Fundamentals of Machine Learning

Unit 5

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 is a type of machine learning in which models are trained using unlabeled dataset and are allowed to act on that data without any supervision.

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.

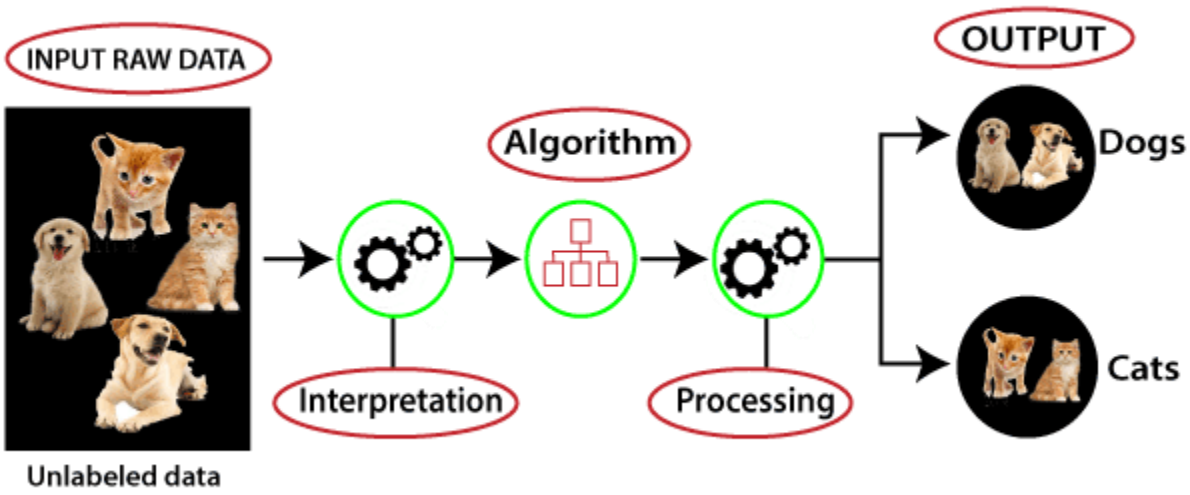
Why use Unsupervised Learning?

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:

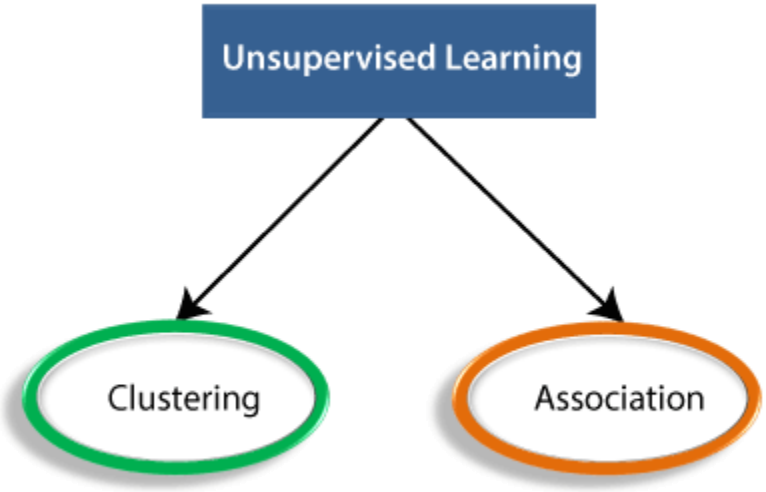


Here, we have taken an unlabeled input data, which means it is not categorized and corresponding outputs are also not given. Now, this unlabeled input data is fed to the machine learning model in order to train it. Firstly, it will interpret the raw data to find the hidden patterns from the data and 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.

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.

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.

