K-Means Clustering

Agenda

1. Discussion Questions
2. Unsupervised Learning and Clustering
3. Common Distance Metrics
4. Scaling
5. K-Means Clustering
6. Optimal number of clusters
7. Pros & cons

Questions to discuss

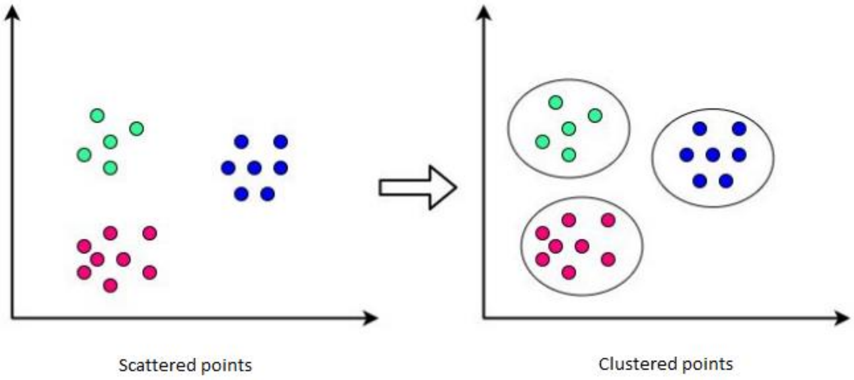
1. What is Unsupervised Learning and Clustering?
2. What is K-Means Clustering and how it works?
3. How to find the optimal number of clusters?
4. What are the pros and cons of K-Means Clustering?

Unsupervised Learning

- Unsupervised Learning is a class of Machine Learning techniques to find the patterns in data.
- The data given to unsupervised algorithms are not labeled, which means only the input variables (X) are given with no corresponding output variable (y).
- Involves training of an algorithm using information that is neither classified nor labeled.
- No defined dependent and independent variables.
- Patterns in the data are used to identify/group similar observations

Clustering

- The objective is to group a set of objects in such a way that objects in the same group are more similar to each other than to those in other groups
- It involves ensuring that the distance between data points in a cluster is very low compared to the distance between 2 clusters.
- This kind of algorithm captures the hidden patterns in data to find the underlying structure and discover new insights.
- The similarity between data points is determined by the distance between them, which can be measured using different distance metrics

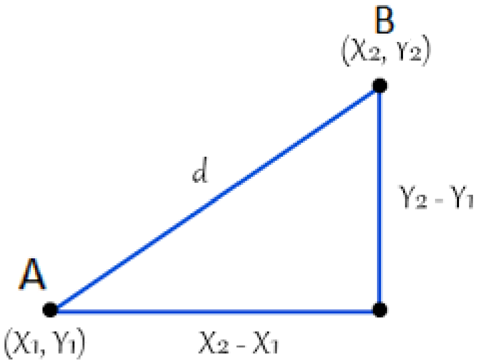


Common Distance Metrics

- **Euclidean Distance Metrics**

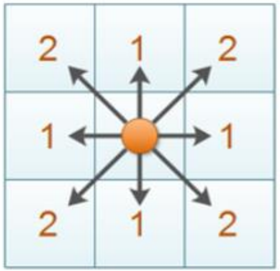
$$\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

Euclidean (A,B) = $\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$



- **Manhattan distances**

$$|x_1 - x_2| + |y_1 - y_2|$$

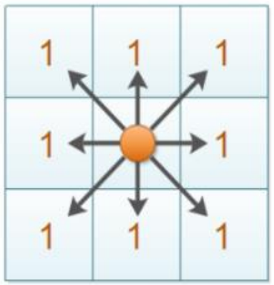


$$|x_1 - x_2| + |y_1 - y_2|$$

Common Distance Metrics

- <u>Chebyshev distance</u>

$$\max(|x_1 - x_2|, |y_1 - y_2|)$$



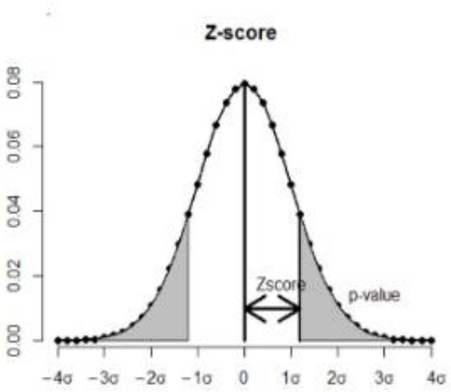
$$\max(|x_1 - x_2|, |y_1 - y_2|)$$

- <u>Minkowski distance</u>

$$\left(\sum_{i=1}^{n} |x_i - y_i|^p\right)^{\frac{1}{p}}$$

Scaling the data

- It is important to normalize the data using either Z-score or StandardScaler before performing K-means clustering
- This ensures that the different attributes in the data are of the same scale



