Clustering in Machine Learning

Clustering or cluster analysis is a machine learning technique, which groups the unlabelled dataset. It can be defined as **"A way of grouping the data points into different clusters, consisting of similar data points. The objects with the possible similarities remain in a group that has less or no similarities with another group."**

It does it by finding some similar patterns in the unlabelled dataset such as shape, size, color, behavior, etc., and divides them as per the presence and absence of those similar patterns.

It is an unsupervised learning method, hence no supervision is provided to the algorithm, and it deals with the unlabeled dataset.

After applying this clustering technique, each cluster or group is provided with a cluster-ID. ML system can use this id to simplify the processing of large and complex datasets.

The clustering technique is commonly used for **statistical data analysis.**

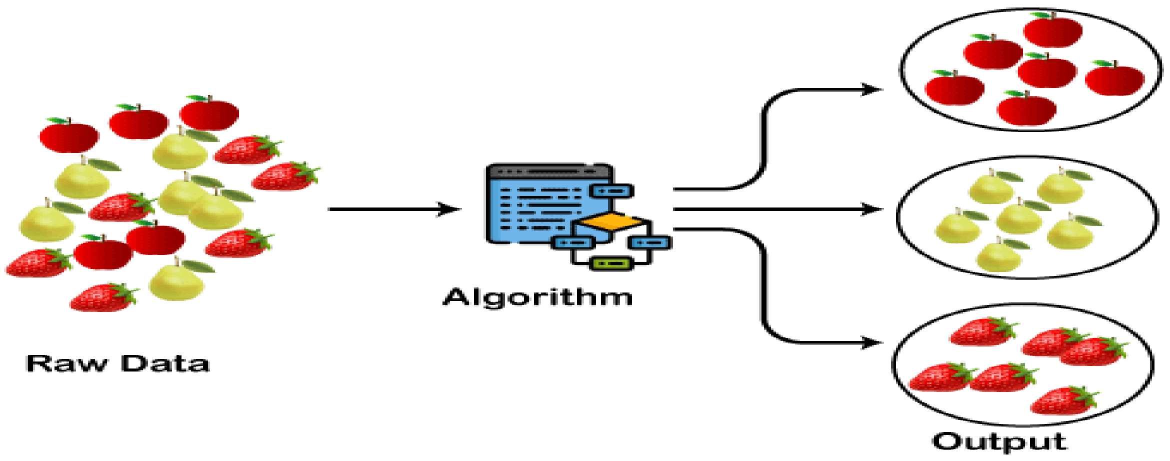
Note: Clustering is somewhere similar to the classification algorithm, but the difference is the type of dataset that we are using. In classification, we work with the labeled data set, whereas in clustering, we work with the unlabelled dataset.

Example: Let's understand the clustering technique with the real-world example of Mall: When we visit any shopping mall, we can observe that the things with similar usage are grouped together. Such as the t-shirts are grouped in one section, and trousers are at other sections, similarly, at vegetable sections, apples, bananas, Mangoes, etc., are grouped in separate sections, so that we can easily find out the things. The clustering technique also works in the same way. Other examples of clustering are grouping documents according to the topic.

The clustering technique can be widely used in various tasks. Some most common uses of this technique are:

- Market Segmentation
- Statistical data analysis
- Social network analysis
- Image segmentation
- Anomaly detection, etc.

The below diagram explains the working of the clustering algorithm. We can see the different fruits are divided into several groups with similar properties.



Types of Clustering Methods

The clustering methods are broadly divided into **Hard clustering** (datapoint belongs to only one group) and **Soft Clustering** (data points can belong to another group also). But there are also other various approaches of Clustering exist. Below are the main clustering methods used in Machine learning:

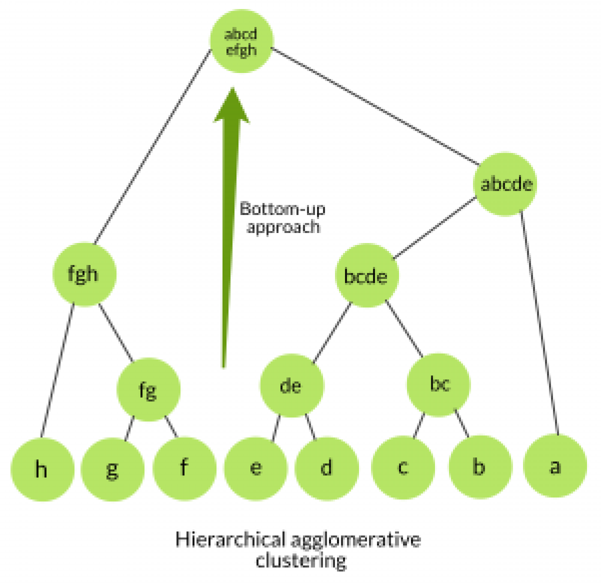
1. **Partitioning Clustering**
2. **Density-Based Clustering**
3. **Distribution Model-Based Clustering**
4. **Hierarchical Clustering**
5. **Fuzzy Clustering**

Basically, there are two types of hierarchical cluster analysis strategies –

1. Agglomerative Clustering: Also known as bottom-up approach or hierarchical agglomerative clustering (HAC). A structure that is more informative than the unstructured set of clusters returned by flat clustering. This clustering algorithm does not require us to prespecify the number of clusters. Bottom-up algorithms treat each data as a singleton cluster at the outset and then successively agglomerates pairs of clusters until all clusters have been merged into a single cluster that contains all data.

Algorithm :

```
given a dataset ($d_1$, $d_2$, $d_3$, ....$d_N$) of size N
# compute the distance matrix
for i=1 to N:
  # as the distance matrix is symmetric about
  # the primary diagonal so we compute only lower
  # part of the primary diagonal
  for j=1 to i:
    dis_mat[i][j] = distance[$d_i$, $d_j$]
each data point is a singleton cluster**repeat**
  merge the two cluster having minimum distance
  update the distance matrix**until** only a single cluster remains
```



Python implementation of the above algorithm using the scikit-learn library:

- Python3

```
from sklearn.cluster import AgglomerativeClustering
import numpy as np

# randomly chosen dataset
X = np.array([[1, 2], [1, 4], [1, 0],
              [4, 2], [4, 4], [4, 0]])

# here we need to mention the number of clusters
# otherwise the result will be a single cluster
# containing all the data
clustering = AgglomerativeClustering(n_clusters = 2).fit(X)

# print the class labels
print(clustering.labels_)
```

Output :

```
[1, 1, 1, 0, 0, 0]
```

2. Divisive clustering: Also known as a top-down approach. This algorithm also does not require to prespecify the number of clusters. Top-down clustering requires a method for splitting a cluster that contains the whole data and proceeds by splitting clusters recursively until individual data have been split into singleton clusters.

Algorithm :

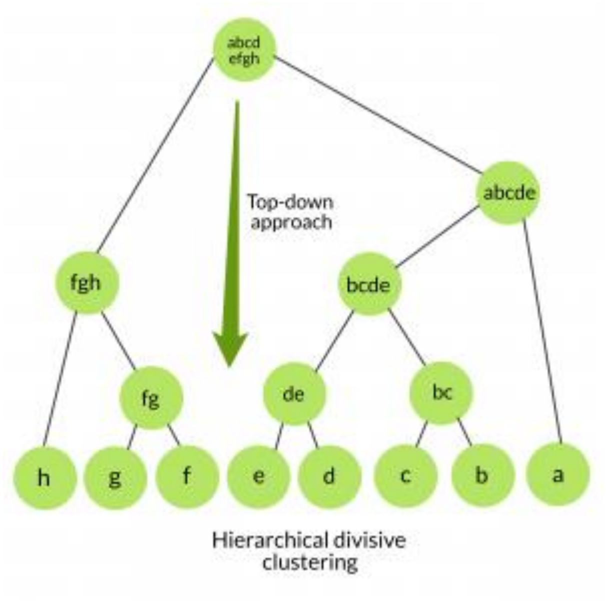
given a dataset (d_1, d_2, d_3, ...d_N) of size N

at the top we have all data in one cluster

the cluster is split using a flat clustering method eg. K-Means etc**repeat**

choose the best cluster among all the clusters to split

split that cluster by the flat clustering algorithm**until** each data is in its own singleton cluster



