Machine Learning
Unit-4 Notes
Session: 2023-24 (EVEN-24)

Branch: CSE **Semester: 6th sem**

Syllabus: Unsupervised Learning
Introduction Clustering, K-means clustering. Apriori algorithm and associations rule, anomaly detection algorithm, Hierarchical clustering, K-Medoids.

4.1 Unsupervised Learning
We learned supervised machine learning in which models are trained using labeled data under the supervision of training data. But there may be many cases in which we do not have labeled data and need to find the hidden patterns from the given dataset. So, to solve such types of cases in machine learning, we need unsupervised learning techniques.

What is Unsupervised Learning?

As the name suggests, unsupervised learning is a machine learning technique in which models are not supervised using training dataset. Instead, models itself find the hidden patterns and insights from the given data. It can be compared to learning which takes place in the human brain while learning new things. It can be defined as:

Unsupervised learning cannot be directly applied to a regression or classification problem because unlike supervised learning, we have the input data but no corresponding output data. The goal of unsupervised learning is to find the underlying structure of dataset, group that data according to similarities, and represent that dataset in a compressed format**.**

Example: Suppose the unsupervised learning algorithm is given an input dataset containing images of different types of cats and dogs. The algorithm is never trained upon the given dataset, which means it does not have any idea about the features of the dataset. The task of the unsupervised learning algorithm is to identify the image features on their own. Unsupervised learning algorithm will perform this task by clustering the image dataset into the groups according to similarities between images.

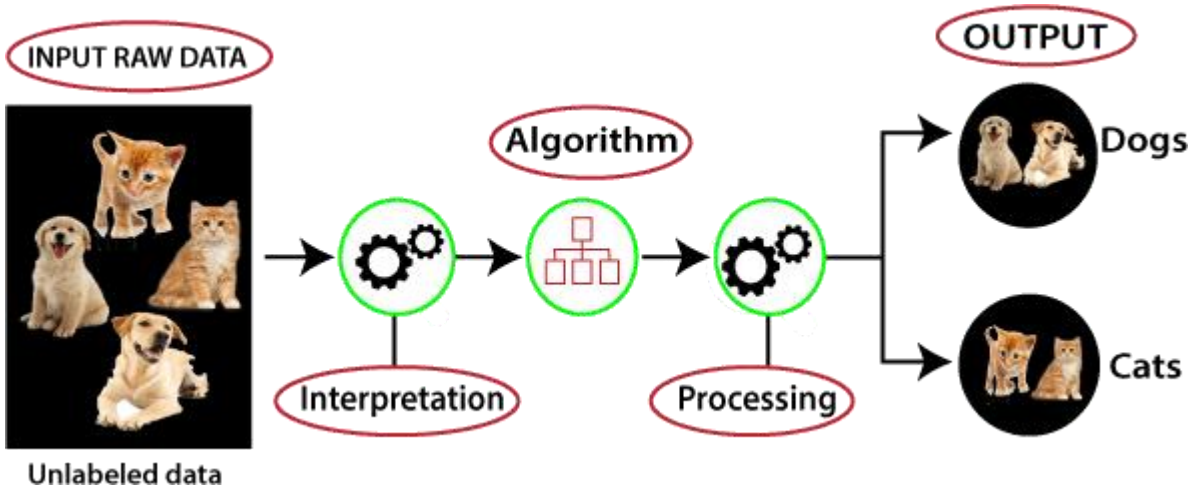
Why use Unsupervised Learning?

Below are some main reasons which describe the importance of Unsupervised Learning:

- Unsupervised learning is helpful for finding useful insights from the data.
- Unsupervised learning is much similar as a human learns to think by their own experiences, which makes it closer to the real AI.
- Unsupervised learning works on unlabeled and uncategorized data which make unsupervised learning more important.
- In real-world, we do not always have input data with the corresponding output so to solve such cases, we need unsupervised learning.

Working of Unsupervised Learning

Working of unsupervised learning can be understood by the below diagram:

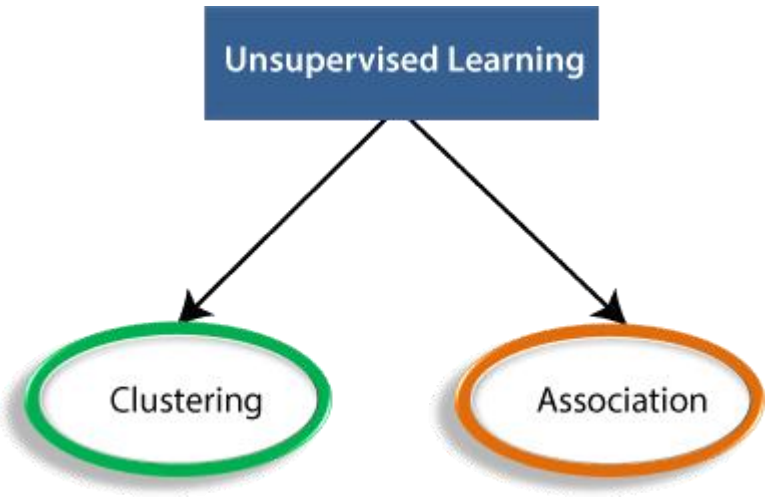


Here, we have taken an unlabeled input data, which means it is not categorized and corresponding outputs are also not given. Now, this unlabeled input data is fed to the machine learning model in order to train it. Firstly, it will interpret the raw data to find the hidden patterns from the data and then will apply suitable algorithms such as k-means clustering, Decision tree, etc.

Once it applies the suitable algorithm, the algorithm divides the data objects into groups according to the similarities and difference between the objects.

Types of Unsupervised Learning Algorithm:

The unsupervised learning algorithm can be further categorized into two types of problems:



- **Clustering**: Clustering is a method of grouping the objects into clusters such that objects with most similarities remains into a group and has less or no similarities with the objects of another group. Cluster analysis finds the commonalities between the data objects and categorizes them as per the presence and absence of those commonalities.

- **Association**: An association rule is an unsupervised learning method which is used for finding the relationships between variables in the large database. It determines the set of items that occurs together in the dataset. Association rule makes marketing strategy more effective. Such as people who buy X item (suppose a bread) are also tend to purchase Y (Butter/Jam) item. A typical example of Association rule is Market Basket Analysis.

Unsupervised Learning algorithms:

Below is the list of some popular unsupervised learning algorithms:

- K-means clustering
- KNN (k-nearest neighbors)
- Hierarchal clustering
- Anomaly detection
- Neural Networks
- Principle Component Analysis
- Independent Component Analysis
- Apriori algorithm
- Singular value decomposition

Advantages of Unsupervised Learning

- Unsupervised learning is used for more complex tasks as compared to supervised learning because, in unsupervised learning, we don't have labeled input data.
- Unsupervised learning is preferable as it is easy to get unlabeled data in comparison to labeled data.

Disadvantages of Unsupervised Learning

- Unsupervised learning is intrinsically more difficult than supervised learning as it does not have corresponding output.
- The result of the unsupervised learning algorithm might be less accurate as input data is not labeled, and algorithms do not know the exact output in advance.

4.2 Introduction Clustering

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.

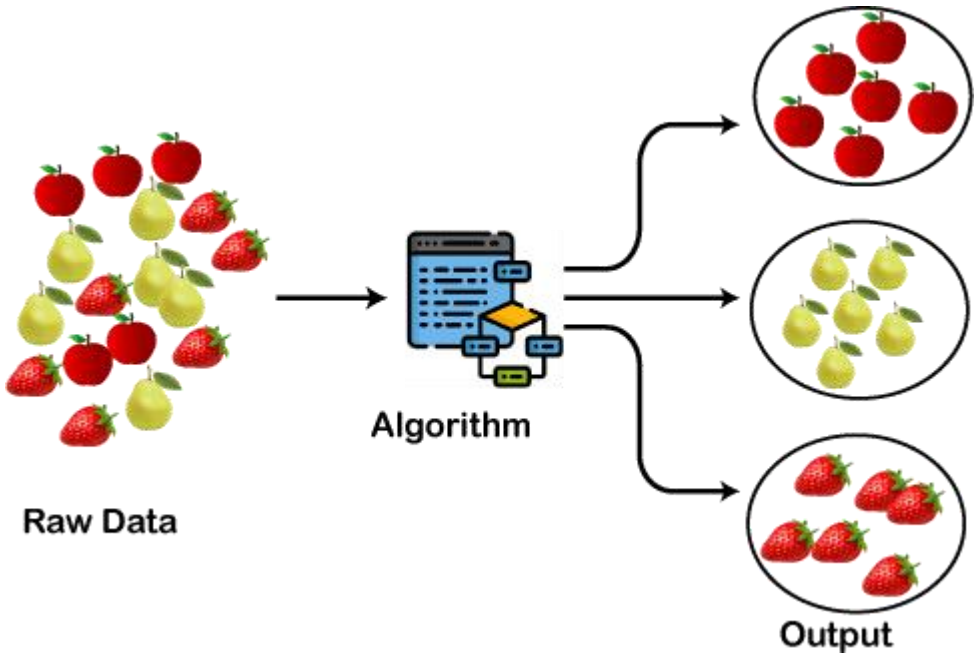
Example: Let's understand the clustering technique with the real-world example of Mall: When we visit any shopping mall, we can observe that the things with similar usage are grouped together. Such as the t-shirts are grouped in one section, and trousers are at other sections, similarly, at vegetable 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.

Apart from these general usages, it is used by the **Amazon** in its recommendation system to provide the recommendations as per the past search of products. **Netflix** also uses this technique to recommend the movies and web-series to its users as per the watch history.

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:

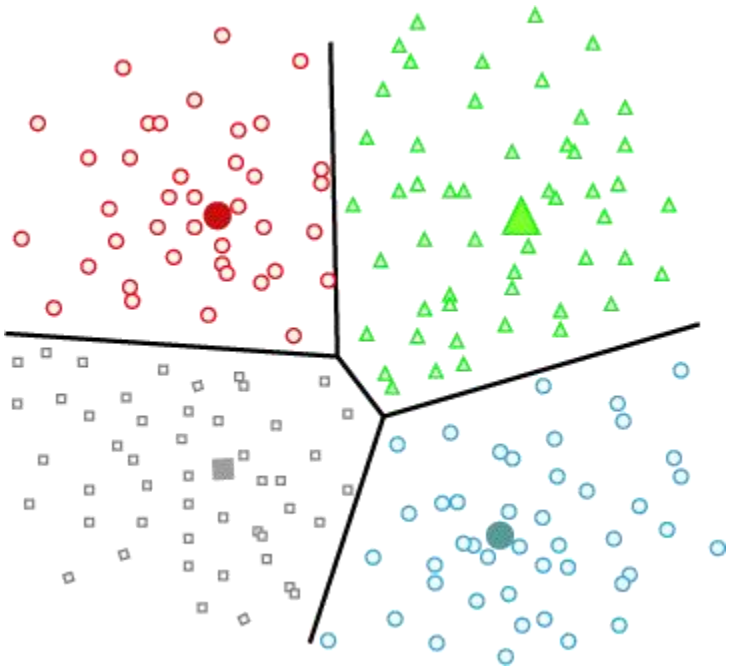
1. **Partitioning Clustering**

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

Partitioning Clustering

It is a type of clustering that divides the data into non-hierarchical groups. It is also known as the **centroid-based method**. The most common example of partitioning clustering is the **K-Means Clustering algorithm**.

