Machine learning

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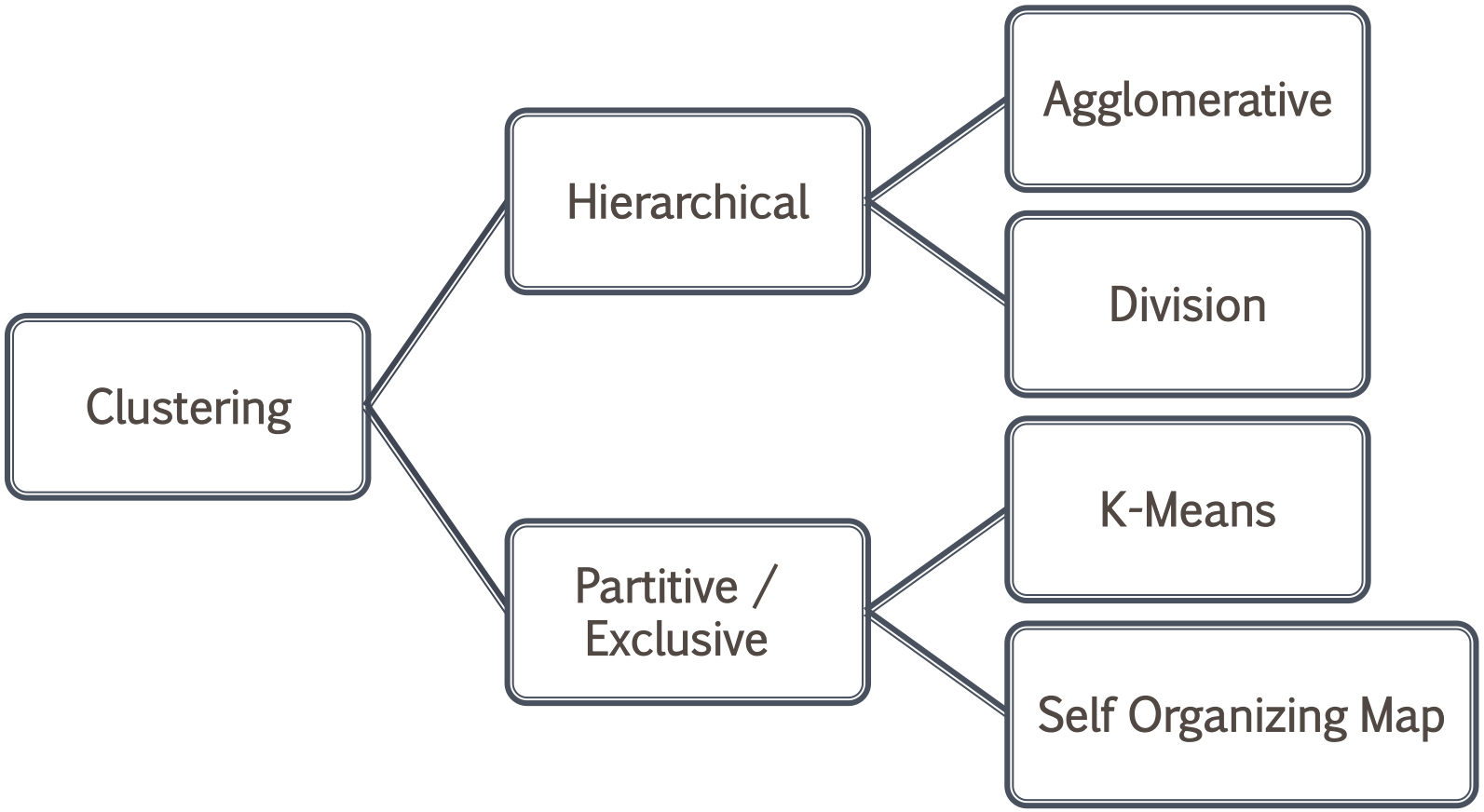
