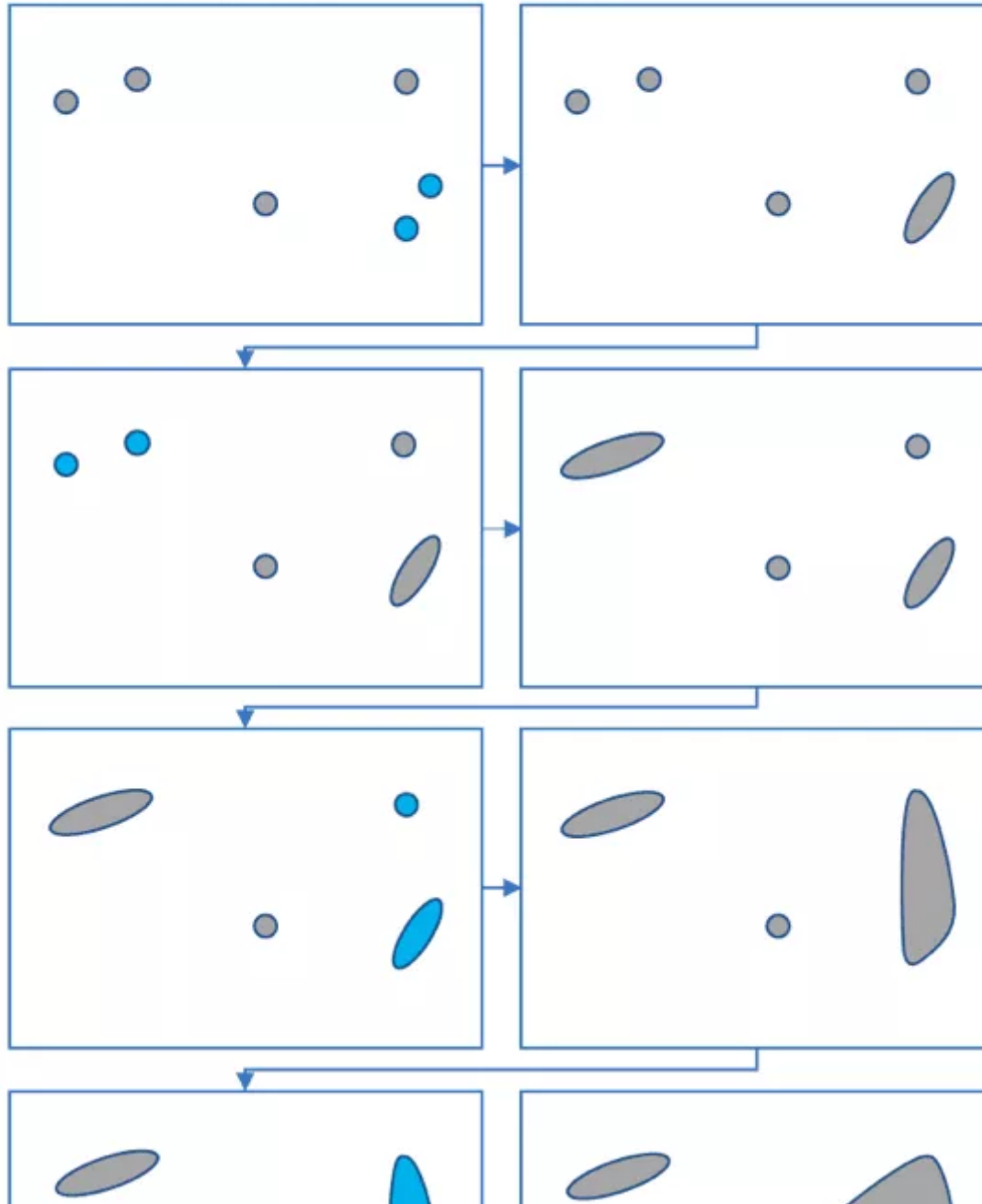
Cons

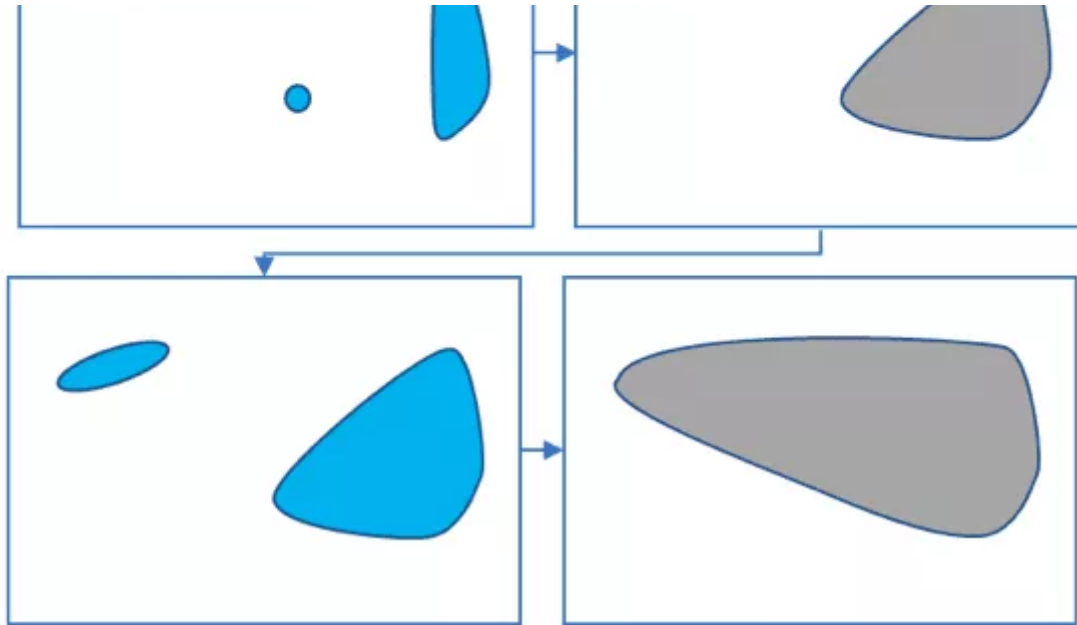
Once a decision is made to combine two clusters, it can't be undone Too slow for large data sets, $O(n^2 \log(n))$

▼ How its Work

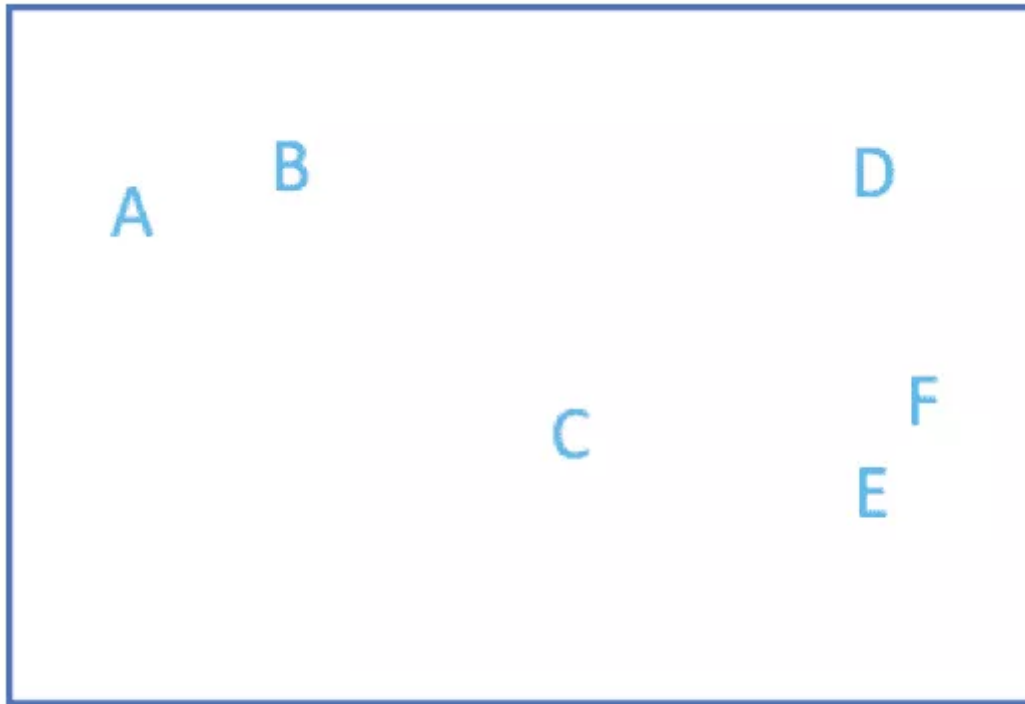
Identify the two clusters that are **closest** together

Merge the two most similar clusters

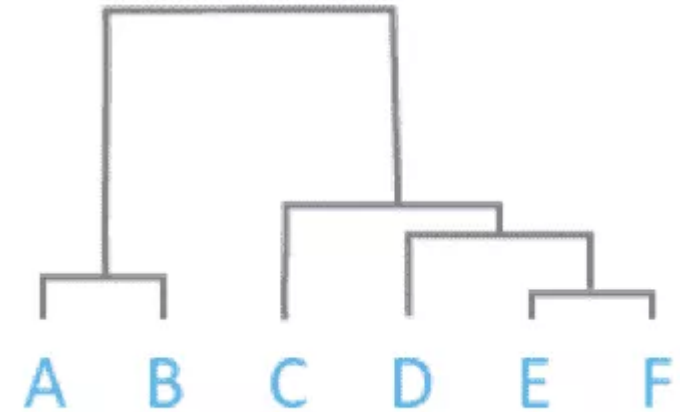




The main output of Hierarchical Clustering is a dendrogram, which shows the hierarchical relationship between the clusters:



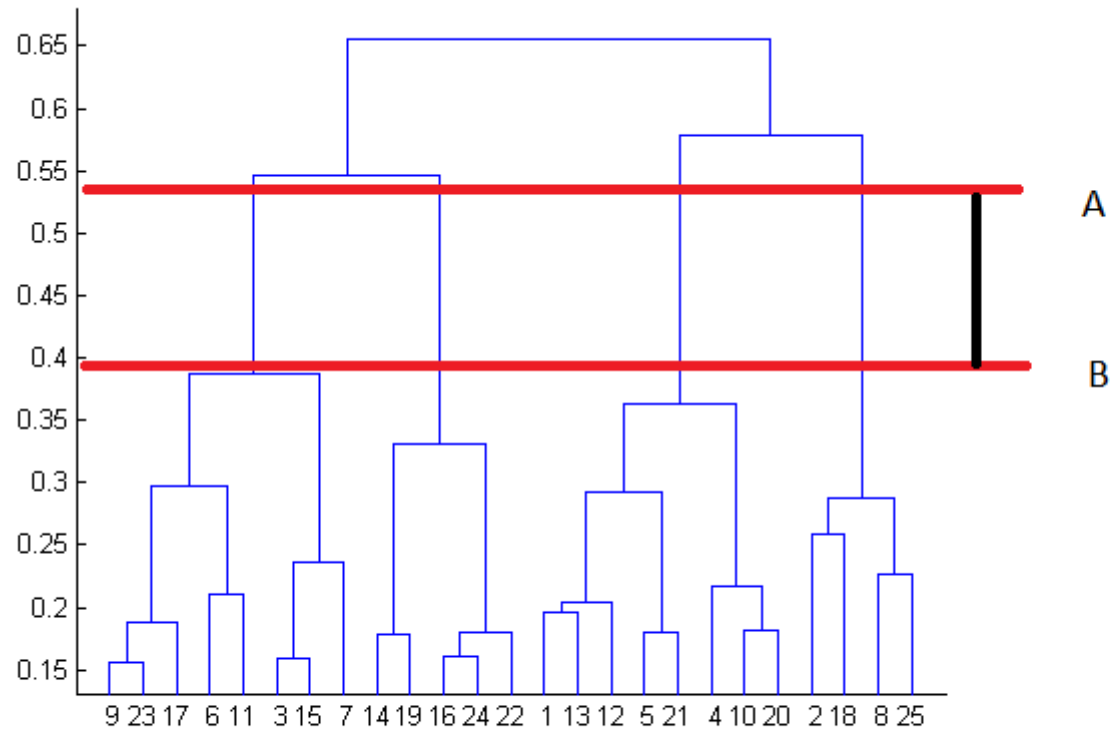
Dendrogram



▼ Dendrograms

We can use a dendrogram to visualize the history of groupings and figure out the optimal number of clusters.

1. Determine the largest vertical distance that doesn't intersect any of the other clusters
2. Draw a horizontal line at both extremities
3. The optimal number of clusters is equal to the number of vertical lines going through the horizontal line For eg., in the below case, best choice for no. of clusters will be 4.



► Linkage Criteria

Similar to gradient descent, you can tweak certain parameters to get drastically different results.

[] ↳ 5 cells hidden

Python loc() function

The loc() function is label based data selecting method which means that we have to pass the name of the row or column which we want to select. This method includes the last element of the range passed in it, unlike iloc(). loc() can accept the boolean data unlike iloc(). Many

Python iloc() function

The iloc() function is an indexed-based selecting method which means that we have to pass an integer index in the method to select a specific row/column. This method does not include the last element of the range passed in it unlike loc(). iloc() does not accept the boolean data unlike loc(). Operations performed using iloc() are:

Example 1:

Selecting rows using integer indices

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```
# selecting 0th, 2th, 4th, and 7th index rows
display(dataset.iloc[[0, 2, 4, 7]])
```

	CustomerID	Genre	Age	Annual Income (k\$)	Spending Score (1-100)
0	1	Male	19	15	39
2	3	Female	20	16	6
4	5	Female	31	17	40
7	8	Female	23	18	94

