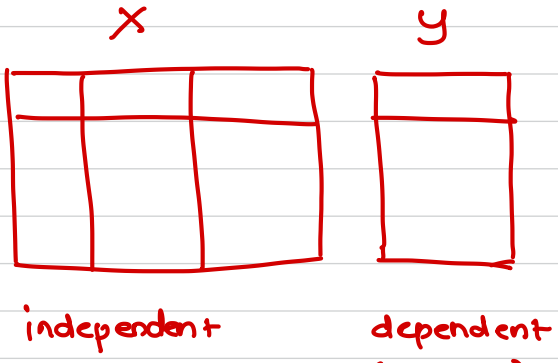
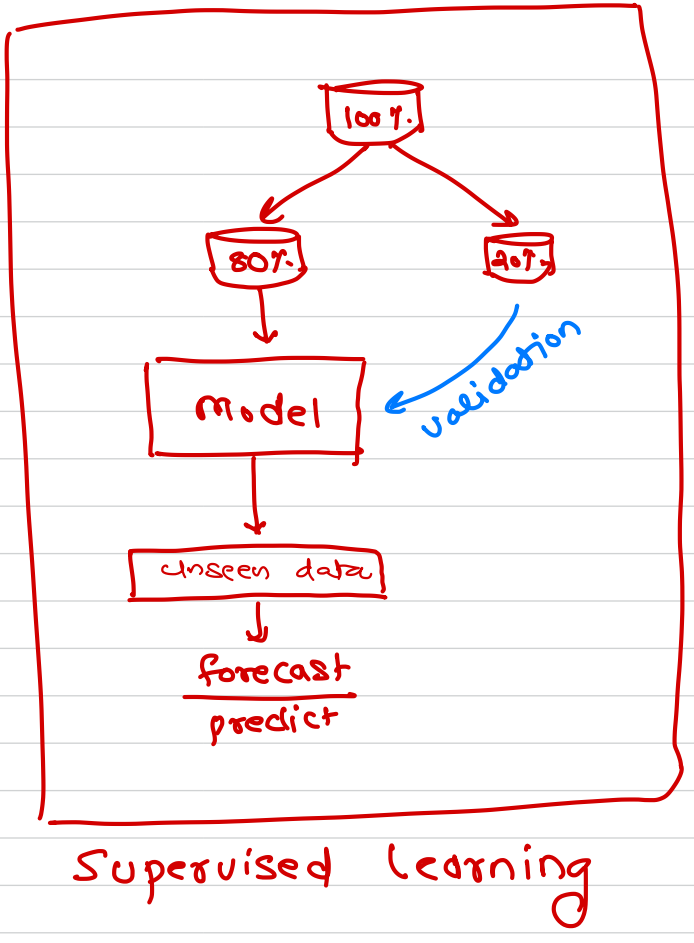
Machine Learning