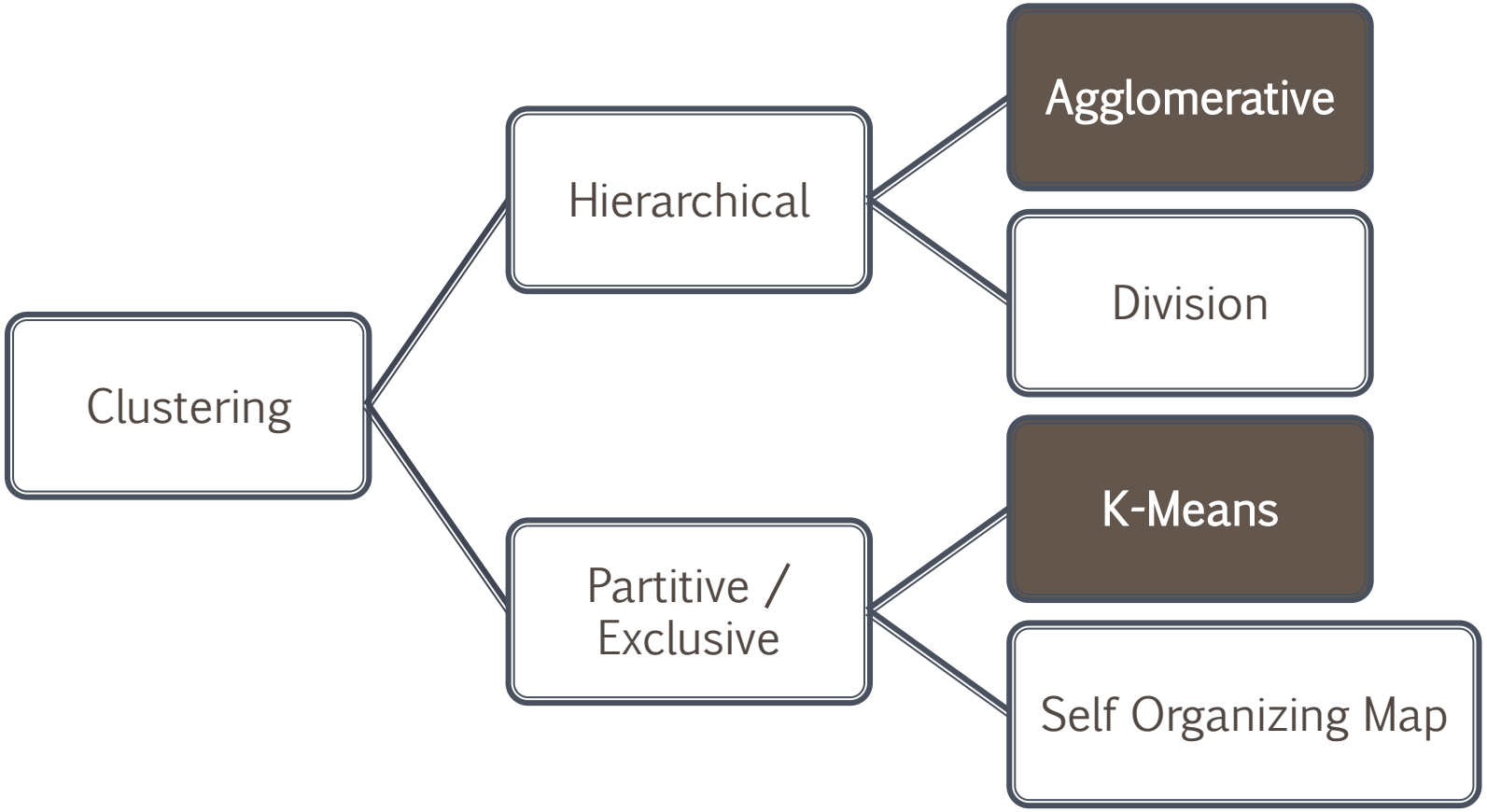
Lecture 11: Clustering Part2 (Agglomerative)