```
x=dataset.iloc[:2,-1:]
```

x

Spending Score (1-100)

0	39
1	81

```
X = dataset.iloc[:, [3, 4]].values
```

```
X
```

```
[ 70, 40],
[ 76, 87],
[ 77, 12],
[ 77, 97],
[ 77, 36],
[ 77, 74],
[ 78, 22],
[ 78, 90],
[ 78, 17],
[ 78, 88],
[ 78, 20],
[ 78, 76],
[ 78, 16],
[ 78, 89],
[ 78,  1],
[ 78, 78],
[ 78,  1],
[ 78, 73],
[ 79, 35],
[ 79, 83],
[ 81,  5],
[ 81, 93],
[ 85, 26],
[ 85, 75],
[ 86, 20],
[ 86, 95],
[ 87, 27],
[ 87, 63],
[ 87, 13],
[ 87, 75],
```

```
[ 87, 10],  
[ 87, 92],  
[ 88, 13],  
[ 88, 86],  
[ 88, 15],  
[ 88, 69],  
[ 93, 14],  
[ 93, 90],  
[ 97, 32],  
[ 97, 86],  
[ 98, 15],  
[ 98, 88],  
[ 99, 39],  
[ 99, 97],  
[101, 24],  
[101, 68],  
[103, 17],  
[103, 85],  
[103, 23],  
[103, 69],  
[113,  8],  
[113, 91],  
[120, 16],  
[120, 79],  
[126, 28],  
[126, 74],  
[137, 18],  
[137, 83]])
```

▼ Training the Hierarchical Clustering model on the dataset

```
from sklearn.cluster import AgglomerativeClustering  
hc = AgglomerativeClustering(n_clusters = 5, affinity = 'euclidean', linkage = 'ward')
```

y_hc

n_clusters int

affinity

linkage{'ward', 'complete', 'average', 'single'}, default='ward'

'single' uses the minimum of the distances between all observations of the two sets.

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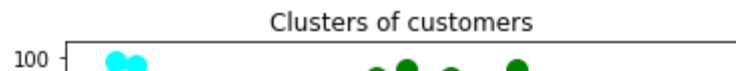
```
print(hc)
```

```
AgglomerativeClustering(n_clusters=5)
```

▼ Visualising the clusters

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```
plt.scatter(X[y_hc == 0, 0], X[y_hc == 0, 1], s = 100, c = 'red', label = 'Cluster 1')
plt.scatter(X[y_hc == 1, 0], X[y_hc == 1, 1], s = 100, c = 'blue', label = 'Cluster 2')
plt.scatter(X[y_hc == 2, 0], X[y_hc == 2, 1], s = 100, c = 'green', label = 'Cluster 3')
plt.scatter(X[y_hc == 3, 0], X[y_hc == 3, 1], s = 100, c = 'cyan', label = 'Cluster 4')
plt.scatter(X[y_hc == 4, 0], X[y_hc == 4, 1], s = 100, c = 'magenta', label = 'Cluster 5')
plt.title('Clusters of customers')
plt.xlabel('Annual Income (k$)')
plt.ylabel('Spending Score (1-100)')
plt.legend()
plt.show()
```



How does it work?

We will use Agglomerative Clustering, a type of hierarchical clustering that follows a bottom up approach.

We begin by treating each data point as its own cluster. Then, we join clusters together that have the shortest distance between them to create larger clusters.

This step is repeated until one large cluster is formed containing all of the data points.

Hierarchical clustering requires us to decide on both a distance and linkage method.

We will use euclidean distance and the Ward linkage method, which attempts to minimize the variance between clusters.

▼ Example

Start by visualizing some data points:

```
import numpy as np
import matplotlib.pyplot as plt

x = [4, 5, 10, 4, 3, 11, 14, 6, 10, 12]
y = [21, 19, 24, 17, 16, 25, 24, 22, 21, 21]

plt.scatter(x, y)
plt.show()
```



Now we compute the ward linkage using euclidean distance, and visualize it using a dendrogram:

Example

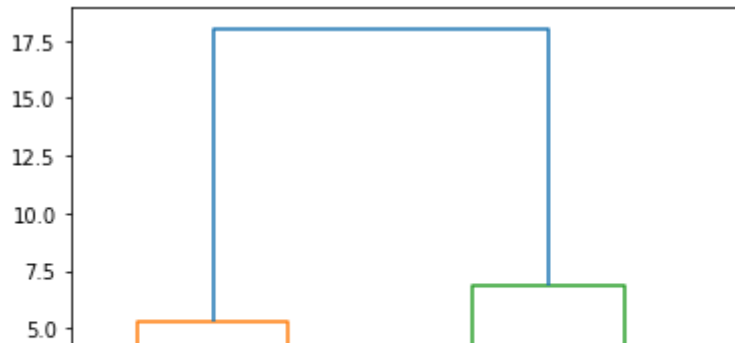
```
import numpy as np
import matplotlib.pyplot as plt
from scipy.cluster.hierarchy import dendrogram, linkage

x = [4, 5, 10, 4, 3, 11, 14, 6, 10, 12]
y = [21, 19, 24, 17, 16, 25, 24, 22, 21, 21]

data = list(zip(x, y))

linkage_data = linkage(data, method='ward', metric='euclidean')
dendrogram(linkage_data)

plt.show()
```

Here, we do the same thing with Python's scikit-learn library. Then, visualize on a 2-dimensional plot:

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.cluster import AgglomerativeClustering

x = [4, 5, 10, 4, 3, 11, 14, 6, 10, 12]
y = [21, 19, 24, 17, 16, 25, 24, 22, 21, 21]

data = list(zip(x, y))

hierarchical_cluster = AgglomerativeClustering(n_clusters=2, affinity='euclidean', linkage='ward')
labels = hierarchical_cluster.fit_predict(data)

plt.scatter(x, y, c=labels)
plt.show()
```



▼ Example Explained

Import the modules you need.

1. import numpy as np
2. import matplotlib.pyplot as plt
3. from scipy.cluster.hierarchy import dendrogram, linkage
4. from sklearn.cluster import AgglomerativeClustering

Create arrays that resemble two variables in a dataset.

Note that while we only have two variables here, this method will work with any number of variables:

```
x = [4, 5, 10, 4, 3, 11, 14, 6, 10, 12]
y = [21, 19, 24, 17, 16, 25, 24, 22, 21, 21]
```

▼ Turn the data into a set of points:

```
data = list(zip(x, y))
print(data)
```

```
[(4, 21), (5, 19), (10, 24), (4, 17), (3, 16), (11, 25), (14, 24), (6, 22), (10, 21), (12, 21)]
```

Compute the linkage between all of the different points.

Here we use a simple euclidean distance measure and Ward's linkage, which seeks to minimize the variance between clusters.

In complete-link (or complete linkage) hierarchical clustering, we merge in each step the two clusters whose merger has the smallest diameter (or: the two clusters with the smallest maximum pairwise distance).

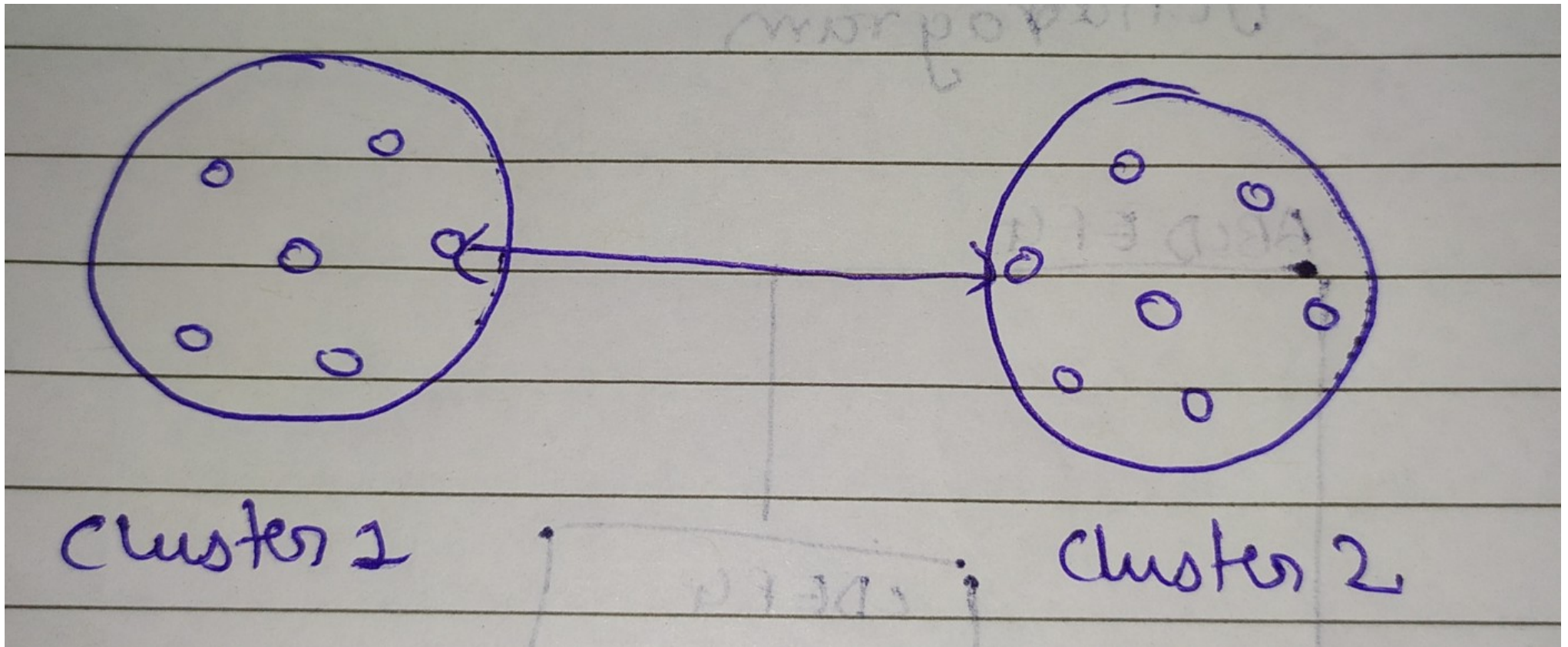
In single-link (or single linkage) hierarchical clustering, we merge in each step the two clusters whose two closest members have the smallest distance (or: the two clusters with the smallest minimum pairwise distance).

Complete-link clustering can also be described using the concept of clique. Let d_n be the diameter of the cluster created in step n of complete-link clustering. Define graph $G(n)$ as the graph that links all data points with a distance of at most d_n . Then the clusters after step n are the cliques of $G(n)$. This motivates the term complete-link clustering.

Let's understand all four linkage used in calculating distance between Clusters:

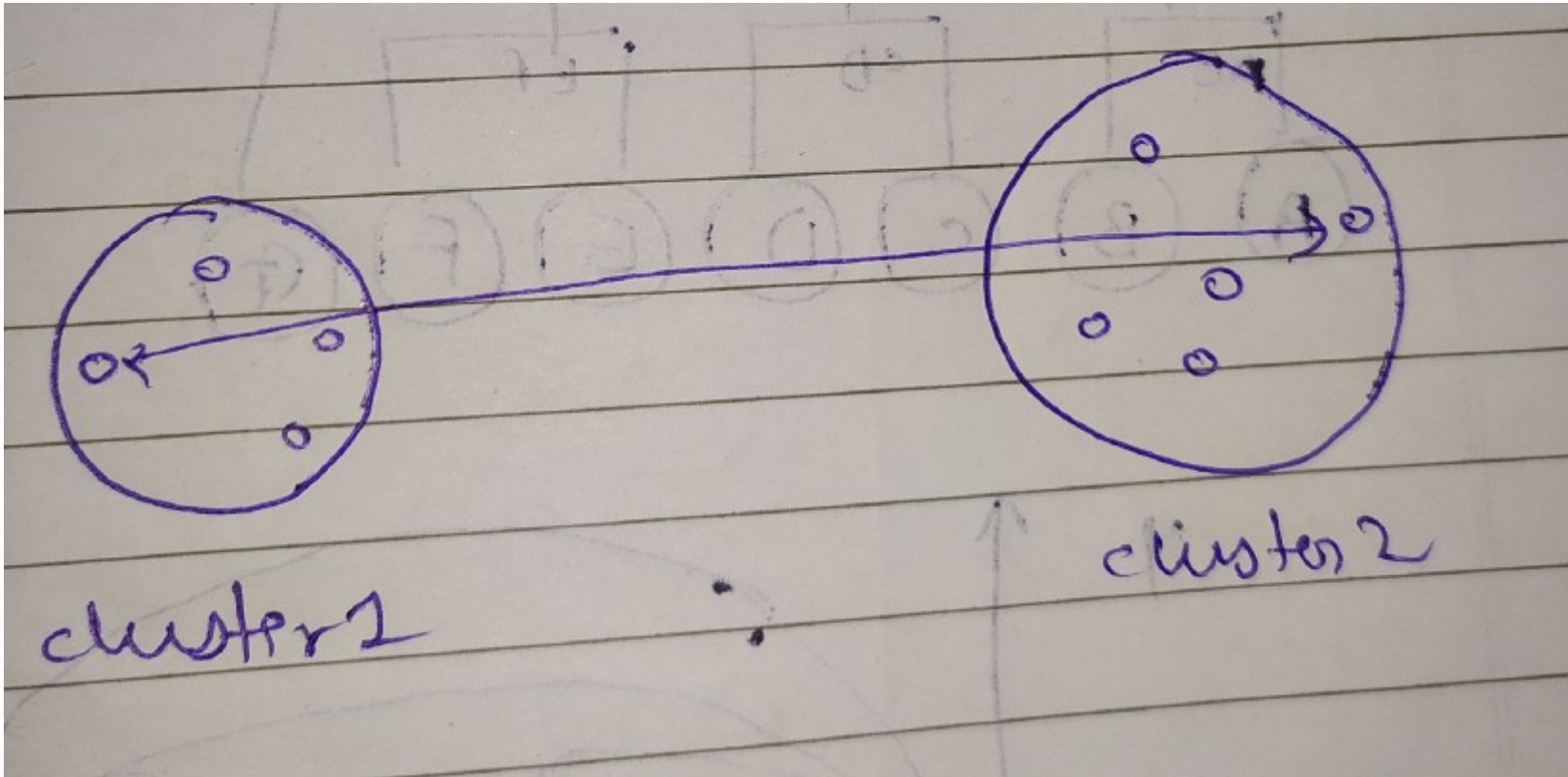
Single linkage:

Single linkage returns minimum distance between two point , where each points belong to two different clusters



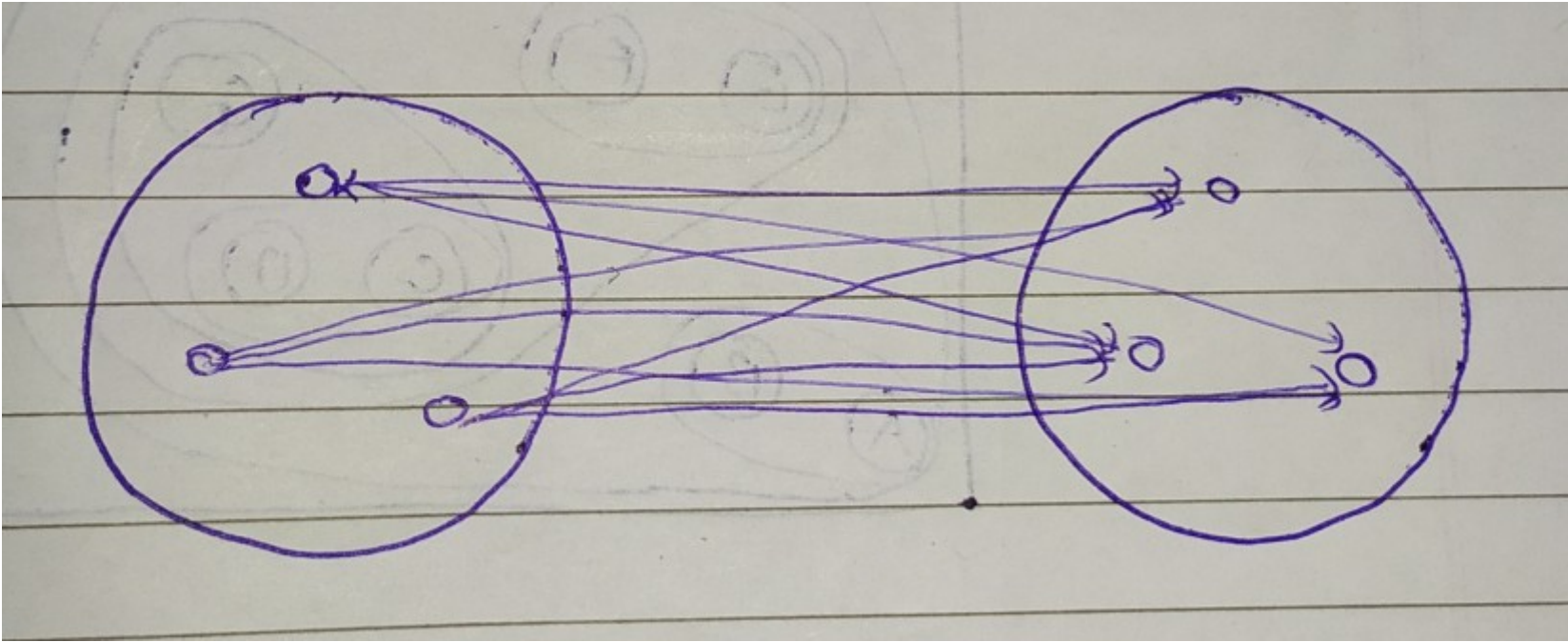
2. Complete linkage:

It returns the maximum distance between each data point.



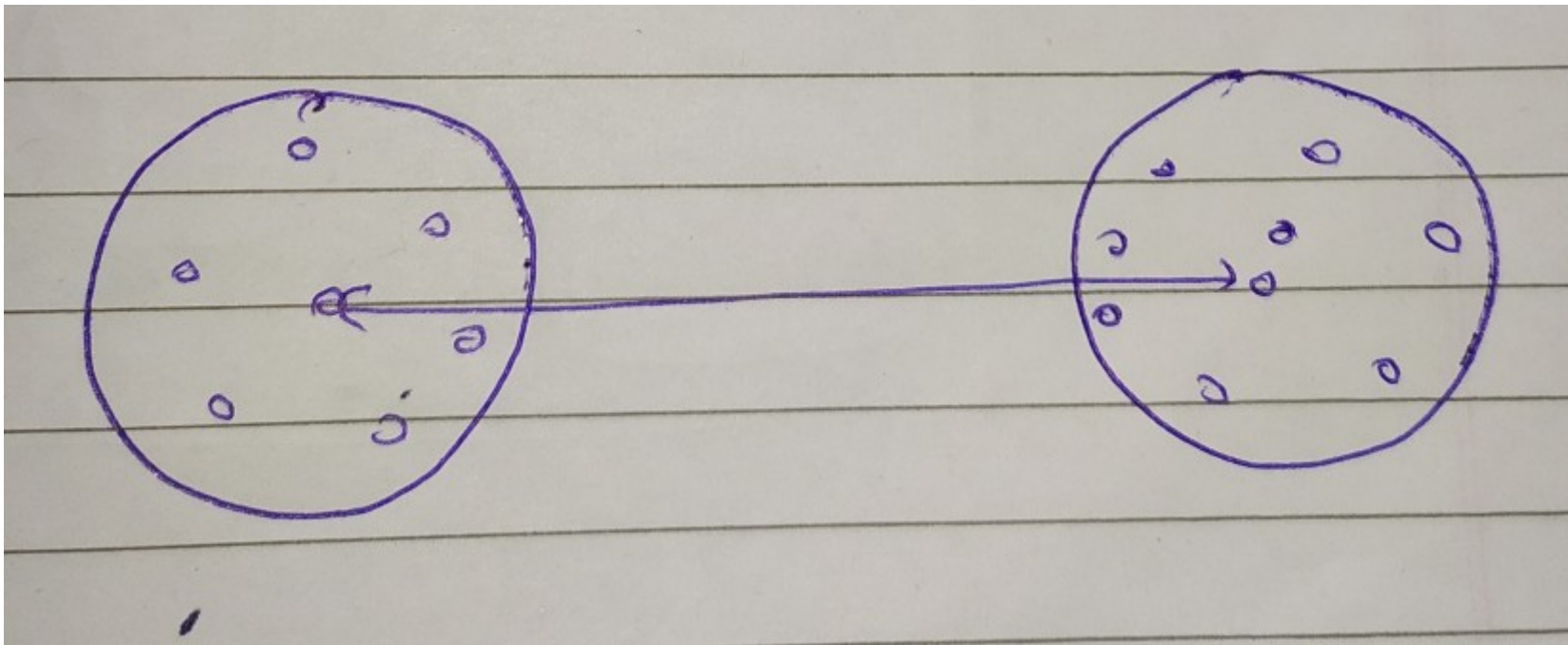
3. Average linkage:

It returns the average of distances between all pairs of data point .



▼ 4. Centroid linkage

It returns the distance between centroid of Clusters.



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What is Ward's Method? Ward's method (a.k.a. Minimum variance method or Ward's Minimum Variance Clustering Method) is an alternative to single-link clustering. Popular in fields like linguistics, it's liked because it usually creates compact, even-sized clusters (Szmrecsanyi, 2012).

Like most other clustering methods, Ward's method is computationally intensive. However, Ward's has significantly fewer computations than other methods. The drawback is this usually results in less than optimal clusters. That said, the resulting clusters are usually good enough for most purposes.

Sum of Squares Index, E Like other clustering methods, Ward's method starts with n clusters, each containing a single object. These n clusters are combined to make one cluster containing all objects. At each step, the process makes a new cluster that minimizes variance, measured by

an index called E (also called the sum of squares index).

At each step, the following calculations are made to find E:

Find the mean of each cluster.

Calculate the distance between each object in a particular cluster, and that cluster's mean.

Square the differences from Step 2.

Sum (add up) the squared values from Step 3.

Add up all the sums of squares from Step 4.

▼ `linkage_data = linkage(data, method='ward', metric='euclidean')`

Finally, plot the results in a dendrogram.

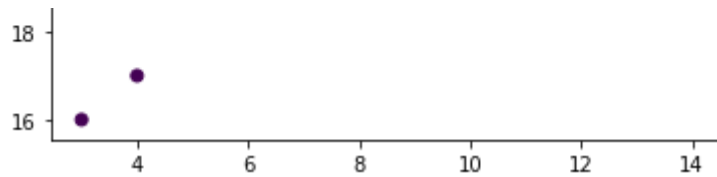
This plot will show us the hierarchy of clusters from the bottom (individual points) to the top (a single cluster consisting of all data points).

`plt.show()` lets us visualize the dendrogram instead of just the raw linkage data.

```
dendrogram(linkage_data)
plt.show()
```




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