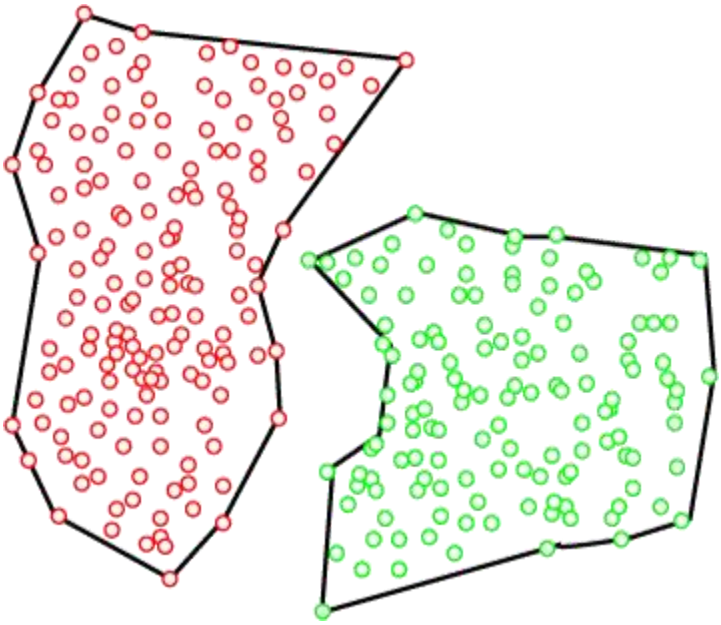
In this type, the dataset is divided into a set of k groups, where K is used to define the number of pre-defined groups. The cluster center is created in such a way that the distance between the data points of one cluster is minimum as compared to another cluster centroid.



Density-Based Clustering

The density-based clustering method connects the highly-dense areas into clusters, and the arbitrarily shaped distributions are formed as long as the dense region can be connected. This algorithm does it by identifying different clusters in the dataset and connects the areas of high densities into clusters. The dense areas in data space are divided from each other by sparser areas.

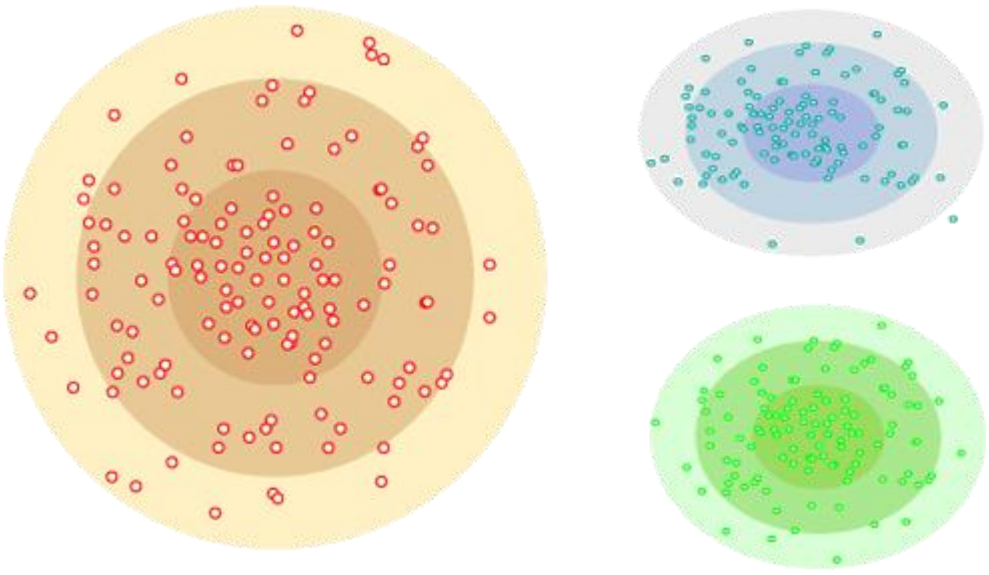
These algorithms can face difficulty in clustering the data points if the dataset has varying densities and high dimensions.



Distribution Model-Based Clustering

In the distribution model-based clustering method, the data is divided based on the probability of how a dataset belongs to a particular distribution. The grouping is done by assuming some distributions commonly **Gaussian Distribution**.

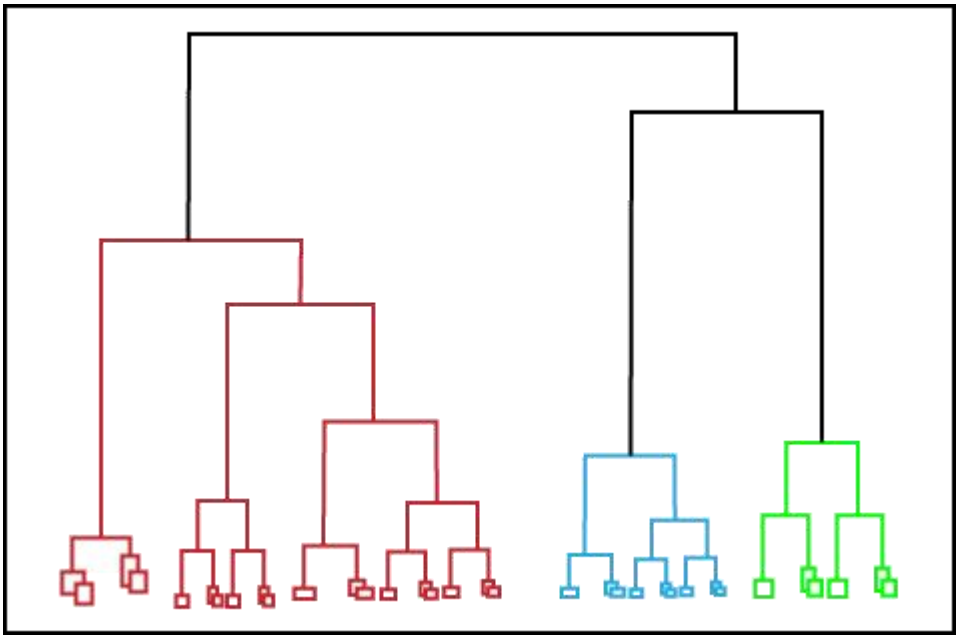
The example of this type is the **Expectation-Maximization Clustering algorithm** that uses Gaussian Mixture Models (GMM).



Hierarchical Clustering

Hierarchical clustering can be used as an alternative for the partitioned clustering as there is no requirement of pre-specifying the number of clusters to be created. In this technique, the dataset is divided into clusters to create a tree-like structure, which is also called a **dendrogram**. The observations or any number of clusters can be

selected by cutting the tree at the correct level. The most common example of this method is the **Agglomerative Hierarchical algorithm**.



Fuzzy Clustering

Fuzzy clustering is a type of soft method in which a data object may belong to more than one group or cluster. Each dataset has a set of membership coefficients, which depend on the degree of membership to be in a cluster. **Fuzzy C-means algorithm** is the example of this type of clustering; it is sometimes also known as the Fuzzy k-means algorithm.

Clustering Algorithms

The Clustering algorithms can be divided based on their models that are explained above. There are different types of clustering algorithms published, but only a few are commonly used. The clustering algorithm is based on the kind of data that we are using. Such as, some algorithms need to guess the number of clusters in the given dataset, whereas some are required to find the minimum distance between the observation of the dataset.

Here we are discussing mainly popular Clustering algorithms that are widely used in machine learning:

1. **K-Means algorithm:** The k-means algorithm is one of the most popular clustering algorithms. It classifies the dataset by dividing the samples into different clusters of equal variances. The number of clusters must be specified in this algorithm. It is fast with fewer computations required, with the linear complexity of **O(n).**
2. **Mean-shift algorithm:** Mean-shift algorithm tries to find the dense areas in the smooth density of data points. It is an example of a centroid-based model, that works on updating the candidates for centroid to be the center of the points within a given region.
3. **DBSCAN Algorithm:** It stands **for Density-Based Spatial Clustering of Applications with Noise**. It is an example of a density-based model similar to the mean-shift, but with some remarkable advantages. In

this algorithm, the areas of high density are separated by the areas of low density. Because of this, the clusters can be found in any arbitrary shape.

4. **Expectation-Maximization Clustering using GMM:** This algorithm can be used as an alternative for the k-means algorithm or for those cases where K-means can be failed. In GMM, it is assumed that the data points are Gaussian distributed.
5. **Agglomerative Hierarchical algorithm:** The Agglomerative hierarchical algorithm performs the bottom-up hierarchical clustering. In this, each data point is treated as a single cluster at the outset and then successively merged. The cluster hierarchy can be represented as a tree-structure.
6. **Affinity Propagation:** It is different from other clustering algorithms as it does not require to specify the number of clusters. In this, each data point sends a message between the pair of data points until convergence. It has $O(N^2T)$ time complexity, which is the main drawback of this algorithm.

Applications of Clustering

Below are some commonly known applications of clustering technique in Machine Learning:

- **In Identification of Cancer Cells:** The clustering algorithms are widely used for the identification of cancerous cells. It divides the cancerous and non-cancerous data sets into different groups.
- **In Search Engines:** Search engines also work on the clustering technique. The search result appears based on the closest object to the search query. It does it by grouping similar data objects in one group that is far from the other dissimilar objects. The accurate result of a query depends on the quality of the clustering algorithm used.
- **Customer Segmentation:** It is used in market research to segment the customers based on their choice and preferences.
- **In Biology:** It is used in the biology stream to classify different species of plants and animals using the image recognition technique.
- **In Land Use:** The clustering technique is used in identifying the area of similar lands use in the GIS database. This can be very useful to find that for what purpose the particular land should be used, that means for which purpose it is more suitable.

4.3 K-means clustering

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.