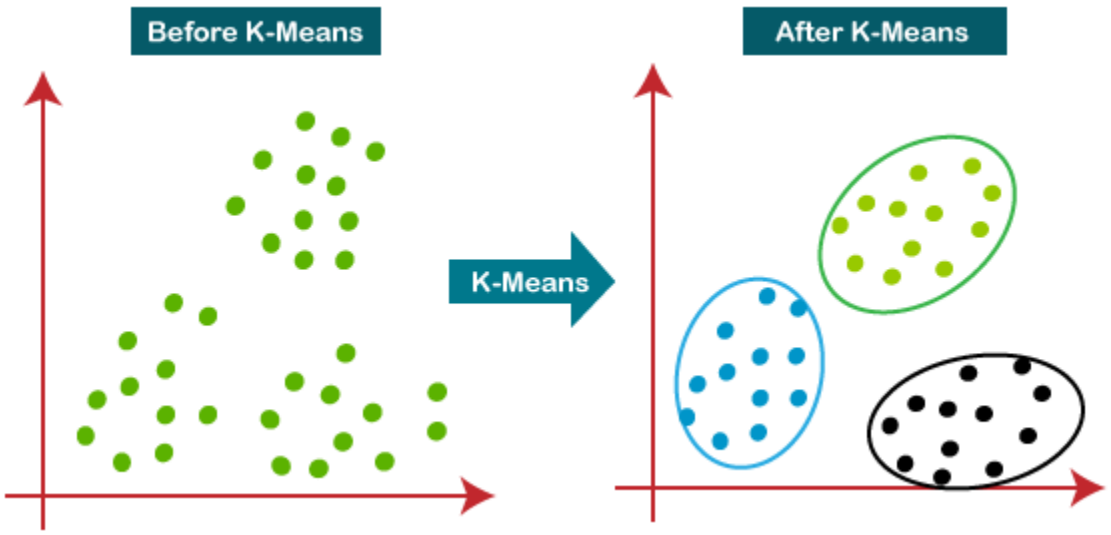
The algorithm takes the unlabeled dataset as input, divides the dataset into k-number of clusters, and repeats the process until it does not find the best clusters. The value of k should be predetermined in this algorithm.

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.

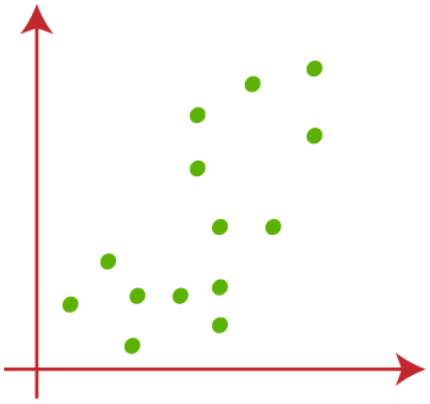
Step-5: Repeat the third steps, which means reassign each datapoint to the new closest centroid of each cluster.

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

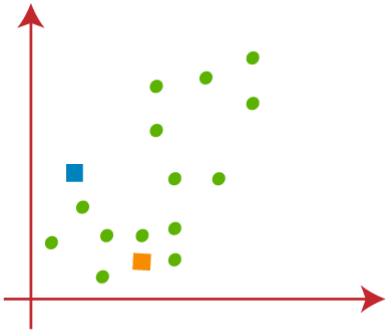
Step-7: The model is ready.

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:

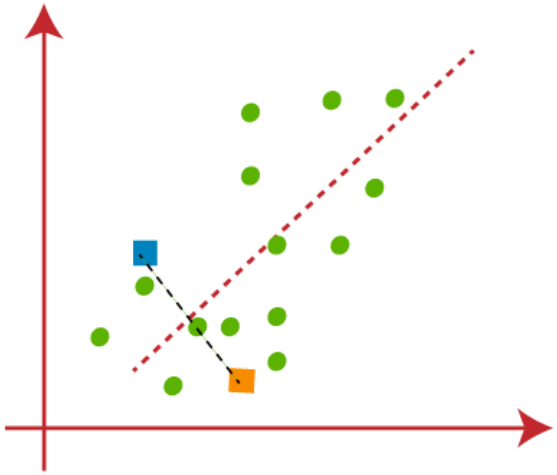


- Let's take number k of clusters, i.e., K=2, to identify the dataset and to put them into different clusters. It means here we will try to group these datasets into two different clusters.
- We need to choose some random k points or centroid to form the cluster. These points can be either the points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