Two main groups of clustering algorithms



Two main groups of clustering algorithms

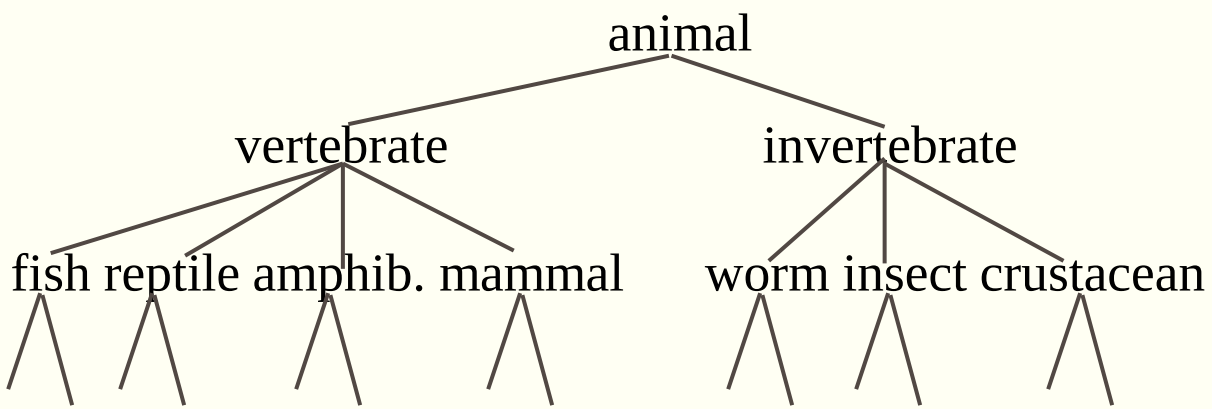


Hierarchical Clustering Algorithms

- Two main types of hierarchical clustering
  - **Agglomerative:** Bottom-up approach
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - **Divisive:** Top-down approach
    - Start with one, all-inclusive cluster
    - At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
  - Merge or split one cluster at a time

Hierarchical Clustering

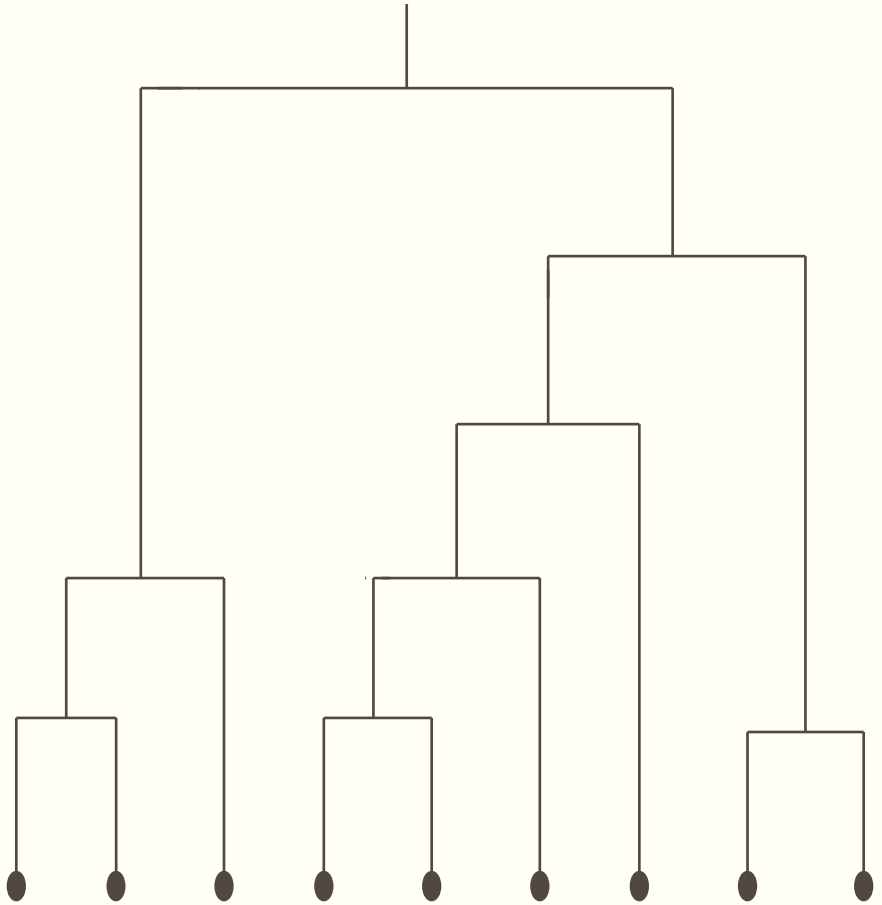
- Build a tree-based hierarchical taxonomy (*dendrogram*) from a set of documents.



- One approach: recursive application of a partitional clustering algorithm.

Dendrogram: Hierarchical Clustering

- Clustering obtained by cutting the dendrogram at a desired level: each connected component forms a cluster.



Hierarchical Agglomerative Clustering (HAC)

- Starts with each doc in a separate cluster
  - then repeatedly joins the *closest pair* of clusters, until there is only one cluster.
- The history of merging forms a binary tree or hierarchy.

