L09 Hierarchical clustering

Simpsons slides from Tom Mitchell & Ziv Bar-Joseph (CMU 10-601)

Jason Fleischer

Two Types of Clustering

- **Partitional algorithms:** Construct various partitions and then evaluate them by some criterion
- **Hierarchical algorithms:** Create a hierarchical decomposition of the set of objects using some criterion (focus of this class)

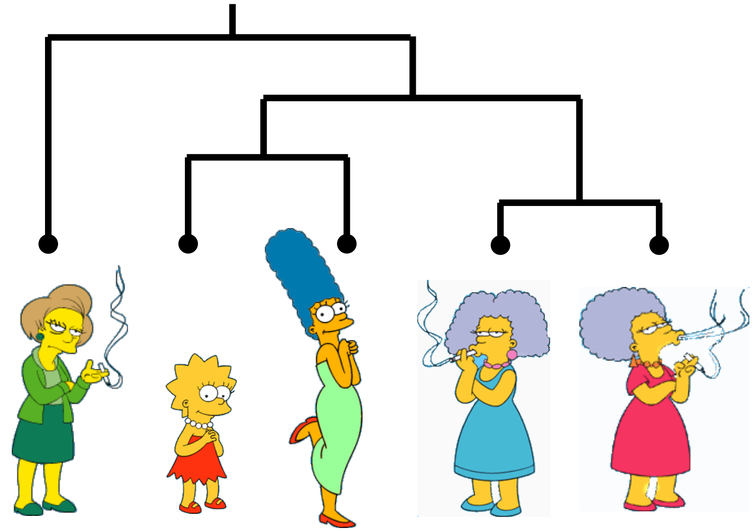