Clustering



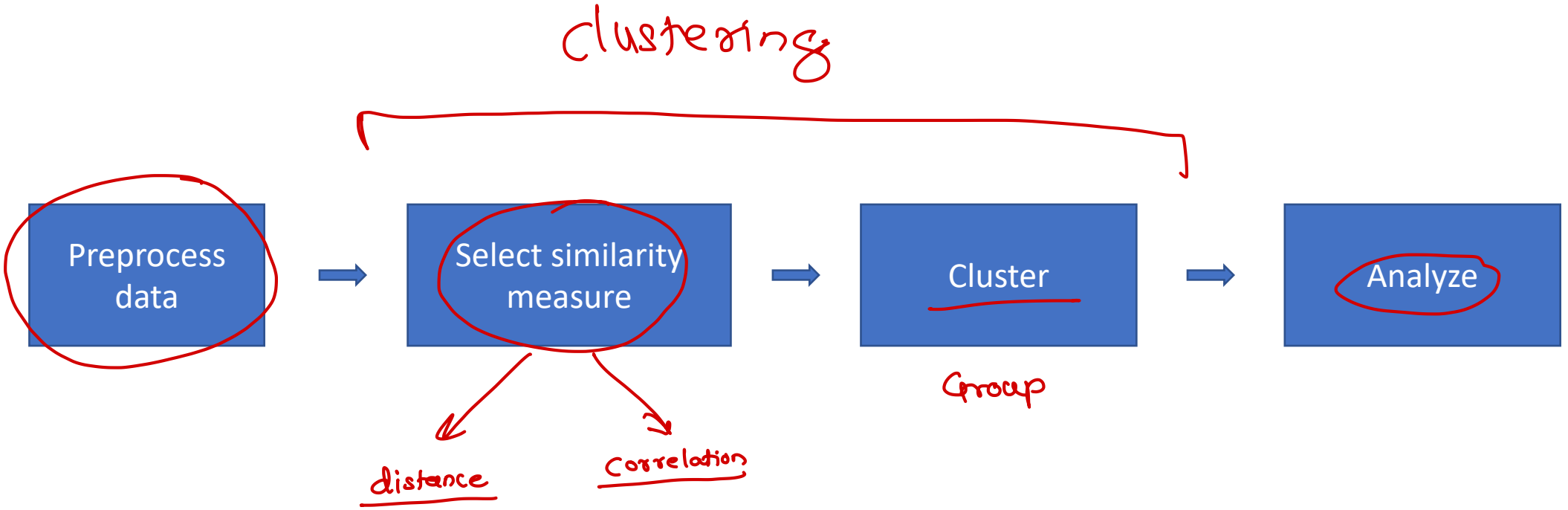


Supervised learning

Overview

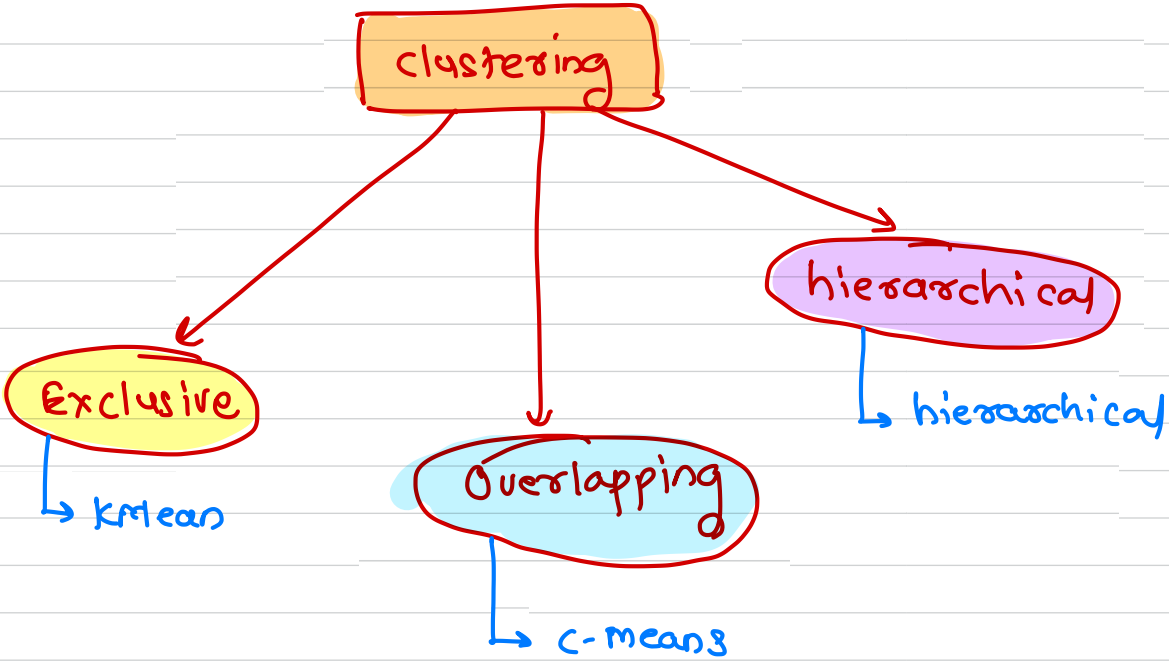
- **Clustering** is one of the most common exploratory data analysis technique used to get an intuition about the structure of the data
- It can be defined as the task of identifying subgroups in the data such that data points in the same subgroup (cluster) are very similar while data points in different clusters are very different
- In other words, we try to find homogeneous subgroups within the data such that data points in each cluster are as similar as possible according to a similarity measure such as euclidean-based distance or correlation-based distance
- The decision of which similarity measure to use is application-specific
- Unlike supervised learning, clustering is considered an unsupervised learning method since we don't have the ground truth to compare the output of the clustering algorithm to the true labels to evaluate its performance

Overview


clustering
Preprocess data
Select similarity measure
Cluster
Analyze
Group
distance
correlation

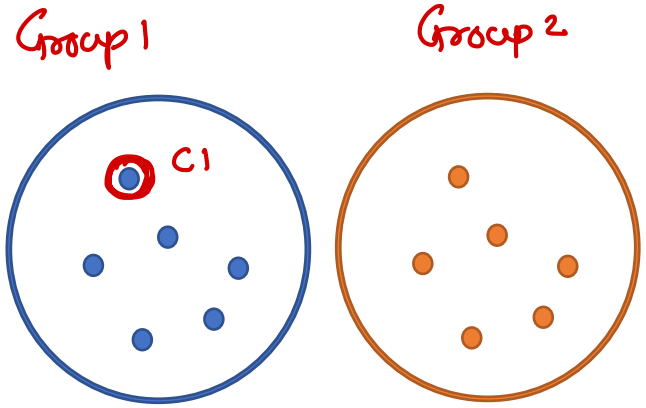
Use Cases

- Marketing
  - Discovering groups in customer databases like who makes long-distance calls or who are earning more or who are spending more
- Insurance
  - Identifying groups of insurance policy holder with high claim rate
- Land use
  - Identification of areas of similar land use in GIS database