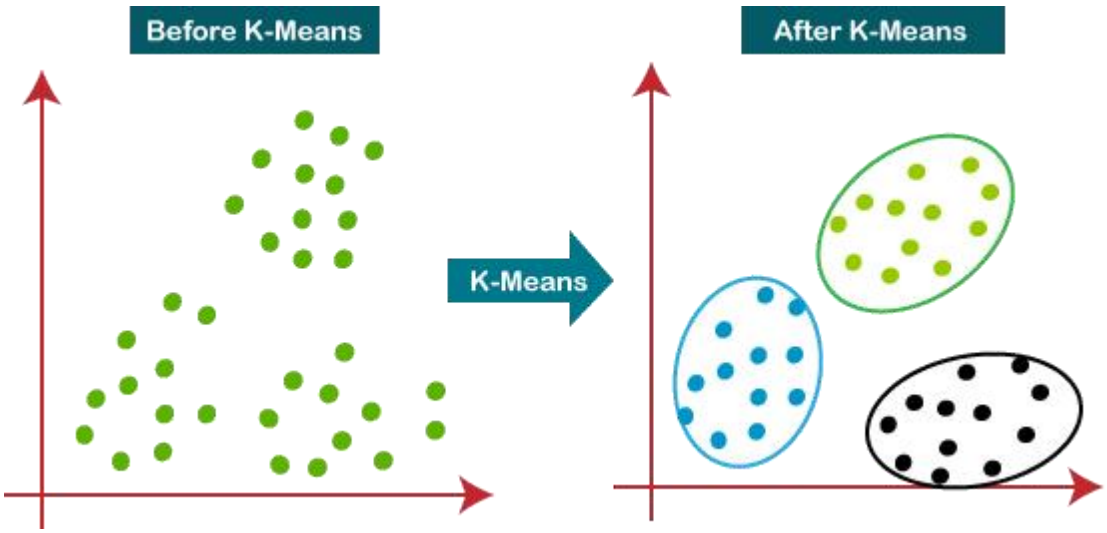
The algorithm takes the unlabeled dataset as input, divides the dataset into k-number of clusters, and repeats the process until it does not find the best clusters. The value of k should be predetermined in this algorithm.

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.

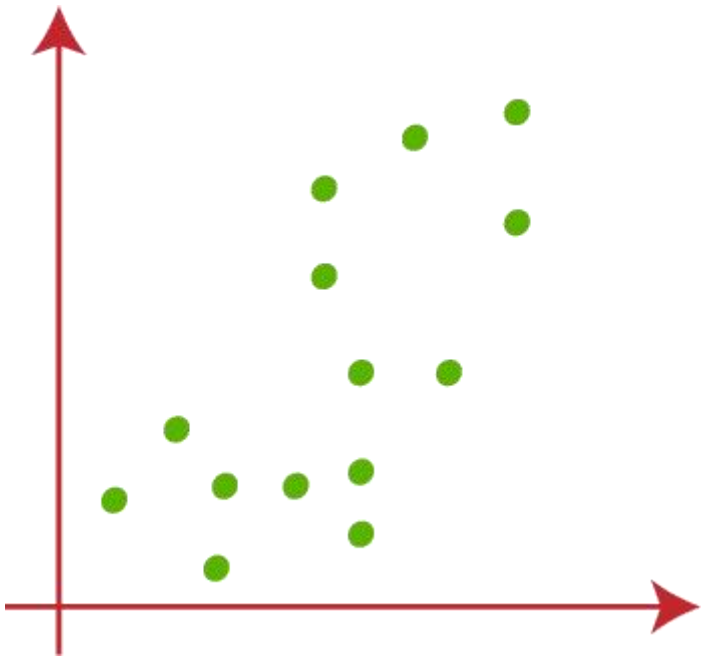
Step-5: Repeat the third steps, which means reassign each datapoint to the new closest centroid of each cluster.

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

Step-7: The model is ready.

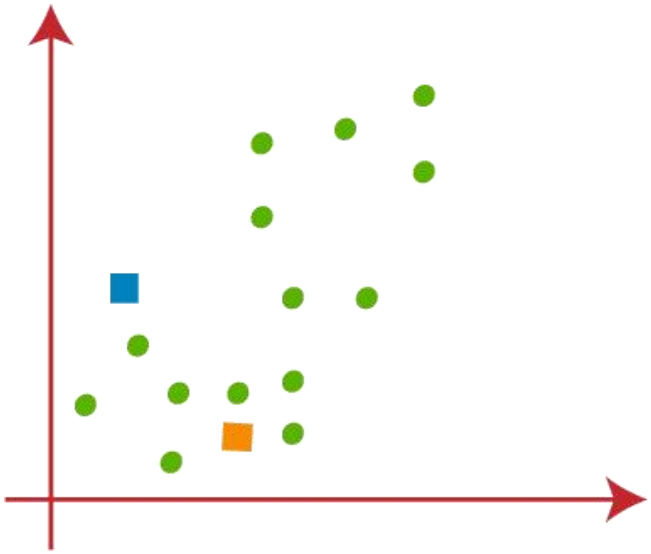
Let's understand the above steps by considering the visual plots:

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

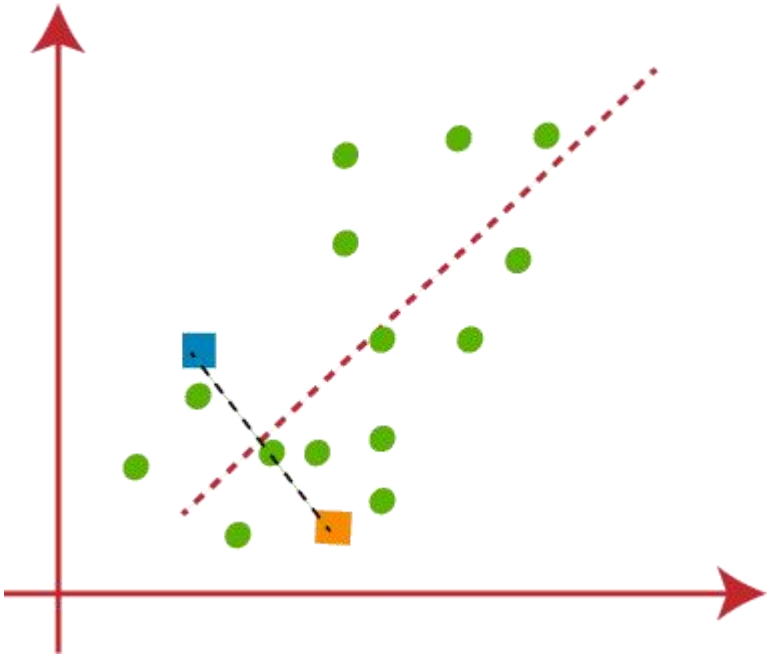


- Let's take number k of clusters, i.e., K=2, to identify the dataset and to put them into different clusters. It means here we will try to group these datasets into two different clusters.
- We need to choose some random k points or centroid to form the cluster. These points can be either the points from the dataset or any other point. So, here we are selecting the below two points as k points

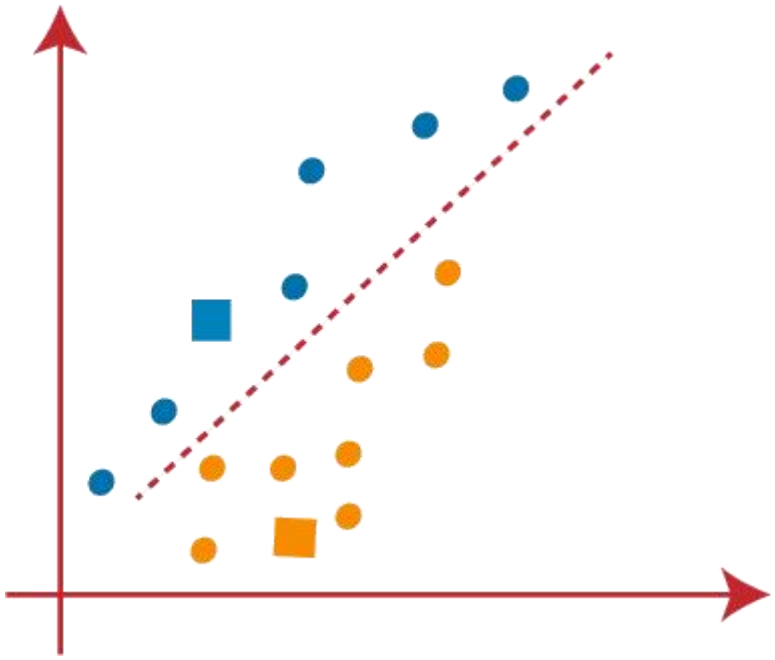
which are not the part of our dataset. Consider the below image:



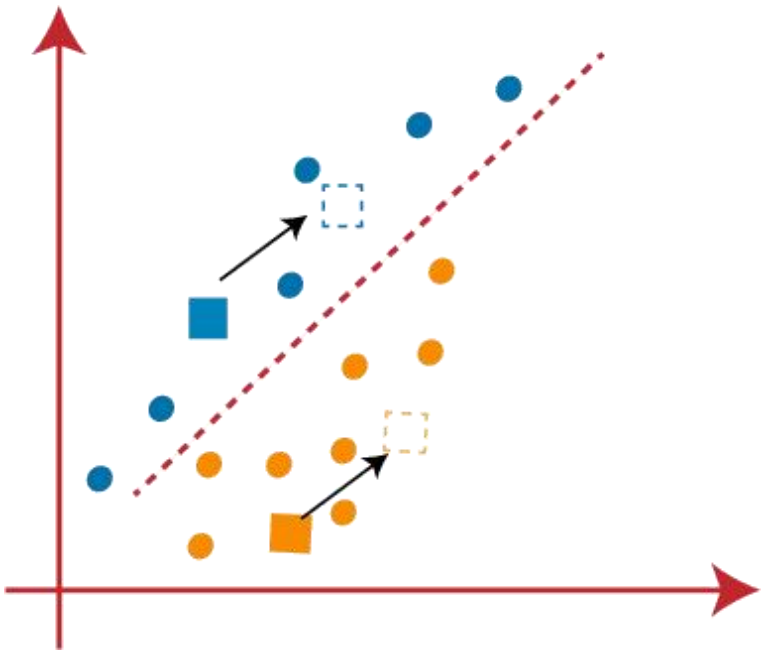
- Now we will assign each data point of the scatter plot to its closest K-point or centroid. We will compute it by applying some mathematics that we have studied to calculate the distance between two points. So, we will draw a median between both the centroids. Consider the below image:



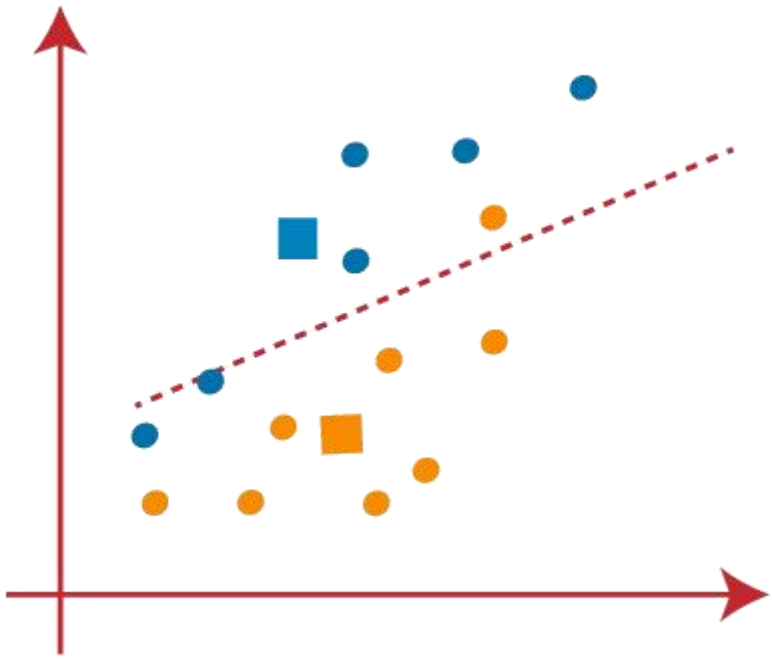
From the above image, it is clear that points left side of the line is near to the K1 or blue centroid, and points to the right of the line are close to the yellow centroid. Let's color them as blue and yellow for clear visualization.