Score

Mean

$$Z = \frac{x - \mu}{\sigma}$$

SD

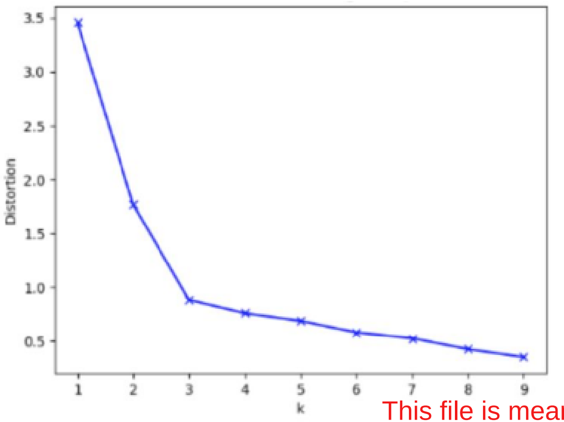
K-Means Clustering

- K-Means is one of the most common clustering techniques
- It is a centroid-based clustering algorithm where the objective is to find K clusters / groups
- The working of K-means clustering can be summarized as follows:
    - Step 1: Initialize the K random centroids or K points
    - Step 2: For each data point, calculate the Euclidean distance of it from randomly chosen K centroids and assign each point to a minimum distance cluster.
    - Step 3: Update the centroid by using newly assigned data points to the cluster by calculating the average of data points.
    - Step 4: Repeat the above process for a given no. of iterations or until the centroid allocation no longer changes

- Large K produces smaller groups and small K produces larger groups

Optimal Number of Clusters: Elbow Method

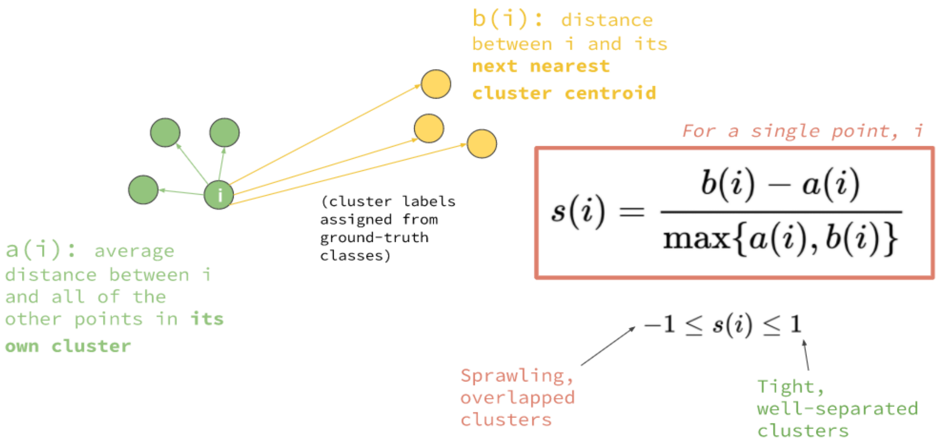
- There is no method to define the exact value of K
- The Elbow method is the most popular and well-known method to find the optimal no. of clusters
- This method is based on plotting the value of the cost function against different values of K
- The point where the distortion declines most is said to be the elbow point and defines the optimal number of clusters for the dataset



- In the example here, you can that the distortion decreases most at 3
- Hence, the optimal value of K will be 3 for performing the clustering

Optimal Number of Clusters: Silhouette Score

- The silhouette score is a metric which indicates the goodness of clustering algorithms
- It values range between -1 to +1
  - 1 indicates tight, well-separated clusters
  - 0 indicates clusters not well separable
  - -1 indicates data points of one cluster is more closer to centroid of another cluster than the centroid of its own cluster
- **Silhouette score = (b-a)/max(a,b)**
  - a = average intra-cluster distance i.e., the average distance between each point within a cluster.
  - b = average inter-cluster distance i.e., the average distance between all clusters.



Pros and Cons

Pros:

- Can be implemented with ease and it is faster than other clustering algorithms
- Works great on large scale data
- Results guarantee convergence
- Easily works with new examples

Cons:

- Sensitive to outliers
- Quite difficult to determine the number of clusters
- Sensitive to initialization of cluster centers

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Happy Learning !