clustering
Exclusive
kMean
Overlapping
C-means
hierarchical
hierarchical

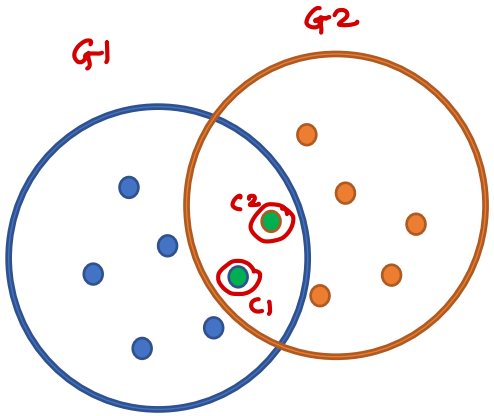
Types

- **Exclusive clustering**
  - An item belongs exclusively to one cluster and not several
  - E.g. K-Means clustering



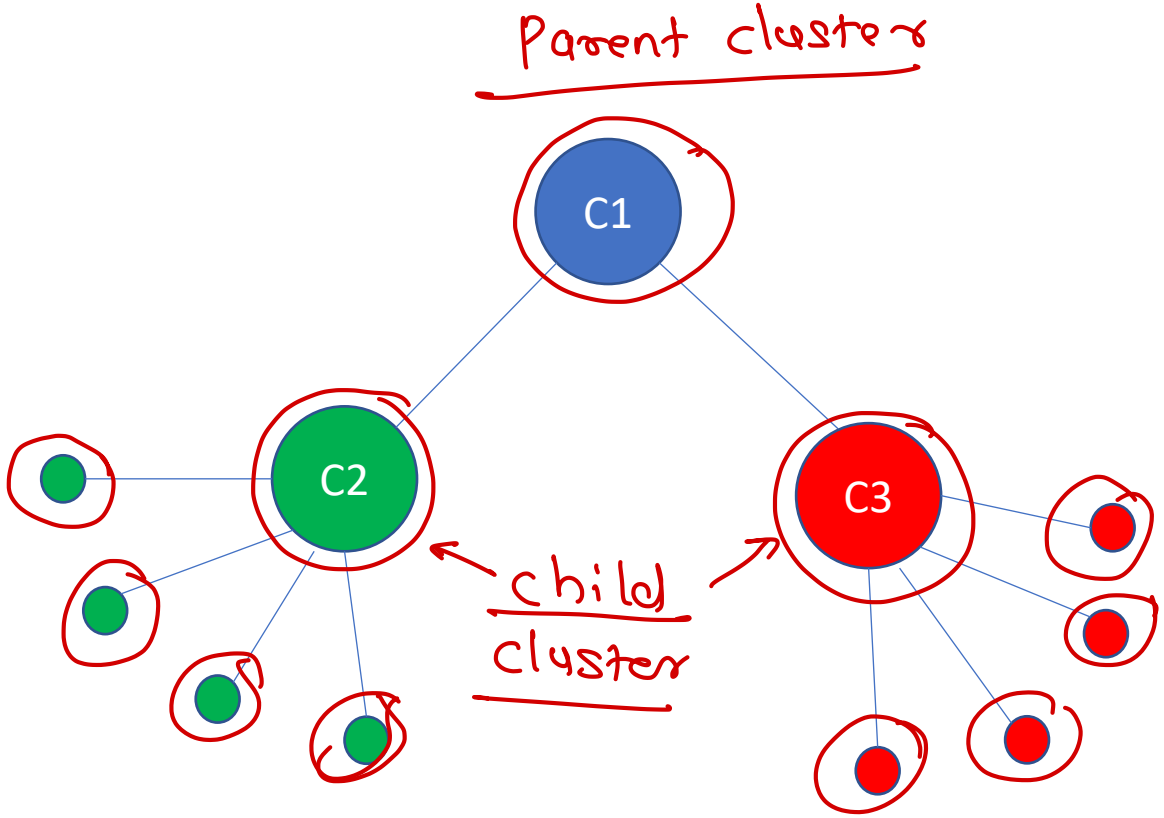
Types

- **Overlapping clustering**
  - An Item can belong to multiple clusters
  - Its degree of association with each cluster is known
  - E.g. Fuzzy/C-means clustering



Types

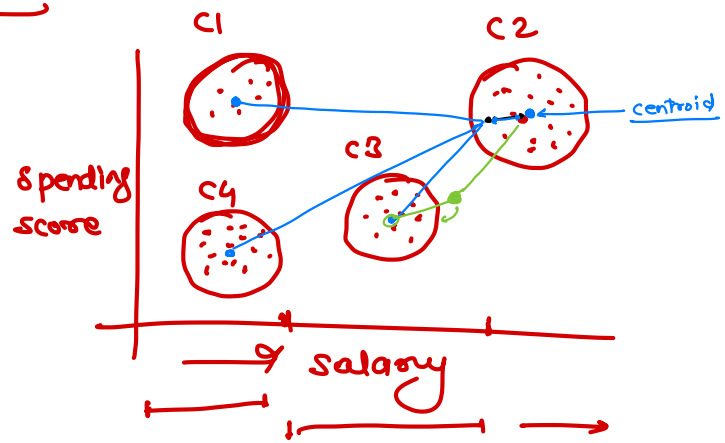
- Hierarchical clustering
  - When two clusters have a parent child relationship
  - It forms a tree like structure
  - E.g. Hierarchical clustering



KMeans

Overview

- **Kmeans** algorithm is an iterative algorithm that tries to partition the dataset into distinct non-overlapping subgroups (clusters) where each data point belongs to **only one group**
- It tries to make the inter-cluster data points as similar as possible while also keeping the clusters as different (far) as possible
- It assigns data points to a cluster such that the sum of the squared distance between the data points and the cluster's centroid (arithmetic mean of all the data points that belong to that cluster) is at the minimum
- The less variation we have within clusters, the more homogeneous (similar) the data points are within the same cluster



How does it work?

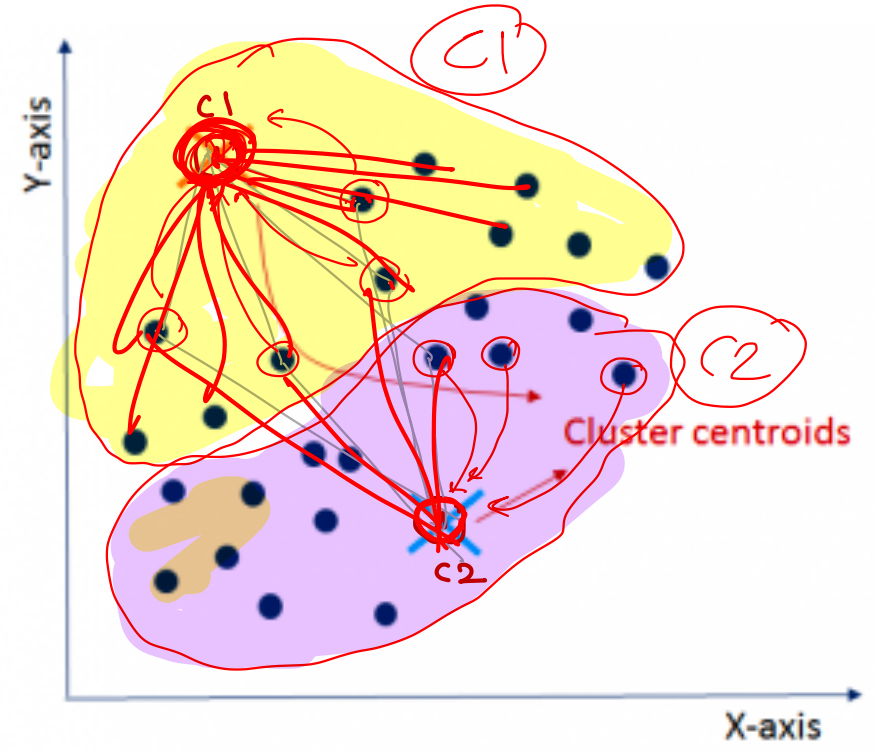
- Specify number of clusters *K*
- Initialize centroids by first shuffling the dataset and then randomly selecting *K* data points for the centroids without replacement
- Keep iterating until there is no change to the centroids. i.e assignment of data points to clusters isn't changing
- Compute the sum of the squared distance between data points and all centroids
- Assign each data point to the closest cluster (centroid)
- Compute the centroids for the clusters by taking the average of the all data points that belong to each cluster

K-Means Clustering - Algorithm

- **Initialization**
  - randomly initialise two points called the cluster centroids