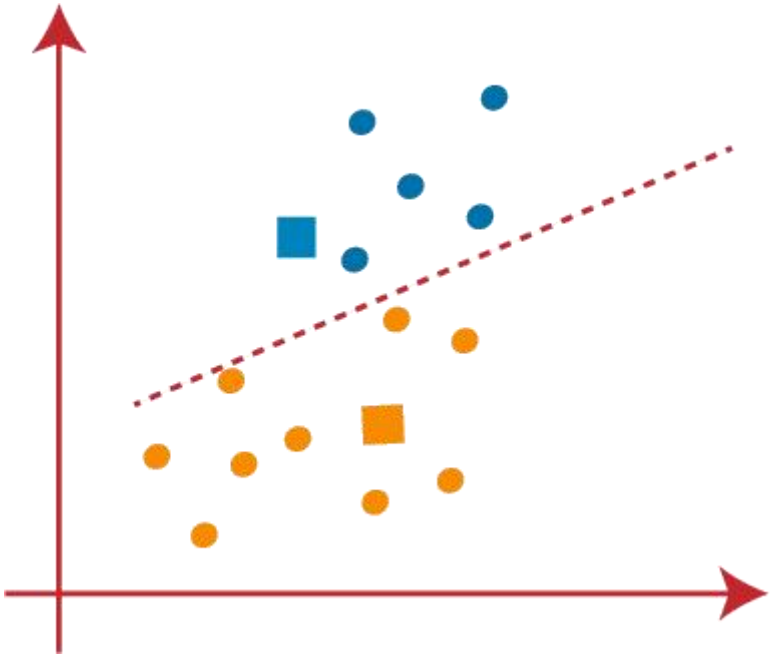
- As we need to find the closest cluster, so we will repeat the process by choosing **a new centroid**. To choose the new centroids, we will compute the center of gravity of these centroids, and will find new centroids as below:



- 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:

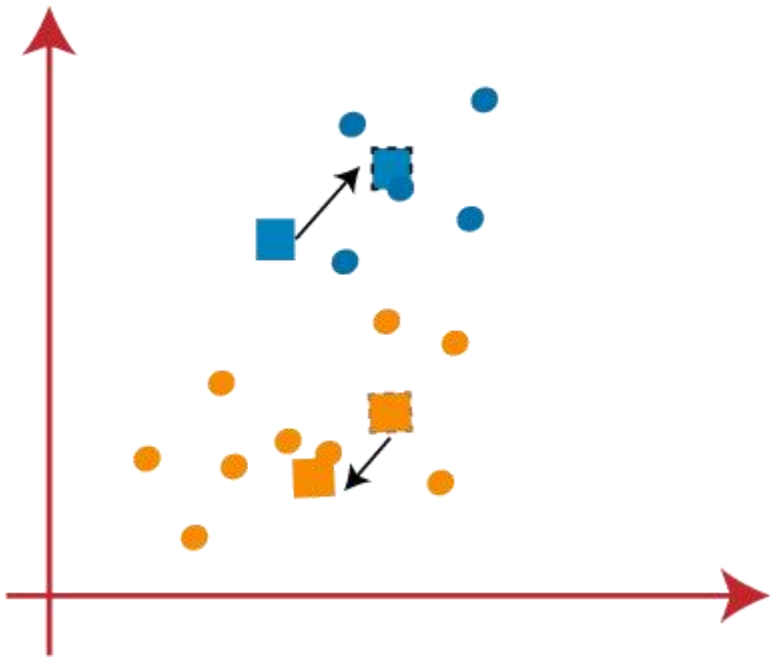


From the above image, we can see, one yellow point is on the left side of the line, and two blue points are right to the line. So, these three points will be assigned to new centroids.

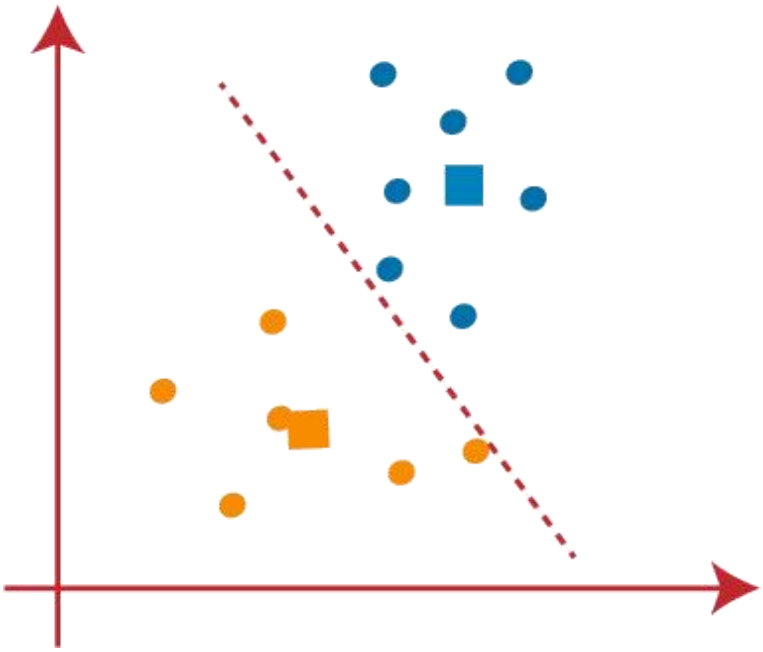


As reassignment has taken place, so we will again go to the step-4, which is finding new centroids or K-points.

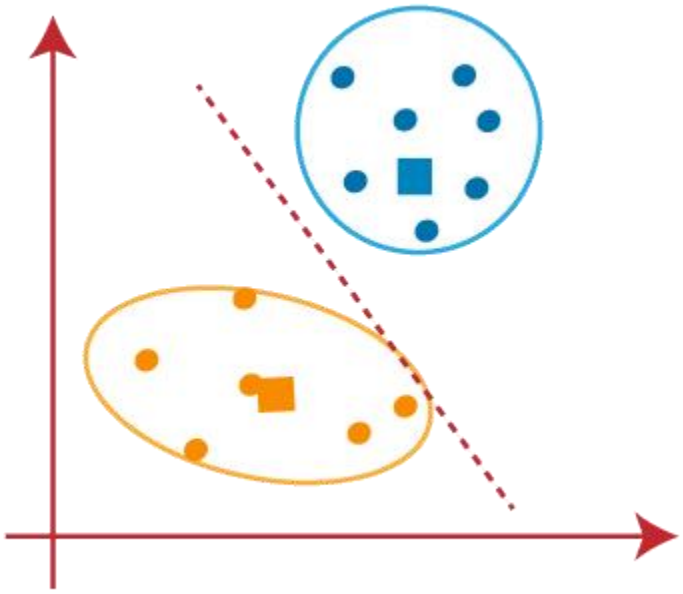
- We will repeat the process by finding the center of gravity of centroids, so the new centroids will be as shown in the below image:



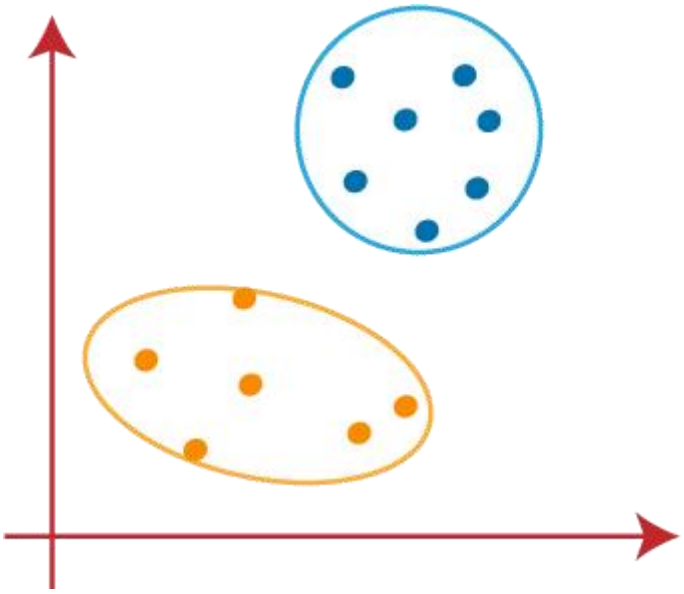
- As we got the new centroids so again will draw the median line and reassign the data points. So, the image will be:



- 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:



4.4 Apriori algorithm and Associations rule

The Apriori algorithm uses frequent itemsets to generate association rules, and it is designed to work on the databases that contain transactions. With the help of these association rule, it determines how strongly or how weakly two objects are connected. This algorithm uses a **breadth-first search** and **Hash Tree** to calculate the itemset associations efficiently. It is the iterative process for finding the frequent itemsets from the large dataset.

This algorithm was given by the **R. Agrawal** and **Srikant** in the year **1994**. It is mainly used for *market basket analysis* and helps to find those products that can be bought together. It can also be used in the healthcare field to find drug reactions for patients.

What is Frequent Itemset?

Frequent itemsets are those items whose support is greater than the threshold value or user-specified minimum support. It means if A & B are the frequent itemsets together, then individually A and B should also be the frequent itemset.

Suppose there are the two transactions: A= {1,2,3,4,5}, and B= {2,3,7}, in these two transactions, 2 and 3 are the frequent itemsets.

Steps for Apriori Algorithm

Below are the steps for the apriori algorithm:

Step-1: Determine the support of itemsets in the transactional database, and select the minimum support and confidence.

Step-2: Take all supports in the transaction with higher support value than the minimum or selected support value.

Step-3: Find all the rules of these subsets that have higher confidence value than the threshold or minimum confidence.

Step-4: Sort the rules as the decreasing order of lift.

