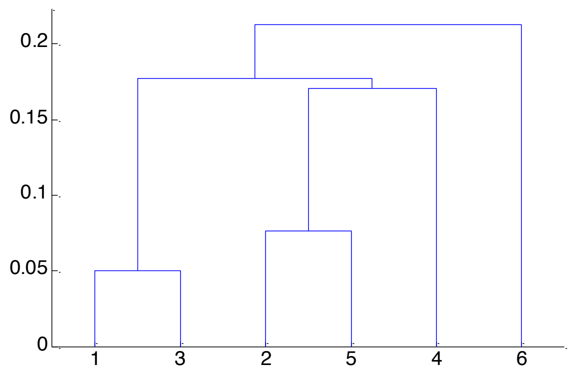
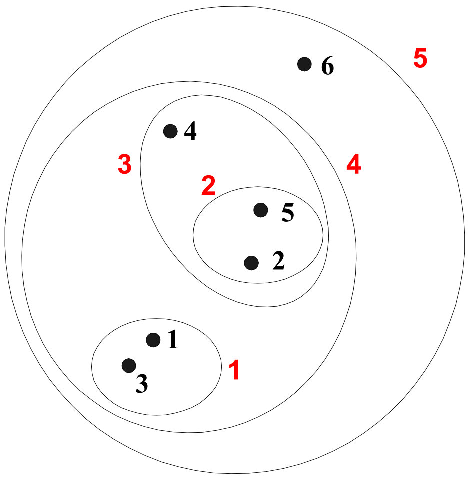
CS 484
Data Mining

Clustering 3

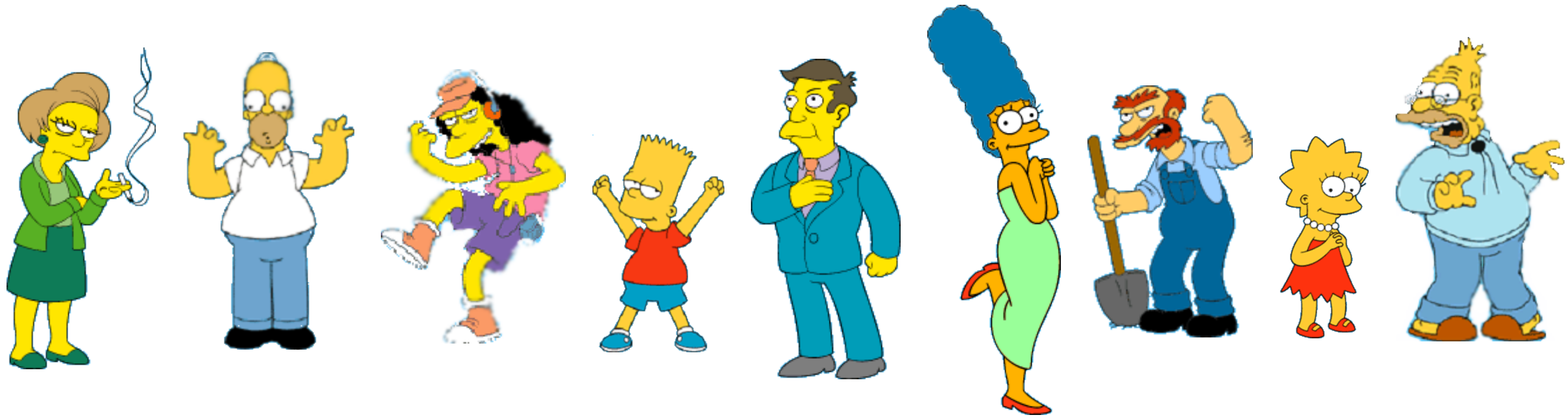
Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
  - A tree like diagram that records the sequences of merges or splits



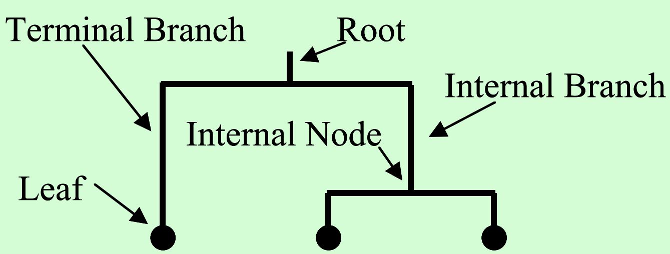


What is a natural grouping among these objects?

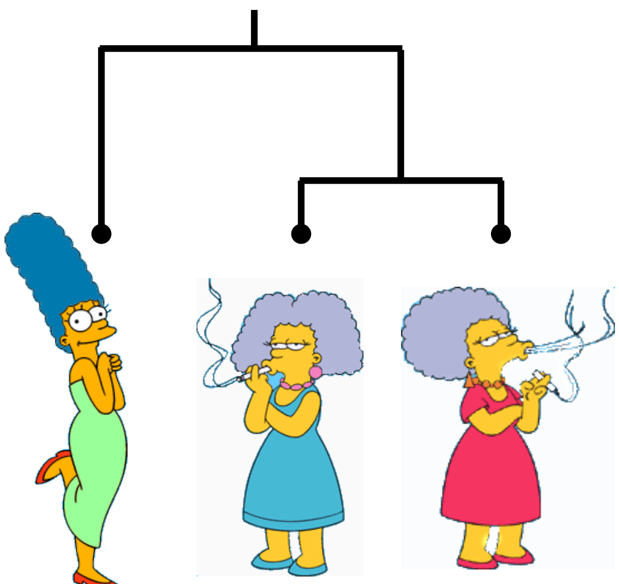


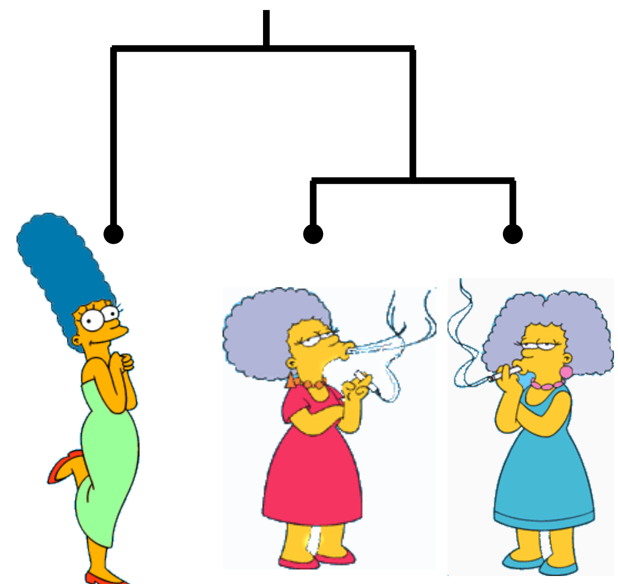
A Useful Tool for Summarizing Similarity Measurements

Dendrogram:

