Hierarchical Clustering

Relationship between Clusters

K-Means Clustering

- We learned about the K-Means Clustering Algorithm, which finds the centroid of the clusters

    1) Initialize centroids at random
    2) Assign observations to the cluster of the nearest centroid
    3) Recalculate the centroids based on the cluster assignment
    4) Repeat Steps 2 and 3 until the cluster assignments stop changing

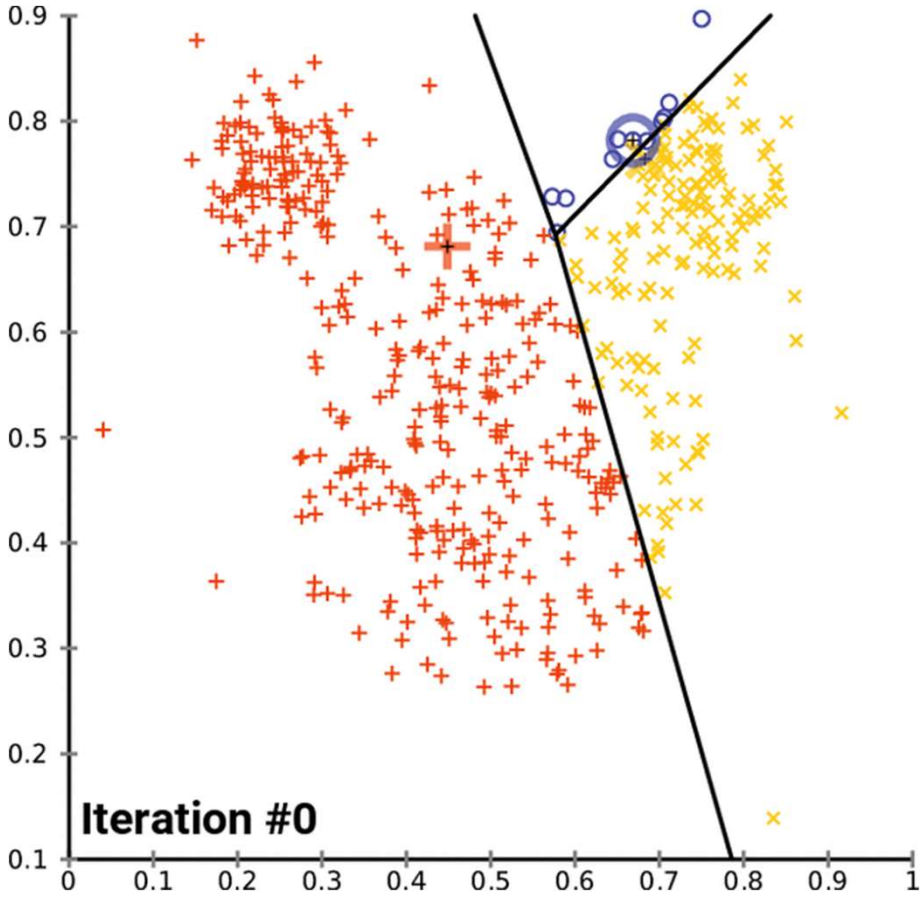


Image Source: Wikipedia

K-Means: Limitations

- It is an iterative based approach that requires us to specify the number of clusters.
    - Determining the optimal number of clusters can be challenging, especially in cases where the data's underlying structure is not well understood.

- Final results can be sensitive to the initial placement of cluster centroids and the choice of the distance metric.

- Assumes that clusters are spherical and isotropic, meaning they have similar sizes and densities in all directions.

- Sensitive to outliers, where outliers can disproportionately influence the position of centroids, leading to suboptimal clustering results.

Hierarchical Clustering

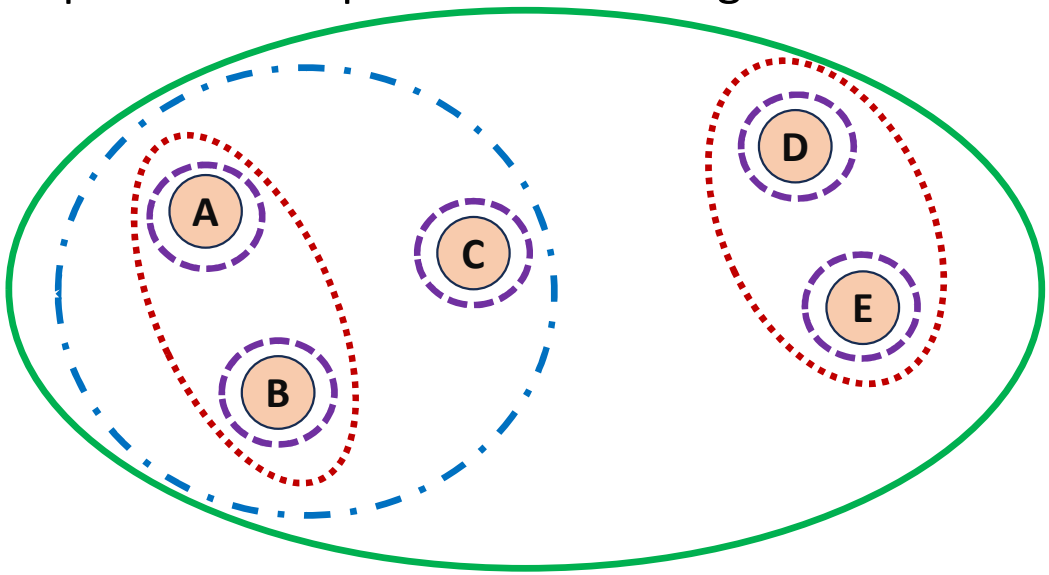
- Hierarchical Clustering - An alternative approach that does not require a pre-specified choice of K, and provides a deterministic answer

- It is based on distances between the data points in contrast to K-means, which focuses on distance from the centroid

    - **Agglomerative/Bottom-Up Clustering**: We recursively merge similar clusters
    - **Divisive / Top-down Clustering**: We recursively sub-divide into dissimilar sub clusters

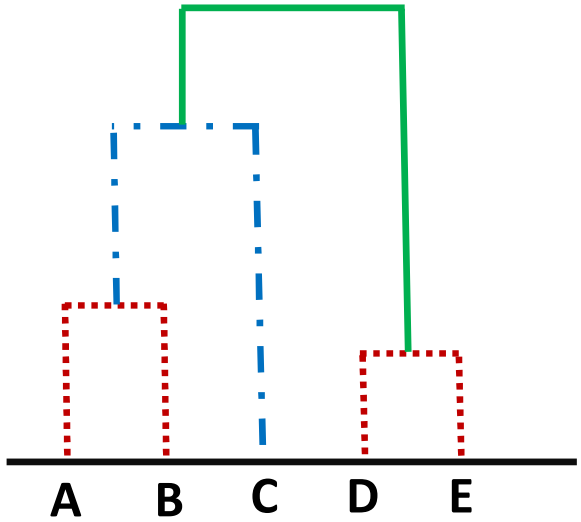
Agglomerative Clustering

- Start with each point in its own cluster
- Identify the two closest clusters (C_i, C_j) - merge them
- Repeat until all points are in a single cluster



- Set threshold τ to 0.
  - $\tau = \tau + \varepsilon$; where ε is a small positive quantity.
  - If the distance between any pair of clusters is < τ, combine them
  - Update all distances from/to the newly formed cluster

✓ To visualize the results we can look at the corresponding dendrogram



y-axis on dendrogram is the distance between the clusters that got merged at that step

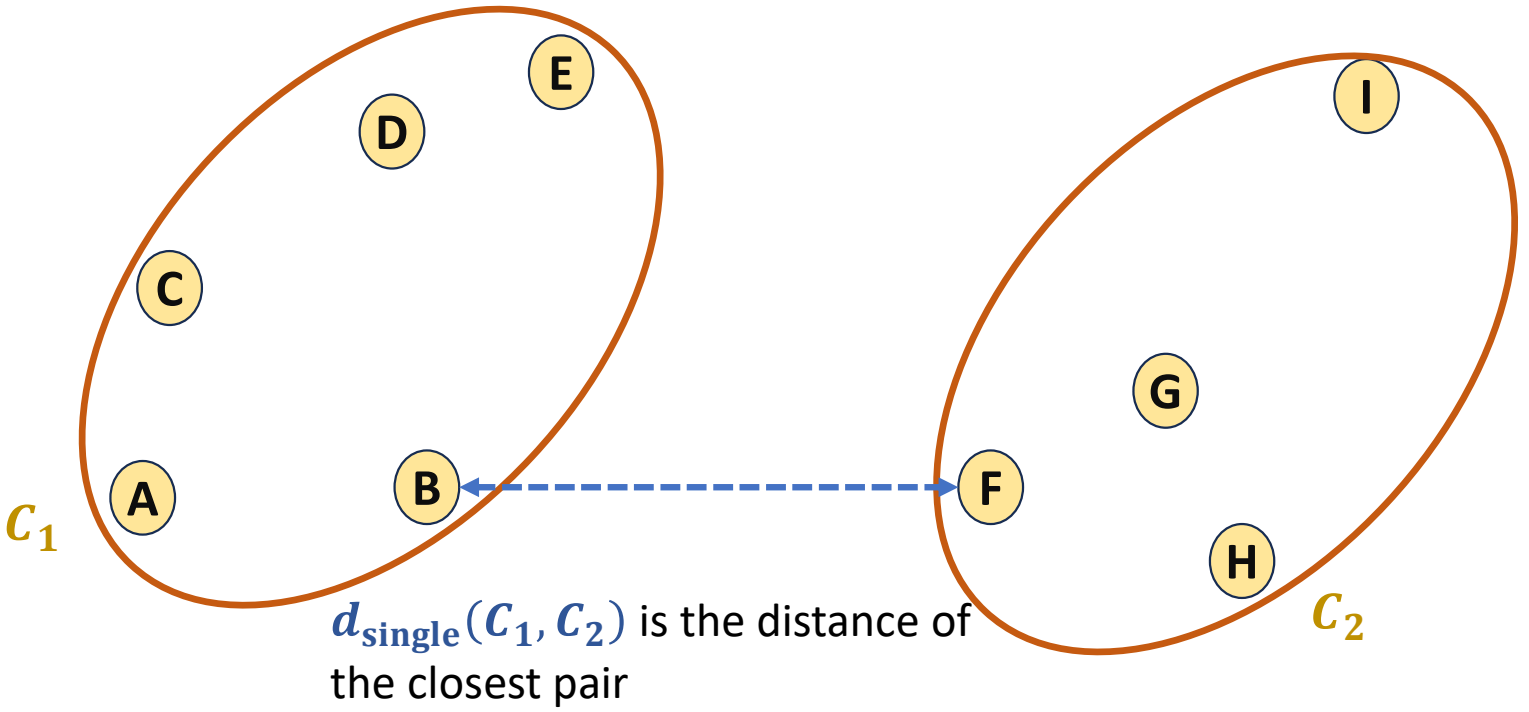
Agglomerative Clustering

- The agglomerative clustering is based on the measurement of the cluster similarity.
    - How do we measure distance between a cluster and a point?
    - How do we measure distance between the two clusters?
- The choice of how to measure distances between clusters is called the linkage.
- Linkage is a dissimilarity measure $\boldsymbol{d(C_i, C_j)}$, between two sets of clusters C_1 and C_2, telling us how different the points in these sets are.
- Different Types:
    - **Single Linkage**: Smallest of the distance between pairs of samples
    - **Complete Linkage**: Largest of the distance between pairs of samples
    - **Average Linkage**: Average of the distance between pairs of samples

Single Linkage

- Single linkage also known as nearest-neighbour linkage measures the dissimilarity between C_1 and C_2, by looking at the smallest dissimilarity between two points in C_1 and C_2.

$$d_{\text{single}}(C_1, C_2) = \min_{i \in C_1, j \in C_2} d(x_i, x_j)$$



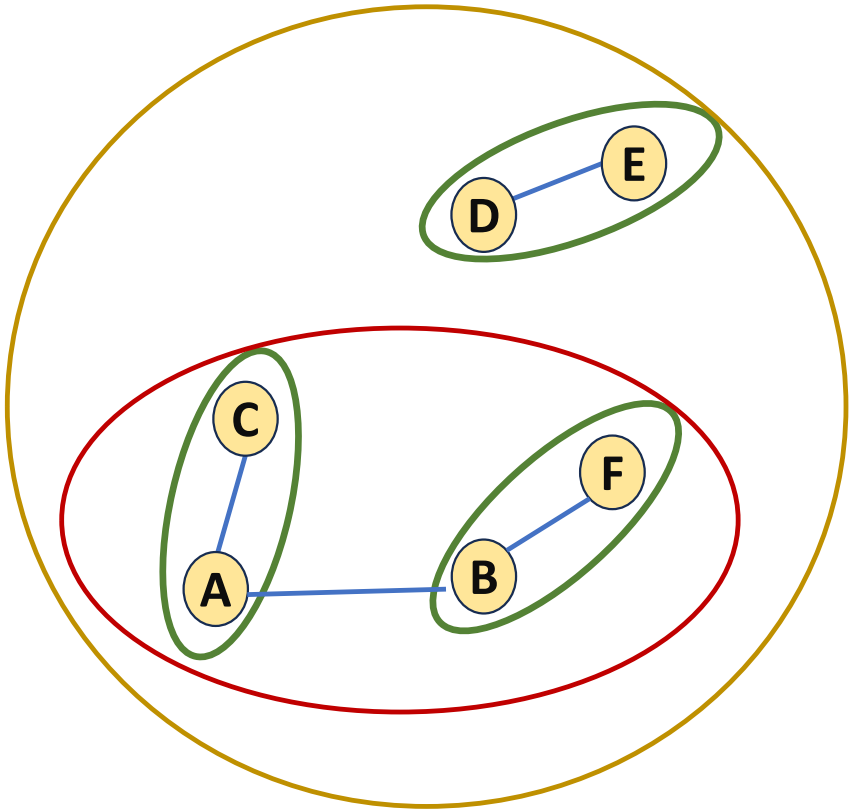
$d_{\text{single}}(C_1, C_2)$ is the distance of the closest pair

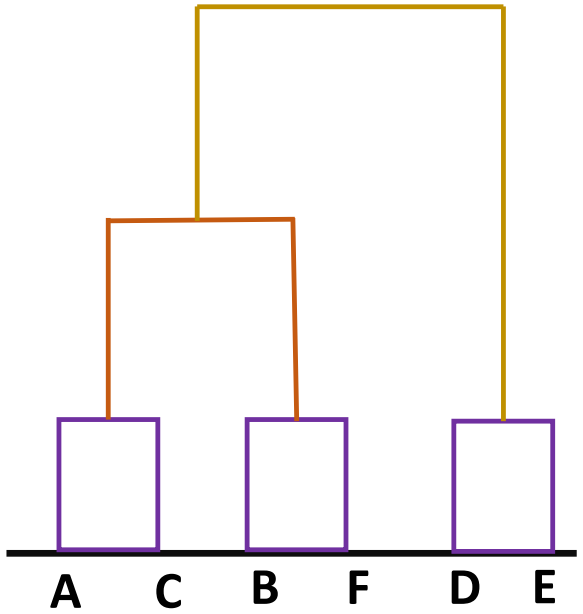
Pros: Can accurately handle non-elliptical shapes.

Cons:

- Sensitive to noise and outliers.
- May yield long extended clusters, with point in clusters being quite dissimilar [Chaining]

Single Linkage

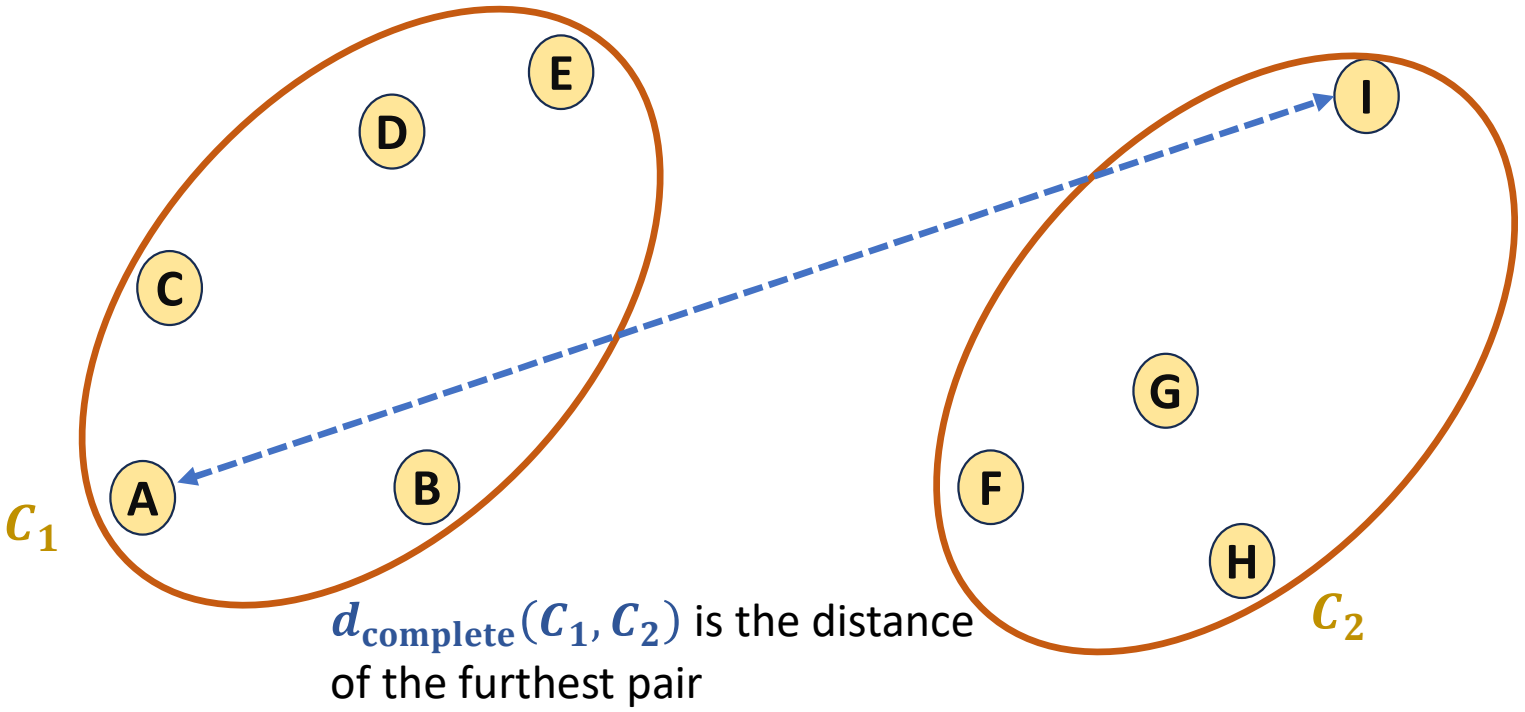




Complete Linkage

- Complete linkage also known as furthest-neighbour linkage measures the dissimilarity between C_1 and C_2, by looking at the largest dissimilarity between two points in C_1 and C_2.

$$d_{\text{complete}}(C_1, C_2) = \max_{i \in C_1, j \in C_2} d(x_i, x_j)$$

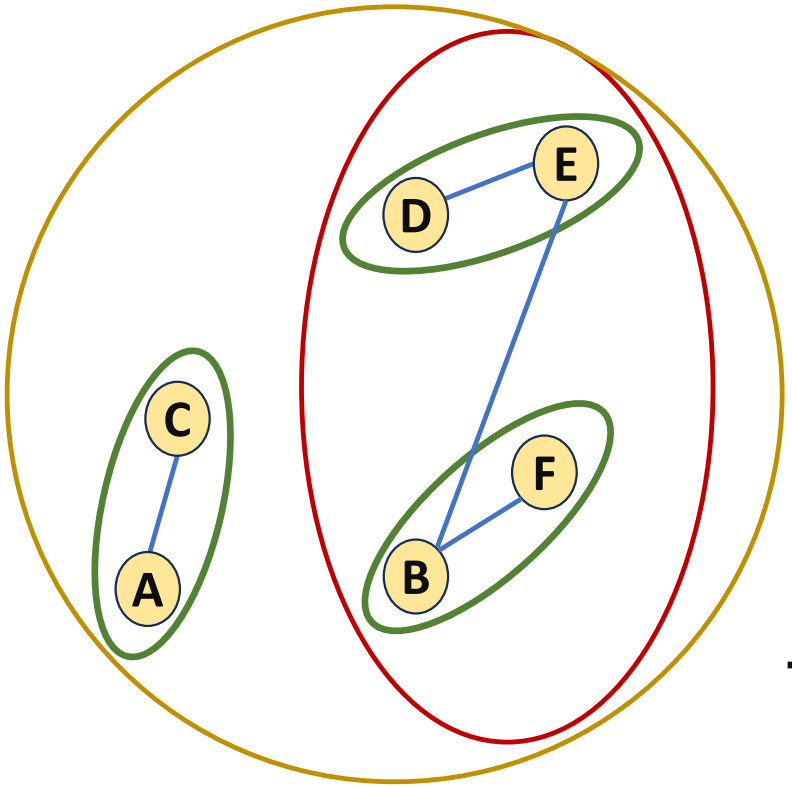


$d_{\text{complete}}(C_1, C_2)$ is the distance of the furthest pair

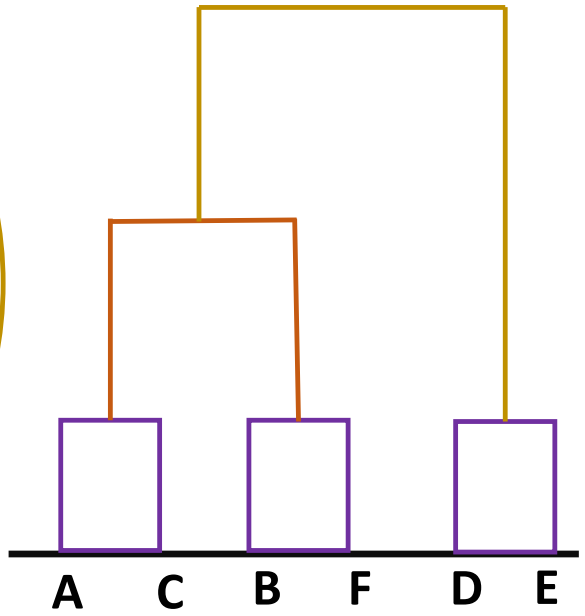
Pros: Less sensitive to noise and outliers.

Cons:
Points in one cluster may be closer to points in another cluster than to any of its own cluster [Crowding]

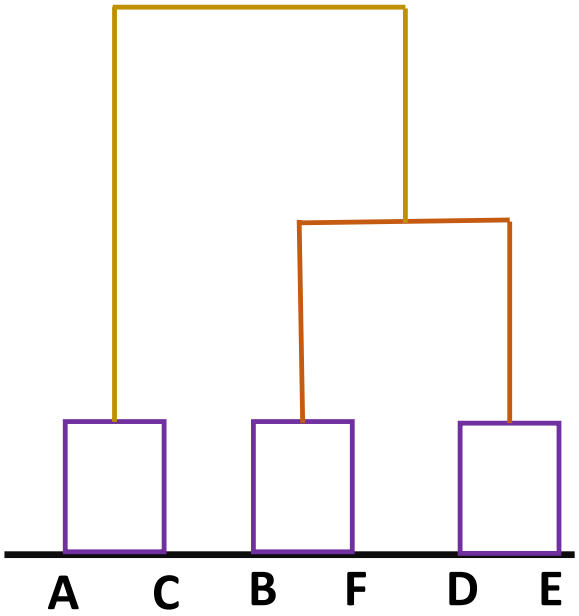
Complete Linkage



Note: The clustering is different depending on the linkage you choose.



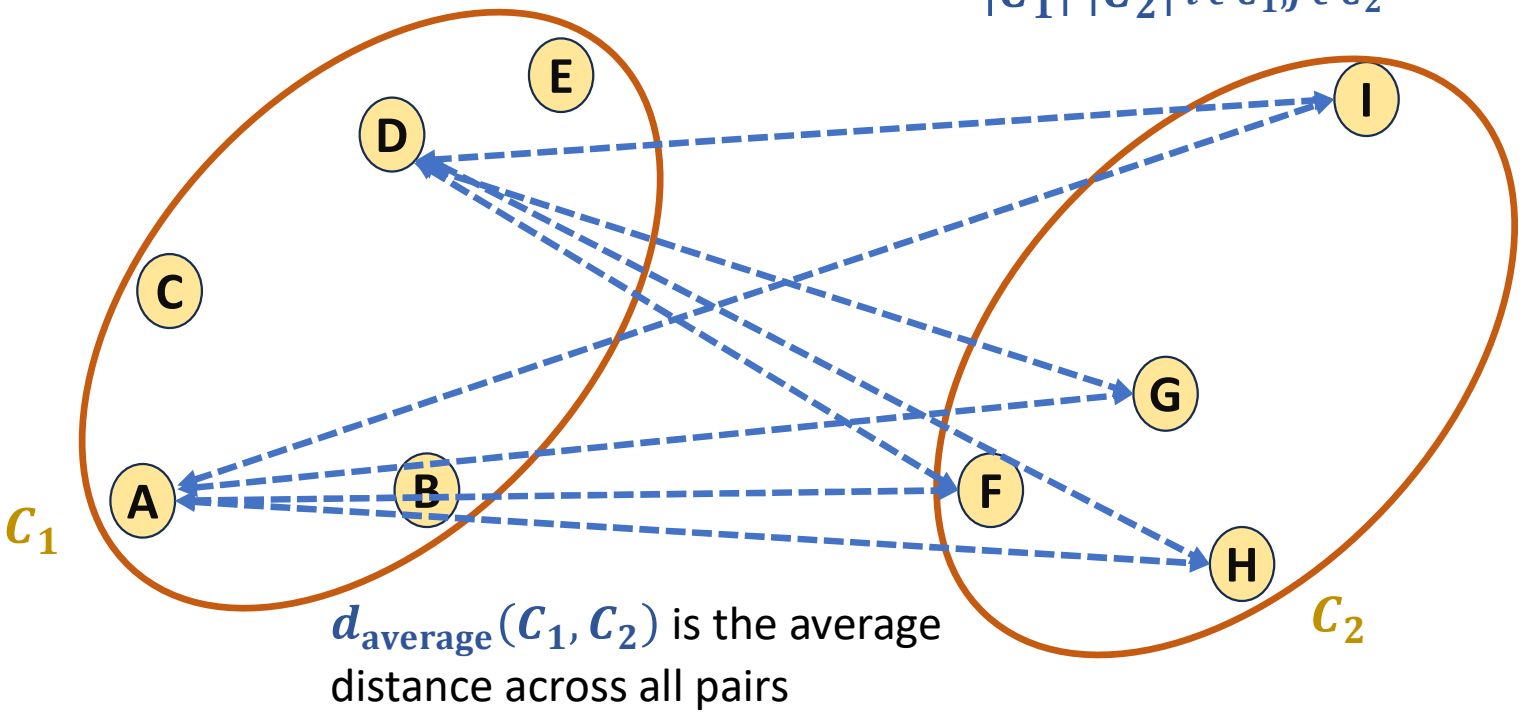
Single Linkage



Average Linkage

- In average linkage the dissimilarity between C_1 and C_2, is the average dissimilarity over all points in C_1 and C_2.

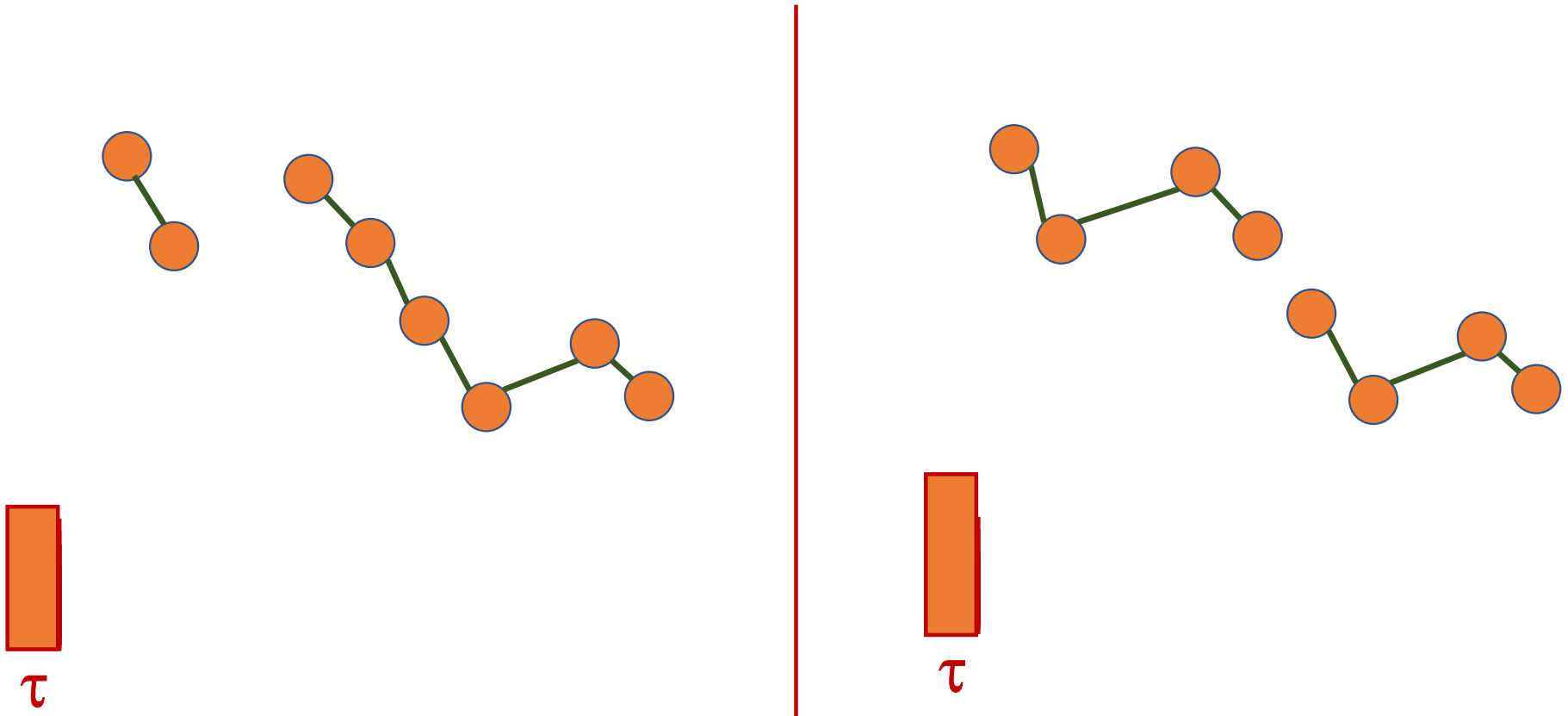
$$d_{\text{average}}(C_1, C_2) = \frac{1}{|C_1|\,|C_2|} \min_{i \in C_1, j \in C_2} d(x_i, x_j)$$



$d_{\text{average}}(C_1, C_2)$ is the average distance across all pairs

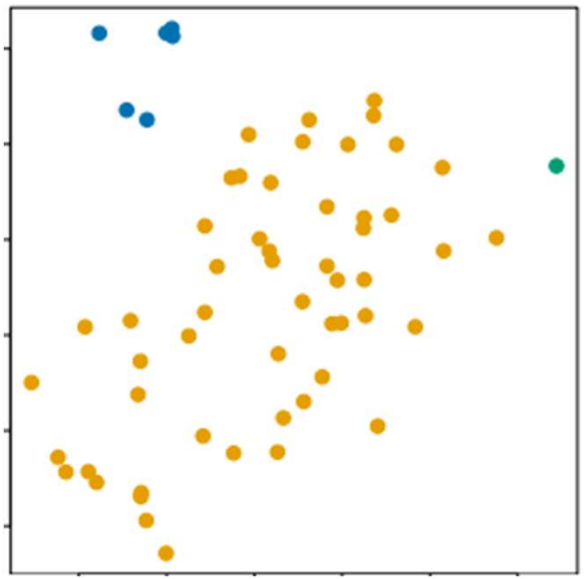
- Tries to strike a balance.
- Clusters tend to be relatively compact and relatively far apart.

Single-Link vs. Complete-Link Clustering

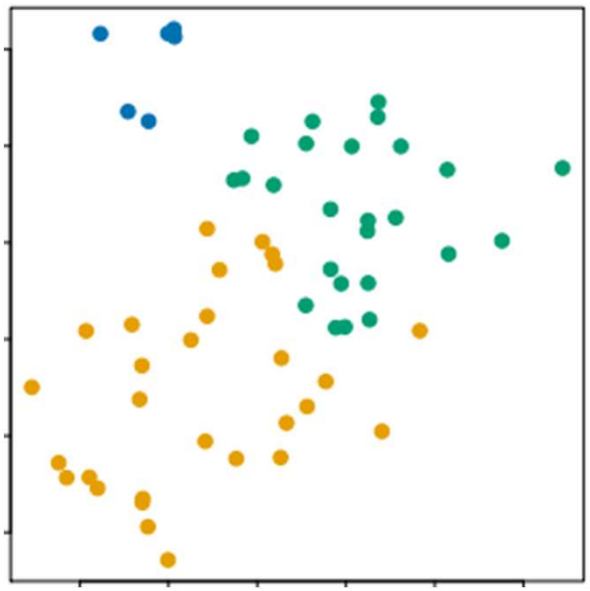


Example of Chaining and Crowding

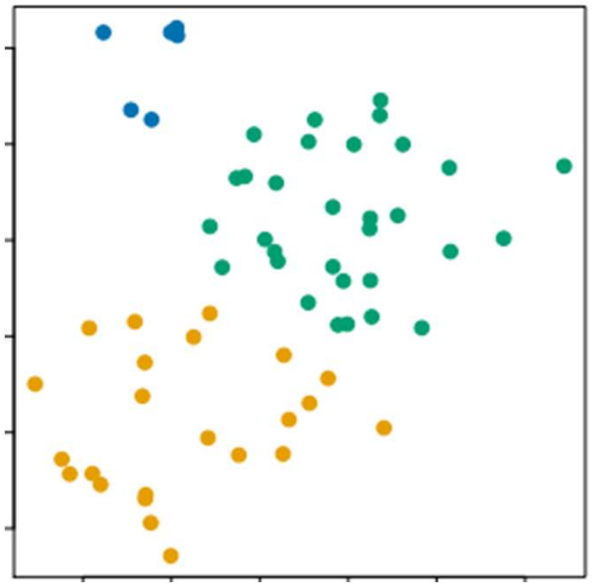
Single Linkage



Complete Linkage



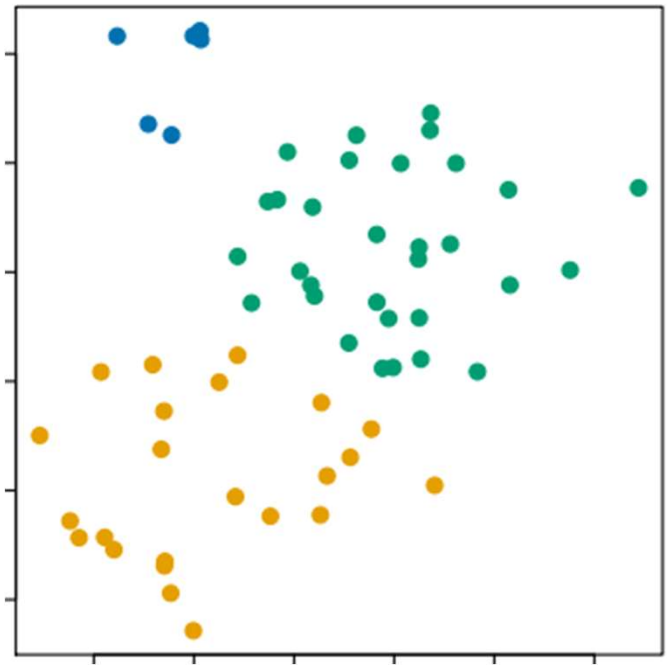
Average Linkage



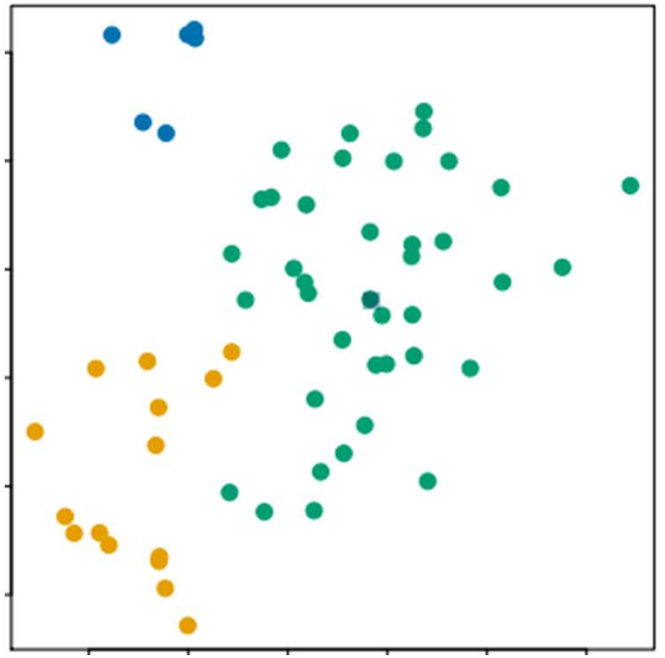
Single linkage reproduces long chain like clusters, while
Complete linkage strives to find compact clusters

Comments on Average Linkage

- The average linkage is not invariant to increasing or decreasing transformations of the dissimilarity matrix d



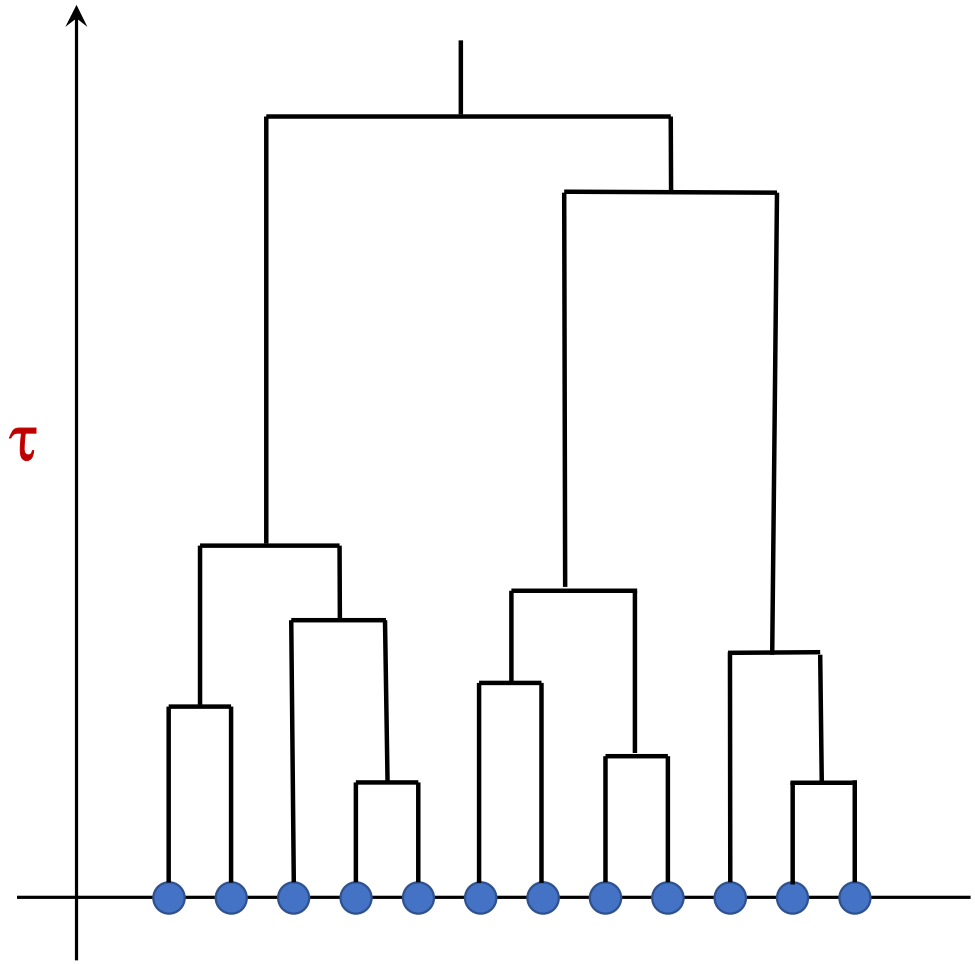
Euclidean Distance: $\mathrm{D} = \left(\left(x_i - x_j \right)^2 + \left(y_i - y_j \right)^2 \right)^{1/2}$



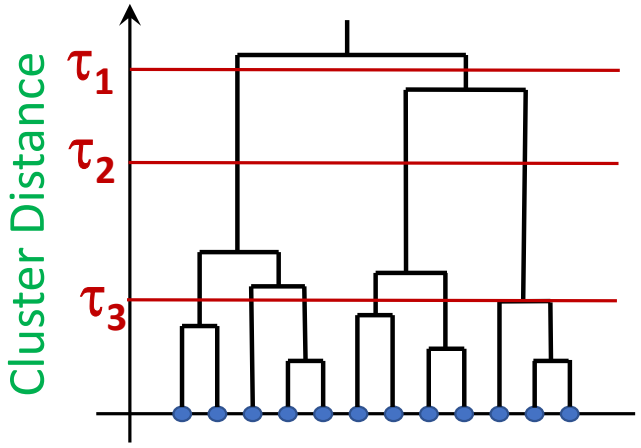
Euclidean Distance: $D^2 = \left(x_i - x_j \right)^2 + \left(y_i - y_j \right)^2$

Dendrograms: Visualizing the Clustering

- A 2-D diagram with all samples arranged along x-axis.
- y-axis represents the distance threshold τ.
- Each sample/cluster has a vertical line until the threshold τ at which they join.

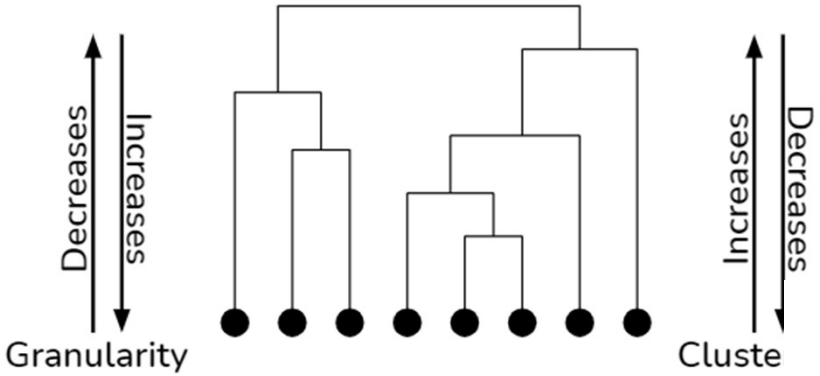


Dendrograms



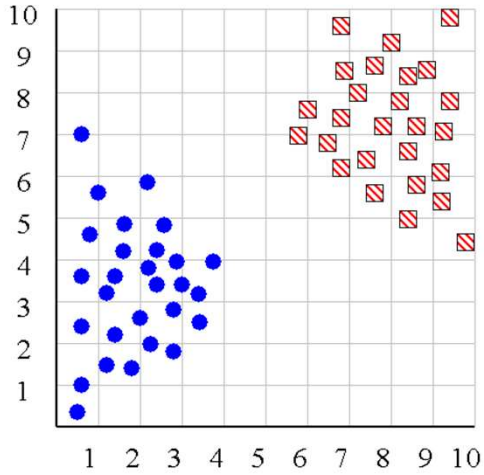
- Dendograms gives a visual representation of the whole hierarchical clustering process.
  - Allows the user to make the final decision
- Applicable irrespective of the dimensionality of the original samples
- One can create multiple clustering based on the choice of threshold
- Can be used with any distance metric and cluster distance measurement strategy (single, complete, average)
- Effective and intuitive cluster validity measure.

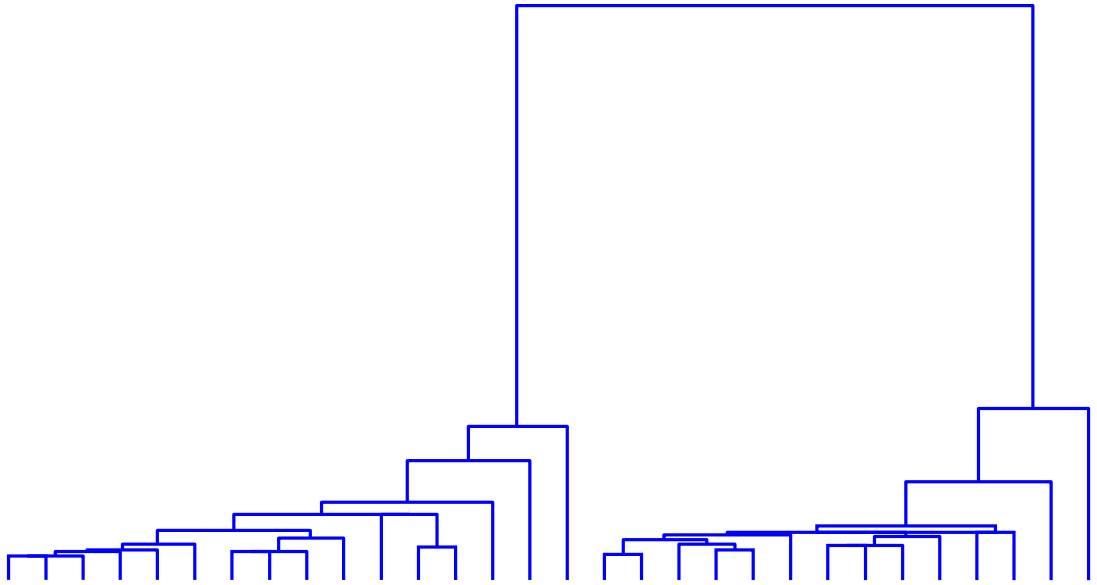
K measure from Dendrogram



Effect of granularity and cluster size while traversing in the dendrogram

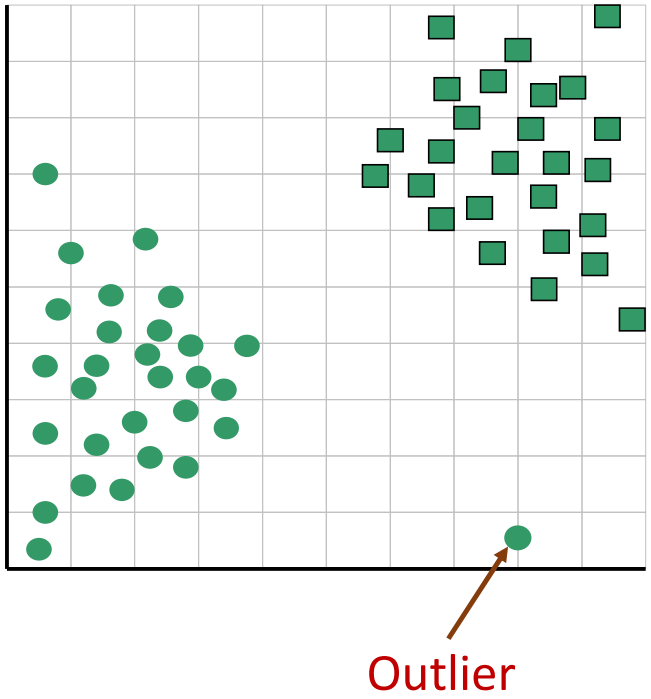
Image Source: https://towardsdatascience.com

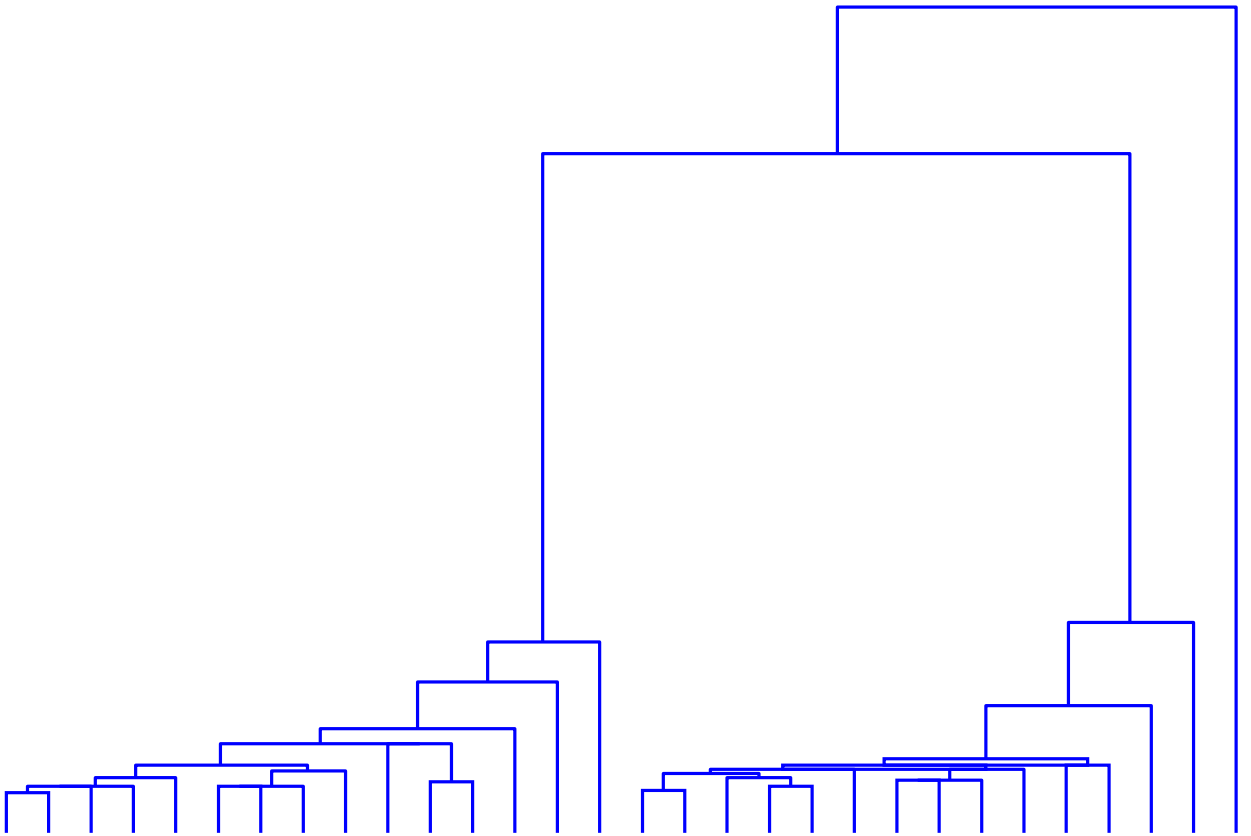




Outlier Detection With Dendrogram

The single isolated branch is suggestive of a data point that is very different to all others

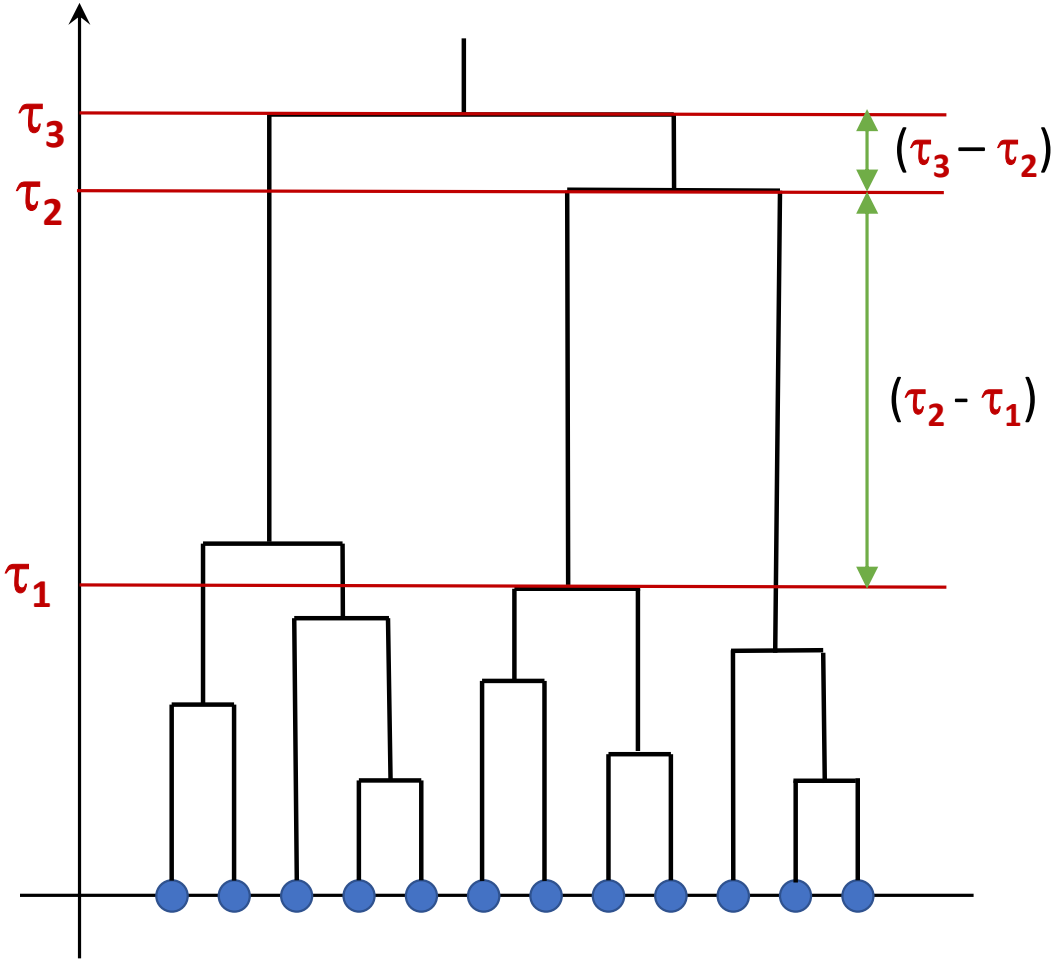




Based on slide by Eamonn Keogh

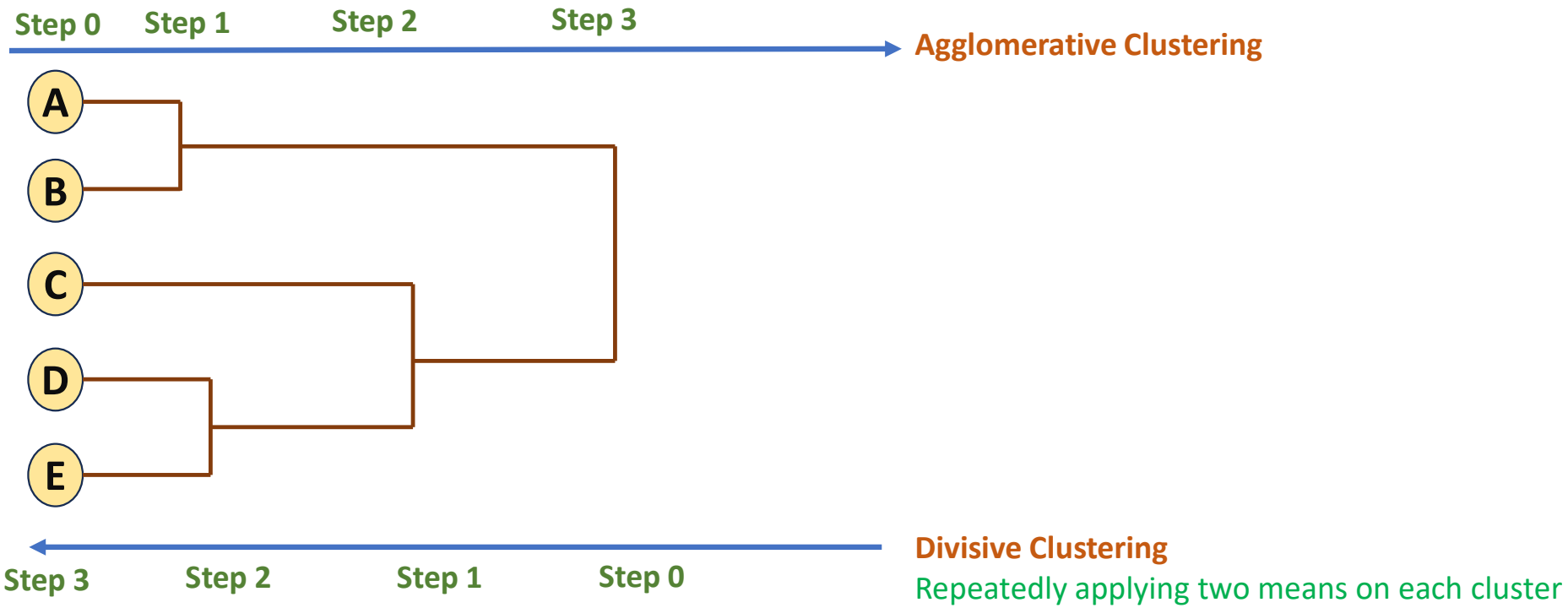
Lifetime and Cluster Validity

- Lifetime
  - The time ($\tau_2 - \tau_1$),from birth to death of a specific set of clusters
  - The interval of τ during which a specific clustering prevails
- Larger lifetime indicates that the clusters are stables over a larger range on distance threshold and hence more valid



Divisive Clustering

- Divisive Clustering groups data samples in a top-down fashion



Divisive Clustering

- Start with all data in one cluster

- Repeat until all clusters are singletons/until no dissimilarity remains between clusters

1) Choose one cluster C_k with the largest dissimilarity among its datapoints
   $C_k = \arg\max_{i \neq j} D_{ij}$
2) Divide the selected cluster into two subclusters using different splitting criteria, such as partitioning the cluster along the dimension that maximizes the inter-cluster dissimilarity or using clustering algorithms like K-means to partition the cluster.
3) Update the cluster structure by replacing the original cluster with the two newly formed subclusters.
4) Repeat steps 1-3 until a stopping criteria is met.

Agglomerative vs. Divisive

Agglomerative Clustering
Bottom-Up Approach
Computationally Efficient
Robustness to initialization
Ease of Interpretation
Chaining Effect
Sensitivity to distance metric

Divisive Clustering
Top-down Approach
Computationally Expensive
Sensitivity to Initialization
Potential for Global Optimum
Less Sensitive to Local Structure
Difficulty in Handling Noise

Hierarchical Clustering: Notes

- Generalizes the clustering process to a hierarchy of cluster labels, which is an inherent nature of the real-world
- We looked into a few basic, yet effective ones
  - Improvements: BIRCH (scalable), ROCK (categorical), CHAMELEON
- Cluster validity allows one to select a specific slice of the hierarchy of clusters
- The approaches need a distance/similarity function between a pair of samples (need not be a simple metric like Euclidean)
- Sensitive to outliers and distance metrics