Note: the resulting clusters are still “hard” and induce a partition

HOW THE AGGLOMERATIVE ALGORITHM WORK?

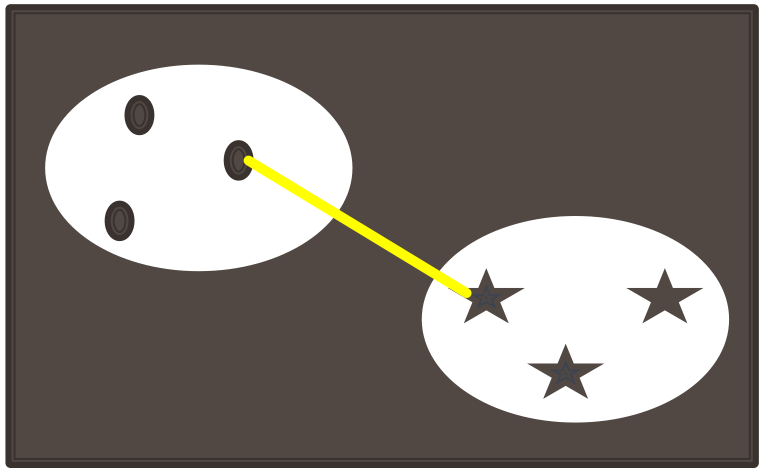
Given a set of N items to be clustered, and an N*N distance (or similarity) matrix, the basic process of hierarchical clustering (defined by S.C. Johnson in 1967) is this:

- 1- Start by assigning each item to a cluster, so that if you have N items, you now have N clusters, each containing just one item. Let the distances (similarities) between the clusters the same as the distances (similarities) between the items they contain.
- 2- Find the closest (most similar) pair of clusters and merge them into a single cluster, so that now you have one cluster less.
- 3- Compute distances (similarities) between the new cluster and each of the old clusters.
- 4- Repeat steps 2 and 3 until all items are clustered into a single cluster of size N.

STEP 3: CAN BE DONE IN DIFFERENT WAYS

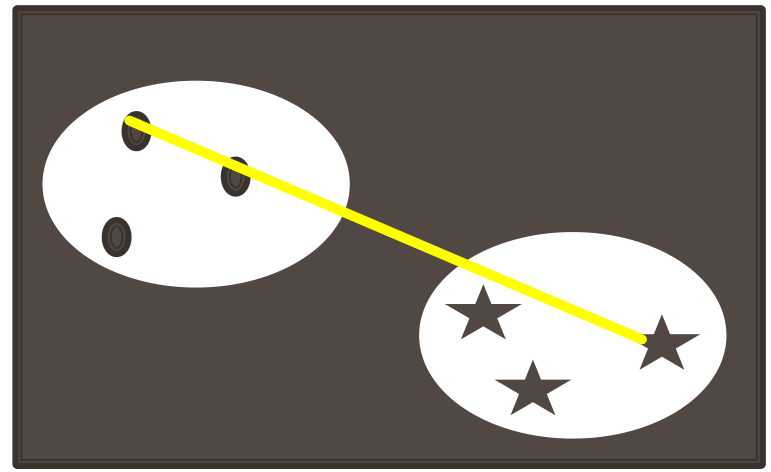
- **Single-linkage clustering** (also called the minimum distance method), we consider the distance between one cluster and another cluster to be equal to the shortest distance from any member of one cluster to any member of the other cluster.

$$D_{sl}(C_i, C_j) = \min_{x,y} \{ d(x, y) \mid x \in C_i, y \in C_j \}$$



- ***Complete-linkage* clustering** (also called the *diameter* or *maximum* method), we consider the distance between one cluster and another cluster to be equal to the greatest distance from any member of one cluster to any member of the other cluster.