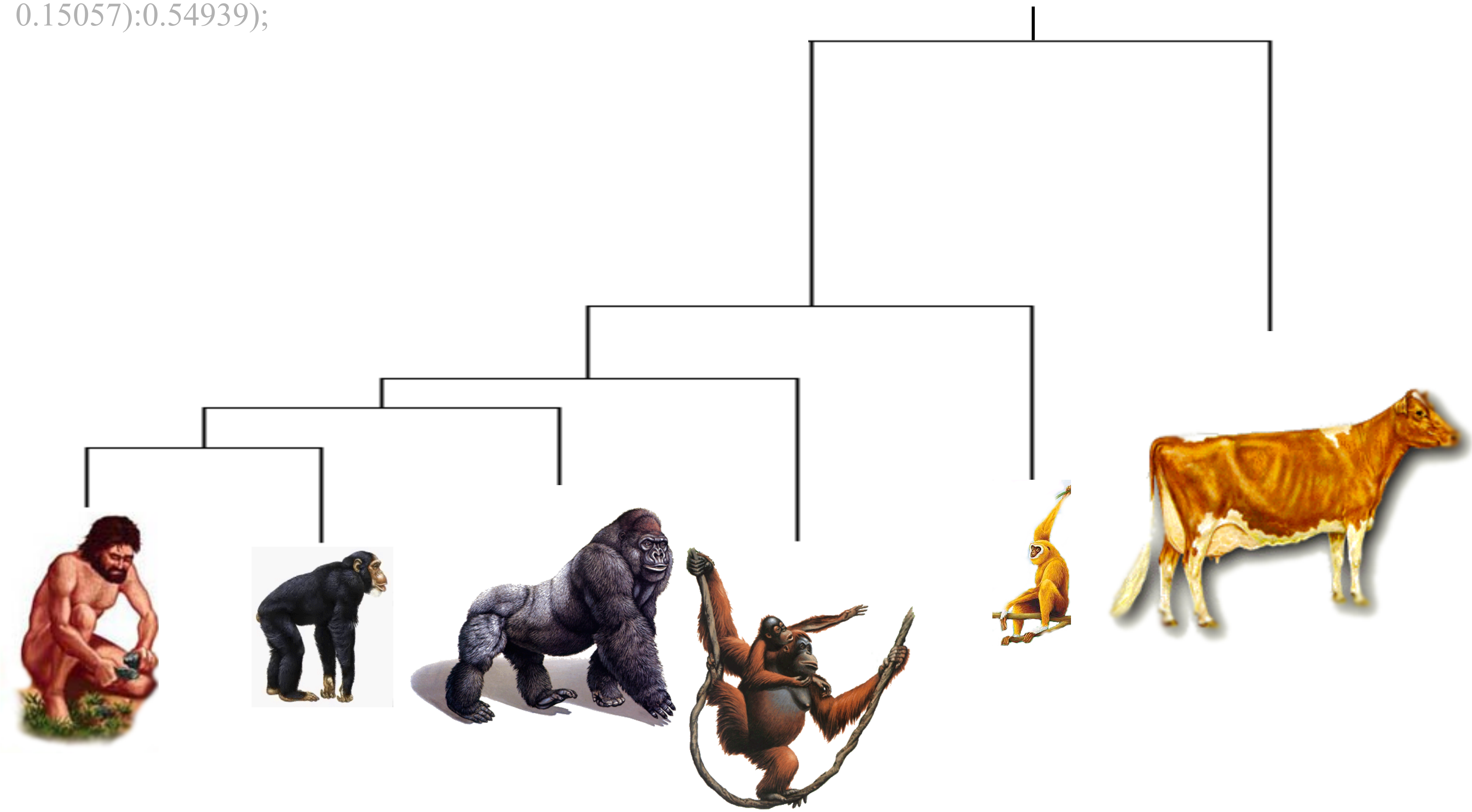


The similarity between two objects in a dendrogram is represented as the height of the lowest internal node they share.



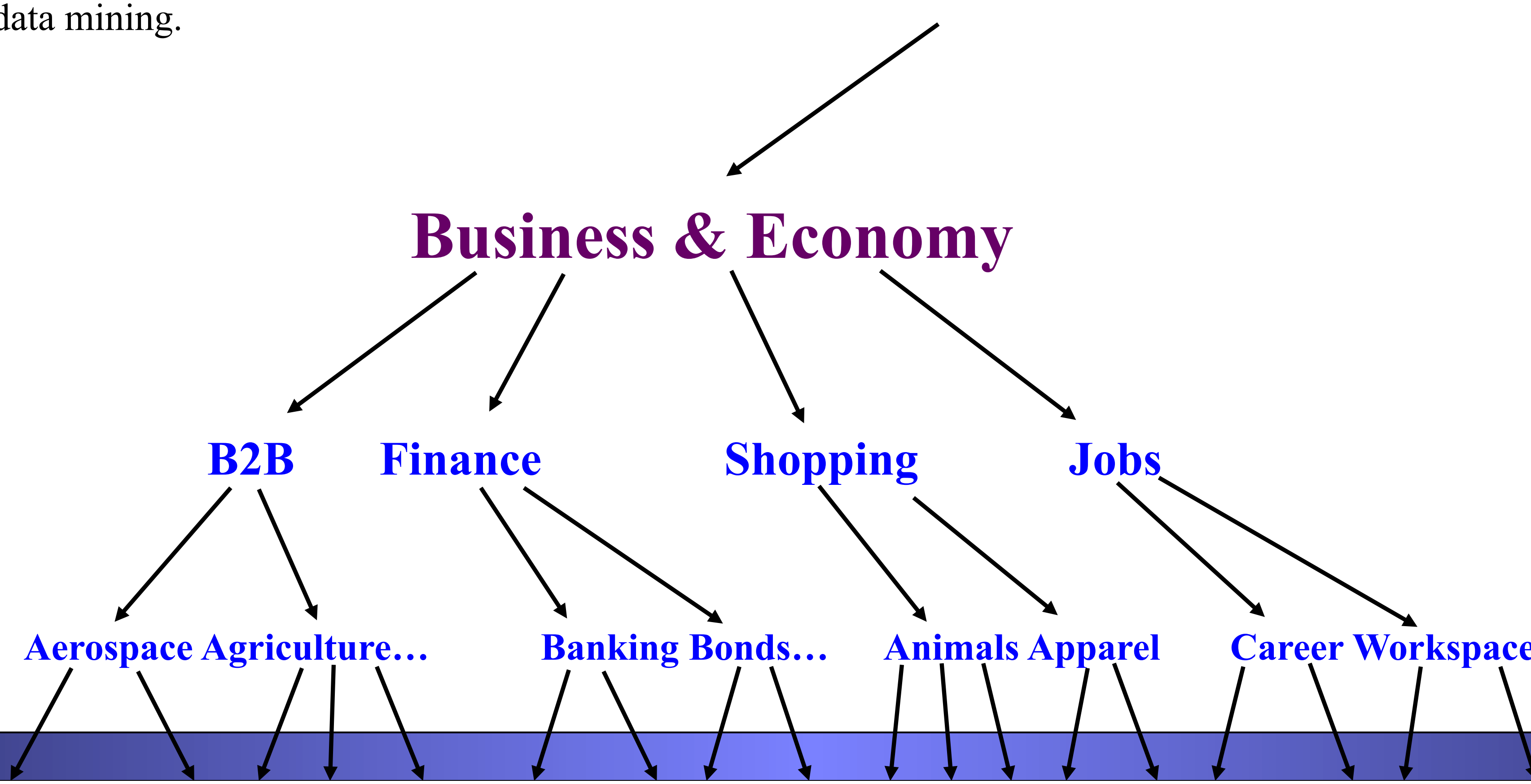


(Bovine:0.69395,(Gibbon:0.36079,(Orangutan:0.33636,(Gorilla:0.17147,(Chimp:0.19268,Human:0.11927):0.08386):0.06124):0.15057):0.54939);

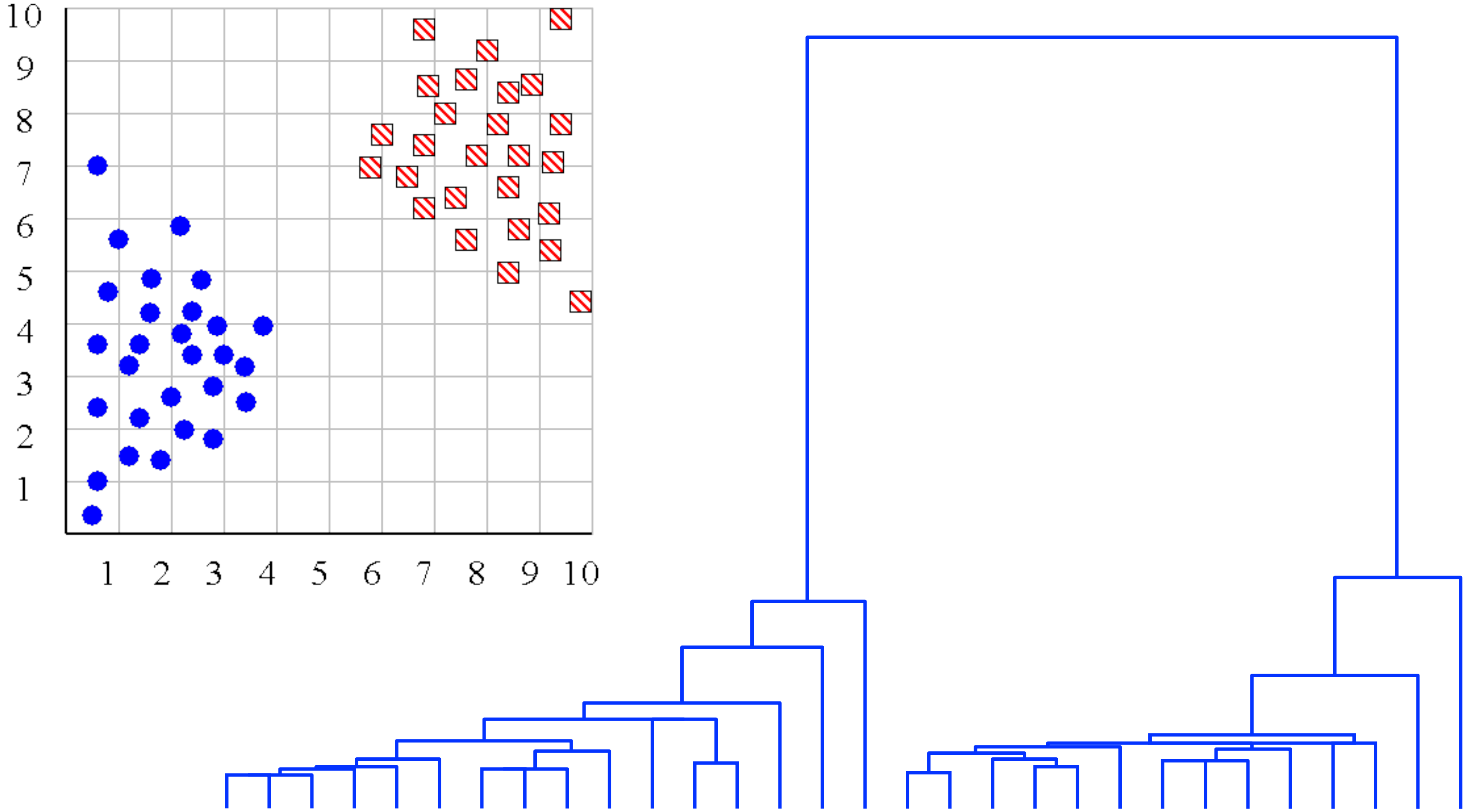


Note that hierarchies are commonly used to organize information, for example in a web portal.

Yahoo's hierarchy is manually created, we will focus on automatic creation of hierarchies in data mining.

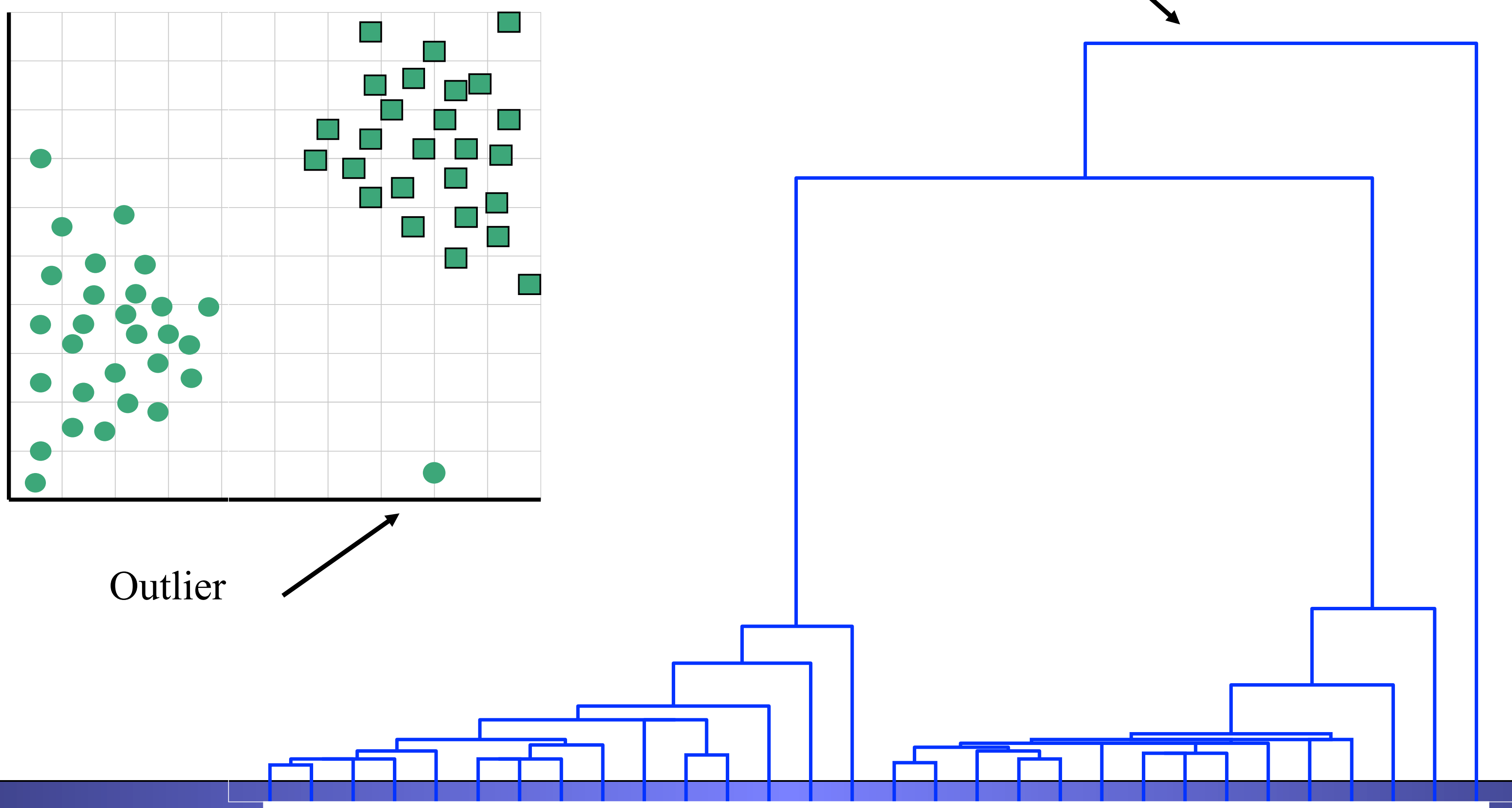


We can look at the dendrogram to determine the "correct" number of clusters. In this case, the two highly separated subtrees are highly suggestive of two clusters. (Things are rarely this clear cut, unfortunately)



One potential use of a dendrogram is to detect outliers

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



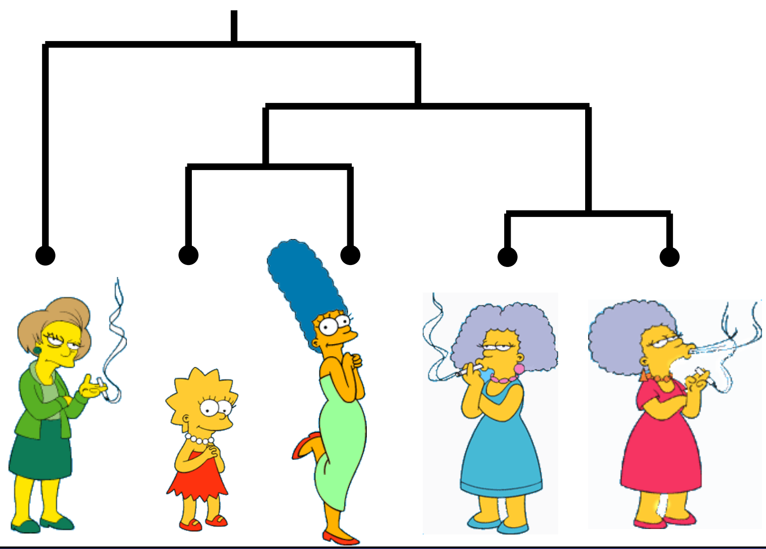
Strengths of Hierarchical Clustering

- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by 'cutting' the dendrogram at the proper level
- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

Hierarchical Clustering

The number of dendrograms with n leafs $= (2n-3)!/[(2^{(n-2)})(n-2)!]$

Number of Leafs	Number of Possible Dendrograms
2	1
3	3
4	15
5	105
...	…
10	34,459,425



Since we cannot test all possible trees we will have to heuristic search of all possible trees. We could do this..

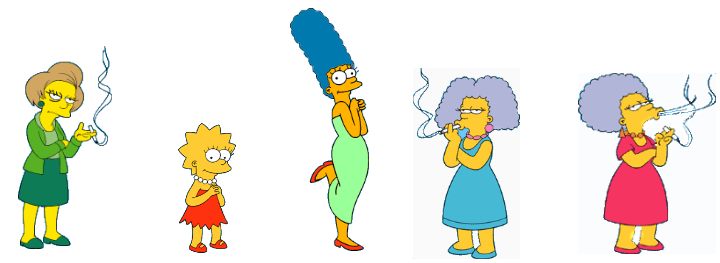
Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.

Top-Down (divisive): Starting with all the data in a single cluster, consider every possible way to divide the cluster into two. Choose the best division and recursively operate on both sides.

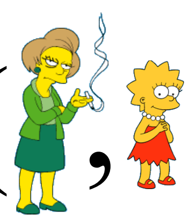
Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique
- Basic algorithm is straightforward
  - Compute the proximity matrix
  - Let each data point be a cluster
  - Repeat
    - Merge the two closest clusters
    - Update the proximity matrix
  - Until only a single cluster remains
  -
- Key operation is the computation of the proximity of two clusters
  - Different approaches to defining the distance between clusters distinguish the different algorithms

We begin with a distance matrix which contains the distances between every pair of objects in our database.



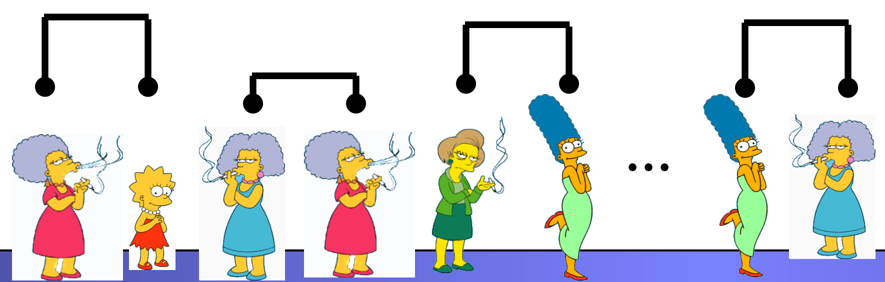
0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
				0

D() = 8

D() = 1

Bottom-Up (agglomerative):
Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.

Consider all possible merges…



Choose the best

Bottom-Up (agglomerative):

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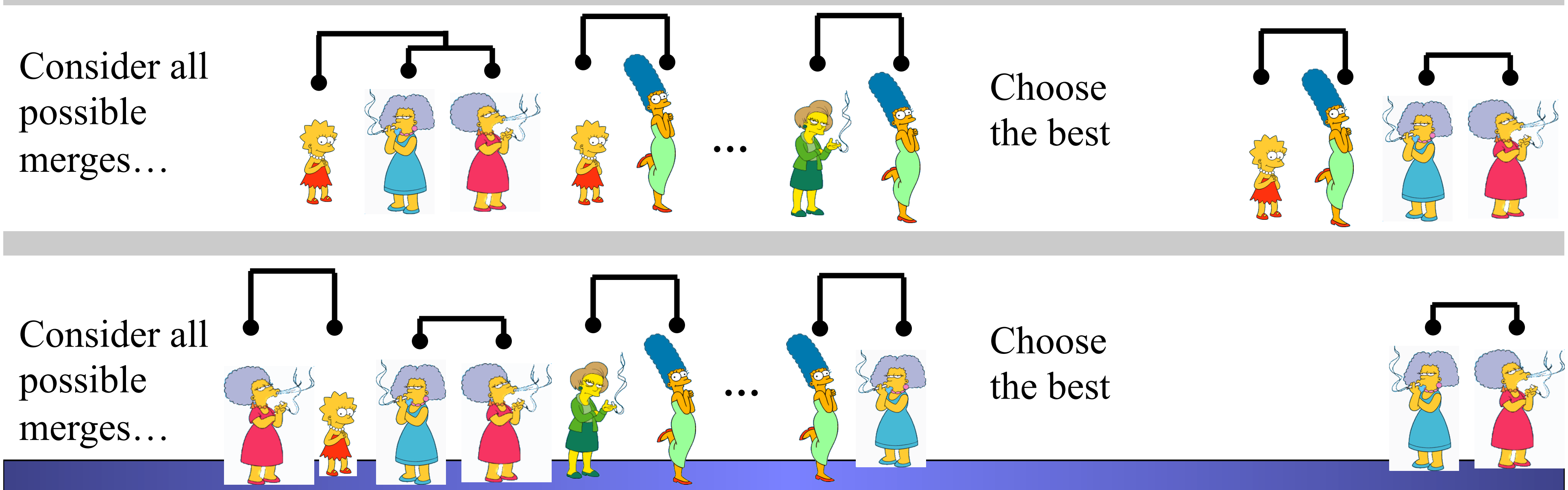

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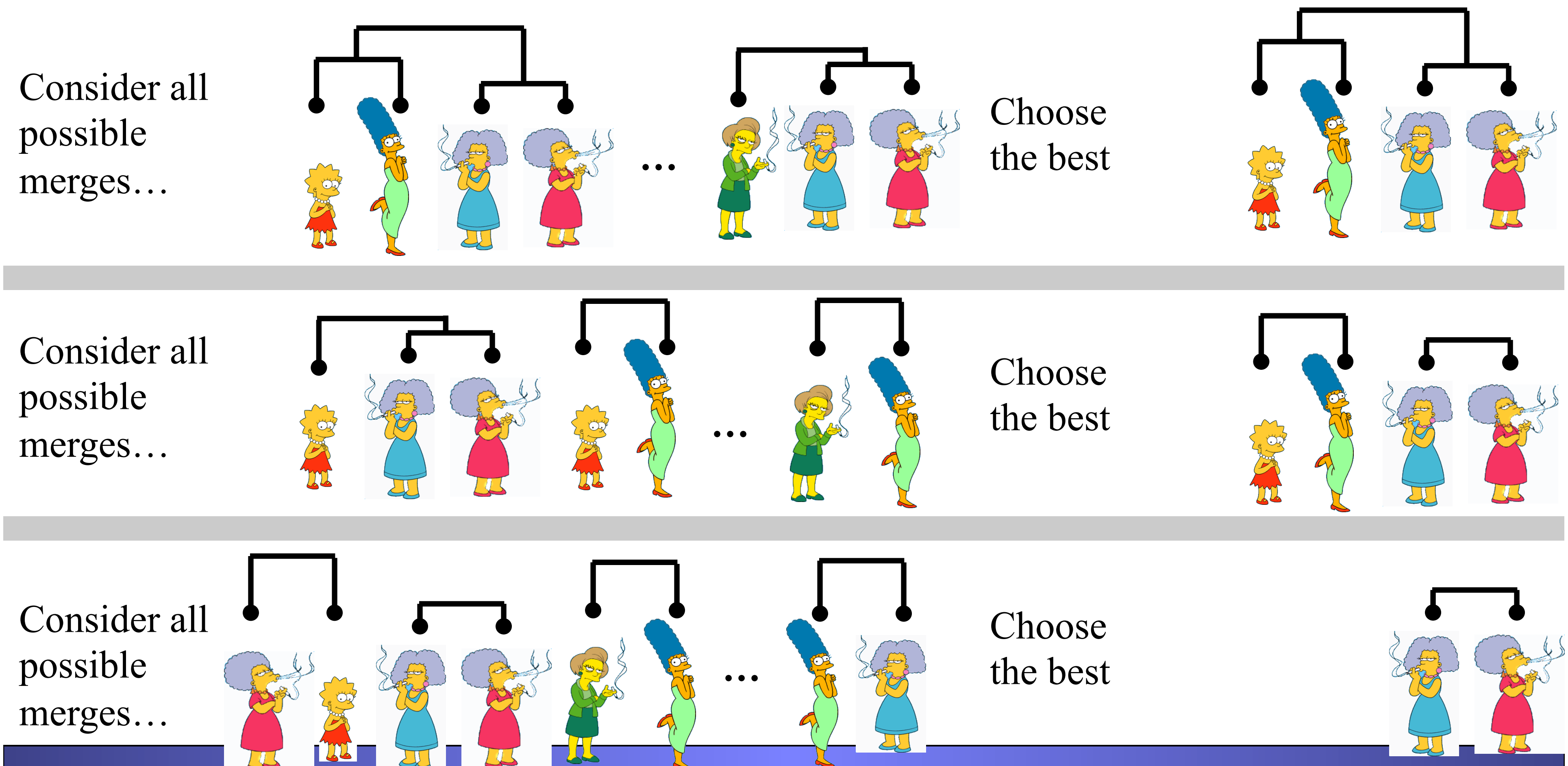

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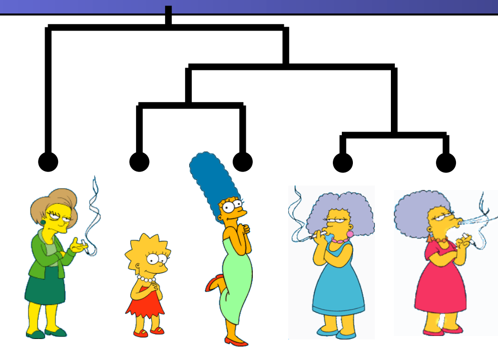

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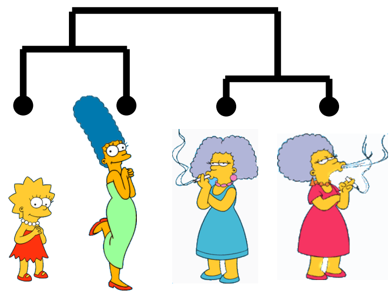

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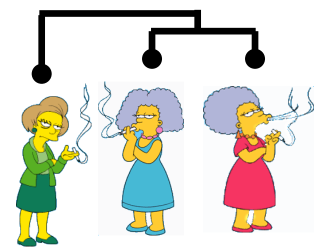
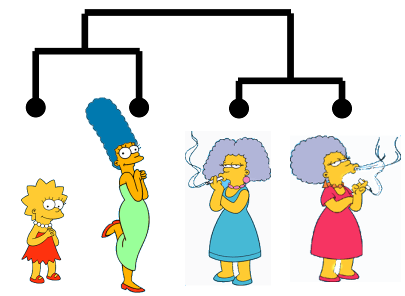
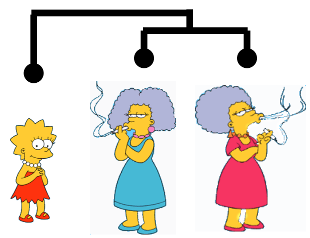
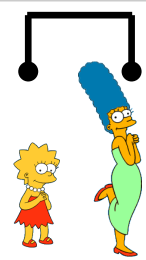


Choose the best



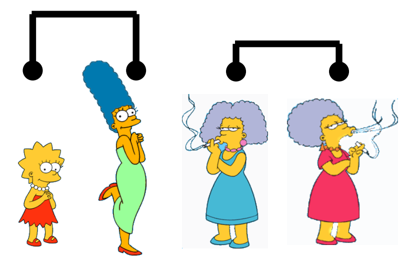
Consider all possible merges…





…

Choose the best



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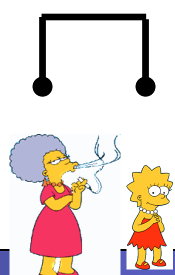
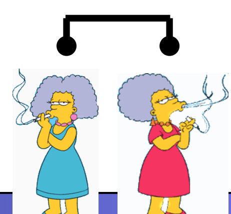


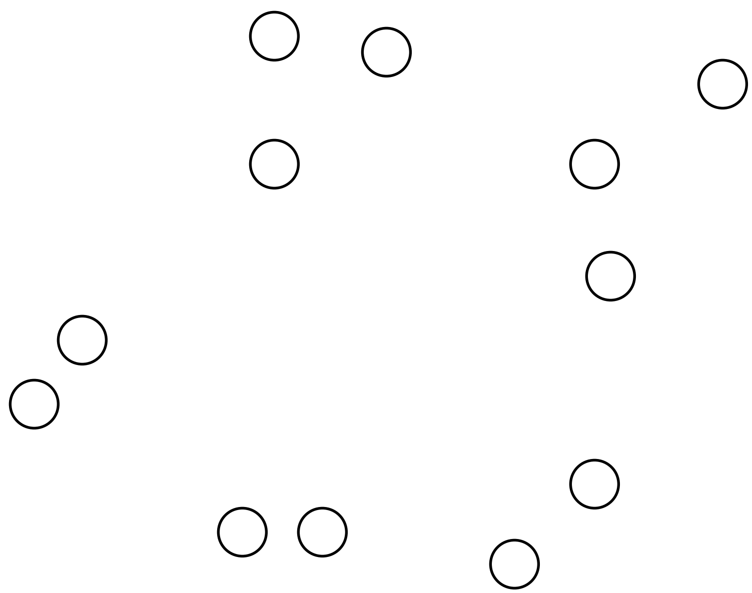


…

Choose the best

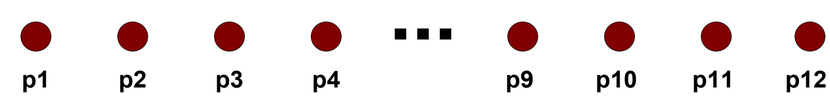
Starting Situation

- Start with clusters of individual points and a proximity matrix



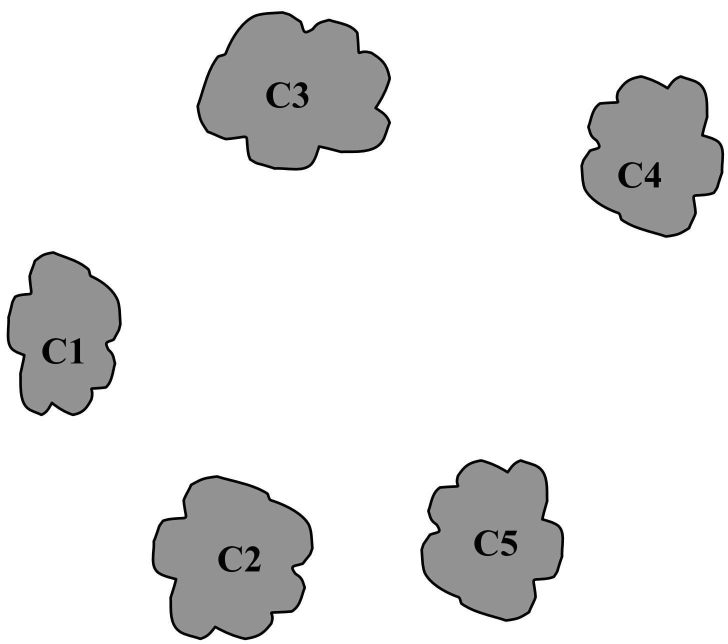
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
. . .						

Proximity Matrix



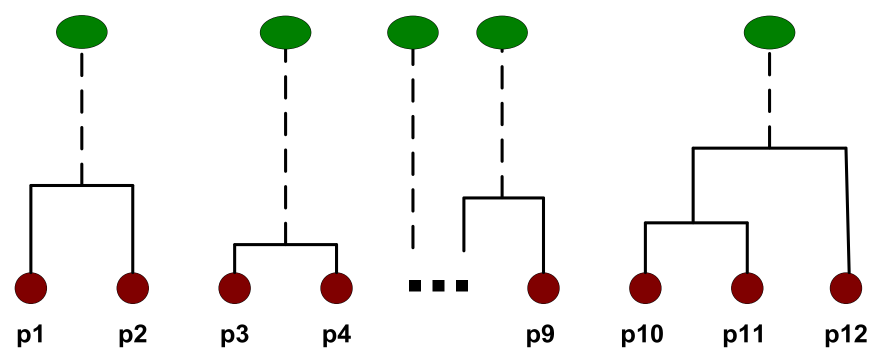
Intermediate Situation

- After some merging steps, we have some clusters



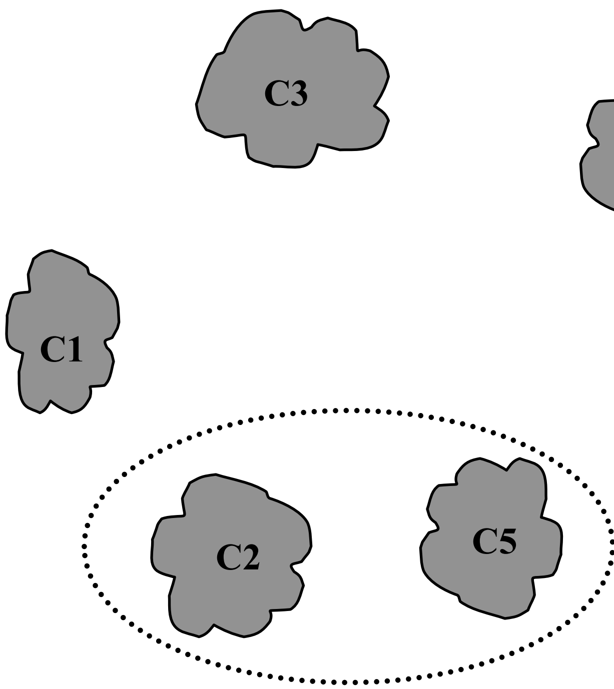
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

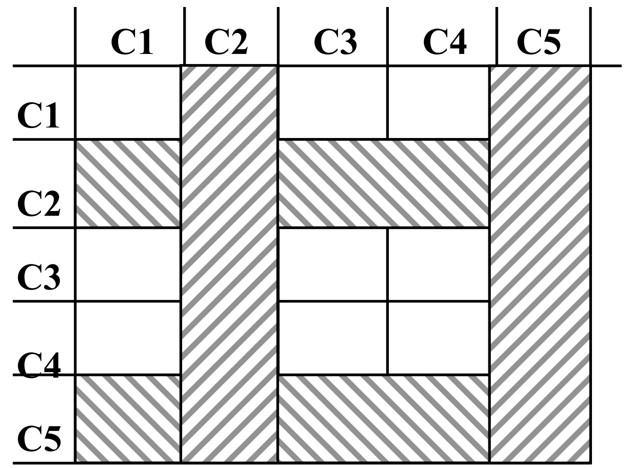
Proximity Matrix



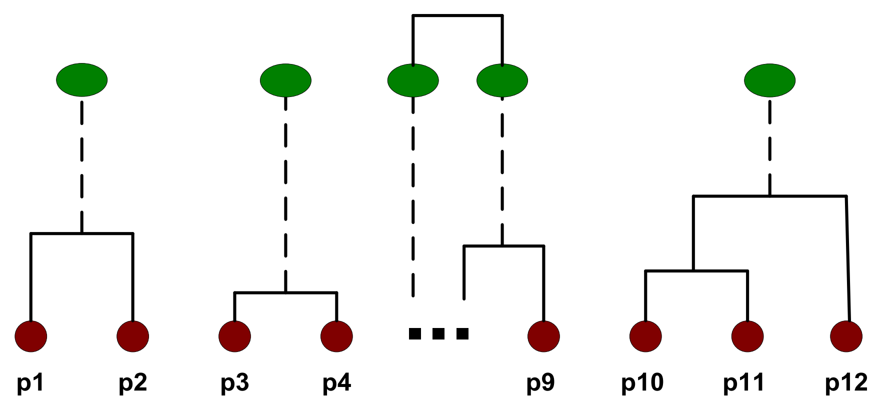
Intermediate Situation

- We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.



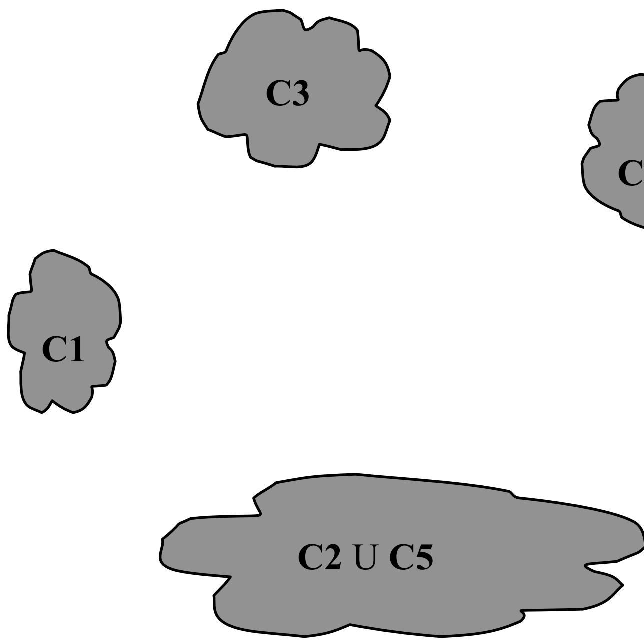


Proximity Matrix



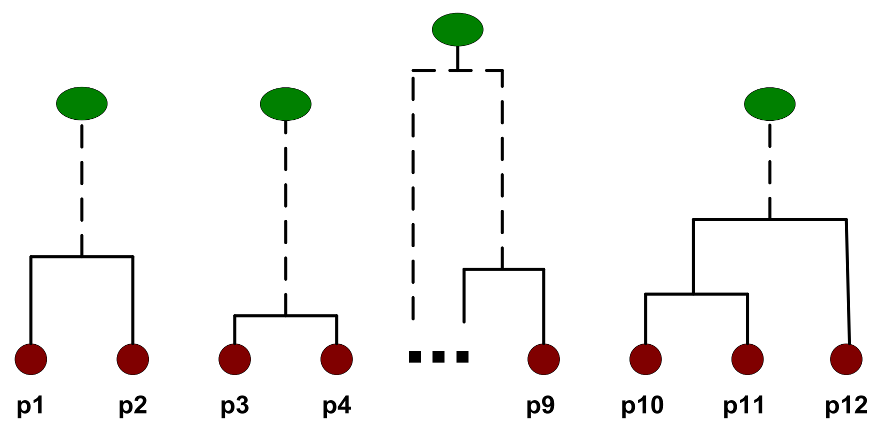
After Merging

- The question is “How do we update the proximity matrix?”



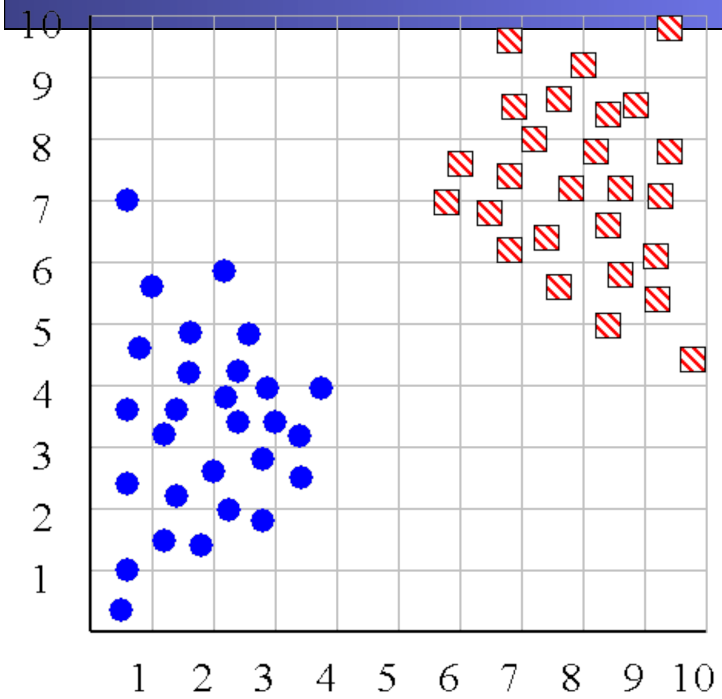
	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

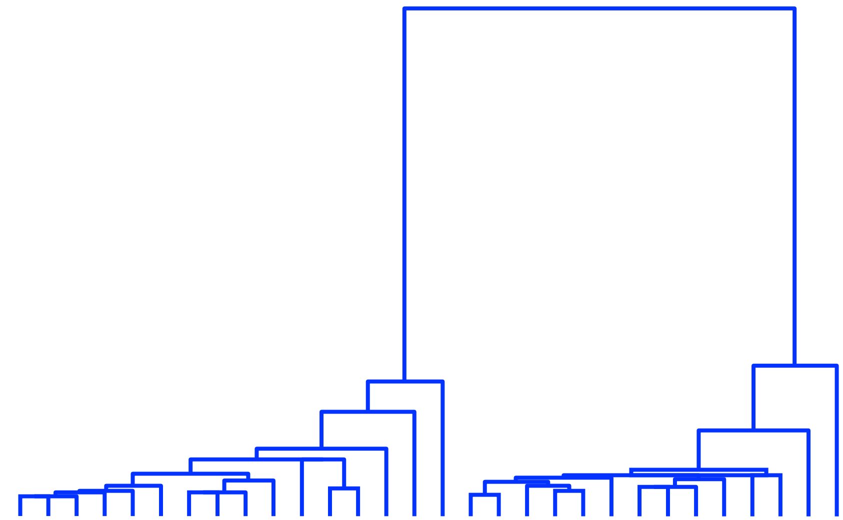
Proximity Matrix



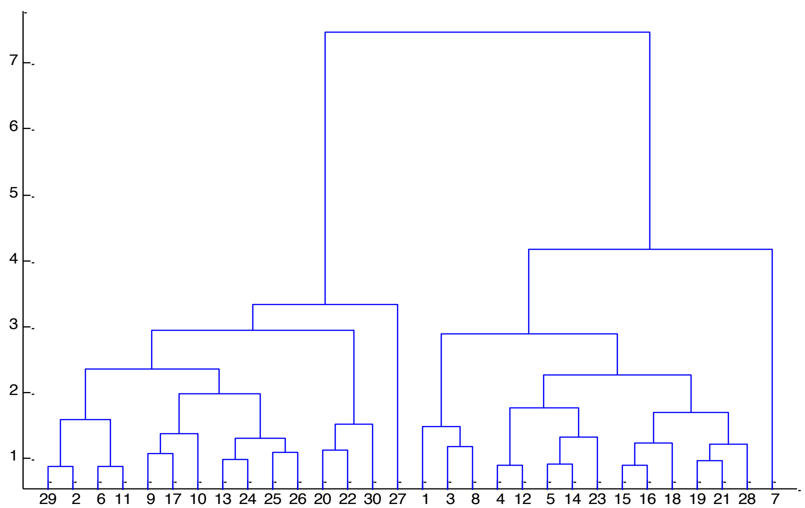
We know how to measure the distance between two objects, but defining the distance between an object and a cluster, or defining the distance between two clusters is non obvious.

- **MIN or Single linkage (nearest neighbor):** In this method the distance between two clusters is determined by the distance of the two closest objects (nearest neighbors) in the different clusters.
- **MAX or Complete linkage (furthest neighbor):** In this method, the distances between clusters are determined by the greatest distance between any two objects in the different clusters (i.e., by the "furthest neighbors").
- **Group average linkage:** In this method, the distance between two clusters is calculated as the average distance between all pairs of objects in the two different clusters.
- **Distance between centroids:** In this method, the distance between two clusters is determined by the distance between their respective centroids.
- **Wards Linkage**: In this method, we try to minimize the variance of the merged clusters

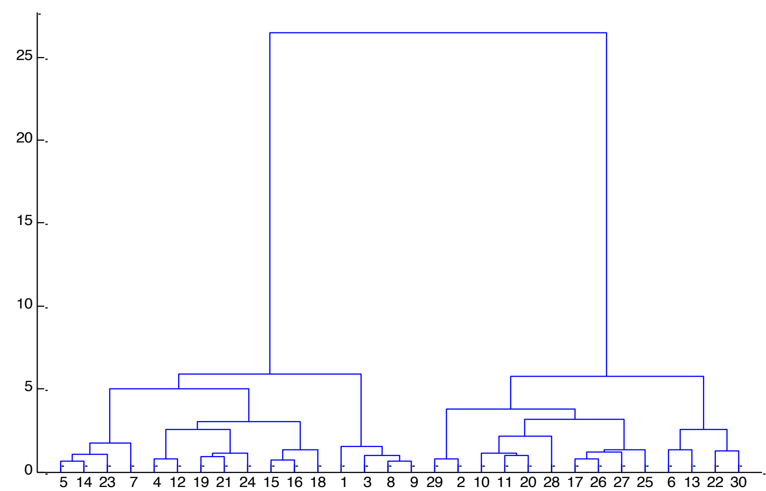




Single linkage

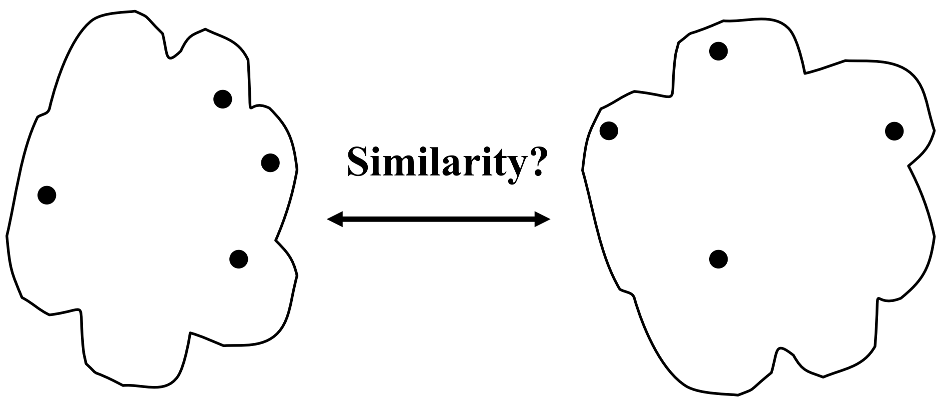


Average linkage



Wards linkage

How to Define Inter-Cluster Similarity

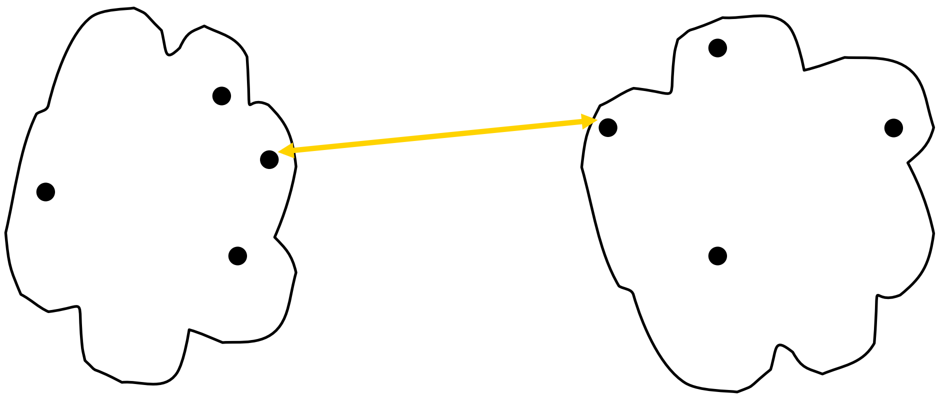


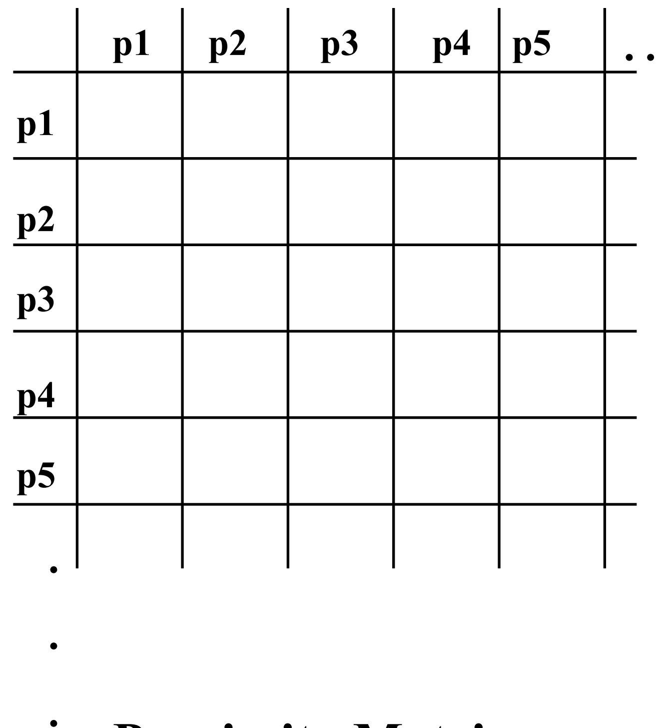
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
. . .						

Proximity Matrix

- MIN (single linkage)
- MAX (complete linkage)
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
  - Ward's Method uses squared error

How to Define Inter-Cluster Similarity





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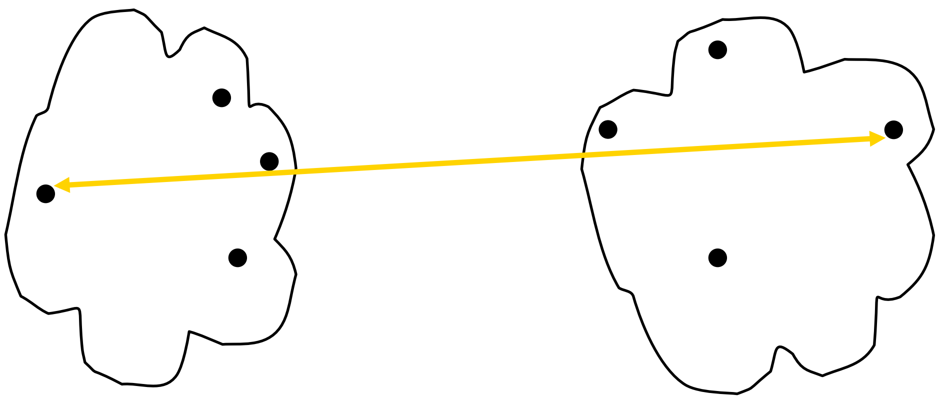

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	p1	p2	p3	p4	p5	. . .
p1						
p2						
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p5						
.						
.						
.						

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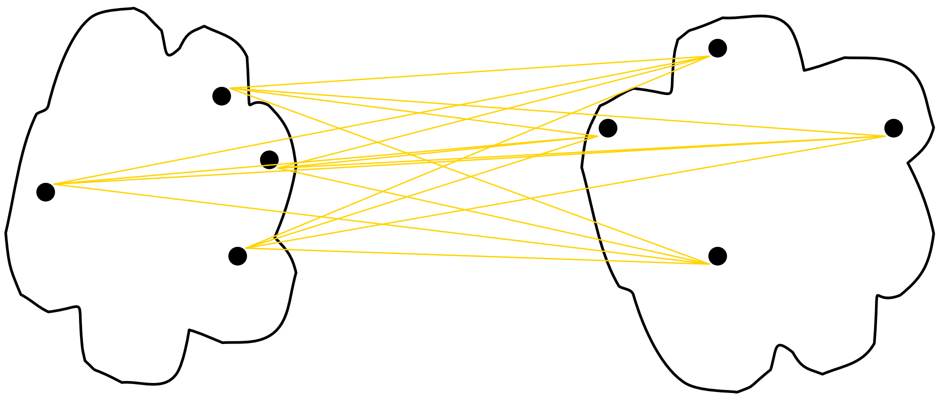

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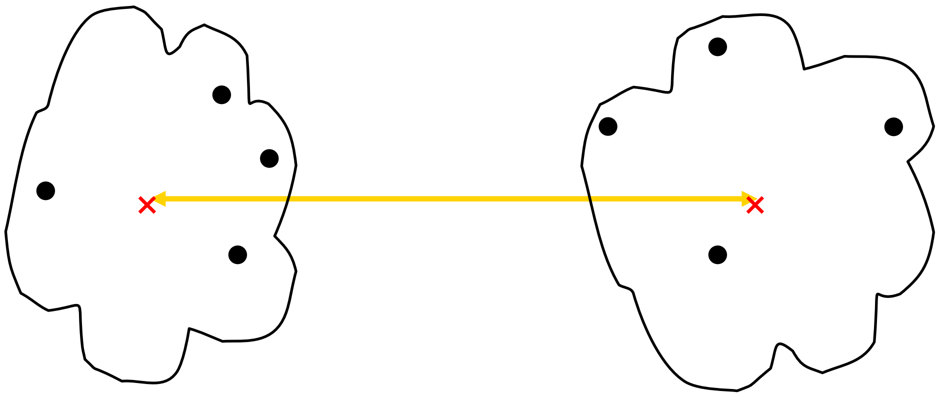
How to Define Inter-Cluster Similarity