Apriori Algorithm Working

We will understand the apriori algorithm using an example and mathematical calculation:

Example: Suppose we have the following dataset that has various transactions, and from this dataset, we need to find the frequent itemsets and generate the association rules using the Apriori algorithm:

TID	ITEMSETS
T1	A, B
T2	B, D
T3	B, C
T4	A, B, D
T5	A, C
T6	B, C
T7	A, C
T8	A, B, C, E
T9	A, B, C

Given: Minimum Support= 2, Minimum Confidence= 50%

Solution:

Step-1: Calculating C1 and L1:

- In the first step, we will create a table that contains support count (The frequency of each itemset individually in the dataset) of each itemset in the given dataset. This table is called the **Candidate set or C1.**

Itemset	Support_Count
A	6
B	7
C	5
D	2
E	1

- Now, we will take out all the itemsets that have the greater support count that the Minimum Support (2). It will give us the table for the **frequent itemset L1.** Since all the itemsets have greater or equal support count than the minimum support, except the E, so E itemset will be removed.

Itemset	Support_Count
A	6
B	7
C	5
D	2

Step-2: Candidate Generation C2, and L2:

- In this step, we will generate C2 with the help of L1. In C2, we will create the pair of the itemsets of L1 in the form of subsets.
- After creating the subsets, we will again find the support count from the main transaction table of datasets, i.e., how many times these pairs have occurred together in the given dataset. So, we will get the below table for C2:

Itemset	Support_Count
{A, B}	4
{A,C}	4
{A, D}	1
{B, C}	4
{B, D}	2
{C, D}	0

- Again, we need to compare the C2 Support count with the minimum support count, and after comparing, the itemset with less support count will be eliminated from the table C2. It will give us the below table for

L2

Itemset	Support_Count
{A, B}	4
{A, C}	4
{B, C}	4
{B, D}	2

A, B, C, D

Step-3: Candidate generation C3, and L3:

- For C3, we will repeat the same two processes, but now we will form the C3 table with subsets of three itemsets together, and will calculate the support count from the dataset. It will give the below table:

Itemset	Support_Count
{A, B, C}	2
{B, C, D}	1
{A, C, D}	0
{A, B, D}	0

- Now we will create the L3 table. As we can see from the above C3 table, there is only one combination of itemset that has support count equal to the minimum support count. So, the L3 will have only one combination, i.e., **{A, B, C}.**

Step-4: Finding the association rules for the subsets:

To generate the association rules, first, we will create a new table with the possible rules from the occurred combination {A, B.C}. For all the rules, we will calculate the Confidence using formula **sup(A ^B)/A.** After calculating the confidence value for all rules, we will exclude the rules that have less confidence than the minimum threshold(50%).

Consider the below table:

Rules	Support	Confidence
A ^B → C	2	Sup{(A ^B) ^C}/sup(A ^B)= 2/4=0.5=50%
B^C → A	2	Sup{(B^C) ^A}/sup(B ^C)= 2/4=0.5=50%
A^C → B	2	Sup{(A ^C) ^B}/sup(A ^C)= 2/4=0.5=50%
C→ A ^B	2	Sup{(C^(A ^B)}/sup(C)= 2/5=0.4=40%
A→ B^C	2	Sup{(A^(B ^C)}/sup(A)= 2/6=0.33=33.33%
B→ B^C	2	Sup{(B^(B ^C)}/sup(B)= 2/7=0.28=28%

As the given threshold or minimum confidence is 50%, so the first three rules **A ^B → C, B^C → A, and A^C → B** can be considered as the strong association rules for the given problem.

Advantages of Apriori Algorithm

- This is easy to understand algorithm
- The join and prune steps of the algorithm can be easily implemented on large datasets.

Disadvantages of Apriori Algorithm

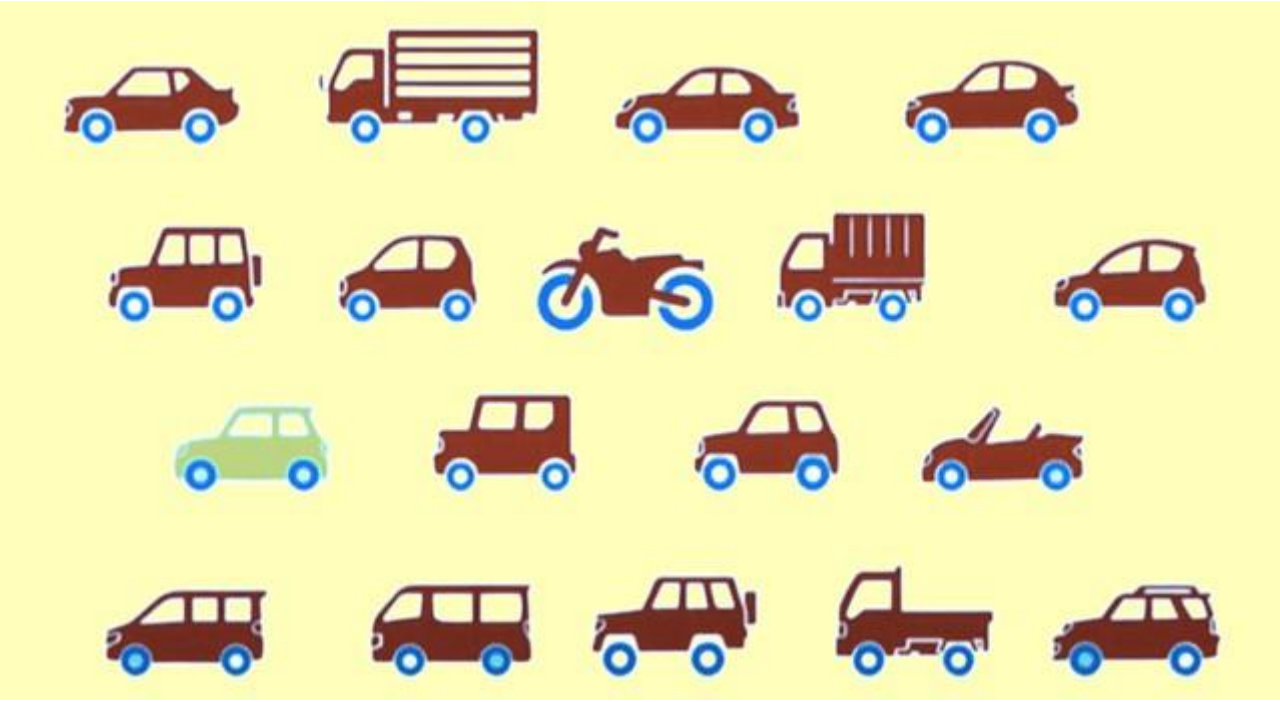
- The apriori algorithm works slow compared to other algorithms.
- The overall performance can be reduced as it scans the database for multiple times.
- The time complexity and space complexity of the apriori algorithm is $O(2^D)$, which is very high. Here D represents the horizontal width present in the database.

4.5 Anomaly detection algorithm

Anomaly detection is a process of finding those rare items, data points, events, or observations that make suspicions by being different from the rest data points or observations. Anomaly detection is also known as outlier detection.

Generally, anomalous data is related to some kind of problems such as bank fraud, medical problems, malfunctioning equipment, etc.

Finding an anomaly is the ability to define what is normal? For example, in the below image, the yellow vehicle is an anomaly among all red vehicles.



Types of Anomaly Detection

1. Point Anomaly

A tuple within the dataset can be said as a Point anomaly if it is far away from the rest of the data.

Example: An example of a point anomaly is a sudden transaction of a huge amount from a credit card.

2. Contextual Anomaly

Contextual anomaly is also known as conditional outliers. If a particular observation is different from other data points, then it is known as a contextual Anomaly. In such types of anomalies, an anomaly in one context may not be an anomaly in another context.

3. Collective Anomaly

Collective anomalies occur when a data point within a set is anomalous for the whole dataset, and such values are known as collective outliers. In such anomalies, specific or individual values are not anomalous as a whole or contextually.

Categories of Anomaly detection techniques

Anomaly detection techniques are broadly categorized into three types:

1. **Supervised Anomaly detection**
2. **Unsupervised Anomaly detection**

Supervised Anomaly Detection

Supervised Anomaly detection needs the labeled training data, which contains both normal and anomalous data for creating a predictive model. Some of the common supervised methods are neural networks, support vector machines, k-nearest neighbors, Bayesian networks, decision trees, etc.

K-nearest neighbor is one of the popular nonparametric techniques, which find the approximate distance between different points on the input vector. This is one of the best anomaly detection methods. Another popular model is the Bayesian network, which is used for anomaly detection when combined with statistical schemes. This model encodes a probabilistic relationship among variable interests.

Supervised anomaly detection techniques have different advantages, such as the capability of encoding interdependencies between variables and of predicting events; it also provides the ability to incorporate both prior knowledge and data.

Unsupervised Anomaly Detection

Unsupervised Anomaly detection does not require labeled training data. These techniques are based on two assumptions, which are,

- Most of the network connections are from normal traffic, and only a small amount of data is abnormal.
- Malicious traffic is statistically different from normal traffic.

On the basis of these assumptions, data clusters of similar data points that occur frequently are assumed to be normal traffic, and those data groups that are infrequent are considered abnormal or malicious.

Some of the common unsupervised anomaly detection algorithms are self-organizing maps (SOM), K-means, C-means, expectation-maximization meta-algorithm (EM), adaptive resonance theory (ART), and one-class support

vector machines. SOM, or Self-organizing map, is a popular technique that aims to reduce the dimension of data visualization.

Anomaly detection can effectively help in catching the fraud, discovering strange activity in large and complex Big Data sets. This can prove to be useful in areas such as banking security, natural sciences, medicine, and marketing, which are prone to malicious activities. With machine learning, an organization can intensify search and increase the effectiveness of its digital business initiatives.

Need of Anomaly Detection

1. Anomaly detection for application performance

Application performance of any company can either generate or reduce workforce productivity and revenue. General or traditional approaches for monitoring the application performance allow to react to issues, but still business used to suffer, and hence it affects the user. But with the help of anomaly detection using machine learning, it is easy to identify and resolve the application performance issues before they affect the business as well as users.

Anomaly detection using machine learning algorithms can simply correlate data with corresponding application performance metrics and find out the complete knowledge of the issue. There are different industries that also employ anomaly detection techniques for their businesses, such as **Telco, Adtech**, etc.

2. Anomaly detection for product quality

It is not enough for product managers to trust another department for taking care of required monitoring and alerts. It is always required for product managers to be able to trust that product will work smoothly. It is because the product always needs changes, from each version release to new feature upgradation, and generates anomalies. If you don't properly monitor these anomalies, it may cause millions of revenues lost and can also affect the brand reputation.