Hierarchical Agglomerative *vs* Divisive clustering –

a. Divisive clustering is more *complex* as compared to agglomerative clustering, as in the case of divisive clustering we need a flat clustering method as “subroutine” to split each cluster until we have each data having its own singleton cluster.

b. Divisive clustering is more *efficient* if we do not generate a complete hierarchy all the way down to individual data leaves. The time complexity of a naive agglomerative clustering is **$O(n^3)$** because we exhaustively scan the N x N matrix dist_mat for the lowest distance in each of N-1 iterations. Using priority queue data structure we can reduce this complexity to **$O(n^2 \log n)$**. By using some more optimizations it can be brought down to **$O(n^2)$**. Whereas for divisive clustering given a fixed number of top levels, using an efficient flat algorithm like K-Means, divisive algorithms are linear in the number of patterns and clusters.

c. A divisive algorithm is also more *accurate*. Agglomerative clustering makes decisions by considering the local patterns or neighbor points without initially taking into account the global distribution of data. These early decisions cannot be undone. whereas divisive clustering takes into consideration the global distribution of data when making top-level partitioning decisions.

K-Means Clustering Algorithm

K-Means Clustering is an unsupervised learning algorithm that is used to solve the clustering problems in machine learning or data science. In this topic, we will learn what is K-means clustering algorithm, how the algorithm works, along with the Python implementation of k-means clustering.

What is K-Means Algorithm?

K-Means Clustering is an Unsupervised Learning algorithm, which groups the unlabeled dataset into different clusters. Here K defines the number of pre-defined clusters that need to be created in the process, as if K=2, there will be two clusters, and for K=3, there will be three clusters, and so on.

> It is an iterative algorithm that divides the unlabeled dataset into k different clusters in such a way that each dataset belongs only one group that has similar properties.

It allows us to cluster the data into different groups and a convenient way to discover the categories of groups in the unlabeled dataset on its own without the need for any training.

It is a centroid-based algorithm, where each cluster is associated with a centroid. The main aim of this algorithm is to minimize the sum of distances between the data point and their corresponding clusters.

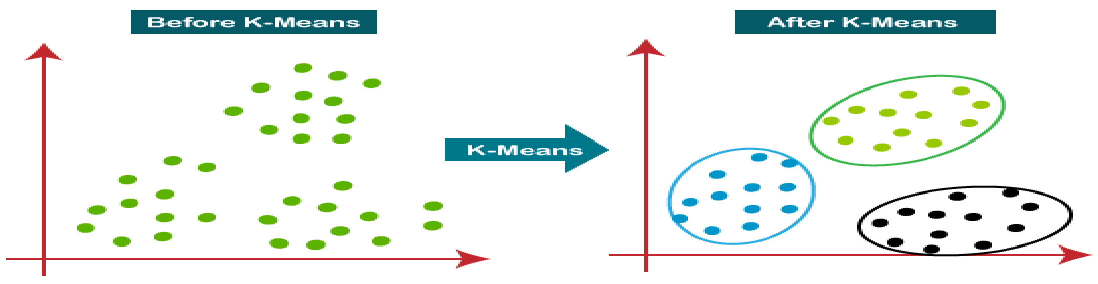
The algorithm takes the unlabeled dataset as input, divides the dataset into k-number of clusters, and repeats the process until it does not find the best clusters. The value of k should be predetermined in this algorithm.

The k-means clustering algorithm mainly performs two tasks:

- Determines the best value for K center points or centroids by an iterative process.
- Assigns each data point to its closest k-center. Those data points which are near to the particular k-center, create a cluster.

Hence each cluster has datapoints with some commonalities, and it is away from other clusters.

The below diagram explains the working of the K-means Clustering Algorithm:



How does the K-Means Algorithm Work?