Bottom up or top down

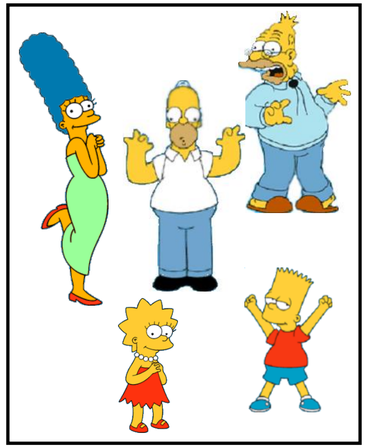
Top down

Hierarchical

Partitional

This is a dendrogram

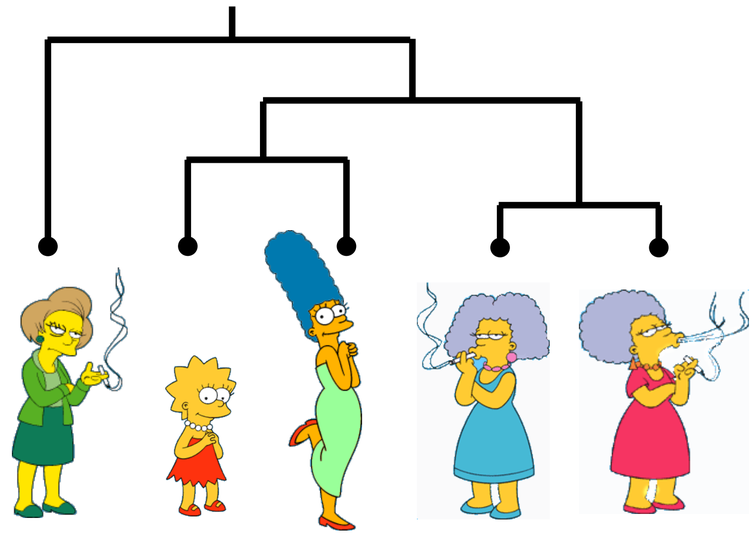




(How-to) Hierarchical Clustering

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

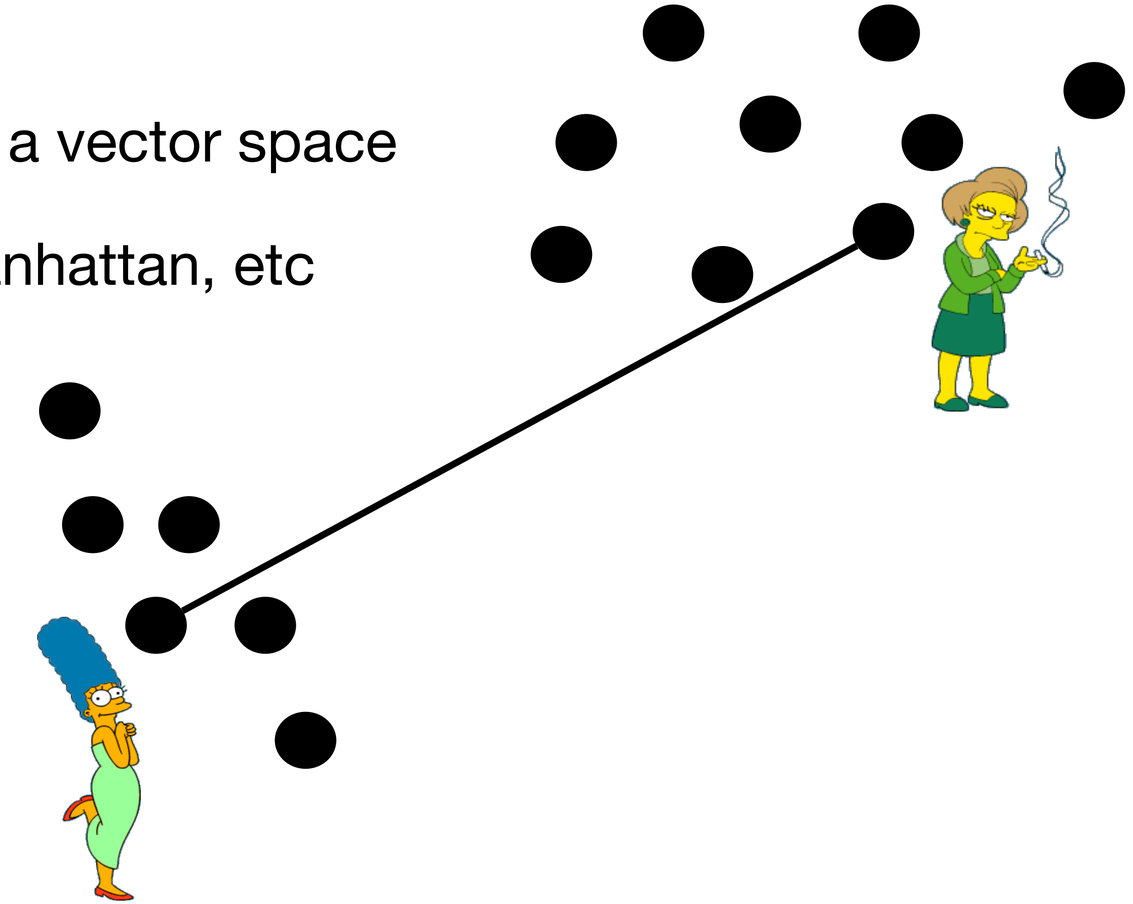


Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.

What is the distance between two datapoints?