3. Anomaly detection for user experience

If you release a faulty version, you may experience a DDoS attack, risk of usage lapses across customer experiences. So, it is required to react to such issues before they impact user experience to reduce the chances of revenue loss.

Proactively streamlining and improving user experiences will help improve customer satisfaction in a variety of industries, including Gaming, online business, etc.

4.6 Hierarchical clustering

Hierarchical clustering is another unsupervised machine learning algorithm, which is used to group the unlabeled datasets into a cluster and also known as **hierarchical cluster analysis** or HCA.

In this algorithm, we develop the hierarchy of clusters in the form of a tree, and this tree-shaped structure is known as the **dendrogram**.

Sometimes the results of K-means clustering and hierarchical clustering may look similar, but they both differ depending on how they work. As there is no requirement to predetermine the number of clusters as we did in the K-Means algorithm.

The hierarchical clustering technique has two approaches:

1. **Agglomerative:** Agglomerative is a **bottom-up** approach, in which the algorithm starts with taking all data points as single clusters and merging them until one cluster is left.
2. **Divisive:** Divisive algorithm is the reverse of the agglomerative algorithm as it is a **top-down approach.**

Why hierarchical clustering?

As we already have other clustering algorithms such as **K-Means Clustering**, then why we need hierarchical clustering? So, as we have seen in the K-means clustering that there are some challenges with this algorithm, which are a predetermined number of clusters, and it always tries to create the clusters of the same size. To solve these two challenges, we can opt for the hierarchical clustering algorithm because, in this algorithm, we don't need to have knowledge about the predefined number of clusters.

In this topic, we will discuss the Agglomerative Hierarchical clustering algorithm.

Agglomerative Hierarchical clustering

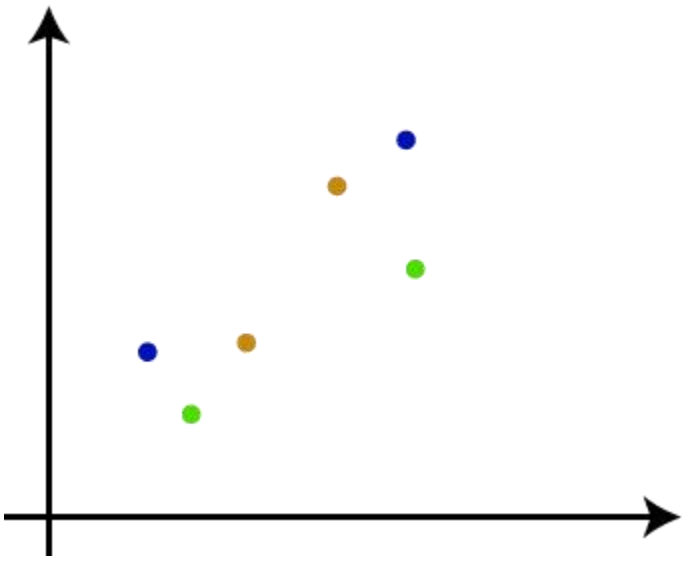
The agglomerative hierarchical clustering algorithm is a popular example of HCA. To group the datasets into clusters, it follows the **bottom-up approach**. It means, this algorithm considers each dataset as a single cluster at the beginning, and then start combining the closest pair of clusters together. It does this until all the clusters are merged into a single cluster that contains all the datasets.

This hierarchy of clusters is represented in the form of the dendrogram.

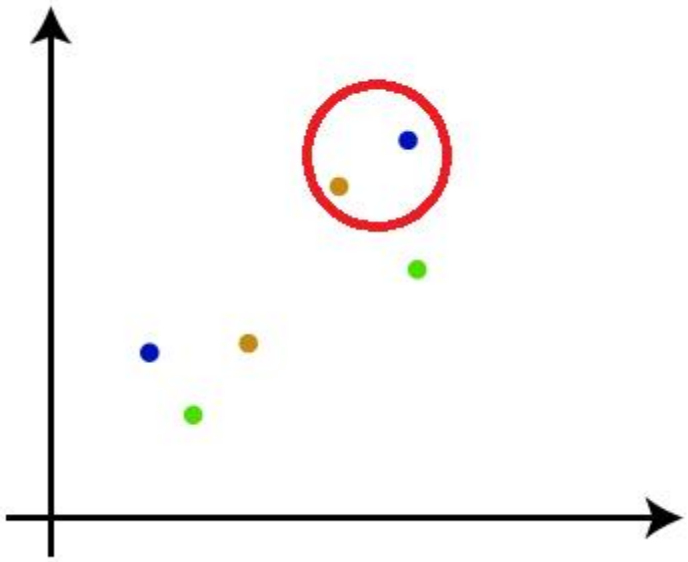
How the Agglomerative Hierarchical clustering Work?

The working of the AHC algorithm can be explained using the below steps:

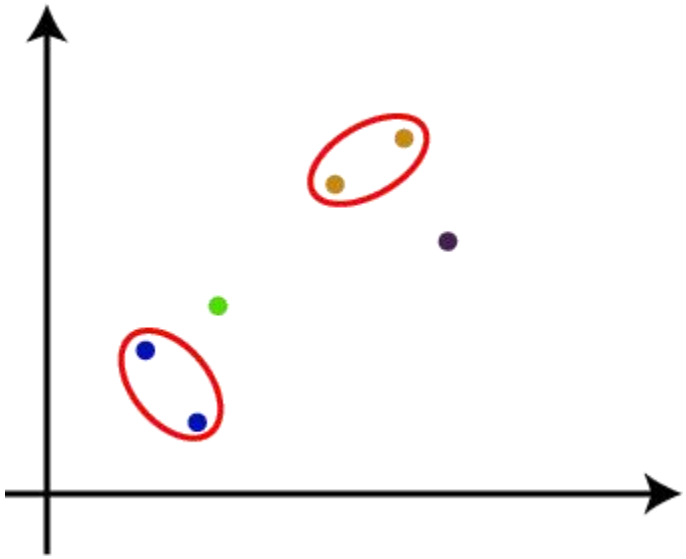
- **Step-1:** Create each data point as a single cluster. Let's say there are N data points, so the number of clusters will also be N.



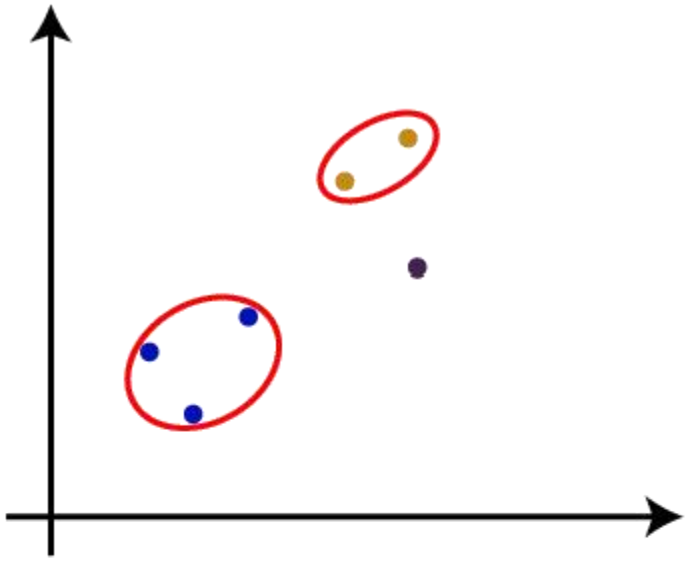
- **Step-2:** Take two closest data points or clusters and merge them to form one cluster. So, there will now be N-1 clusters.

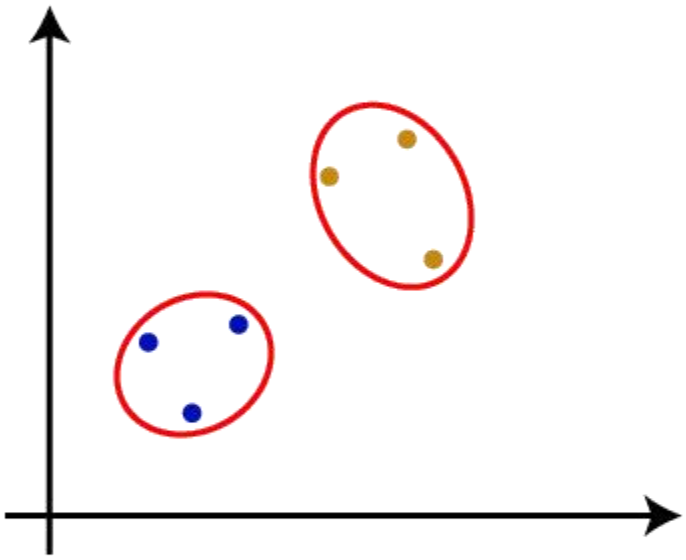


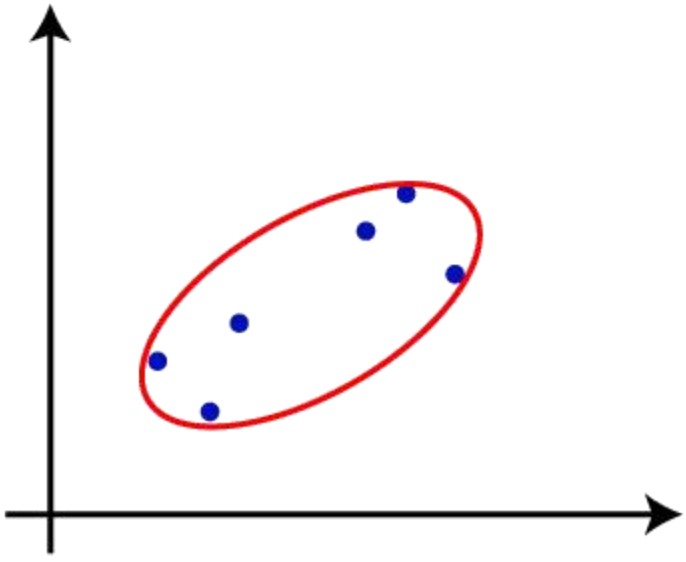
- **Step-3**: Again, take the two closest clusters and merge them together to form one cluster. There will be N-2 clusters.