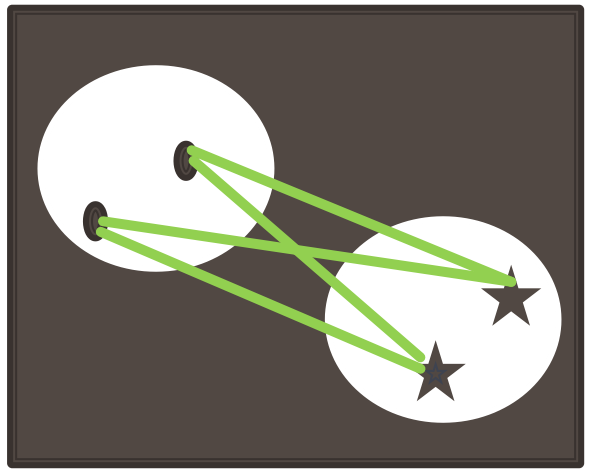
$$D_{cl}(C_i, C_j) = \max_{x,y} \{ d(x, y) \mid x \in C_i, y \in C_j \}$$



STEP 3: CAN BE DONE IN DIFFERENT WAYS

- **Average Linkage**

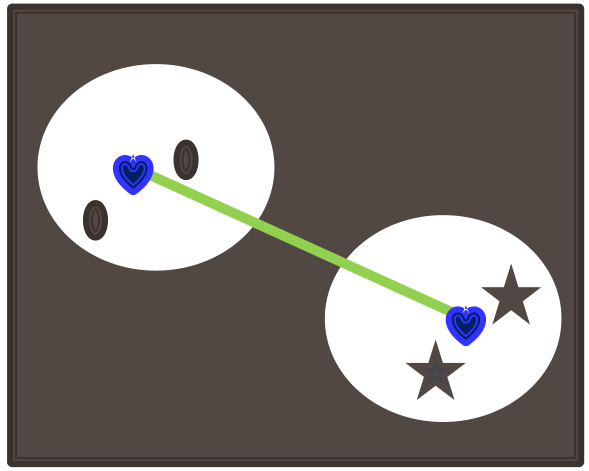
This method involves looking at the distances between all pairs and averages all of these distances. This is also called Unweighted Pair Group Mean Averaging.



$$D_{avg}(C_i, C_j) = \frac{1}{|C_i| \times |C_j|} \sum_{x \in C_i, y \in C_j} d(x, y)$$

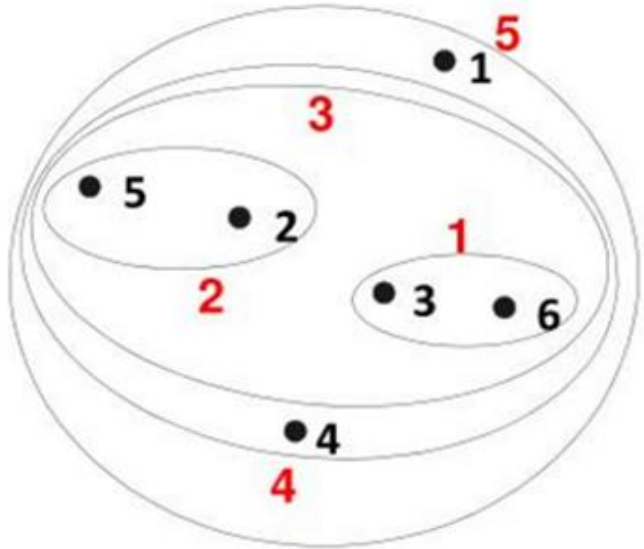
- **Centroid**

Cinteroid distance between clusters $\mathbf{C_i}$ and $\mathbf{C_j}$ is the distance between the centroid $\mathbf{r_i}$ of $\mathbf{C_i}$ and the centroid $\mathbf{r_j}$ of $\mathbf{C_j}$



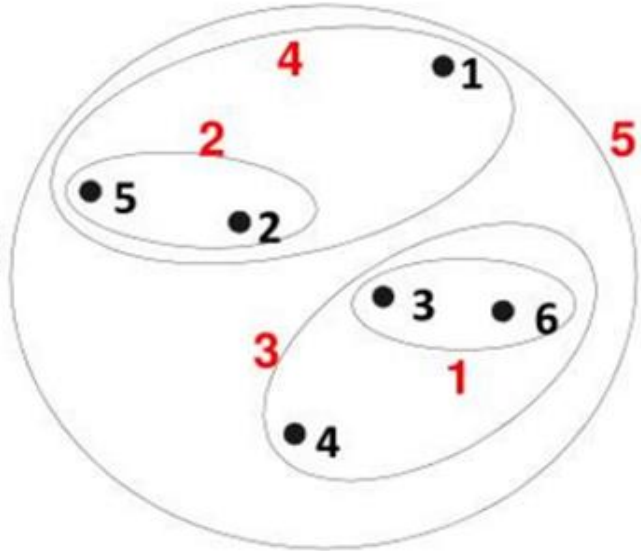
$$D_{centroids}(C_i, C_j) = d(r_i, r_j)$$

