

Initially, All points are separate clusters.

① Hierarchical Clustering

Bottom-up / Agglomerative approach

→ one main disadvantage of K-means is that it needs us to pre-enter the no. of clusters (k).

→ Hierarchical clustering is an alternative approach which does not need us to give the value of k beforehand and also, it creates a beautiful 'tree-based structure' for visualisation.

→ we start by defining any sort of similarity between the datapoints. Generally, we consider Euclidean distance. The points which are closer to each other are more similar than the points which are further away.

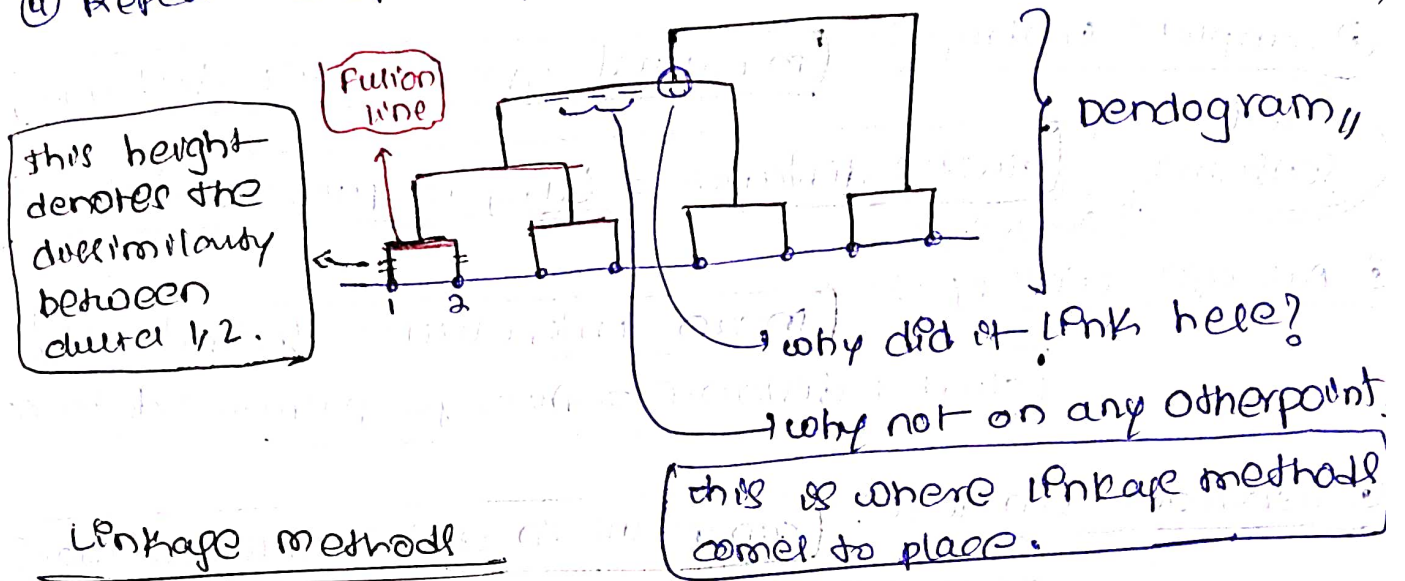
Algorithm

① Begin with n observations and a measure (such as Euclidean distance) of all the $(n-1)/2$ pairwise dissimilarities (distances).
Treat each observation as its own cluster.
So, initially we have n clusters.

② Compare all the distances and put two closest points/clusters in the same cluster.
The dissimilarity between these two clusters indicates the height in the dendrogram at which 'fusion line' should be placed.

③ compute the new pairwise inter-cluster dissimilarity among the remaining clusters.

④ Repeat steps 2 & 3 till we have only one cluster left.



Linkage method

→ Based on pairwise distance, we can now compute a linkage matrix.

The linkage matrix is simply a table listing which pairs of points are merged at what step & what distance.

→ we can cut dendrogram to form flat clusters.

⑥ we know, initially HC starts with clusters consisting of individual points.

→ later it compares the cluster with each other and merges the two "closest cluster".

→ since clusters are pair of points, there are many different kinds of linkage methods.

note

① single linkage

cluster distance = smallest pairwise distance

② complete linkage

(maximal intercluster distance)

less
sensitive

cluster distance = largest pairwise distance

(to outliers)

③ Average linkage

(mean intercluster dissimilarity)

cluster distance = Average pairwise distance

④ centroid linkage

can result in undesirable inversions

cluster distance = distance between the centroids of clusters

⑤ ward's linkage

(Before final merging)

cluster distance = minimize the variance in cluster.

single linkage

(minimal intercluster dissimilarity)

→ single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.

→ cluster distance is the smallest distance b/w any point in cluster ① & any point in cluster ②

→ High sensitive to outliers when forming flat clusters.

→ works well for low-noise data with unusual structures