Unsupervised Learning

Topics covered so far

Unsupervised Learning

- K Means Clustering
- PAM (K Medoids) clustering
- Hierarchical Clustering
- GMM
- DBSCAN

Discussion questions

1. What is K Means Clustering and what are the advantages and disadvantages of using K Means clustering?
2. Why PAM (K Medoids) clustering is a good alternative for K Means clustering?

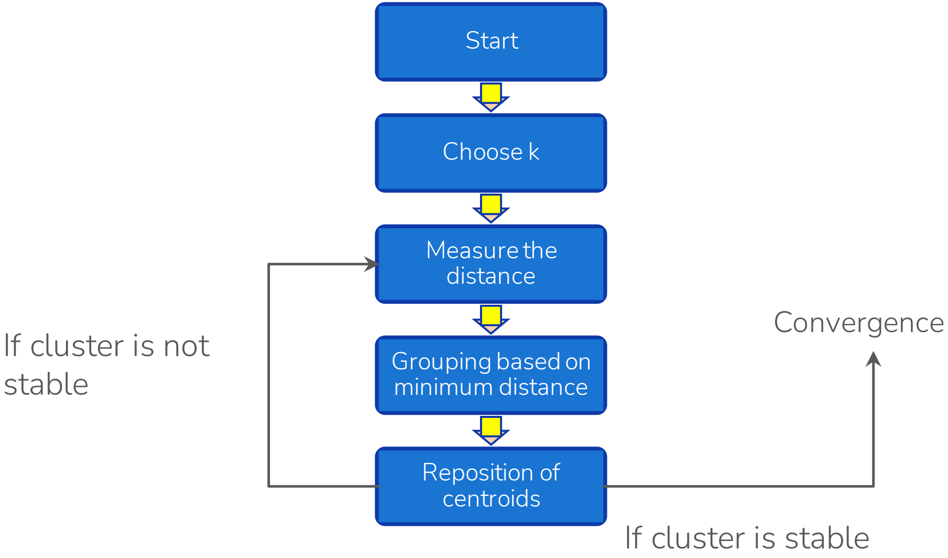
3. What is expectation maximization algorithm and how does it help in GMM clustering?

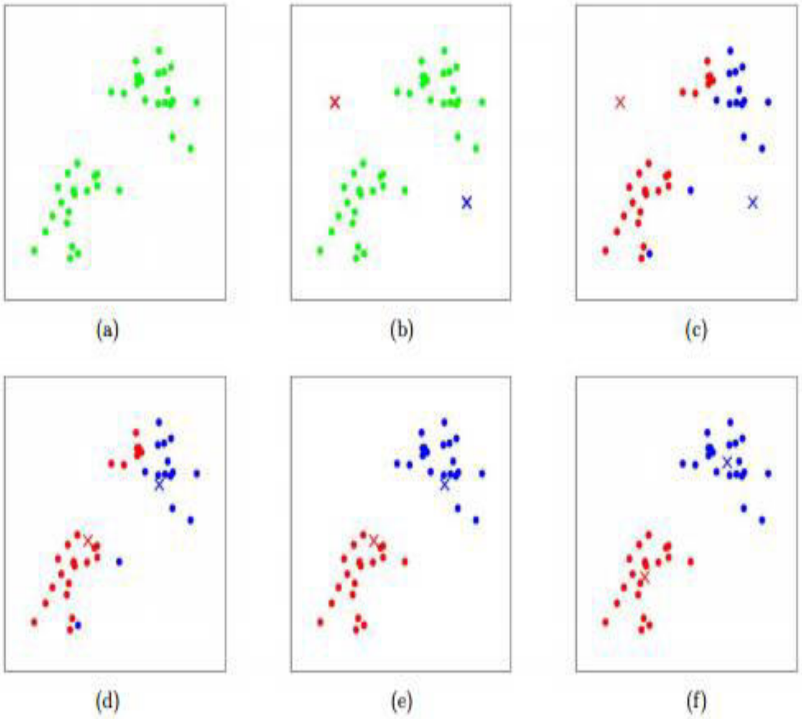
4. What is hierarchical clustering and how do we measure dissimilarity among clusters in hierarchical clustering?

5. How does DBSCAN work and what are the parameters that can be tuned in DBSCAN?

K Means Clustering

K-Means Clustering is an iterative **algorithm** that divides the unlabeled dataset into **k** different **clusters** in such a way that each point in the dataset belongs to only one group that has similar properties.





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Advantages and Disadvantages of using K Means clustering

Advantages:

- K-means is relatively simple to implement
- It scales to large datasets
- It also guarantees convergence
- It can easily adapt to new examples

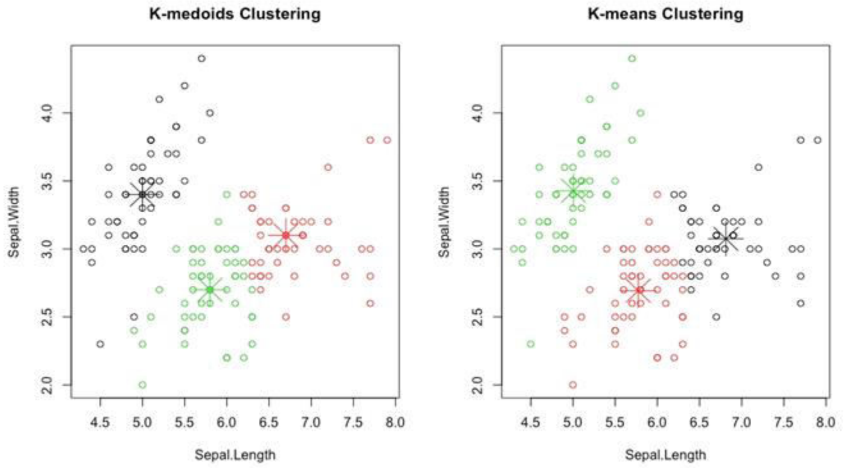
Disadvantages:

- It is difficult to identify the value of k
- k-means has trouble clustering data where clusters are of varying sizes and density
- It can easily get affected by outliers
- It assumes data shape to be spherical in nature and does not perform well on the arbitrary data
- It depends on the initial values assigned to the centroids and gives different results for different initialization

Alternative to K Means - PAM (K Medoids) clustering

- The problem with K means is that the final centroids are not interpretable i.e. centroids are not actual points but the means of the points present in the cluster.
- The idea behind K Medoids clustering is to make the final centroids as actual data points so that they are interpretable.
- In K Medoids, we only change one step from K Means which is to update the centroids. In this process if there are m points in a cluster, swap the previous centroids with all other (m-1) points from the cluster and finalize the point as new centroid which has minimum loss.

- Because of this, unlike K Means it is robust to outliers and converges fast.
- You can see in this image that the centroids in K Medoids are the actual data points represented as the cross, unlike K Means.



Expectation maximization in GMM Clustering

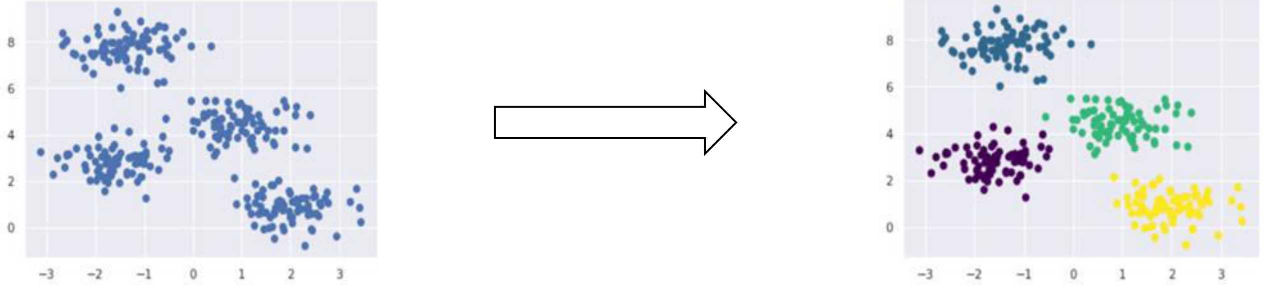
In GMM, we need the parameters of each Gaussian (variance, mean etc.) in order to cluster our data but we need to know which sample belongs to what Gaussian in order to estimate those very same parameters.

That is where we need EM algorithm. There are two steps involved in this algorithm:

1. **The E-step:** It estimates the probability that a given observation to be in a cluster/distribution. This value will be high when the point is assigned to the right cluster and lower otherwise.
2. **The M-step:** In this step we want to maximize the likelihood that each observation came from the distribution

After that we reiterate these two steps and updates the probabilities of an observation to be in a cluster.

Example of GMM clustering



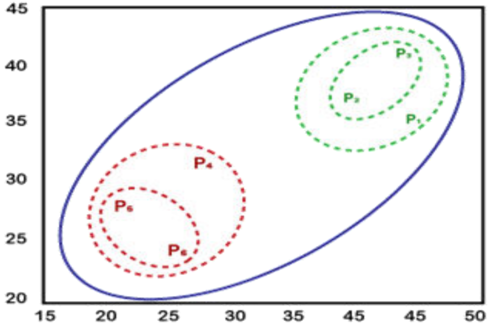
Hierarchical Clustering

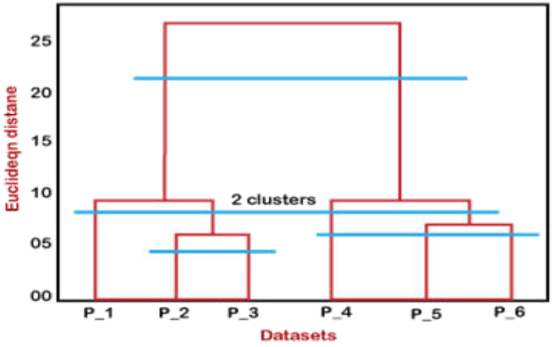
Hierarchical clustering is an unsupervised clustering algorithm which involves creating clusters that have predominant ordering from top to bottom. For e.g: All files and folders on our hard disk are organized in a hierarchy.

The algorithm groups similar objects into groups called ***clusters***. The endpoint is a set of clusters or groups, where each cluster is distinct from each other cluster, and the objects within each cluster are broadly similar to each other.

Steps

- Make each data point a single-point cluster → forms N clusters
- Take the two closest data points and make them one cluster → forms N-1 clusters
- Take the two closest clusters and make them one cluster → Forms N-2 clusters.
- Repeat step-3 until you are left with only one cluster.





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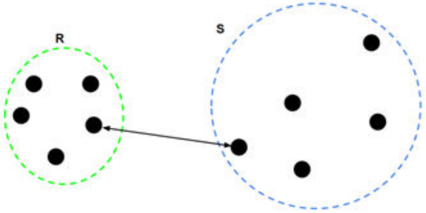
Dissimilarity among clusters in hierarchical clustering

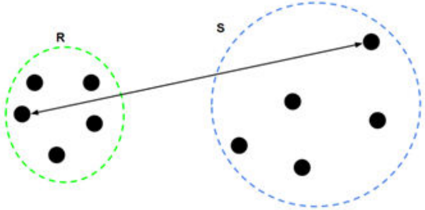
There are following ways by which we can measure dissimilarity among clusters in hierarchical clustering:

- **Single linkage:** It measure the closest pair of points i.e the minimum distance.



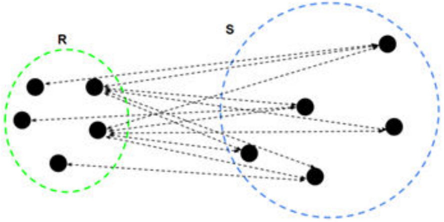
L(R,S) = min(d(i,j)) where i belongs to R and j belongs to S

- **Complete linkage:** It measure the farthest pair of points i.e the maximum distan



L(R,S) = max(d(i,j)) where i belongs t R and j belongs to S

- **Average linkage:** It measure the average dissimilarity over all pairs i.e. the average distance $L(R,S) = \frac{1}{n_R + n_S} \sum_{i=1}^{n_R} \sum_{j=1}^{n_S} D(i,j), i \epsilon R, j \epsilon S$



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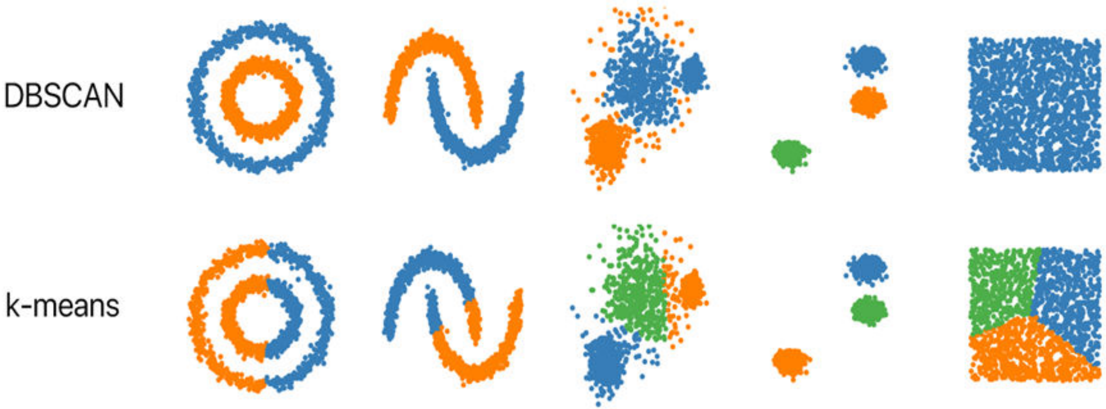
DBSCAN

DBSCAN stands for **D**ensity-**B**ased **S**patial **C**lustering of **A**pplications with **N**oise.

It recognizes groups in the data by looking at the local density of a data point. Unlike K-means, **DBSCAN clustering is not sensitive to outliers** and also does not require the number of clusters to be told beforehand.



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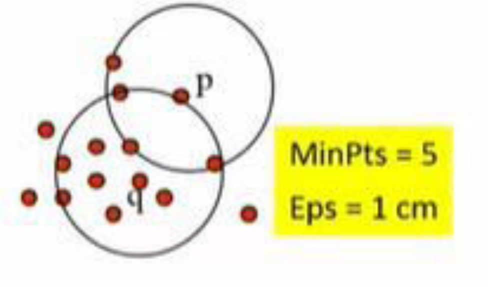
Parameters in DBSCAN

- **eps ('ε'):** It defines the neighborhood around a data point i.e. if the distance between two points is lower or equal to 'eps' then they are considered as neighbors. If the eps value is chosen too small then a large part of the data will be considered as outliers. If it is chosen very large then the clusters will merge and majority of the data points will be in the same clusters. One way to find the eps value is based on the k-distance graph



- **MinPts:** Minimum number of neighbors (data points) within eps radius. Larger the dataset, the larger value of MinPts must be chosen. As a general rule, the minimum MinPts can be derived from the number of dimensions D in the dataset as, MinPts >= D+1. The minimum value of MinPts must be chosen at least

Case Study - Clustering

Great Learning

Happy Learning !