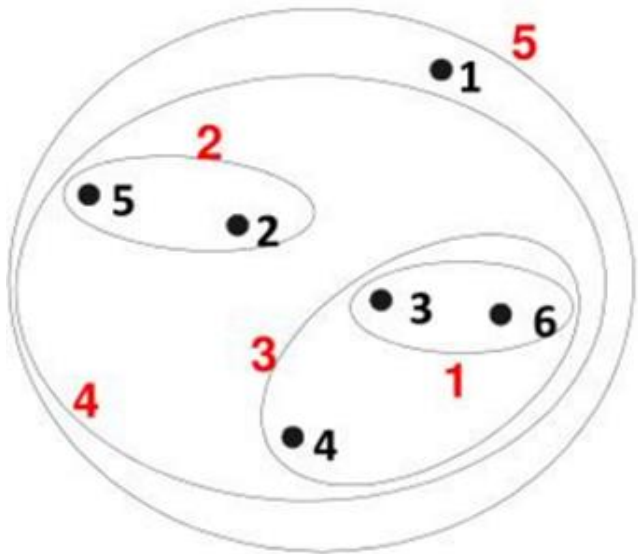
Hierarchical Clustering: Comparison



MIN

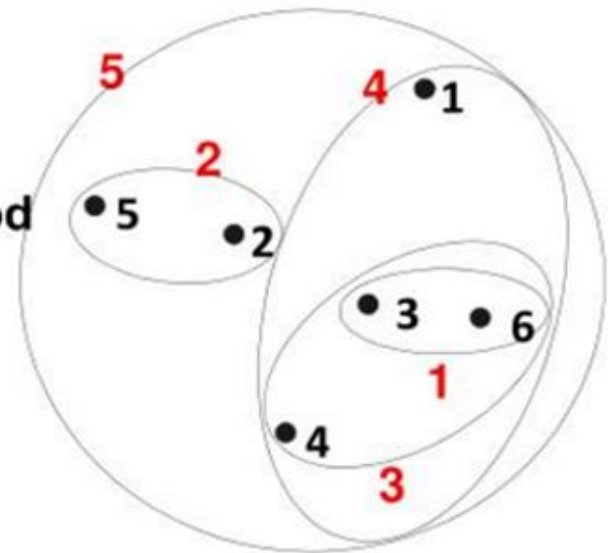
MAX





Group Average

Centroid Method



EXAMPLE

	X1	X2
A	1	1
B	1.5	1.5
C	5	5
D	3	4
E	4	4
F	3	3.5

Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

We have 6 objects and we put each object into one cluster (analogue to put a ball into a basket). Instead of calling them as objects , now we call them clusters . Thus, in the beginning we have 6 clusters. Our goal is to group those 6 clusters such that at the end of the iterations, we will have only single cluster consists of the whole six original objects.

In each step of the iteration, we find the closest pair clusters. In this case, the closest cluster is between cluster F and D with shortest distance of 0.5. Thus, we group cluster D and F into cluster (D, F). Then we update the distance matrix (see distance matrix below). Distance between ungrouped clusters will not change from the original distance matrix.

How to calculate distance between newly grouped clusters (D, F) and other clusters?

- Using the input distance matrix, distance between cluster (D, F) and cluster A is computed as

$$d_{(D,F)\to A} = \min\left(d_{DA}, d_{FA}\right) = \min\left(3.61, 3.20\right) = 3.20$$

- Distance between cluster (D, F) and cluster B is

$$d_{(D,F)\to B} = \min\left(d_{DB}, d_{FB}\right) = \min\left(2.92, 2.50\right) = 2.50$$

- Similarly, distance between cluster (D, F) and cluster C is

$$d_{(D,F)\to C} = \min\left(d_{DC}, d_{FC}\right) = \min\left(2.24, 2.50\right) = 2.24$$

- Finally, distance between cluster E and cluster (D, F) is calculated as

$$d_{E\to(D,F)} = \min\left(d_{ED}, d_{EF}\right) = \min\left(1.00, 1.12\right) = 1.00$$

- Then, the updated distance matrix becomes

Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	3.20	4.24
B	0.71	0.00	4.95	2.50	3.54
C	5.66	4.95	0.00	2.24	1.41
D, F	3.20	2.50	2.24	0.00	1.00
E	4.24	3.54	1.41	1.00	0.00

Dist	A	B	C	D, F	E
A	0.00	0.71	5.66	3.20	4.24
B	0.71	0.00	4.95	2.50	3.54
C	5.66	4.95	0.00	2.24	1.41
D, F	**3.20**	**2.50**	**2.24**	0.00	1.00
E	4.24	3.54	1.41	**1.00**	0.00

Looking at the lower triangular updated distance matrix, we found out that the closest distance between cluster B and cluster A is now 0.71. Thus, we group cluster A and cluster B into a single cluster name (A, B).