Start with a distance metric

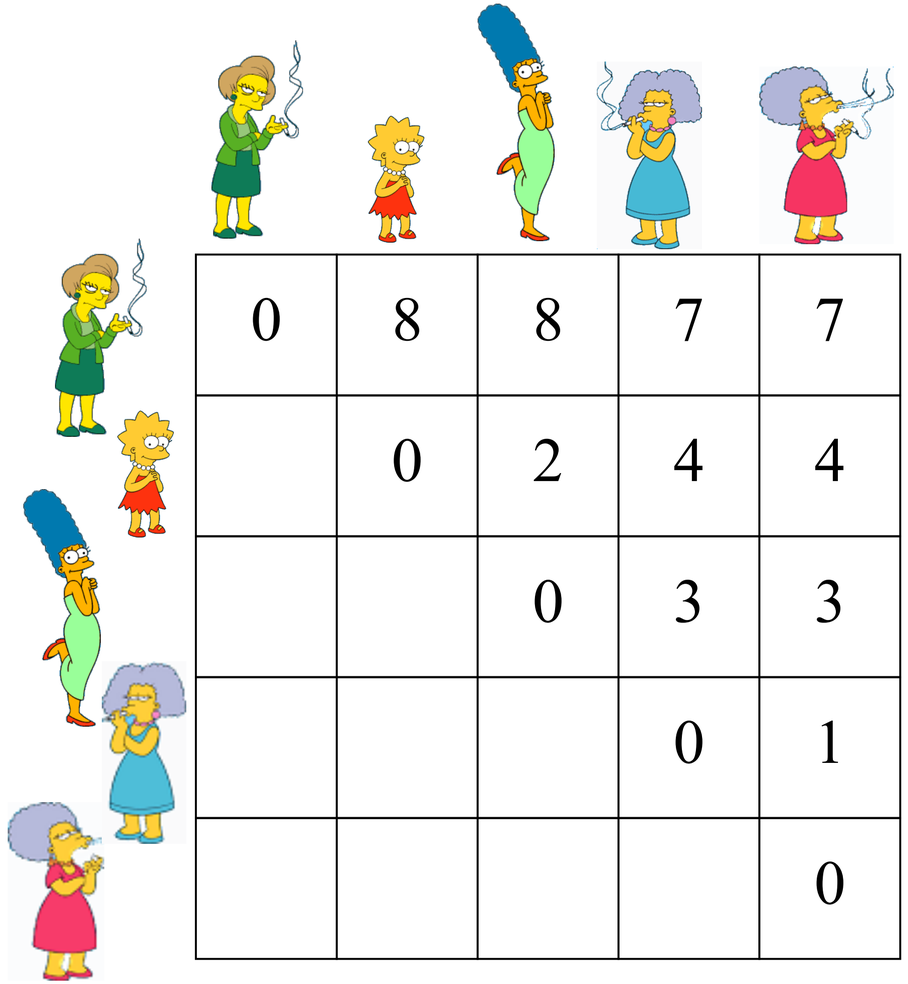
- $d(x, x')$
- Metric operating in a vector space
- e.g., Euclidean, Manhattan, etc



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

D() = 8

D() = 1

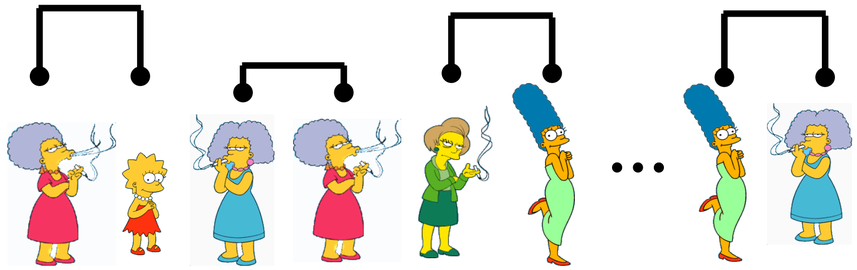


0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
				0

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

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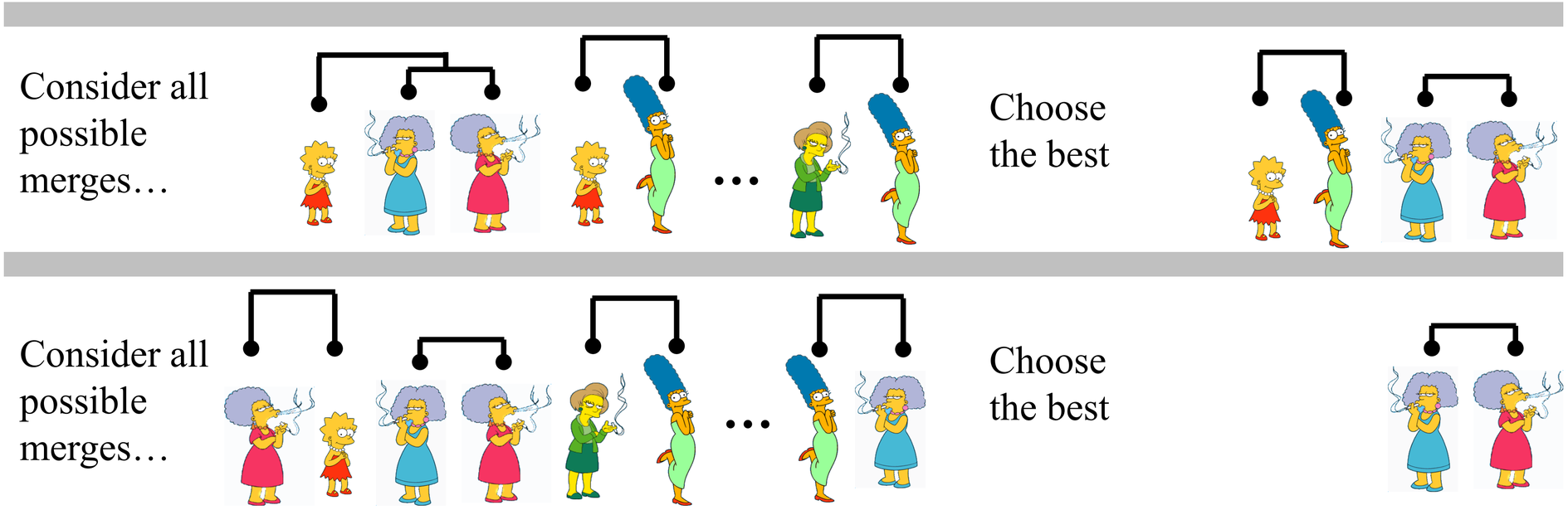