- **Step-4:** Repeat Step 3 until only one cluster left. So, we will get the following clusters. Consider the below images:







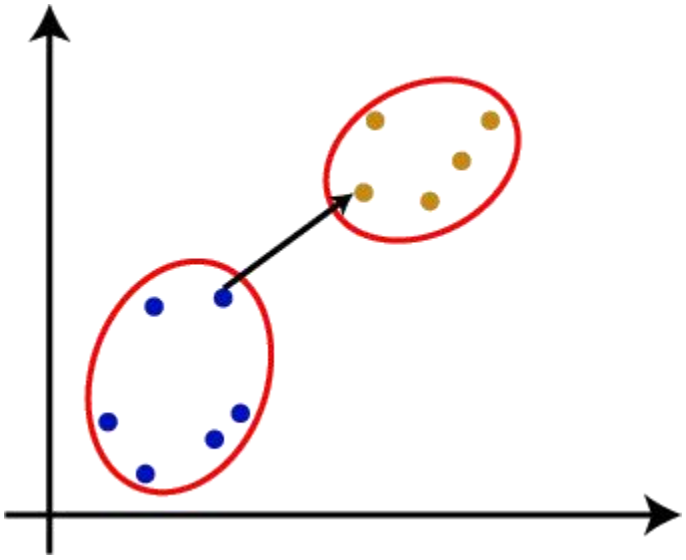
- **Step-5:** Once all the clusters are combined into one big cluster, develop the dendrogram to divide the clusters as per the problem.

Note: To better understand hierarchical clustering, it is advised to have a look on k-means clustering

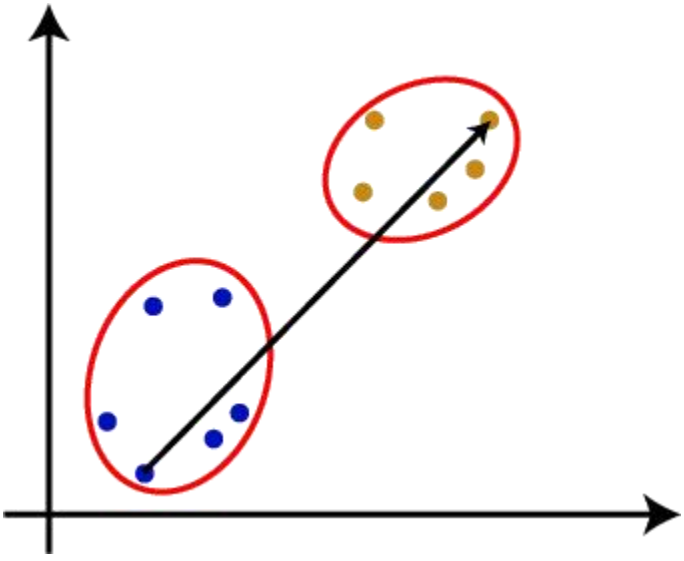
Measure for the distance between two clusters

As we have seen, the **closest distance** between the two clusters is crucial for the hierarchical clustering. There are various ways to calculate the distance between two clusters, and these ways decide the rule for clustering. These measures are called **Linkage methods**. Some of the popular linkage methods are given below:

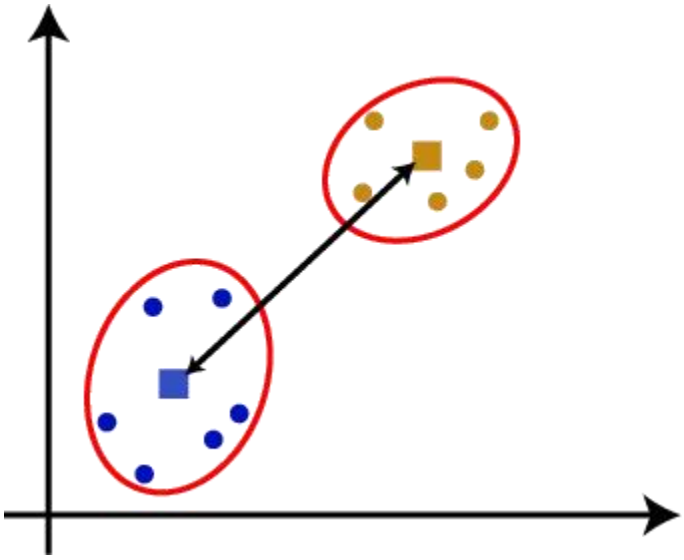
1. **Single Linkage:** It is the Shortest Distance between the closest points of the clusters. Consider the below image:



2. **Complete Linkage:** It is the farthest distance between the two points of two different clusters. It is one of the popular linkage methods as it forms tighter clusters than single-linkage.



3. **Average Linkage:** It is the linkage method in which the distance between each pair of datasets is added up and then divided by the total number of datasets to calculate the average distance between two clusters. It is also one of the most popular linkage methods.
4. **Centroid Linkage:** It is the linkage method in which the distance between the centroid of the clusters is calculated. Consider the below image:

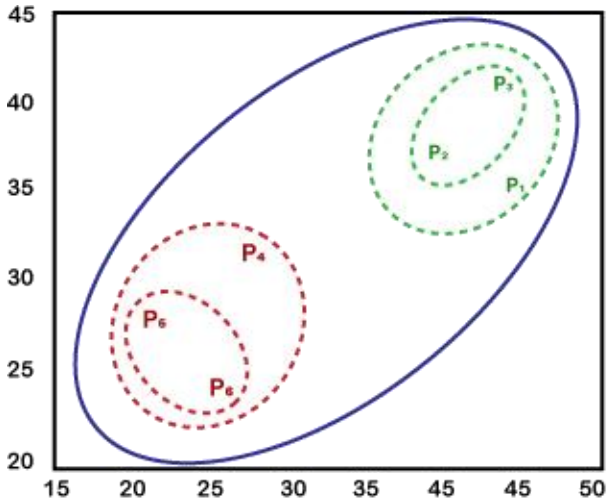


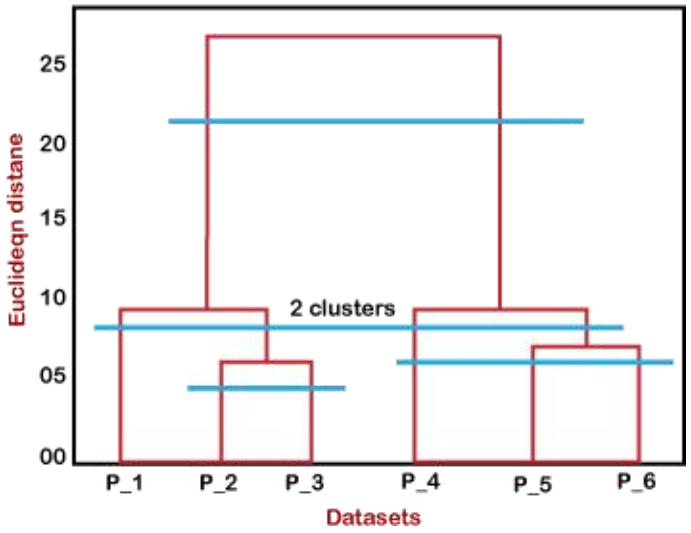
From the above-given approaches, we can apply any of them according to the type of problem or business requirement.

Woking of Dendrogram in Hierarchical clustering

The dendrogram is a tree-like structure that is mainly used to store each step as a memory that the HC algorithm performs. In the dendrogram plot, the Y-axis shows the Euclidean distances between the data points, and the x-axis shows all the data points of the given dataset.

The working of the dendrogram can be explained using the below diagram:





In the above diagram, the left part is showing how clusters are created in agglomerative clustering, and the right part is showing the corresponding dendrogram.

- As we have discussed above, firstly, the datapoints P2 and P3 combine together and form a cluster, correspondingly a dendrogram is created, which connects P2 and P3 with a rectangular shape. The hight is decided according to the Euclidean distance between the data points.
- In the next step, P5 and P6 form a cluster, and the corresponding dendrogram is created. It is higher than of previous, as the Euclidean distance between P5 and P6 is a little bit greater than the P2 and P3.
- Again, two new dendrograms are created that combine P1, P2, and P3 in one dendrogram, and P4, P5, and P6, in another dendrogram.
- At last, the final dendrogram is created that combines all the data points together.

We can cut the dendrogram tree structure at any level as per our requirement.

4.7 K-Medoids

K-Medoids and K-Means are two types of clustering mechanisms in Partition Clustering. First, Clustering is the process of breaking down an abstract group of data points/ objects into classes of similar objects such that all the objects in one cluster have similar traits. , a group of n objects is broken down into k number of clusters based on their similarities.

Two statisticians, Leonard Kaufman, and Peter J. Rousseeuw came up with this method. This tutorial explains what K-Medoids do, their applications, and the difference between K-Means and K-Medoids.

K-medoids is an unsupervised method with unlabelled data to be clustered. It is an improvised version of the K-Means algorithm mainly designed to deal with outlier data sensitivity. Compared to other partitioning algorithms, the algorithm is simple, fast, and easy to implement.

The partitioning will be carried on such that:

1. Each cluster must have at least one object
2. An object must belong to only one cluster

Here is a small recap on K-Means clustering:

In the K-Means algorithm, given the value of k and unlabelled data:

1. Choose k number of random points (Data point from the data set or some other points). These points are also called "**Centroids**" or "**Means**".
2. Assign all the data points in the data set to the closest centroid by applying any distance formula like **Euclidian distance, Manhattan distance,** etc.
3. Now, choose new centroids by calculating the mean of all the data points in the clusters and goto step 2
4. Continue step 3 until no data point changes classification between two iterations.

The problem with the K-Means algorithm is that the algorithm needs to handle outlier data. An outlier is a point different from the rest of the points. All the outlier data points show up in a different cluster and will attract other clusters to merge with it. Outlier data increases the mean of a cluster by up to 10 units. Hence, **K-Means clustering is highly affected by outlier data.**

K-Medoids:

Medoid: A Medoid is a point in the cluster from which the sum of distances to other data points is minimal.

(or)

A Medoid is a point in the cluster from which dissimilarities with all the other points in the clusters are minimal.

Instead of centroids as reference points in K-Means algorithms, the K-Medoids algorithm takes a Medoid as a reference point.

There are three types of algorithms for K-Medoids Clustering:

1. **PAM (Partitioning Around Clustering)**
2. **CLARA (Clustering Large Applications)**
3. **CLARANS (Randomized Clustering Large Applications)**

PAM is the most powerful algorithm of the three algorithms but has the disadvantage of time complexity. The following K-Medoids are performed using PAM. In the further parts, we'll see what CLARA and CLARANS are.