Dist	A,B	C	(D, F)	E
A,B	0	?	?	?
C	?	0	2.24	1.41
(D, F)	?	2.24	0	1.00
E	?	1.41	1.00	0

- Using the input distance matrix (size 6 by 6), distance between cluster C and cluster (D, F) is computed as

$$d_{C\to(A,B)} = \min\left(d_{CA}, d_{CB}\right) = \min\left(5.66, 4.95\right) = 4.95$$

- Distance between cluster (D, F) and cluster (A, B) is the minimum distance between all objects involves in the two clusters

$$d_{(D,F)\to(A,B)} = \min\left(d_{DA}, d_{DB}, d_{FA}, d_{FB}\right) = \min\left(3.61, 2.92, 3.20, 2.50\right) = 2.50$$

- Similarly, distance between cluster E and (A, B) is

$$d_{E\to(A,B)} = \min\left(d_{EA}, d_{EB}\right) = \min\left(4.24, 3.54\right) = 3.54$$

- Then the updated distance matrix is

Min Distance (Single Linkage)

Dist	A,B	C	(D, F)	E
A,B	0	4.95	2.50	3.54
C	4.95	0	2.24	1.41
(D, F)	2.50	2.24	0	1.00
E	3.54	1.41	1.00	0

Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

Observing the lower triangular of the updated distance matrix, we can see that the closest distance between clusters happens between cluster E and (D, F) at distance 1.00. Thus, we cluster them together into cluster ((D, F), E).
The updated distance matrix is given below.

Min Distance (Single Linkage)

Dist	(A,B)	C	(D, F), E
(A,B)	0.00	4.95	2.50
C	4.95	0.00	1.41
(D, F), E	2.50	1.41	0.00

Distance between cluster ((D, F), E) and cluster (A, B) is calculated as

$$d_{((D,F),E)\to(A,B)} = \min\left(d_{DA}, d_{DB}, d_{FA}, d_{FB}, d_{EA}, d_{EB}\right) = \min\left(3.61, 2.92, 3.20, 2.50, 4.24, 3.54\right) = 2.50$$

Distance between cluster ((D, F), E) and cluster C yields the minimum distance of 1.41. This distance is computed as

$$d_{((D,F),E)\to C} = \min\left(d_{DC}, d_{FC}, d_{EC}\right) = \min\left(2.24, 2.50, 1.41\right) = 1.41$$

After that, we merge cluster ((D, F), E) and cluster C into a new cluster name (((D, F), E), C).

The updated distance matrix is shown in the figure below

Min Distance (Single Linkage)

Dist	(A,B)	(D, F), E),C
(A,B)	0.00	2.50
((D, F), E),C	2.50	0.00

The minimum distance of 2.5 is the result of the following computation:

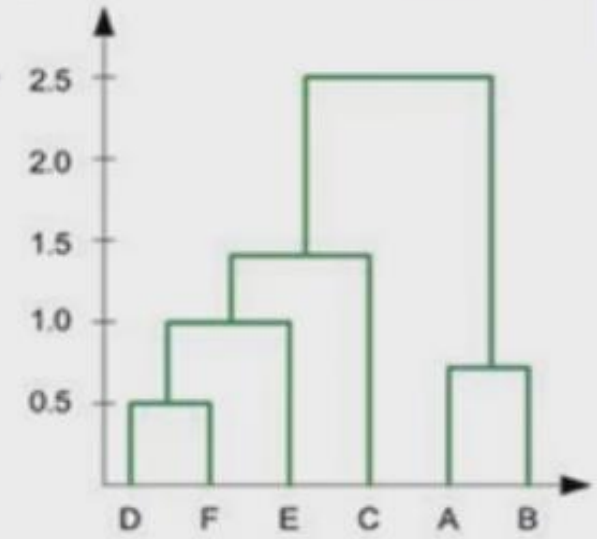
$$d_{(((D,F),E),C)\to(A,B)} = \min\left(d_{DA}, d_{DB}, d_{FA}, d_{FB}, d_{EA}, d_{EB}, d_{CA}, d_{CB}\right)$$

$$d_{(((D,F),E),C)\to(A,B)} = \min\left(3.61, 2.92, 3.20, 2.50, 4.24, 3.54, 5.66, 4.95\right) = 2.50$$

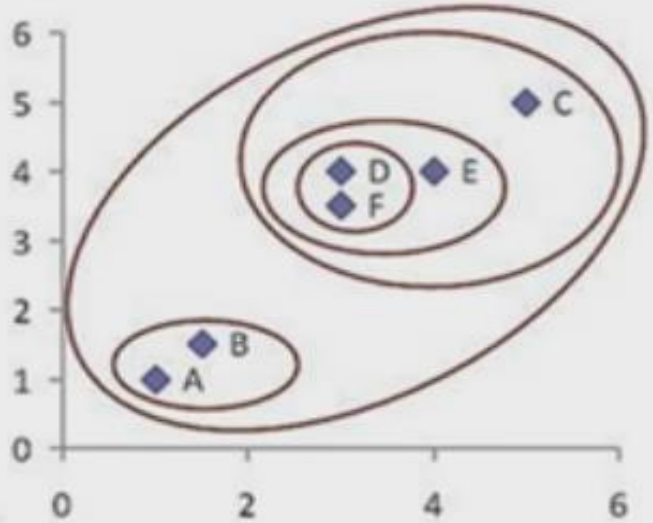
Now if we merge the remaining two clusters, we will get only single cluster contain the whole 6 objects. Thus, our computation is finished. We summarized the results of computation as follow:

1. In the beginning we have 6 clusters: A, B, C, D, E and F
2. We merge cluster D and F into cluster (D, F) at distance 0.50
3. We merge cluster A and cluster B into (A, B) at distance 0.71
4. We merge cluster E and (D, F) into ((D, F), E) at distance 1.00
5. We merge cluster ((D, F), E) and C into (((D, F), E), C) at distance 1.41
6. We merge cluster (((D, F), E), C) and (A, B) into ((((D, F), E), C), (A, B)) at distance 2.50
7. The last cluster contain all the objects, thus conclude the computation

Using this information, we can now draw the final results of a dendogram. The dendogram is drawn based on the distances to merge the clusters above.



* The hierarchy is given as (((D, F), E),C), (A,B). We can also plot the clustering hierarchy into XY space



	X1	X2
A	1	1
B	1.5	1.5
C	5	5
D	3	4
E	4	4
F	3	3.5

What Is A Good Clustering?

- Internal criterion: A good clustering will produce high quality clusters in which:
  - the intra-class (that is, intra-cluster) similarity is high
  - the inter-class similarity is low
  - The measured quality of a clustering depends on both the document representation and the similarity measure used

External criteria for clustering quality

- Quality measured by its ability to discover some or all of the hidden patterns or latent classes in gold standard data
- Assesses a clustering with respect to ground truth … requires *labeled data*
- Assume documents with C gold standard classes, while our clustering algorithms produce K clusters, $\omega_1, \omega_2, \ldots, \omega_K$ with n_i members.

Hierarchical Clustering: Time and Space requirements

- For a dataset **X** consisting of **n** points
- **$O(n^2)$ space**; it requires storing the distance matrix
- **$O(n^3)$ time** in most of the cases
  - There are **n** steps and at each step the size **n^2** distance matrix must be updated and searched
  - Complexity can be reduced to **$O(n^2 \log(n))$** time for some approaches by using appropriate data structures

THE HIERARCHICAL CLUSTERING METHOD

- **Strength**
  - there is no need to specify the number of clusters
  - hierarchical clustering is easy to implement .
  - the dendrogram produced is very useful in understanding the data.
- **Weakness**
  - the algorithm can **never undo any previous steps**. So for example, the algorithm clusters 2 points, and later on we see that the connection was not a good one, the program cannot undo that step.
  - the time complexity for the clustering can result in very long computation times, in comparison with efficient algorithms, such k-Means.
  - if we have a large dataset, it can become difficult to determine the correct number of clusters by the dendrogram.