	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids
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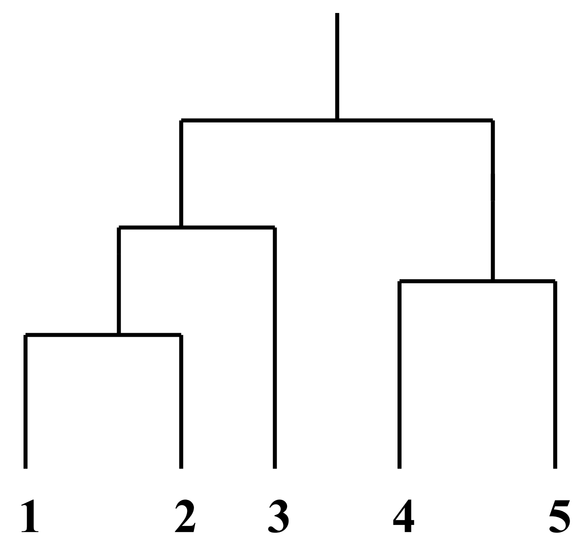
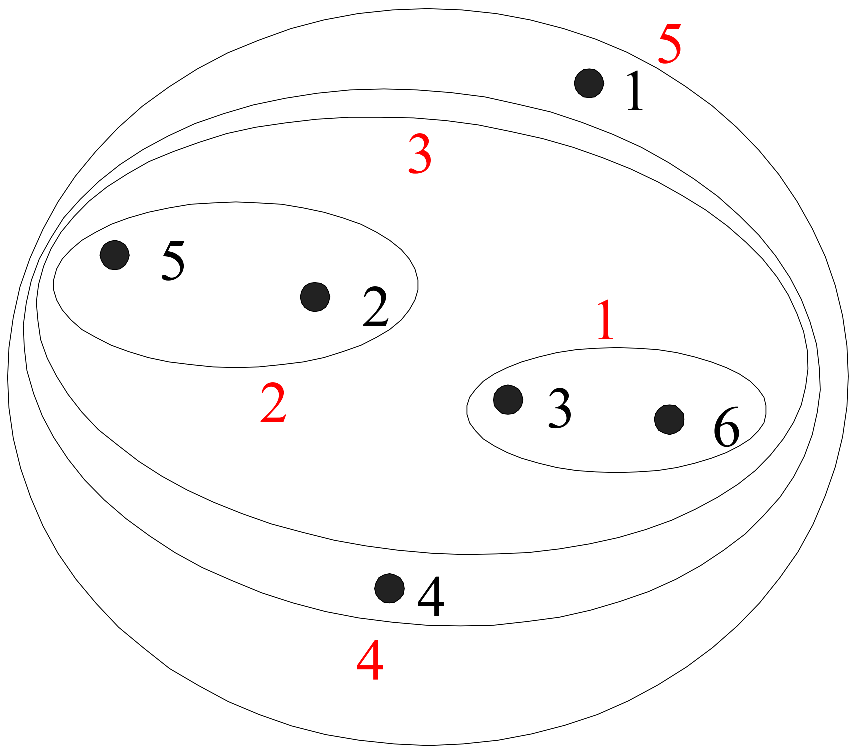
Cluster Similarity: MIN or Single Link

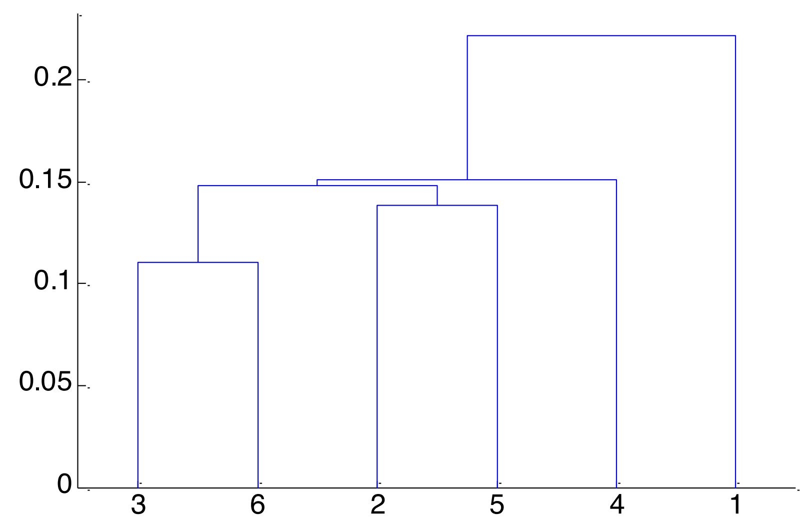
- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph.

	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Hierarchical Clustering: MIN

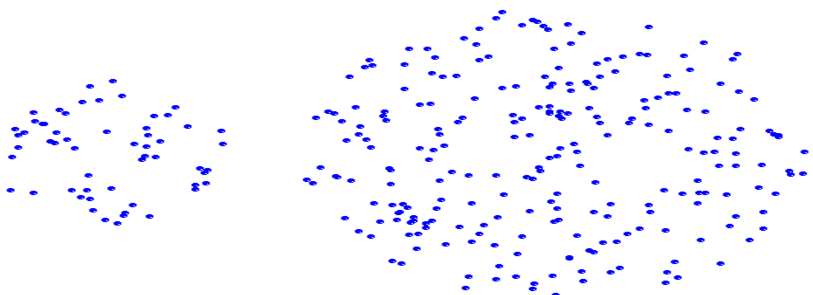




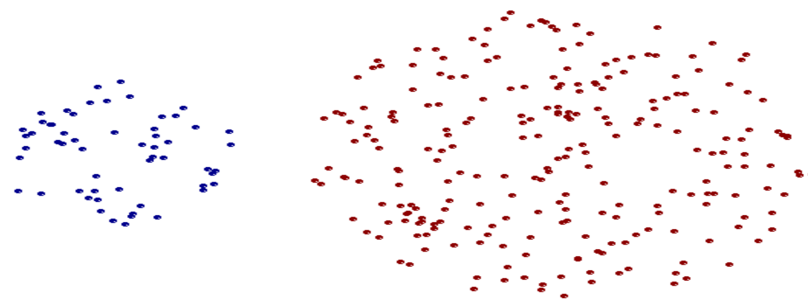
Nested Clusters

Dendrogram

Strength of MIN



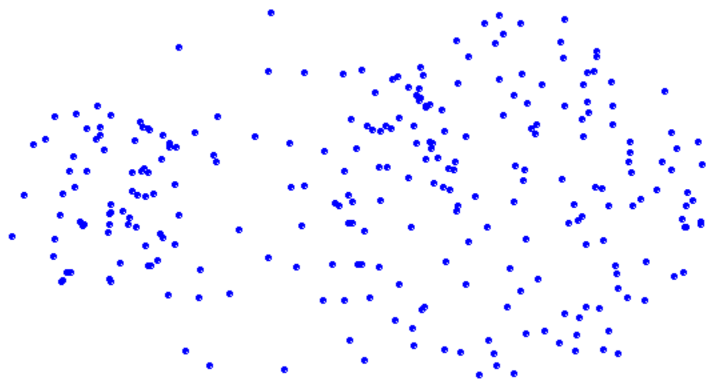
Original Points



Two Clusters

- **Can handle non-elliptical shapes**

Limitations of MIN



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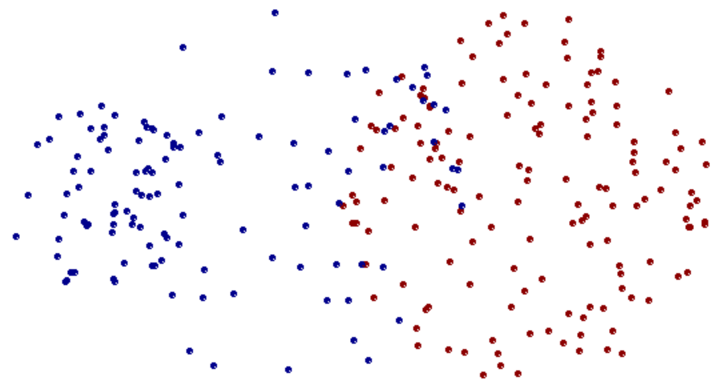

Two Clusters

• **Sensitive to noise and outliers**