The working of the K-Means algorithm is explained in the below steps:

Step-1: Select the number K to decide the number of clusters.

Step-2: Select random K points or centroids. (It can be other from the input dataset).

Step-3: Assign each data point to their closest centroid, which will form the predefined K clusters.

Step-4: Calculate the variance and place a new centroid of each cluster.

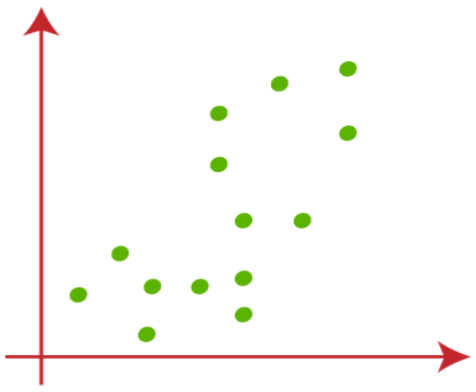
Step-5: Repeat the third steps, which means reassign each datapoint to the new closest centroid of each cluster.

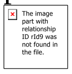
Step-6: If any reassignment occurs, then go to step-4 else go to FINISH.

Step-7: The model is ready.

Let's understand the above steps by considering the visual plots:

Suppose we have two variables M1 and M2. The x-y axis scatter plot of these two variables is given below:



- Let's take number k of clusters, i.e., K=2, to identify the dataset and to put them into different clusters. It means here we will try to group these datasets into two different clusters.
- We need to choose some random k points or centroid to form the cluster. These points can be either the points from the dataset or any other point. So, here we are selecting the below two points as k points, which are not the part of our dataset. Consider the below image:

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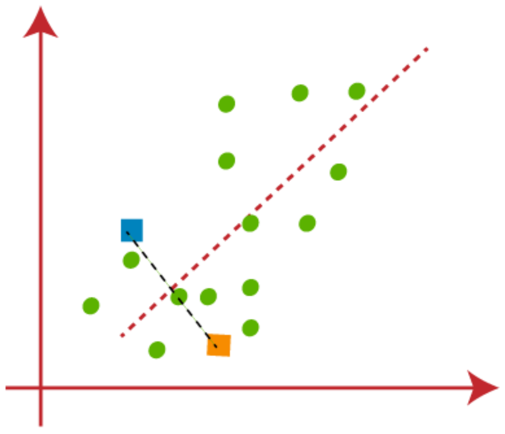
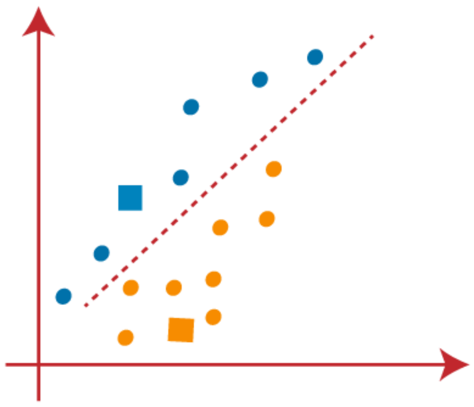
- Now we will assign each data point of the scatter plot to its closest K-point or centroid. We will compute it by applying some mathematics that we have studied to calculate the distance

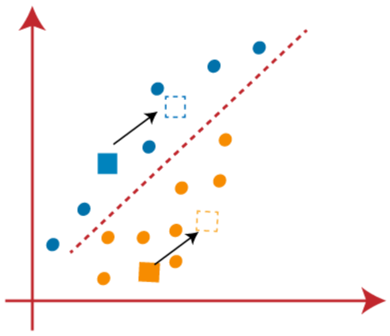
between two points. So, we will draw a median between both the centroids. Consider the below image:



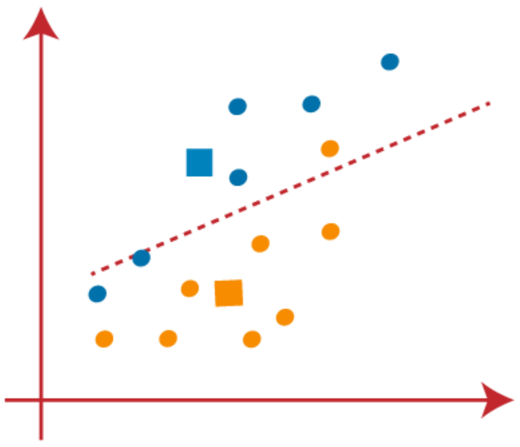
From the above image, it is clear that points left side of the line is near to the K1 or blue centroid, and points to the right of the line are close to the yellow centroid. Let's color them as blue and yellow for clear visualization.



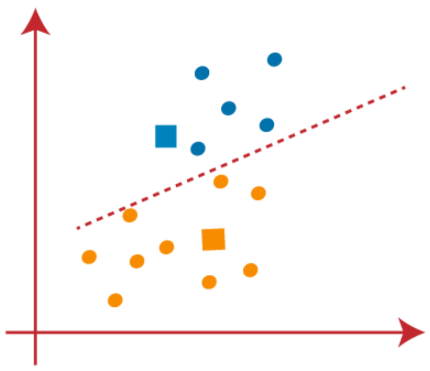
- As we need to find the closest cluster, so we will repeat the process by choosing **a new centroid**. To choose the new centroids, we will compute the center of gravity of these centroids, and will find new centroids as below:



- Next, we will reassign each datapoint to the new centroid. For this, we will repeat the same process of finding a median line. The median will be like below image:

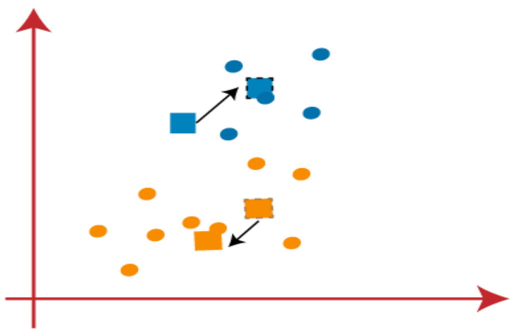


From the above image, we can see, one yellow point is on the left side of the line, and two blue points are right to the line. So, these three points will be assigned to new centroids.

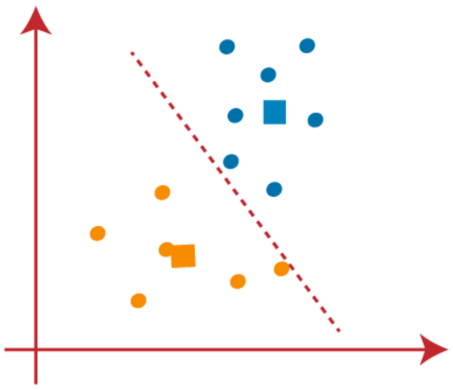


As reassignment has taken place, so we will again go to the step-4, which is finding new centroids or K-points.

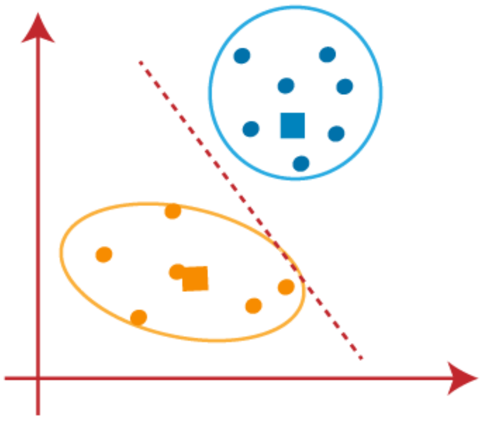
We will repeat the process by finding the center of gravity of centroids, so the new centroids will be as shown in the below image:



- As we got the new centroids so again will draw the median line and reassign the data points. So, the image will be:



- We can see in the above image; there are no dissimilar data points on either side of the line, which means our model is formed. Consider the below image:



As our model is ready, so we can now remove the assumed centroids, and the two final clusters will be as shown in the below image: