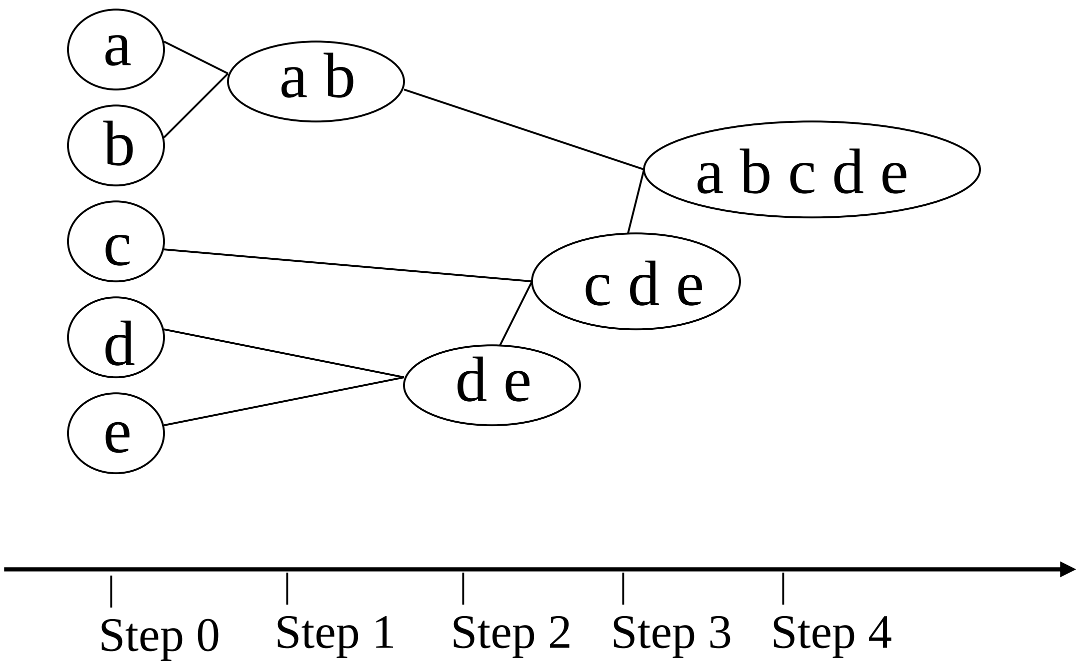
Hierarchical Clustering

- **Agglomerative approach**



bottom-up

Initialization:

Each object is a cluster

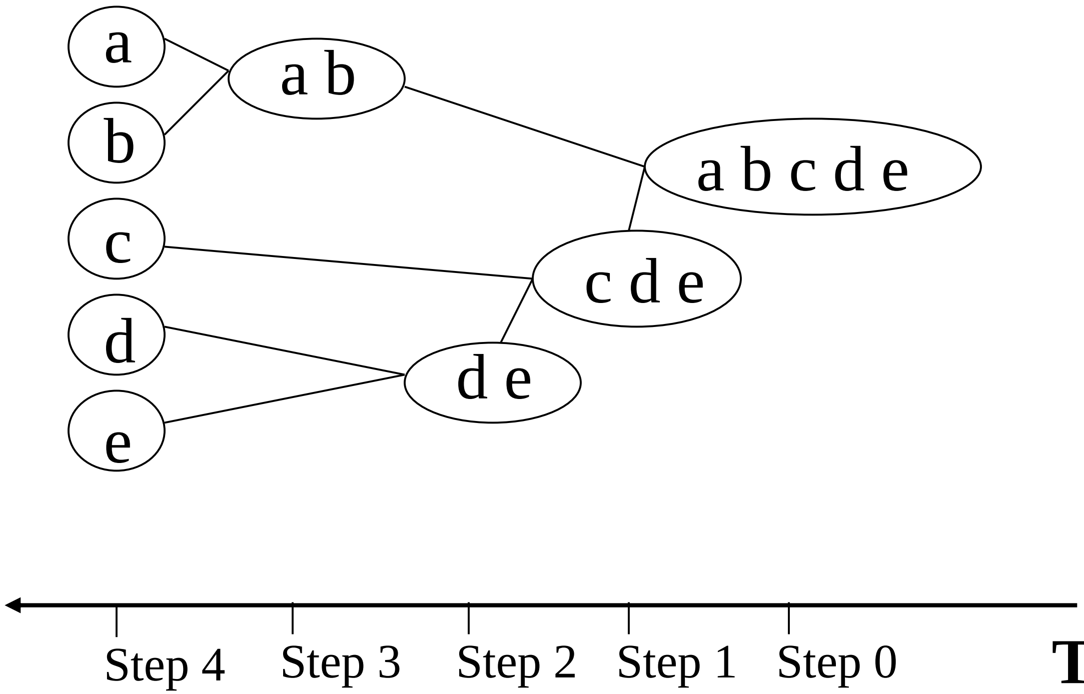
Iteration:

Merge two clusters which are most similar to each other;

Until all objects are merged into a single cluster

Hierarchical Clustering

Divisive Approaches



Top-down

Initialization:

All objects stay in one cluster

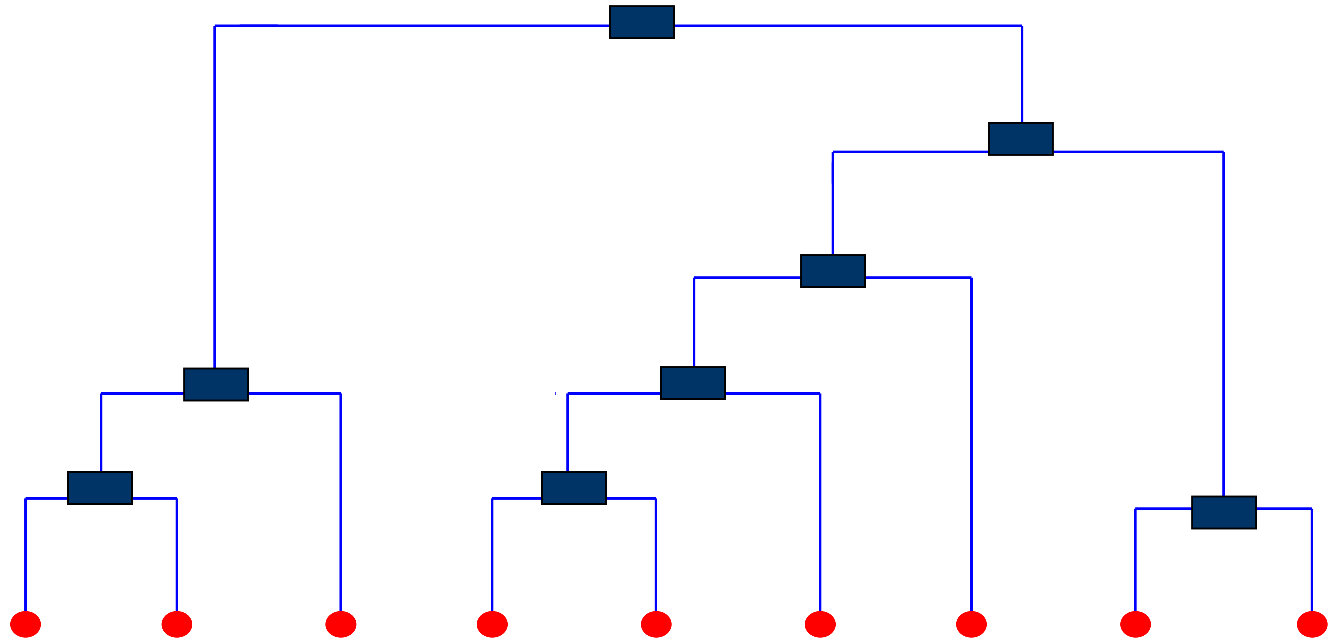
Iteration:

Select a cluster and split it into two sub clusters

Until each leaf cluster contains only one object

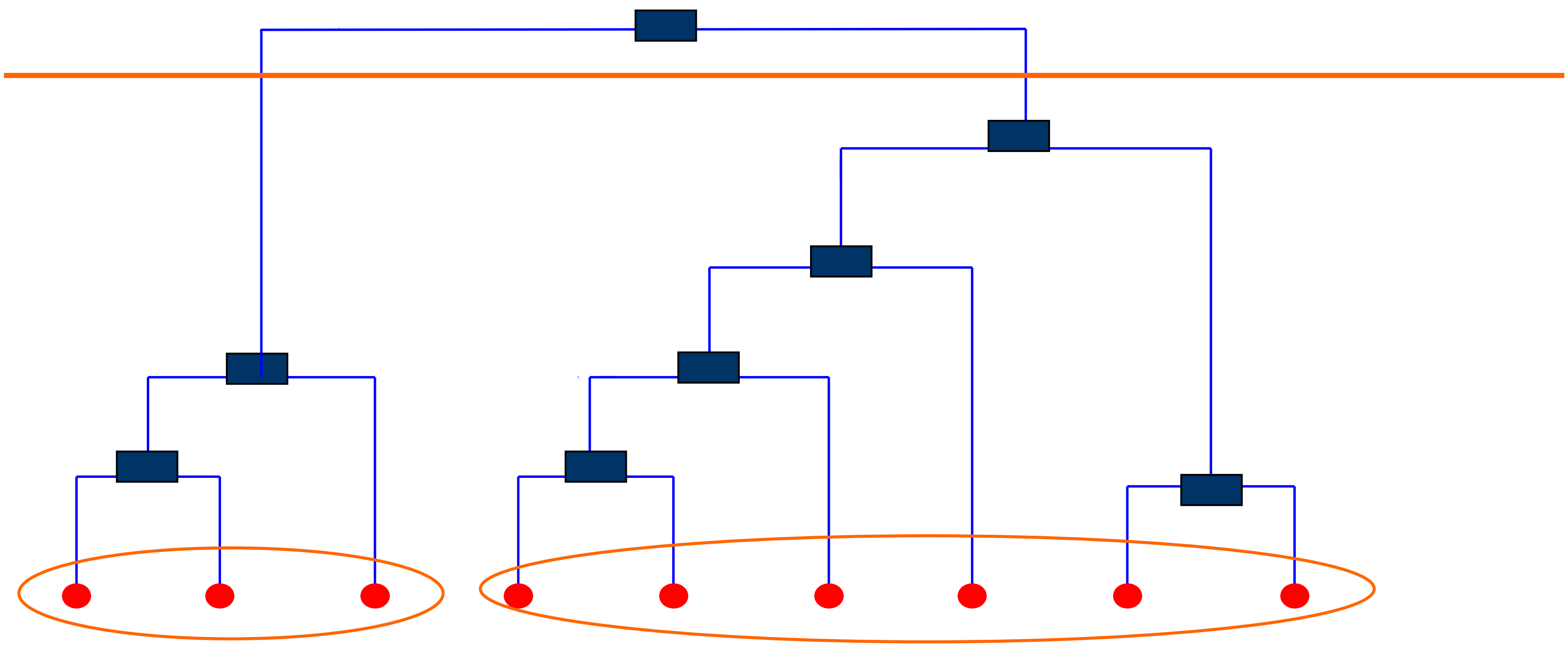
Dendrogram

- A binary tree that shows how clusters are merged/split hierarchically
- Each node on the tree is a cluster; each leaf node is a singleton cluster



Dendrogram

- **A clustering of the data objects is obtained by cutting the *dendrogram* at the desired level, then each connected component forms a cluster**



Dendrogram

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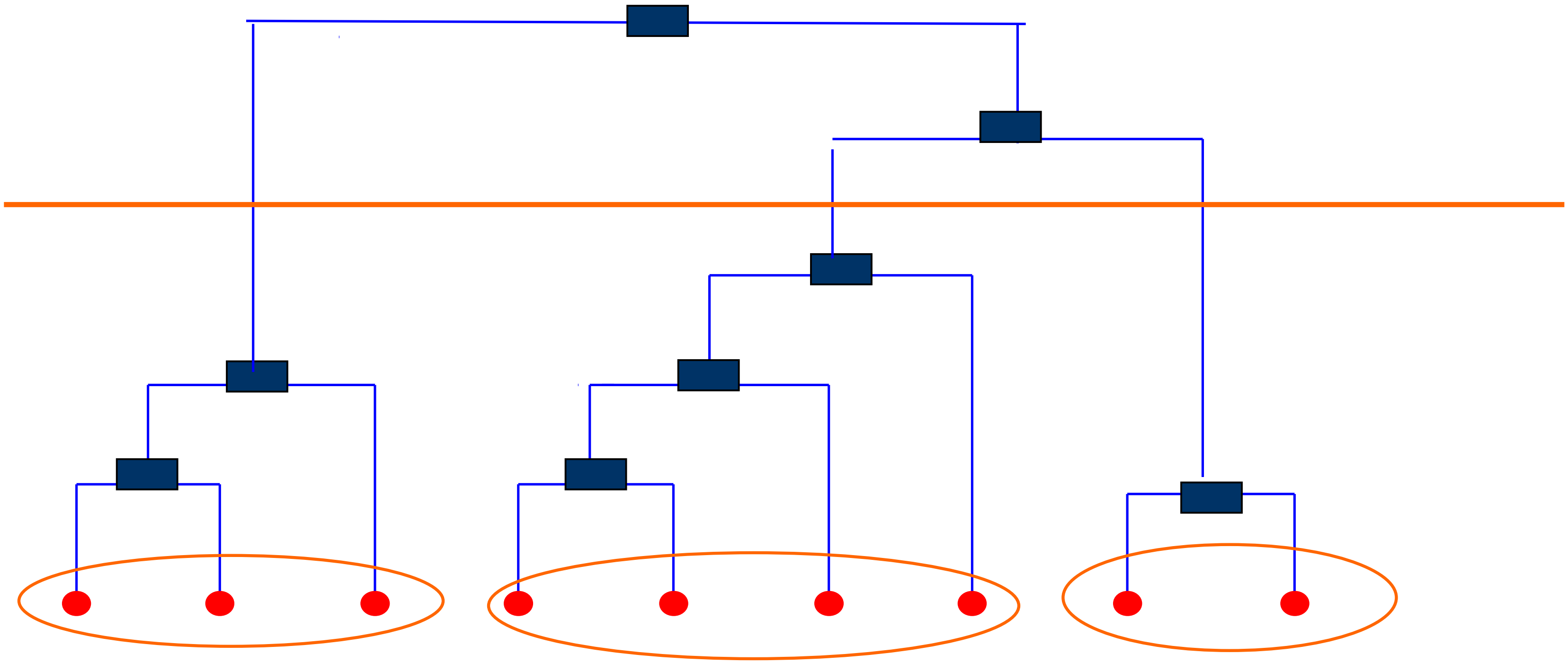
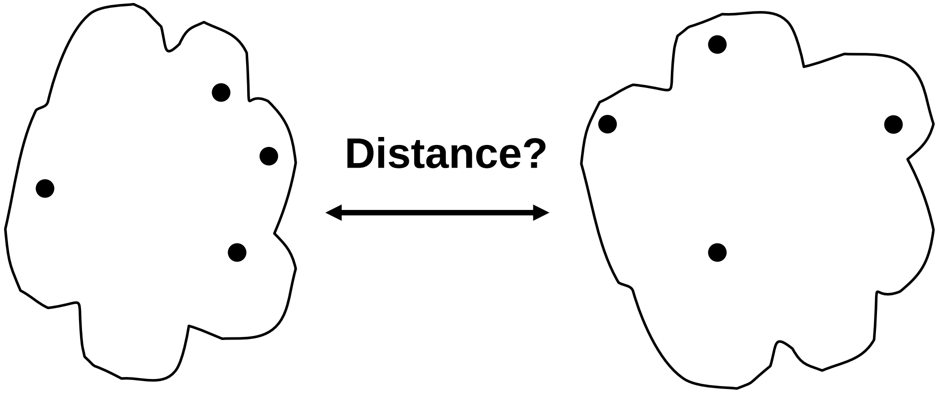


How to Merge Clusters?

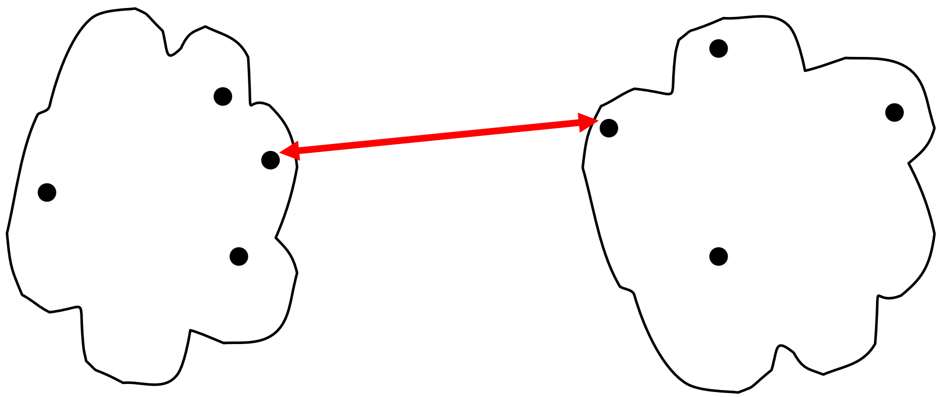
- How to measure the distance between clusters?

  - Single-link
  - Complete-link
  - Average-link
  - Centroid distance



Hint: ***Distance between clusters*** is usually defined on the basis of ***distance between objects.***

How to Define Inter-Cluster Distance

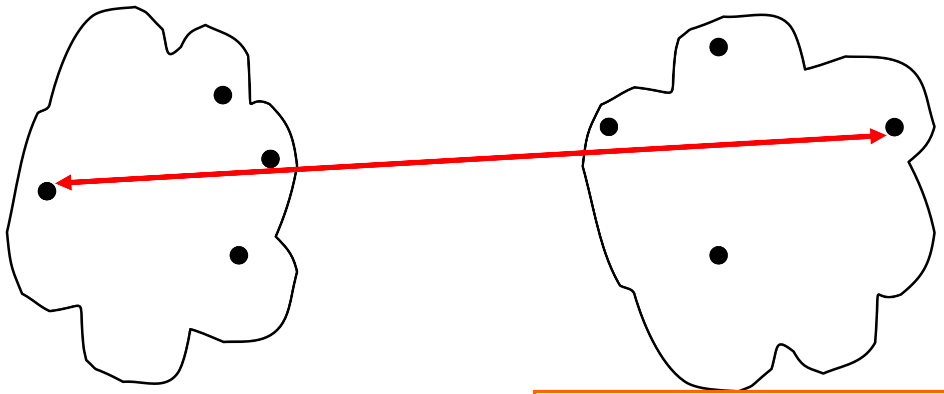


- Single-link
- Complete-link
- Average-link
- Centroid distance

$$\boxed{d_{\min}(C_i, C_j) = \min_{p \in C_i, q \in C_j} d(p, q)}$$

The distance between two clusters is represented by the distance of the ***closest pair of data objects*** belonging to different clusters.

How to Define Inter-Cluster Distance

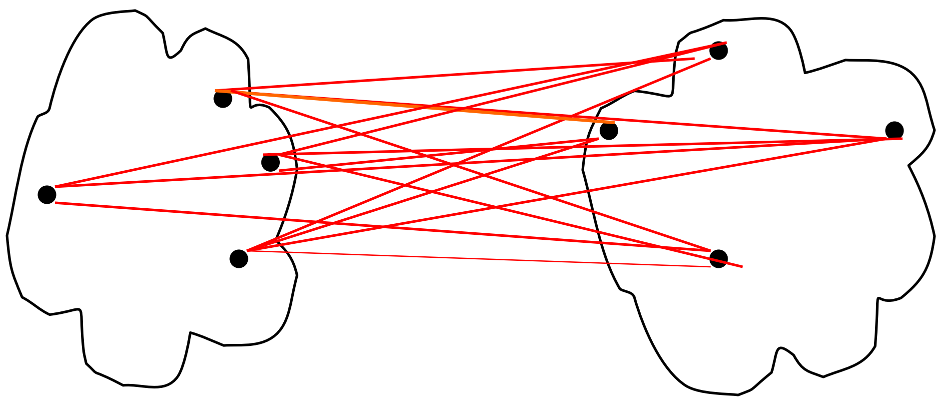


- Single-link
- Complete-link
- Average-link
- Centroid distance

$$d_{\min}(C_i, C_j) = \max_{p \in C_i, q \in C_j} d(p, q)$$

The distance between two clusters is represented by the distance of the ***farthest pair of data objects*** belonging to different clusters.

How to Define Inter-Cluster Distance

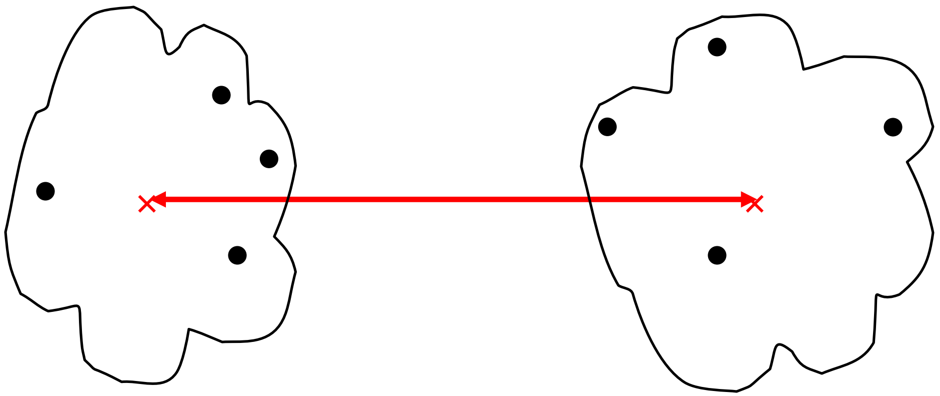


- Single-link
- Complete-link
- Average-link
- Centroid distance

$$d_{\min}(C_i, C_j) = \underset{p \in C_i, q \in C_j}{avg} d(p,q)$$

The distance between two clusters is represented by the ***average*** distance of ***all pairs of data objects*** belonging to different clusters.

How to Define Inter-Cluster Distance



m_i,m_j are the means of C_i, C_j,

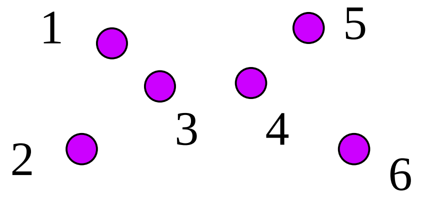
- Single-link
- Complete-link
- Average-link
- Centroid distance

$$d_{mean}(C_i, C_j) = d(m_i, m_j)$$

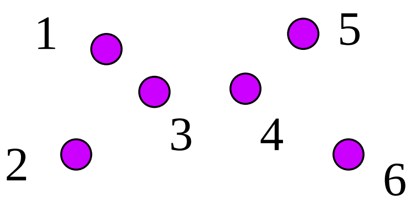
The distance between two clusters is represented by the distance between ***the means of the cluters.***

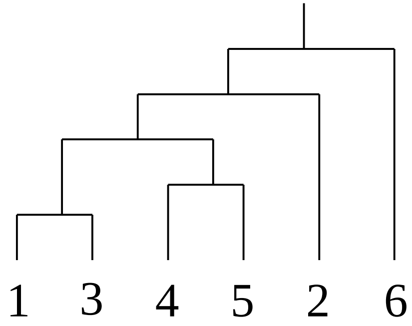
An Example of the Agglomerative Hierarchical Clustering Algorithm

- For the following data set, we will get different clustering results with the single-link and complete-link algorithms.

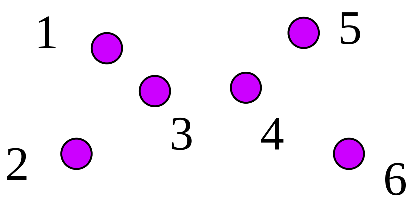


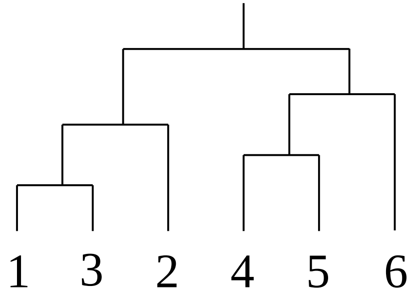
Result of the Single-Link algorithm





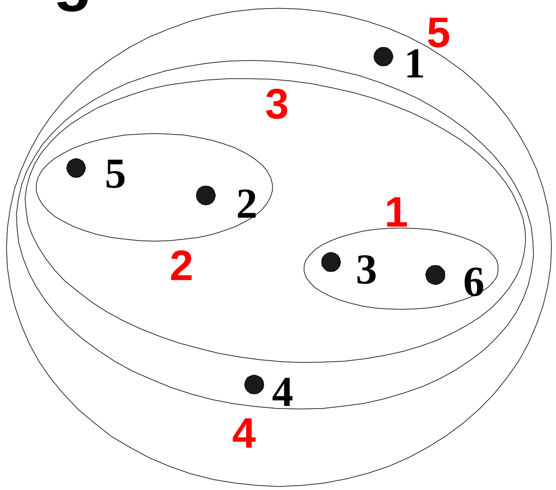
Result of the Complete-Link algorithm



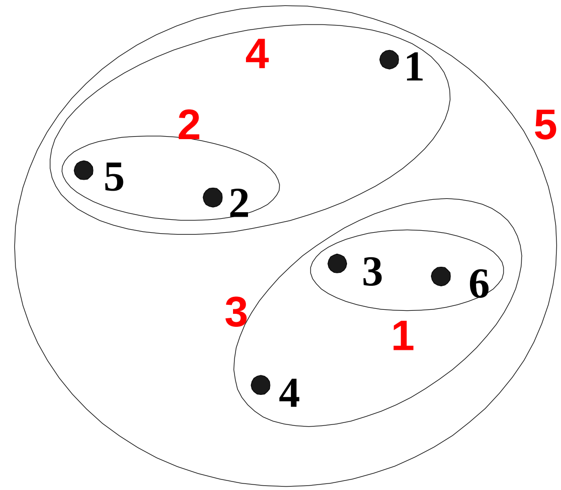


Hierarchical Clustering: Comparison

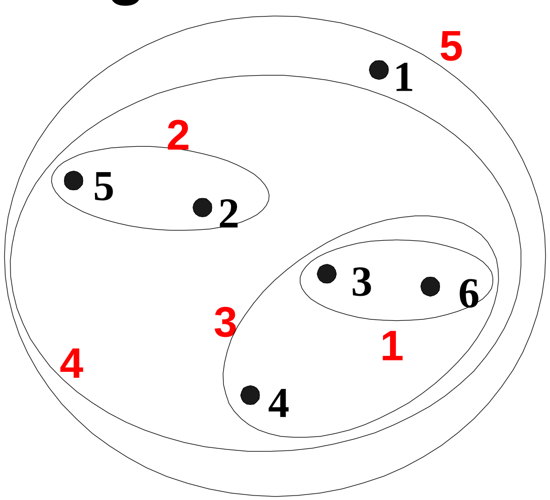
Single-link



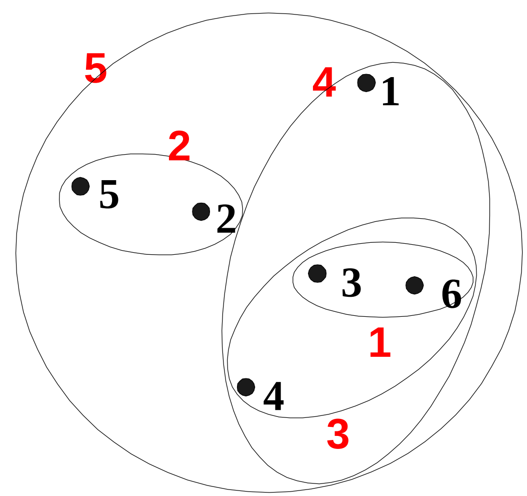
Complete-link



Average-link

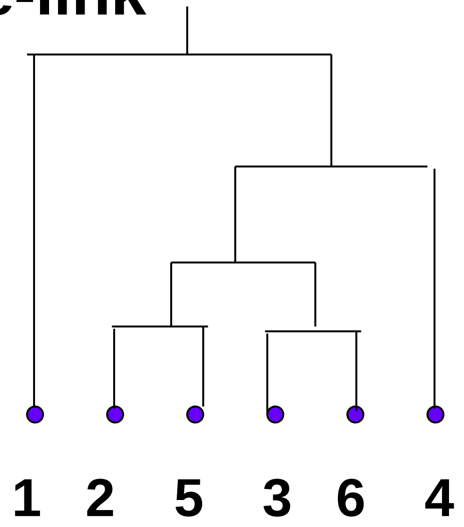


Centroid distance

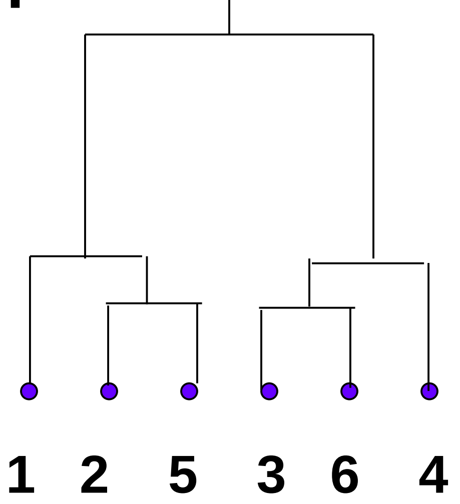


Compare Dendrograms

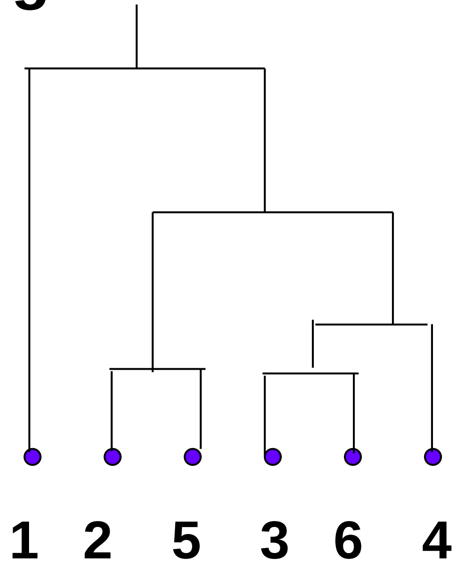
Single-link



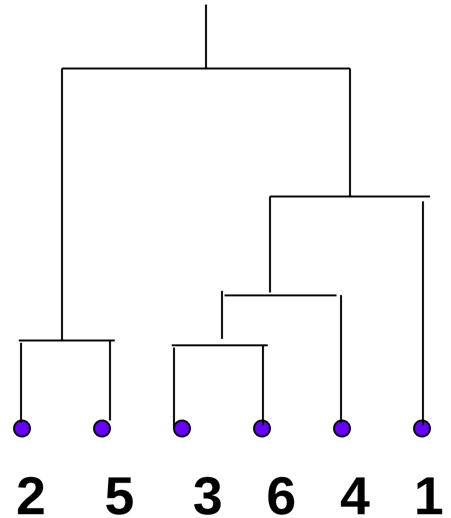
Complete-link



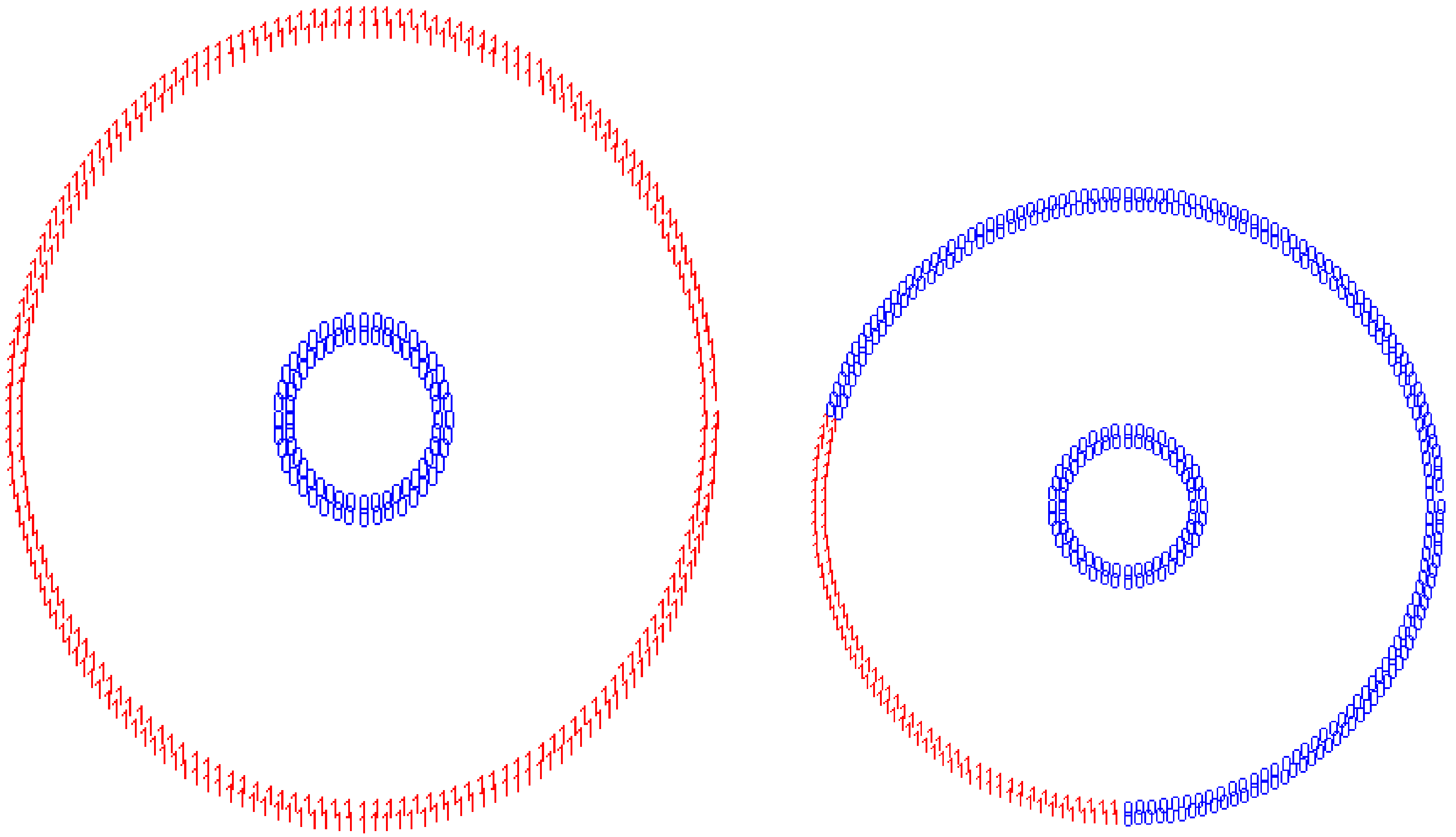
Average-link



Centroid distance

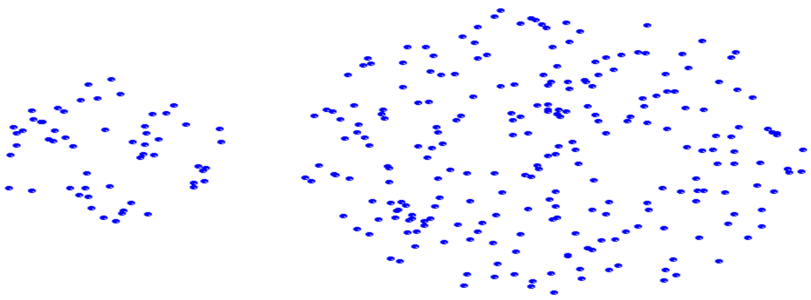


Effect of Bias towards Spherical Clusters

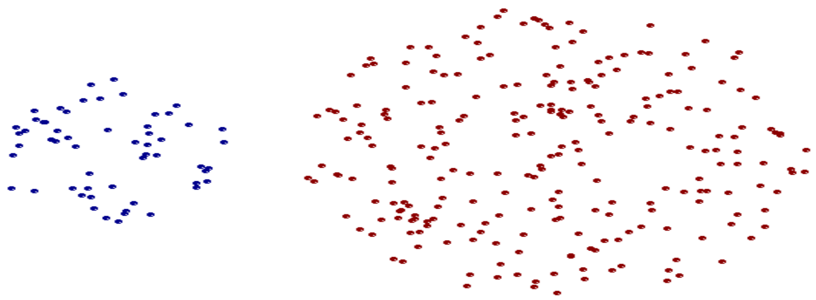


Single-link (2 clusters) Complete-link (2 clusters)

Strength of Single-link



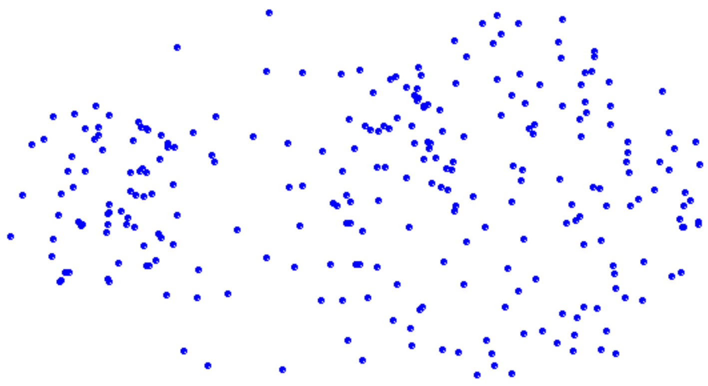
Original Points



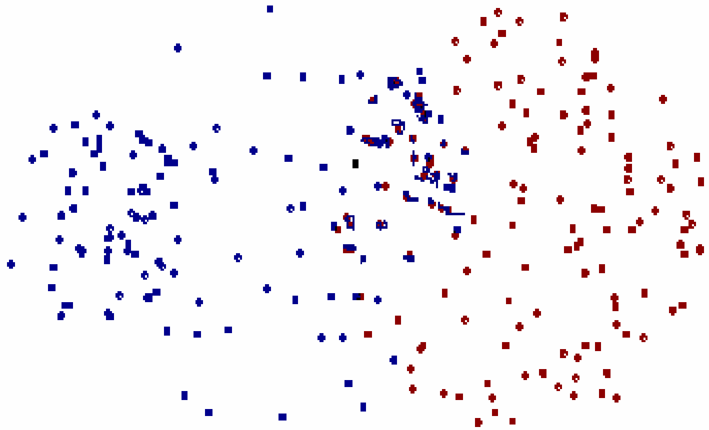
Two Clusters

- **Can handle non-global shapes**

Limitations of Single-Link



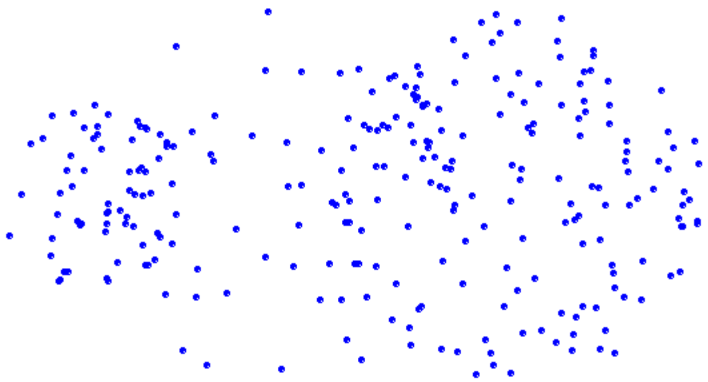
Original Points



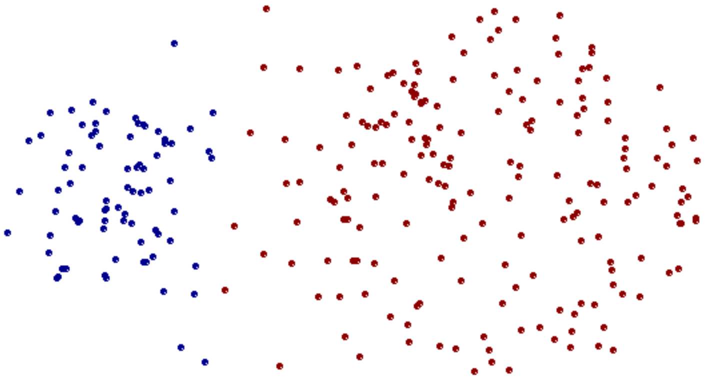
Two Clusters

- Sensitive to noise and outliers

Strength of Complete-link



Original Points



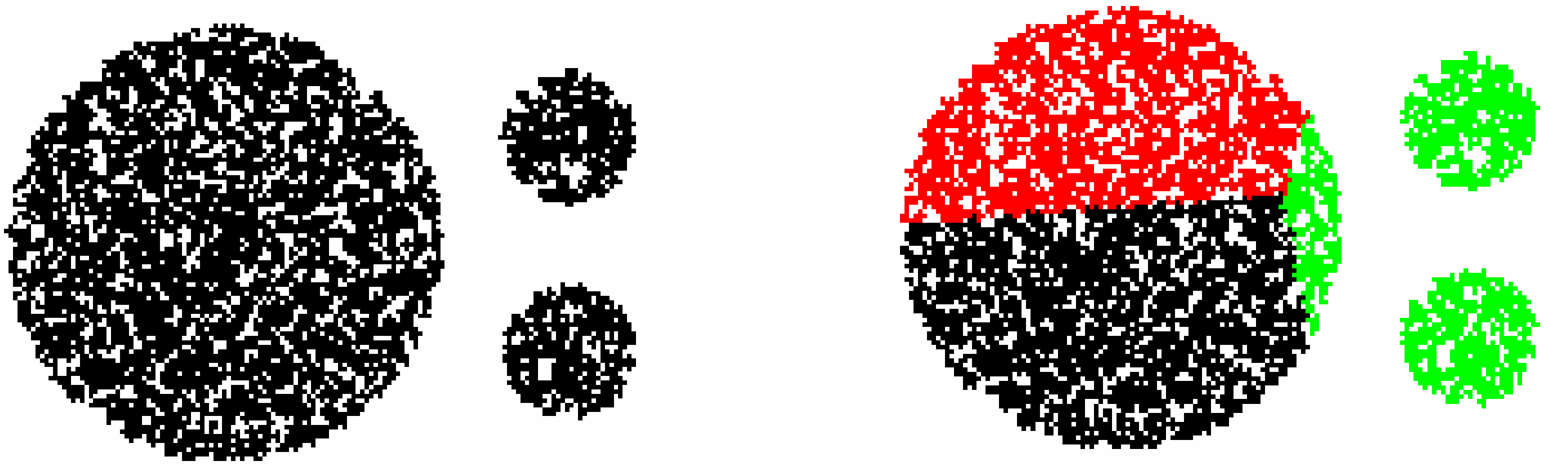
Two Clusters

- Less susceptible to noise and outliers

Which Distance Measure is Better?

- Each method has both advantages and disadvantages; application-dependent, single-link and complete-link are the most common methods
- Single-link
  - Can find irregular-shaped clusters
  - Sensitive to outliers, suffers the so-called chaining effects
- Complete-link, Average-link, and Centroid distance
  - Robust to outliers
  - Tend to break large clusters
  - Prefer spherical clusters

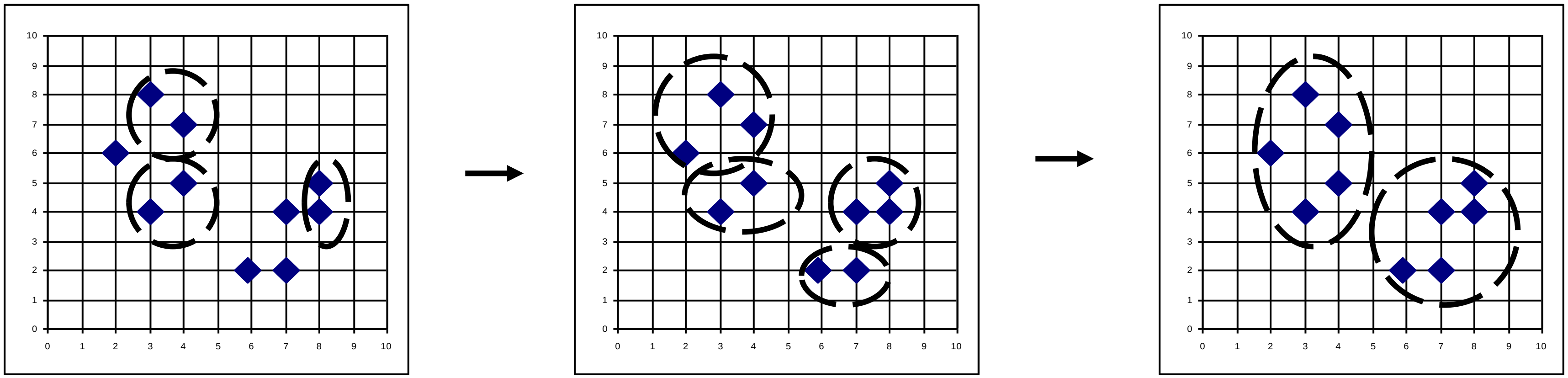
Limitation of Complete-Link, Average-Link, and Centroid Distance



- **The complete-link, average-link, or centroid distance method tend to break the large cluster.**

AGNES (Agglomerative Nesting)

- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical analysis packages; e.g., S+
- Use *single-link method*
- Merge nodes that have *the least* dissimilarity
- Eventually all objects belong to the same cluster

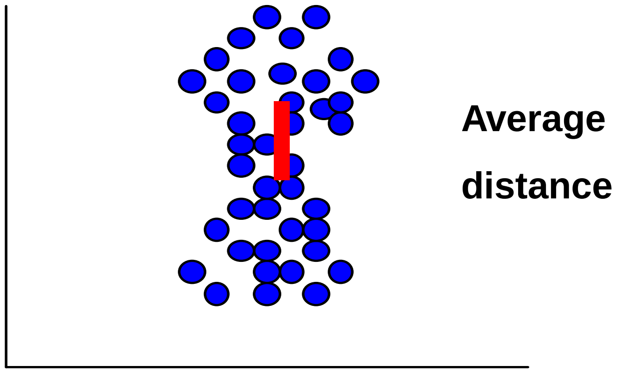


UPGMA

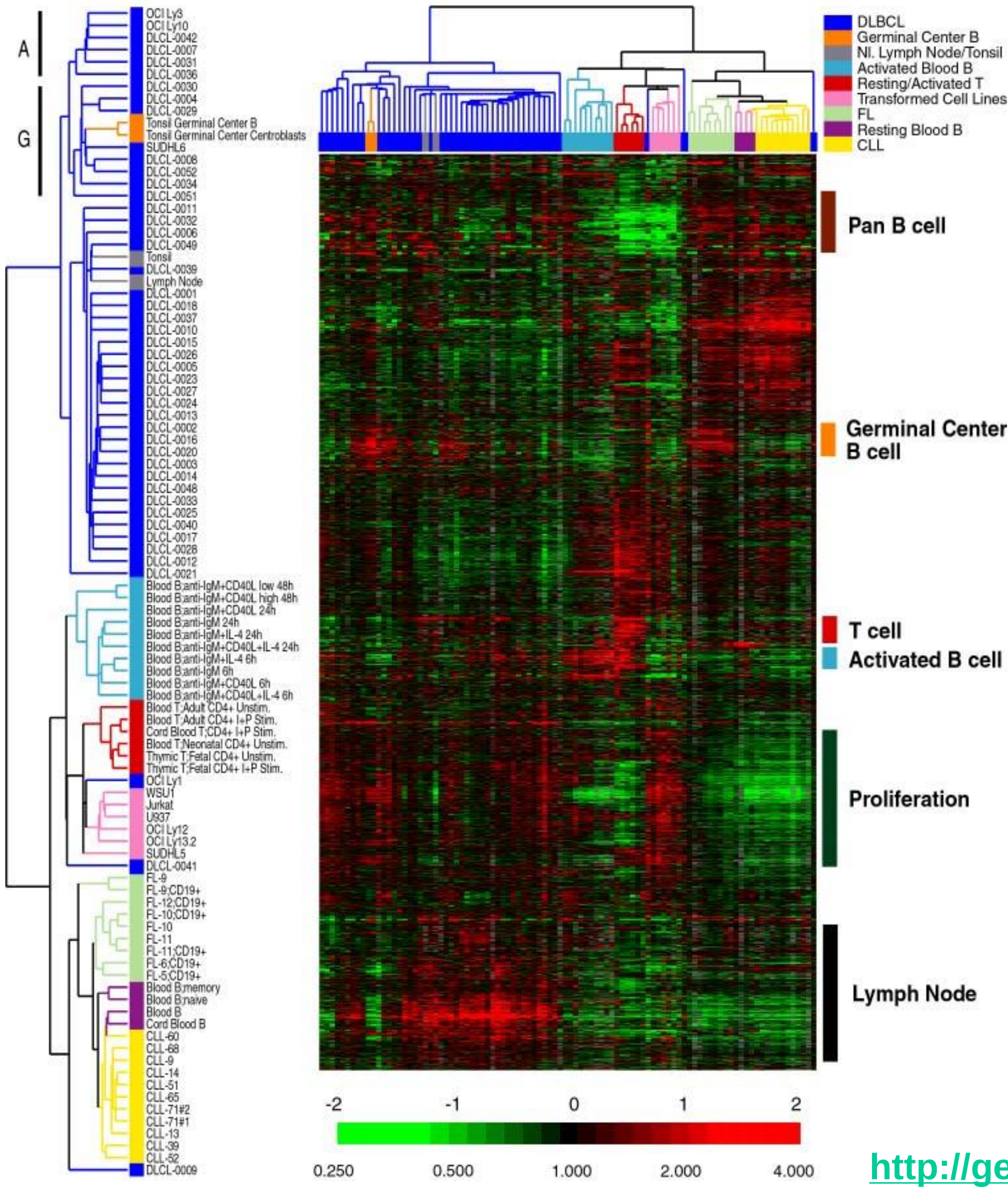
- **UPGMA: Unweighted Pair-Group Method Average.**
- **Merge Strategy:**
  - **Average-link approach;**
  - **The distance between two clusters is measured by the average distance between two objects belonging to different clusters.**

$$d_{avg}(C_i, C_j) = \frac{1}{n_i n_j} \sum_{p \in C_i} \sum_{q \in C_j} d(p, q)$$

n_i,n_j: the number of objects in cluster C_i, C_j.



TreeView



- ❑UPGMA
- ❑ Order the objects
- ❑ The color intensity represents expression level.
- ❑ A large patch of similar color indicates a cluster.

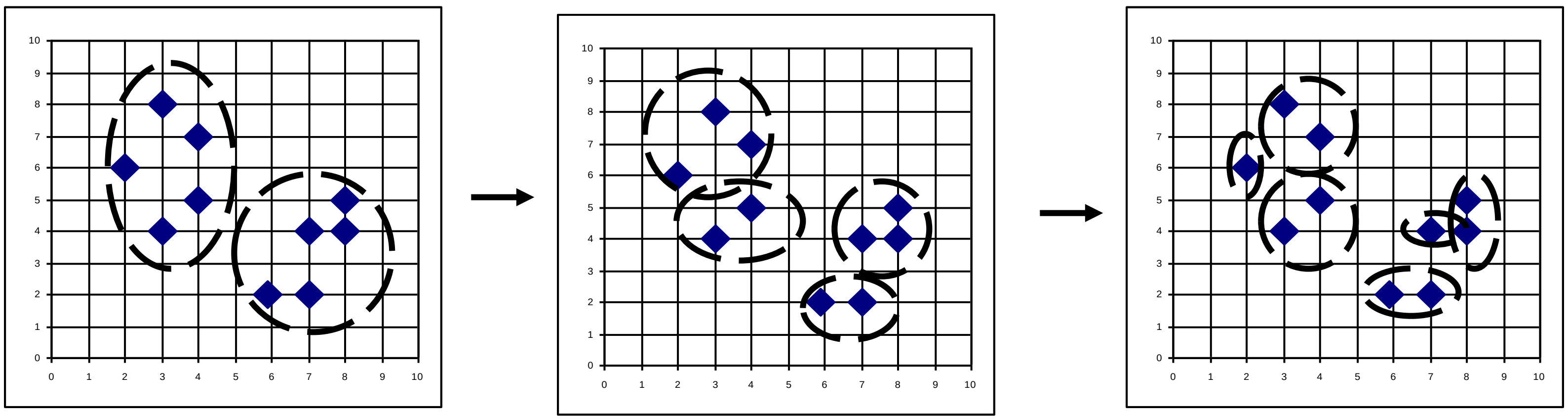
Eisen MB et al. Cluster Analysis and Display of Genome-Wide Expression Patterns. *Proc Natl Acad Sci U S A* 95, 14863-8.

http://rana.lbl.gov/EisenSoftware.htm

http://genome-www.stanford.edu/serum/fig2cluster.html

DIANA (Divisive Analysis)

- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical analysis packages, e.g., S+
- Inverse order of AGNES
- Eventually each node forms a cluster on its own



DIANA- Explored

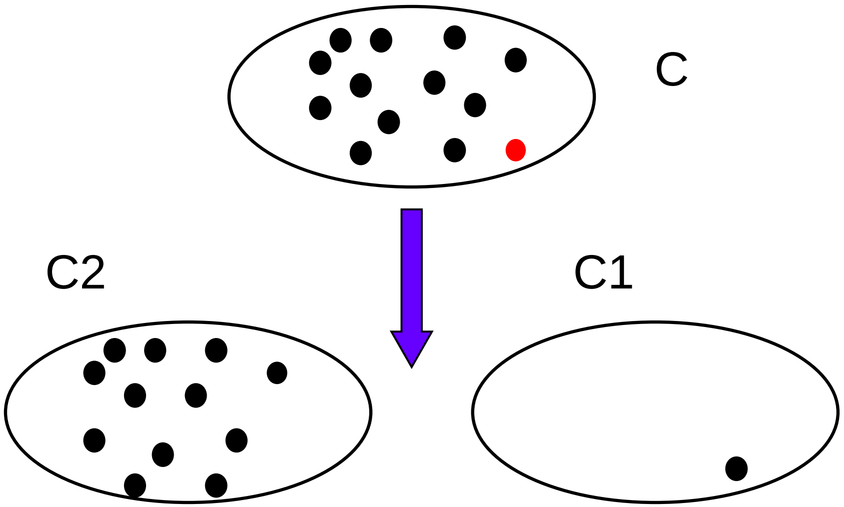
- First, all of the objects form one cluster.
- The cluster is split according to some principle, such as the minimum Euclidean distance between the closest neighboring objects in the cluster.
- The cluster splitting process repeats until, eventually, each new cluster contains a single object or a termination condition is met.

Splitting Process of DIANA

Intialization:

1. **Choose the object O_h which is most dissimilar to other objects in C.**

2. Let C1={O_h}, C2=C-C1.



Splitting Process of DIANA (Cont'd)

Iteration:

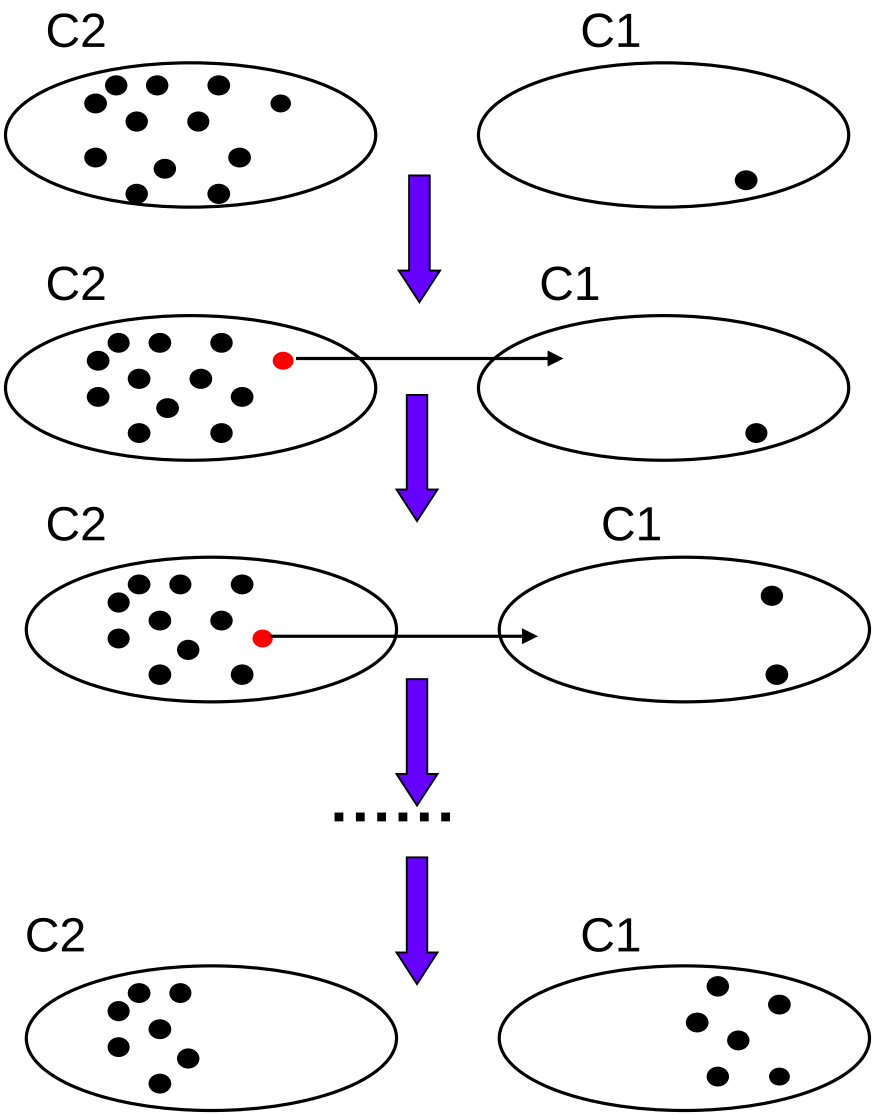
3. For each object Oi in C2, tell whether it is more close to C1 or to other objects in C2

$$D_i = \underset{j \in C_2}{avg}\, d(O_i, O_j) - \underset{j \in C_1}{avg}\, d(O_i, O_j)$$

4. Choose the object O_k with greatest D score.

5. If D_k>0, move Ok from C2 to C1, and repeat 3-5.

6. Otherwise, stop splitting process.



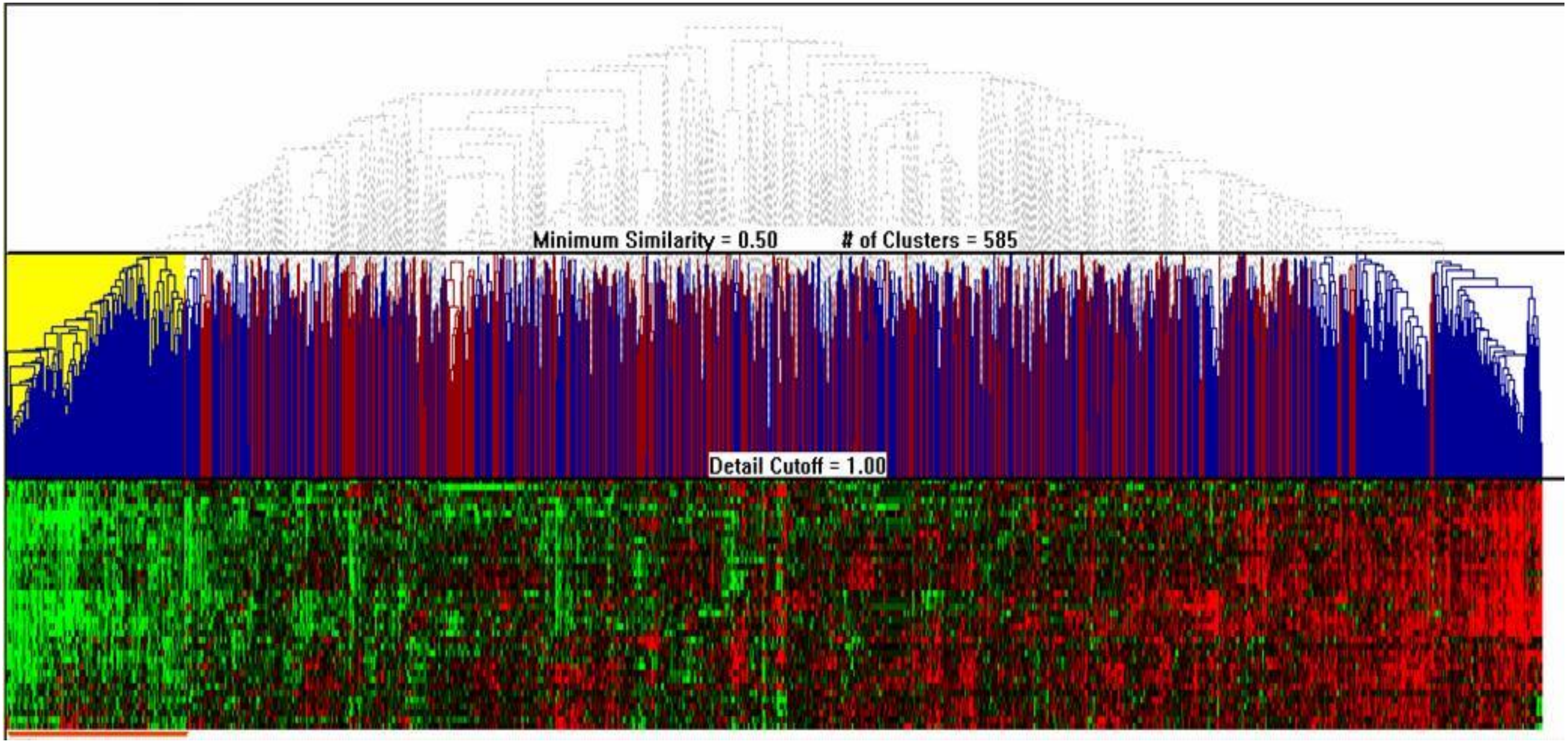
Discussion on Hierarchical Approaches

- Strengths
  - Do not need to input k, the number of clusters
- Weakness
  - Do not scale well; time complexity of at least $O(n^2)$, where n is total number of objects
  - Can never undo what was done previously
- Integration of hierarchical with distance-based clustering
  - BIRCH (1996): uses CF-tree and incrementally adjusts quality of sub-clusters
  - CURE (1998): selects well-scattered points from cluster and then shrinks them towards center of cluster by a specified fraction
  - CHAMELEON (1999): hierarchical clustering using dynamic modeling

How to Derive Clusters from Dendrogram

- **Use global thresholds**
  - **Homogeneity within clusters**
    - **Diameter(C) $\leq$ MaxD**
    - **Avg(sim(O_i,O_j)) $\geq \rho$ (O_i,O_j $\in$ C)**
  - **Separation between clusters**
    - **Inter-cluster distance $\geq \sigma$**
      - **single-link**
      - **complete-link**
      - **…**

Minimum Similarity Threshold



Interactively Exploring Hierarchical Clustering Results, Seo, et al. 2002.

How to Derive Clusters from Dendrogram

- Ask users to derive clusters
  - e.g. TreeView
  - Flexible when user have different requirement of cluster granularity for different parts of data.
  - Inconvenient when data set is large

Coarse granularity

Fine granularity