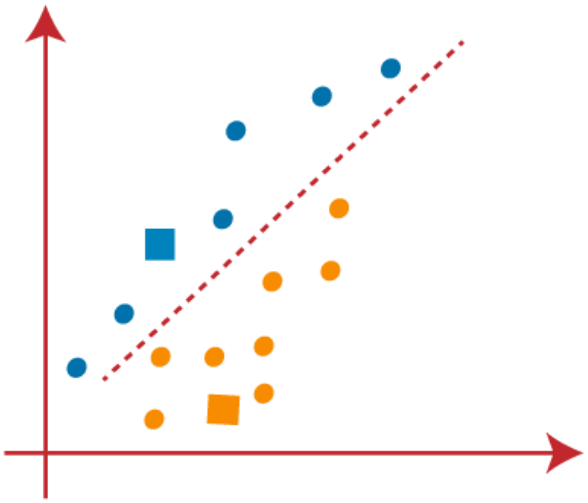


- Now we will assign each data point of the scatter plot to its closest K-point or centroid. We will compute it by applying some mathematics that we have

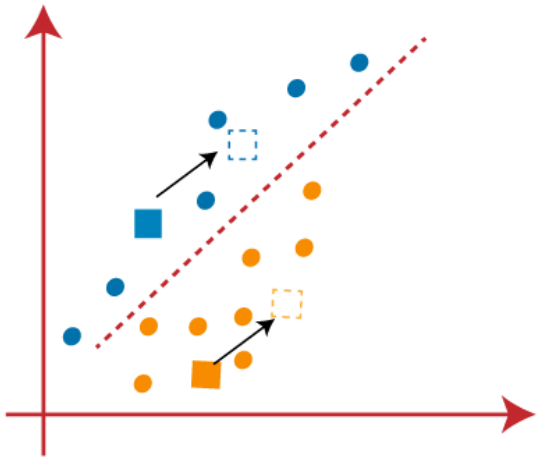
studied to calculate the distance between two points. So, we will draw a median between both the centroids. Consider the below image:



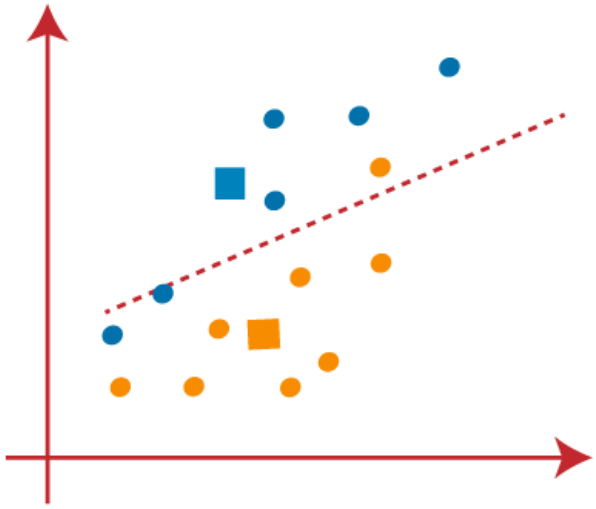
From the above image, it is clear that points left side of the line is near to the K1 or blue centroid, and points to the right of the line are close to the yellow centroid. Let's color them as blue and yellow for clear visualization.



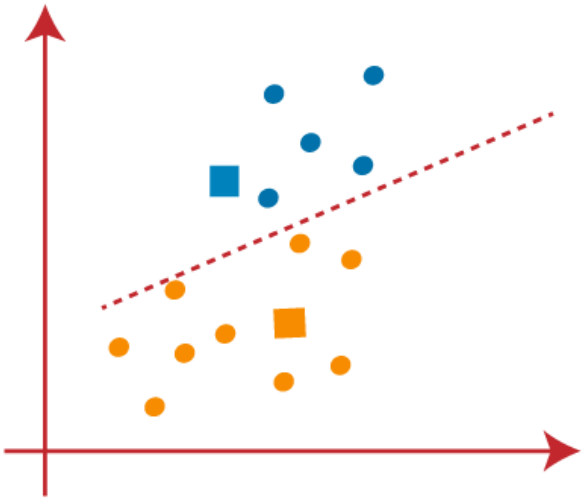
- As we need to find the closest cluster, so we will repeat the process by choosing **a new centroid**. To choose the new centroids, we will compute the center of gravity of these centroids, and will find new centroids as below:



- 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:



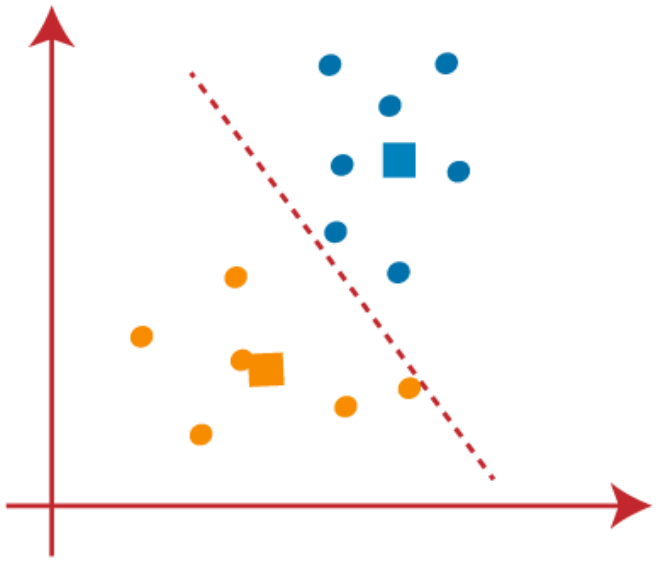
From the above image, we can see, one yellow point is on the left side of the line, and two blue points are right to the line. So, these three points will be assigned to new centroids.



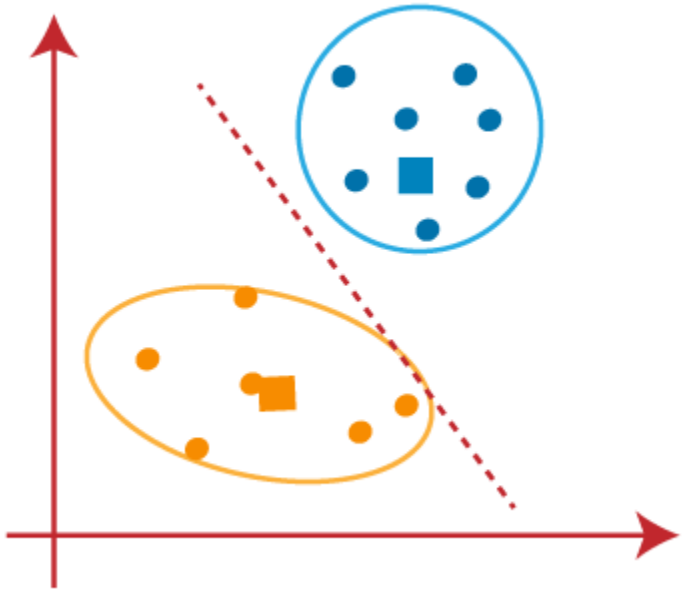
As reassignment has taken place, so we will again go to the step-4, which is finding new centroids or K-points.

- 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:

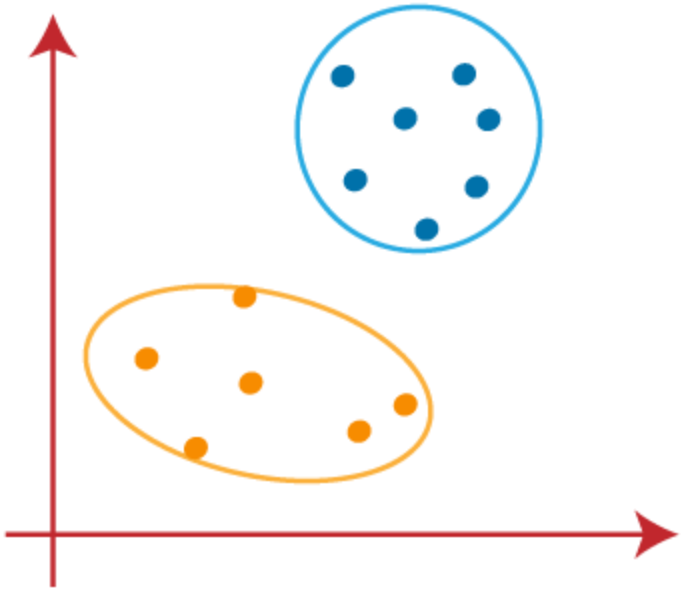
- As we got the new centroids so again will draw the median line and reassign the data points. So, the image will be:



- 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:



How to choose the value of "K number of clusters" in K-means Clustering?