Algorithm:

Given the value of k and unlabelled data:

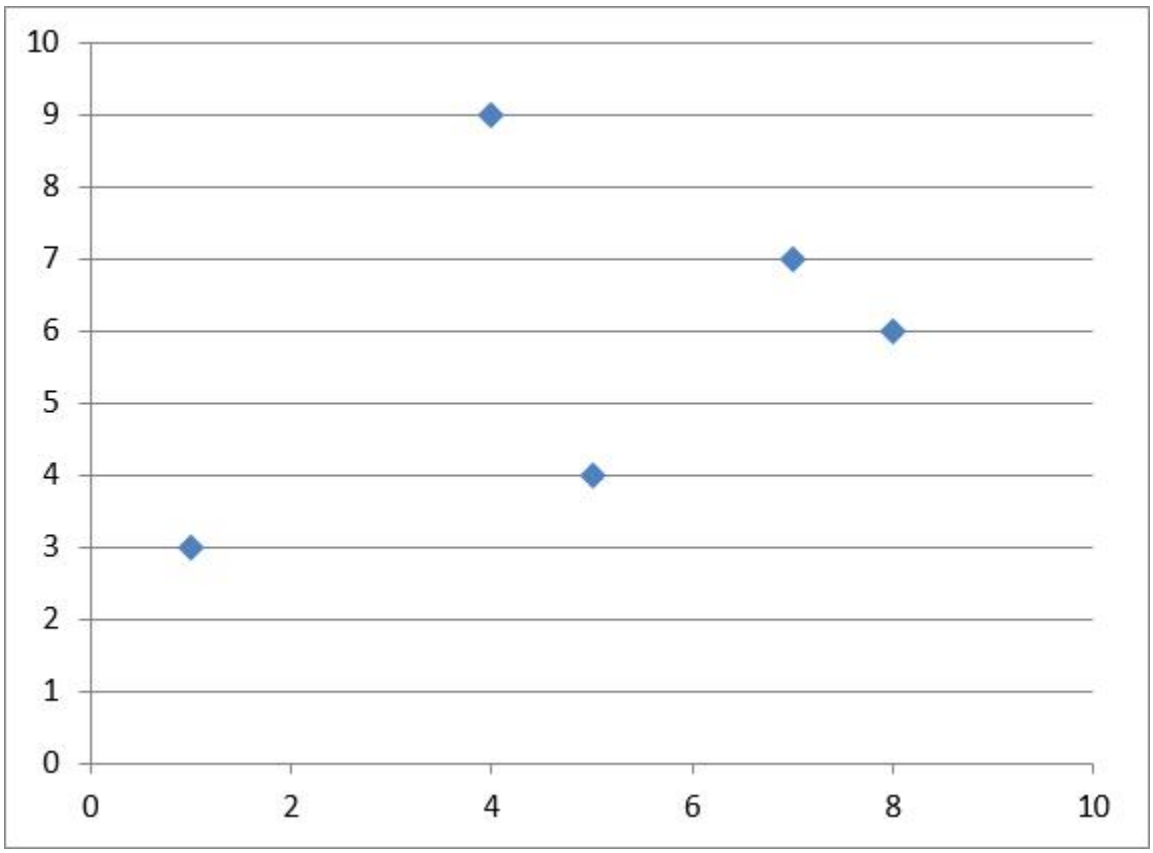
1. Choose k number of random points from the data and assign these k points to k number of clusters. These are the initial medoids.
2. For all the remaining data points, calculate the distance from each medoid and assign it to the cluster with the nearest medoid.
3. Calculate the total cost (Sum of all the distances from all the data points to the medoids)
4. Select a random point as the new medoid and swap it with the previous medoid. Repeat 2 and 3 steps.
5. If the total cost of the new medoid is less than that of the previous medoid, make the new medoid permanent and repeat step 4.
6. If the total cost of the new medoid is greater than the cost of the previous medoid, undo the swap and repeat step 4.
7. The Repetitions have to continue until no change is encountered with new medoids to classify data points.

Here is an example to make the theory clear:

Data set:

	x	y
0	5	4
1	7	7
2	1	3
3	8	6
4	4	9

Scatter plot:



If k is given as 2, we need to break down the data points into 2 clusters.

1. **Initial medoids: M1(1, 3) and M2(4, 9)**
2. Calculation of distances

Manhattan Distance: |x1 - x2| + |y1 - y2|

	x<	y	From M1(1, 3)	From M2(4, 9)
0	5	4	5	6
1	7	7	10	5
2	1	3	-	-
3	8	6	10	7
4	4	9	-	-

Cluster 1: 0

Cluster 2: 1, 3

1. Calculation of total cost:
   (5) + (5 + 7) = 17
2. Random medoid: (5, 4)

M1(5, 4) and M2(4, 9):

	x	y	From M1(5, 4)	From M2(4, 9)
0	5	4	-	-
1	7	7	5	5
2	1	3	5	9
3	8	6	5	7
4	4	9	-	-

Cluster 1: 2, 3

Cluster 2: 1

1. Calculation of total cost:
   (5 + 5) + 5 = 15
   Less than the previous cost
   New medoid: (5, 4).
2. Random medoid: (7, 7)

M1(5, 4) and M2(7, 7)

	x	y	From M1(5, 4)	From M2(7, 7)
0	5	4	-	-
1	7	7	-	-
2	1	3	5	10
3	8	6	5	2
4	4	9	6	5

Cluster 1: 2

Cluster 2: 3, 4

1. Calculation of total cost:
   (5) + (2 + 5) = 12
   Less than the previous cost
   New medoid: (7, 7).
2. Random medoid: (8, 6)

M1(7, 7) and M2(8, 6)

	x	y	From M1(7, 7)	From M2(8, 6)
0	5	4	5	5
1	7	7	-	-
2	1	3	10	10
3	8	6	-	-
4	4	9	5	7

Cluster 1: 4

Cluster 2: 0, 2

1. Calculation of total cost:
   (5) + (5 + 10) = 20
   Greater than the previous cost
   UNDO

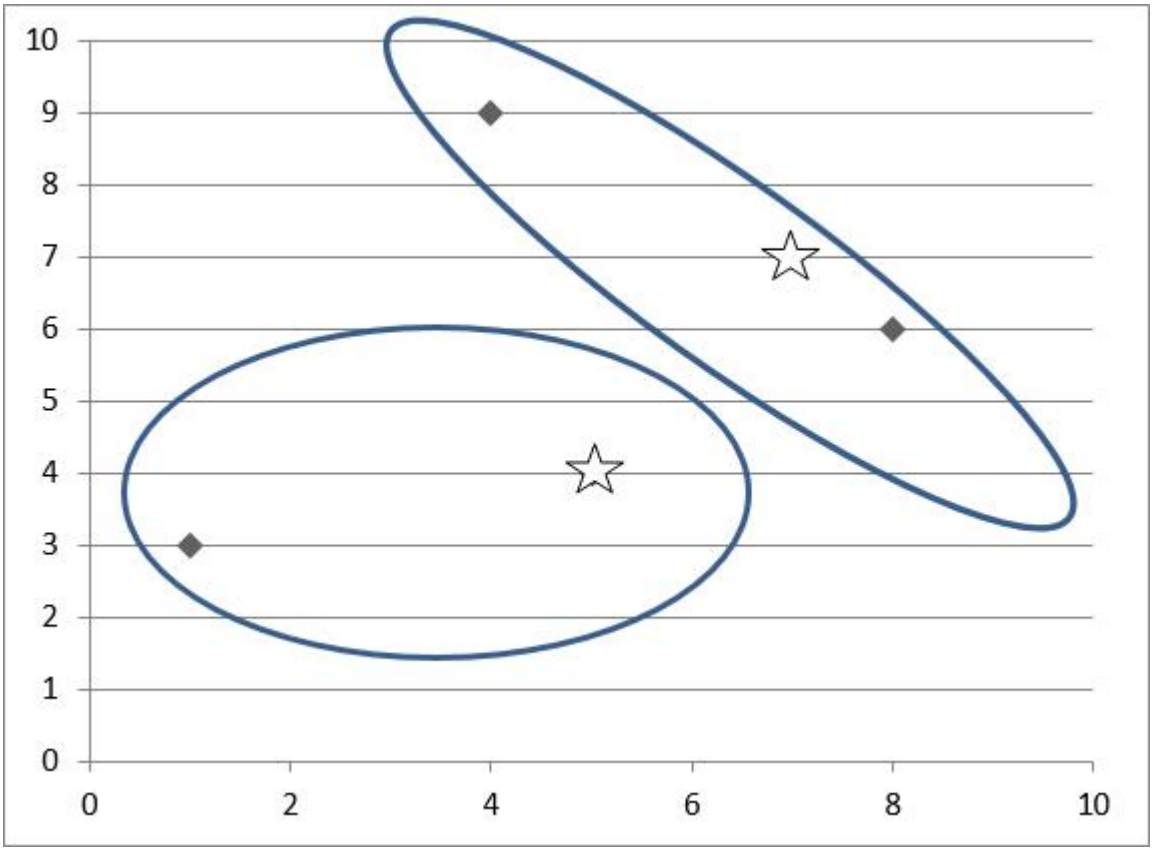
Hence, the final medoids: **M1(5, 4) and M2(7, 7)**

Cluster 1: 2

Cluster 2: 3, 4

Total cost: 12

Clusters:



Limitation of PAM:

Time complexity: $O(k * (n - k)^2)$

Possible combinations for every node: k*(n - k)

Cost for each computation: (n - k)

Total cost: $k*(n - k)^2$

Hence, PAM is suitable and recommended to be used for small data sets.

CLARA:

It is an extension to PAM to support Medoid clustering for large data sets. This algorithm selects **data samples from the data set, applies Pam on each sample, and outputs the best Clustering out of these samples**. This is more effective than PAM. We should ensure that the selected samples aren't biased as they affect the Clustering of the whole data.

CLARANS:

This algorithm selects a sample of neighbors to examine instead of selecting samples from the data set. In every step, it examines the neighbors of every node. The time complexity of this algorithm is $O(n^2)$, and this is the best and most efficient Medoids algorithm of all.

Advantages of using K-Medoids:

1. Deals with noise and outlier data effectively
2. Easily implementable and simple to understand
3. Faster compared to other partitioning algorithms

Disadvantages:

1. Not suitable for Clustering arbitrarily shaped groups of data points.
2. As the initial medoids are chosen randomly, the results might vary based on the choice in different runs.

K-Means and K-Medoids:

K-Means	**K-Medoids**
Both methods are types of Partition Clustering.	
Unsupervised iterative algorithms	
Have to deal with unlabelled data	
Both algorithms group n objects into k clusters based on similar traits where k is pre-defined.	
Inputs: Unlabelled data and the value of k	
Metric of similarity: Euclidian Distance	**Metric of similarity:** Manhattan Distance
Clustering is done based on distance from **centroids.**	Clustering is done based on distance from **medoids.**
A centroid can be a data point or some other point in the cluster	A medoid is always a data point in the cluster.
Can't cope with outlier data	Can manage outlier data too
Sometimes, outlier sensitivity can turn out to be useful	Tendency to ignore meaningful clusters in outlier data

Useful Outlier Clusters:

For suppose, A data set with data on people's income is being clustered to analyze and understand individuals' purchasing and investing behavior within each cluster.

Here outlier data will be people with high incomes-billionaires. All such people tend to purchase and invest more. Hence, a separate cluster for billionaires would be useful in this scenario.

In K-Medoids, It merges this data into the upper-class cluster, which loses the meaningful outlier data in Clustering and is one of the disadvantages of K-Medoids in special situations.