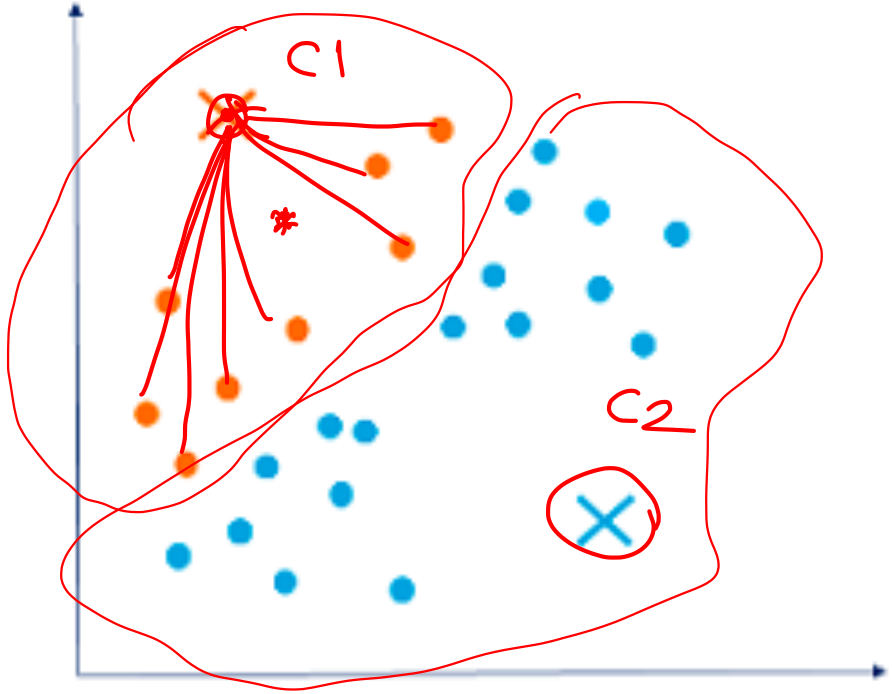
k = 2

Select two random centroids



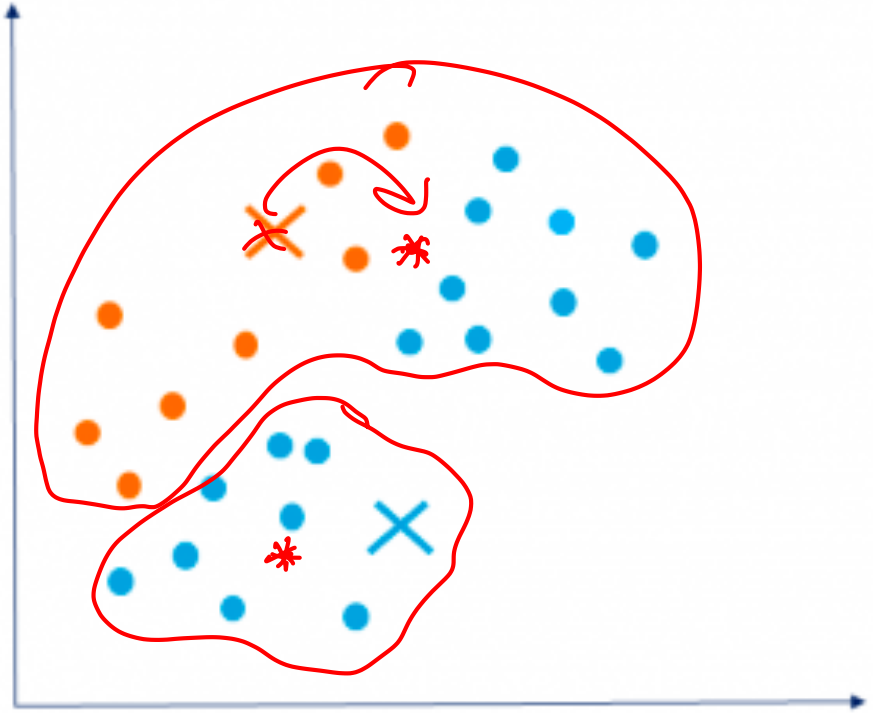
K-Means Clustering - Algorithm

- **Cluster Assignment**
  - Compute the distance between both the points and centroids
  - Depending on the minimum distance from the centroid divide the points into two clusters



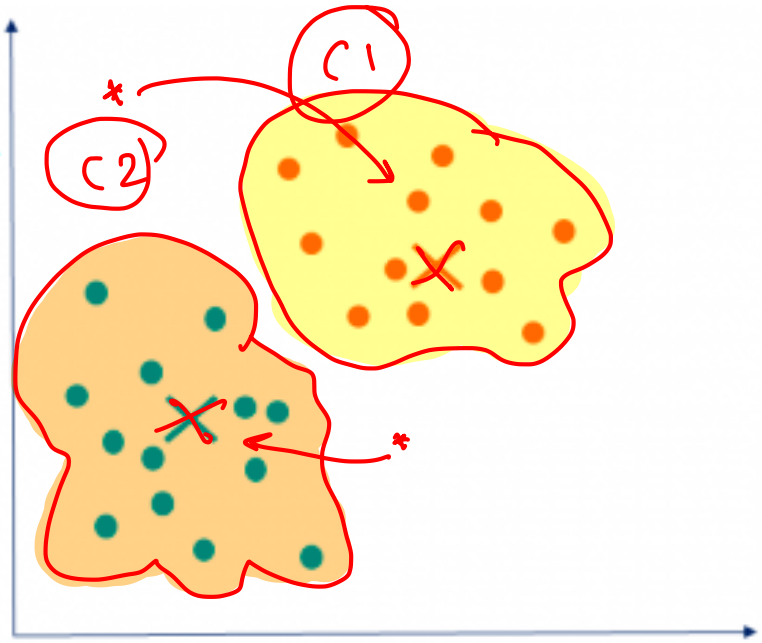
K-Means Clustering - Algorithm

- **Move Centroid**
  - Consider the older centroids are data points
  - Take the older centroid and iteratively reposition them for optimization
- **Optimization**
  - Repeat the steps until the cluster centroids stop changing the positio



K-Means Clustering - Algorithm

- **Convergence**
  - Finally, k-means clustering algorithm converges and divides the data points into two clusters clearly visible in multiple clusters



K-Means Clustering - Example

- Suppose we want to group the visitors to a website using just their age (one-dimensional space) as follows:

15,15,16,19,19,20,20,21,22,28,35,40,41,42,43,44,60,61,65

N = 19

K-Means Clustering - Example

- Initial clusters (random centroid or average)

k = 2

$c_1 = 16$

$c_2 = 22$

$$Distance\ 1 = |x_i - c_1|$$

$$Distance\ 2 = |x_i - c_2|$$

K-Means Clustering - Example

- **Iteration I**

Before:

$c_1 = 16$

$c_2 = 22$

After:

$c_1 = 15.33$

$c_2 = 36.25$

x_i	c_1	c_2	Distance 1	Distance 2	Nearest Cluster	New Centroid
15	16	22	1	7	1	15.33
15	16	22	1	7	1	
16	16	22	0	6	1	
19	16	22	3	3	2	36.25
19	16	22	3	3	2	
20	16	22	4	2	2	
20	16	22	4	2	2	
21	16	22	5	1	2	
22	16	22	6	0	2	
28	16	22	12	6	2	
35	16	22	19	13	2	
40	16	22	24	18	2	
41	16	22	25	19	2	
42	16	22	26	20	2	
43	16	22	27	21	2	
44	16	22	28	22	2	
60	16	22	44	38	2	
61	16	22	45	39	2	
65	16	22	49	43	2	

K-Means Clustering - Example

- **Iteration II**

Before:

$c_1 = 15.33$

$c_2 = 36.25$

After:

$c_1 = 18.56$

$c_2 = 45.9$

x_i	c_1	c_2	Distance 1		Distance 2	Nearest Cluster	New Centroid
15	15.33	36.25	0.33	<	21.25	1	
15	15.33	36.25	0.33	<	21.25	1	
16	15.33	36.25	0.67	<	20.25	1	
19	15.33	36.25	3.67	<	17.25	1	
19	15.33	36.25	3.67	<	17.25	1	**18.56**
20	15.33	36.25	4.67	<	16.25	1	
20	15.33	36.25	4.67	<	16.25	1	
21	15.33	36.25	5.67	<	15.25	1	
22	15.33	36.25	6.67	<	14.25	1	
28	15.33	36.25	12.67	>	8.25	2	
35	15.33	36.25	19.67	>	1.25	2	
40	15.33	36.25	24.67	>	3.75	2	
41	15.33	36.25	25.67	>	4.75	2	
42	15.33	36.25	26.67	>	5.75	2	
43	15.33	36.25	27.67	>	6.75	2	**45.9**
44	15.33	36.25	28.67	>	7.75	2	
60	15.33	36.25	44.67	>	23.75	2	
61	15.33	36.25	45.67	>	24.75	2	
65	15.33	36.25	49.67	>	28.75	2	

K-Means Clustering - Example

- **Iteration III**

Before:

$c_1 = 18.56$

$c_2 = 45.9$

After:

$c_1 = 19.50$

$c_2 = 47.89$

x_i	c_1	c_2	Distance 1	Distance 2	Nearest Cluster	New Centroid
15	18.56	45.9	3.56	30.9	1	
15	18.56	45.9	3.56	30.9	1	
16	18.56	45.9	2.56	29.9	1	
19	18.56	45.9	0.44	26.9	1	
19	18.56	45.9	0.44	26.9	1	19.50
20	18.56	45.9	1.44	25.9	1	
20	18.56	45.9	1.44	25.9	1	
21	18.56	45.9	2.44	24.9	1	
22	18.56	45.9	3.44	23.9	1	
28	18.56	45.9	9.44	17.9	1	
35	18.56	45.9	16.44	10.9	2	
40	18.56	45.9	21.44	5.9	2	
41	18.56	45.9	22.44	4.9	2	
42	18.56	45.9	23.44	3.9	2	
43	18.56	45.9	24.44	2.9	2	47.89
44	18.56	45.9	25.44	1.9	2	
60	18.56	45.9	41.44	14.1	2	
61	18.56	45.9	42.44	15.1	2	
65	18.56	45.9	46.44	19.1	2	

K-Means Clustering - Example

- **Iteration IV**

Before:

$c_1 = 19.50$

$c_2 = 47.89$

After:

$c_1 = 19.50$

$c_2 = 47.89$

x_i	c_1	c_2	Distance 1	Distance 2	Nearest Cluster	New Centroid
15	19.5	47.89	4.50	32.89	1	
15	19.5	47.89	4.50	32.89	1	
16	19.5	47.89	3.50	31.89	1	
19	19.5	47.89	0.50	28.89	1	
19	19.5	47.89	0.50	28.89	1	19.50
20	19.5	47.89	0.50	27.89	1	
20	19.5	47.89	0.50	27.89	1	
21	19.5	47.89	1.50	26.89	1	
22	19.5	47.89	2.50	25.89	1	
28	19.5	47.89	8.50	19.89	1	
35	19.5	47.89	15.50	12.89	2	
40	19.5	47.89	20.50	7.89	2	
41	19.5	47.89	21.50	6.89	2	
42	19.5	47.89	22.50	5.89	2	
43	19.5	47.89	23.50	4.89	2	47.89
44	19.5	47.89	24.50	3.89	2	
60	19.5	47.89	40.50	12.11	2	
61	19.5	47.89	41.50	13.11	2	
65	19.5	47.89	45.50	17.11	2	

K-Means Clustering

- How to find the optimum number of clusters?
  - Elbow Method
  - Purpose Method

Elbow Method

- Total within-cluster variation
  - Also known as Within Sum of Squares (WSS)
  - The sum of squared distances (Euclidean) between the items and the corresponding centroid

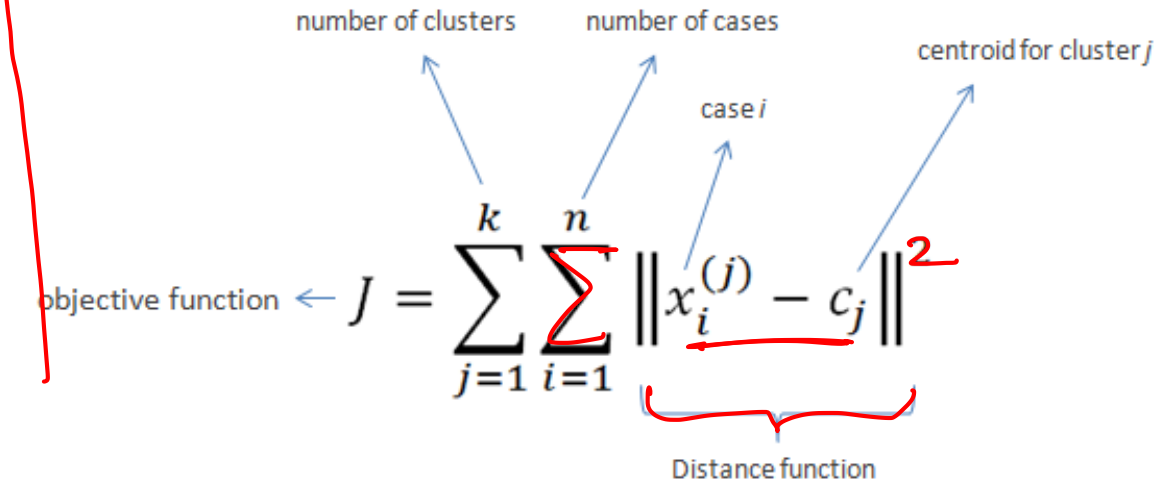
K = 1 = WSS1

K = 2 = WSS2

K = 3 = WSS3

⋮

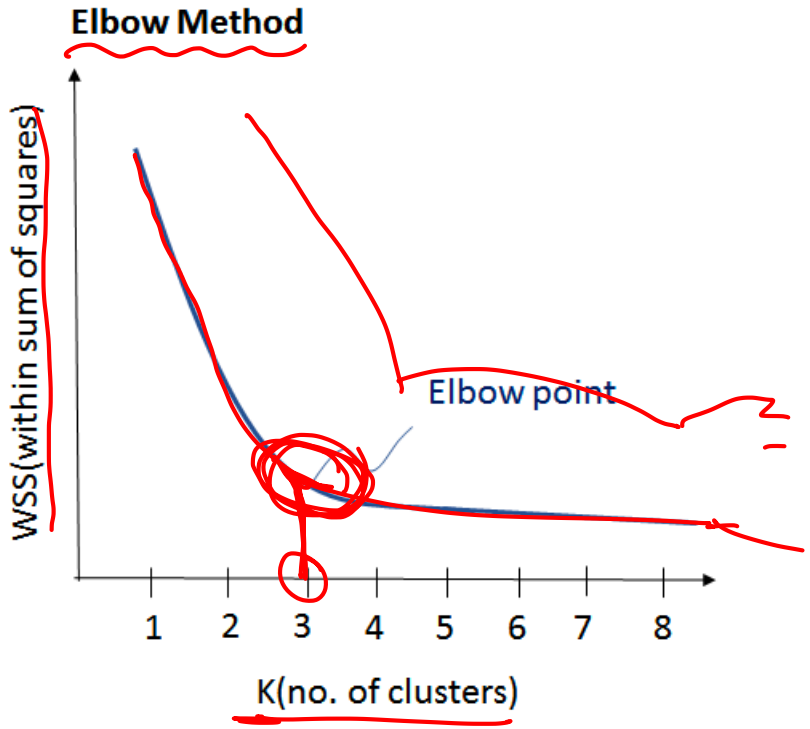
K = 10 = WSS10



Elbow Method

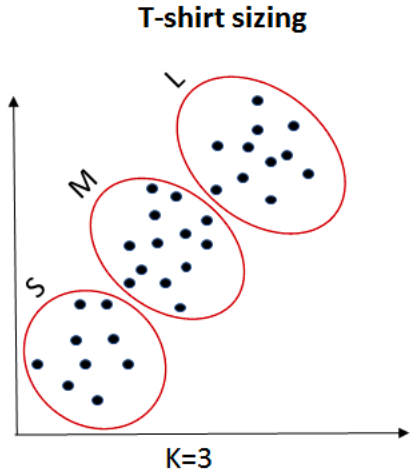
- Draw a curve between WSS (within sum of squares) and the number of clusters

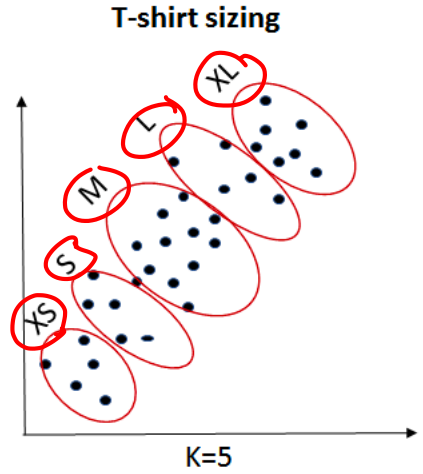
- It is called elbow method because the curve looks like a human arm and the elbow point gives us the optimum number of clusters



Purpose Method

- Get different clusters based on a variety of purposes
- Partition the data on different metrics and see how well it performs for that particular case





- K=3: If you want to provide only 3 sizes(S, M, L) so that prices are cheaper, you will divide the data set into 3 clusters.
- K=5: Now, if you want to provide more comfort and variety to your customers with more sizes (XS, S, M, L, XL), then you will divide the data set into 5 clusters.

Applications

- It is very popular and used in a variety of applications such as market segmentation, document clustering, image segmentation and image compression, etc.

Disadvantages

- It always try to construct a nice spherical shape around the centroid. That means, the minute the clusters have a complicated geometric shapes, kmeans does a poor job in clustering the data
- Doesn't let data points that are far-away from each other share the same cluster even though they obviously belong to the same cluster

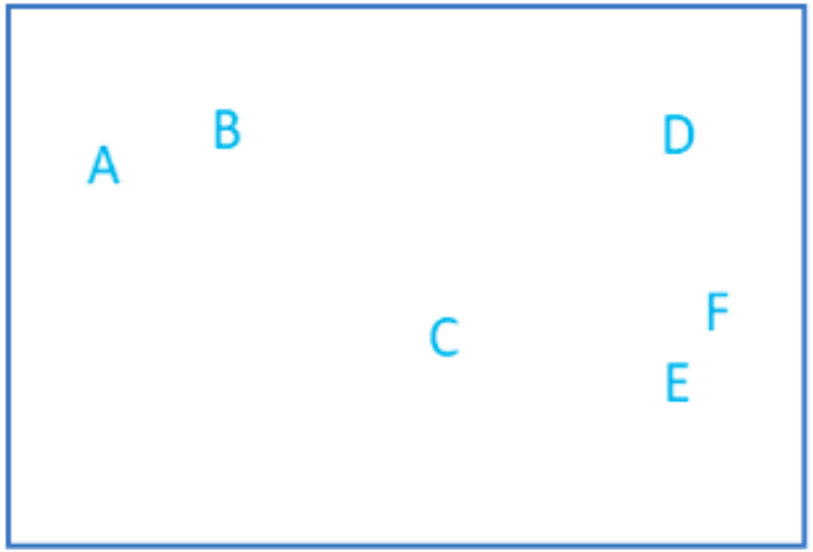
Hierarchical Clustering

Hierarchical Clustering

- Separating data into different groups based on some measure of similarity
- Types
  - Agglomerative
  - Divisive

Hierarchical Clustering

- Dendrogram
  - diagram that shows the hierarchical relationship between objects



Agglomerative Clustering

- Also called as bottom-top clustering as it uses bottom-up approach
- Each data point starts in its own cluster
- These clusters are then joined greedily by taking two most similar clusters together

Agglomerative Clustering

- Start by assigning each item to a cluster
  - if you have N items, you now have N clusters, each containing just one item
- Find the closest (most similar) pair of clusters and merge them into a single cluster, so that now you have one cluster less
- Compute distances (similarities) between the new cluster and each of the old clusters
- Repeat steps 2 and 3 until all items are clustered into a single cluster of size N

Agglomerative Clustering

- Step 3 can be done in different ways
  - Single-linkage
  - Complete-linkage
  - Average-linkage

Agglomerative Clustering

- **Single linkage**
  - Also known as nearest neighbour clustering
  - The distance between two groups is defined as the distance between their two closest members
  - It often yields clusters in which individuals are added sequentially to a single group

Agglomerative Clustering

- **Complete linkage**
  - also known as furthest neighbour clustering
  - the distance between two groups as the distance between their two farthest-apart members

Agglomerative Clustering

- **Average linkage**
  - referred to as the unweighted pair-group method
  - distance between two groups is defined as the average distance between each of their members

Divisive Clustering

- Also called as top-bottom clustering as it uses top-bottom approach
- All data point starts in it's the same cluster
- Then using parametric clustering like k-means divide the cluster into multiple clusters
- For each cluster repeating the process find sub cluster till the desired number of clusters found