The performance of the K-means clustering algorithm depends upon highly efficient clusters that it forms. But choosing the optimal number of clusters is a big task. There are some different ways to find the optimal number of clusters, but here we are discussing the most appropriate method to find the number of clusters or value of K. The method is given below:

Elbow Method

The Elbow method is one of the most popular ways to find the optimal number of clusters. This method uses the concept of WCSS value. **WCSS** stands for **Within Cluster Sum of Squares**, which defines the total variations within a cluster. The formula to calculate the value of WCSS (for 3 clusters) is given below:

$$WCSS= \sum_{Pi \text{ in } Cluster1} distance(P_i\ C_1)^2 + \sum_{Pi \text{ in } Cluster2} distance(P_i\ C_2)^2 + \sum_{Pi \text{ in } CLuster3} distance(P_i\ C_3)^2$$

In the above formula of WCSS,

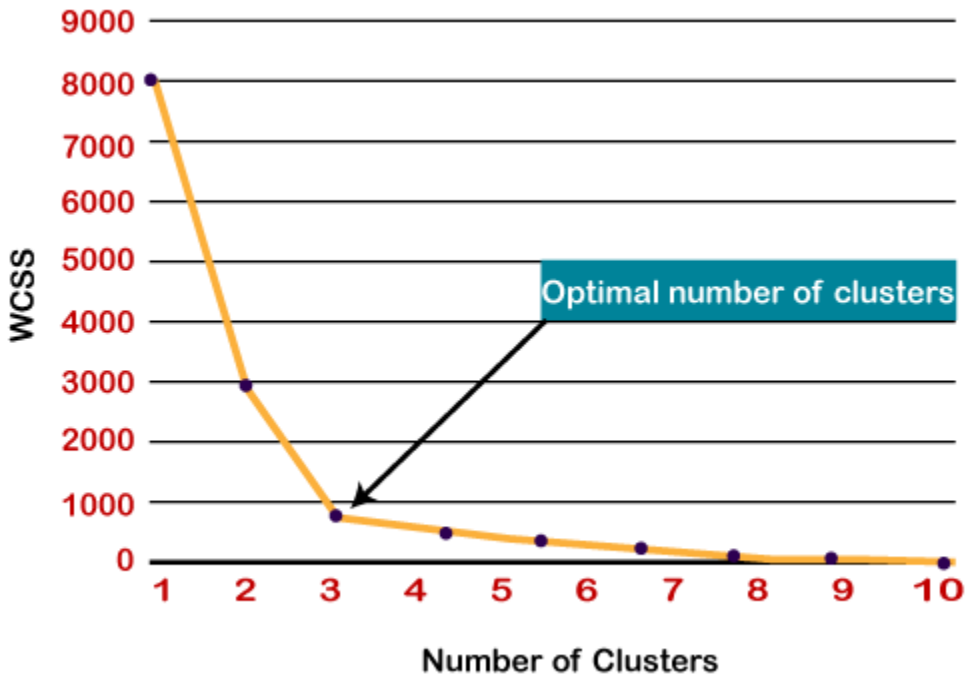
$\sum_{Pi \text{ in } Cluster1} distance(P_i\ C_1)^2$: It is the sum of the square of the distances between each data point and its centroid within a cluster1 and the same for the other two terms.

To measure the distance between data points and centroid, we can use any method such as Euclidean distance or Manhattan distance.

To find the optimal value of clusters, the elbow method follows the below steps:

- It executes the K-means clustering on a given dataset for different K values (ranges from 1-10).
- For each value of K, calculates the WCSS value.
- Plots a curve between calculated WCSS values and the number of clusters K.
- The sharp point of bend or a point of the plot looks like an arm, then that point is considered as the best value of K.

Since the graph shows the sharp bend, which looks like an elbow, hence it is known as the elbow method. The graph for the elbow method looks like the below image:



Apriori Algorithm in Machine Learning:

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.