<u>Foundations of Machine Learning</u> Al2000 and Al5000

FoMI -26 Hierarchical Clustering

> <u>Dr. Konda Reddy Mopuri</u> Department of AI, IIT Hyderabad July-Nov 2025





So far in FoML

- Intro to ML and Probability refresher
- MLE, MAP, and fully Bayesian treatment
- Supervised learning
 - Linear Regression with basis functions
 - Bias-Variance Decomposition
 - Decision Theory three broad classification strategies
 - Neural Networks
- Unsupervised learning
 - K-Means clustering





For today

- Clustering
 - Hierarchical Clustering

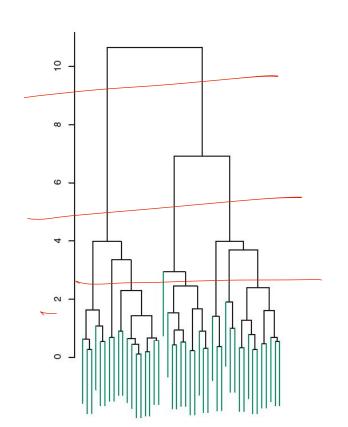
Some of the contents are taken from - Intro to Statistical Learning





- Unlike K-Means, no need to specify the 'K'
- Results in a tree-like representation of the data Dendrogram





Can consider at any level

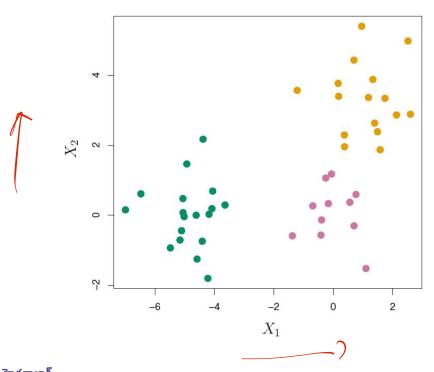


Data-driven Intelligence & Learning Lab

Bottom-up or Agglomerative clustering

- Most common of Hierarchical Clustering
- Builds the Dendrogram starting from the leaves combining the clusters up to the trunk

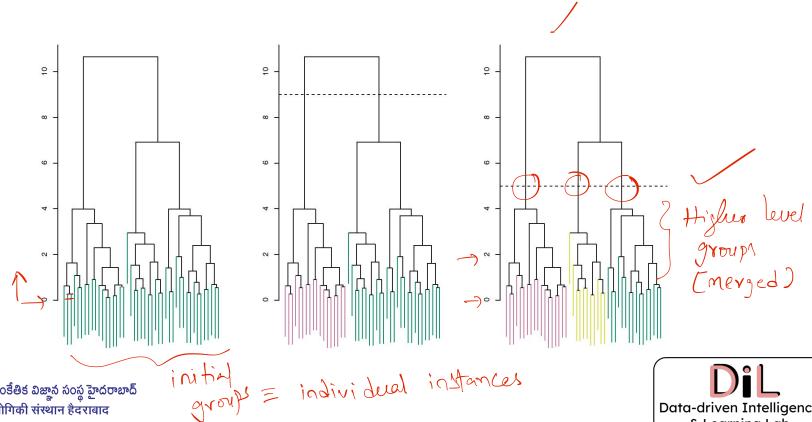




example
2D data
(generaled from
there classes)
Clusters)









భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్ भारतीय प्रौद्योगिकी संस्थान हैदराबाद **Indian Institute of Technology Hyderabad**



- Each leaf represents one of the observations
- As we move up, some leaves begin to fuse into branches
 - Observations that are similar/close to each other

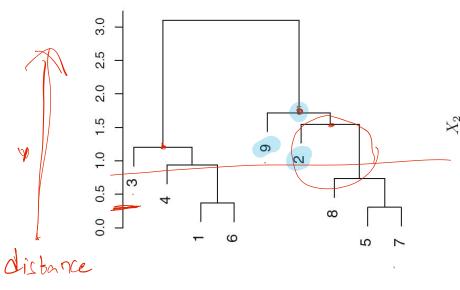


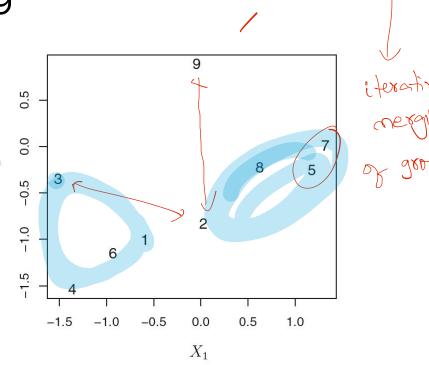


- The earlier the fusion occurs the similar the groups are to each other
- Observations that fuse later are less similar



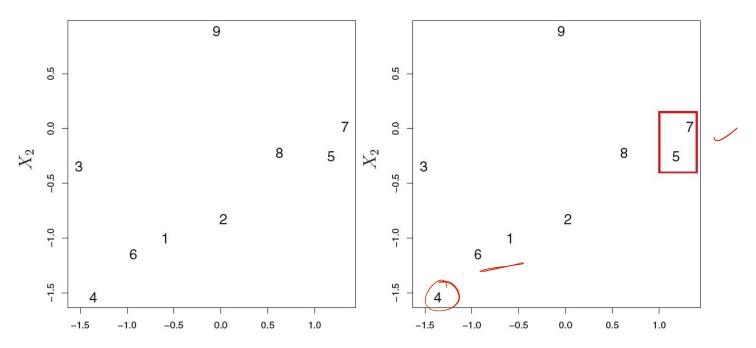






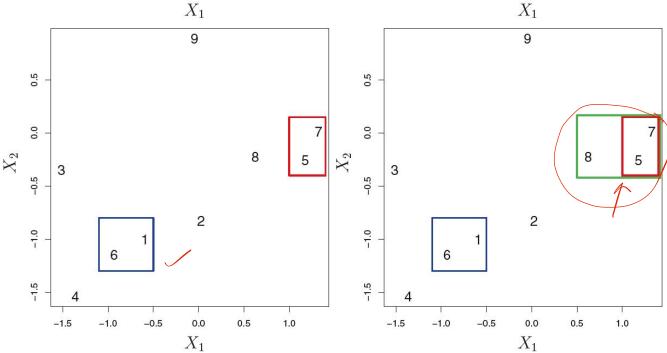


Data-driven Intelligence & Learning Lab











Data-driven Intelligence & Learning Lab

Hierarchical clustering Algorithm

- 1. Begin with n observations and a measure (such as Euclidean distance) of all the $\binom{n}{2} = n(n-1)/2$ pairwise dissimilarities. Treat each observation as its own cluster.
- 2. For $i = n, n 1, \dots, 2$:
 - (a) Examine all pairwise inter-cluster dissimilarities among the *i* clusters and identify the pair of clusters that are least dissimilar (that is, most similar). Fuse these two clusters. The dissimilarity between these two clusters indicates the height in the dendrogram at which the fusion should be placed.
 - (b) Compute the new pairwise inter-cluster dissimilarities among the i-1 remaining clusters.





- Concept of dissimilarity b/w a pair of groups of observations?
- Linkage
 - Complete maximal similarity
 - Single minimal
 - Average average of pairwise similarities
 - Centroid similarity of cluster centers





Next

• GMM for clustering





Rough work