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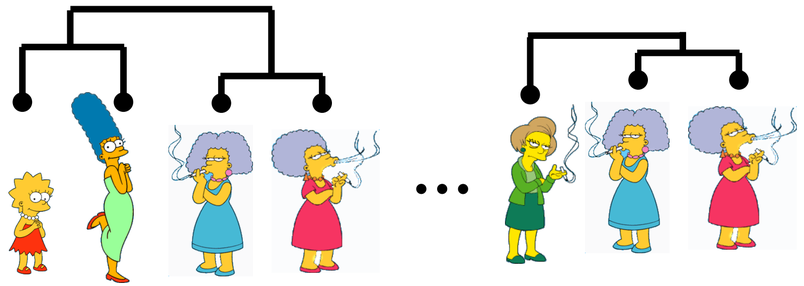
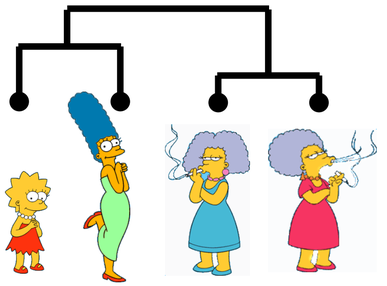


Choose the best



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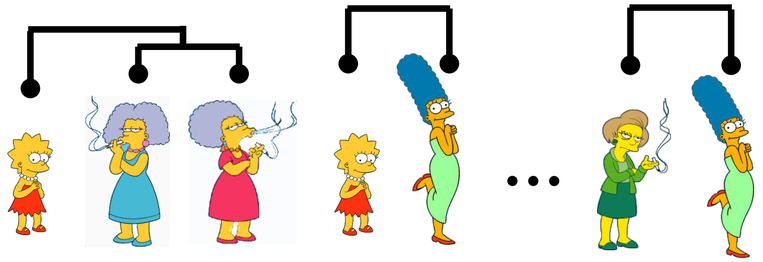
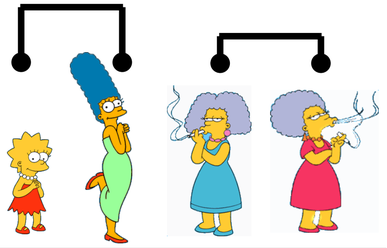


Choose the best



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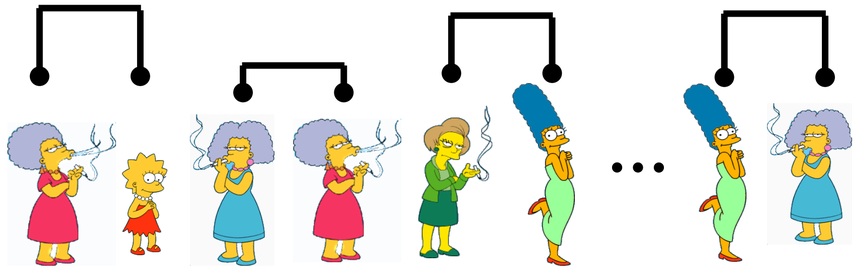

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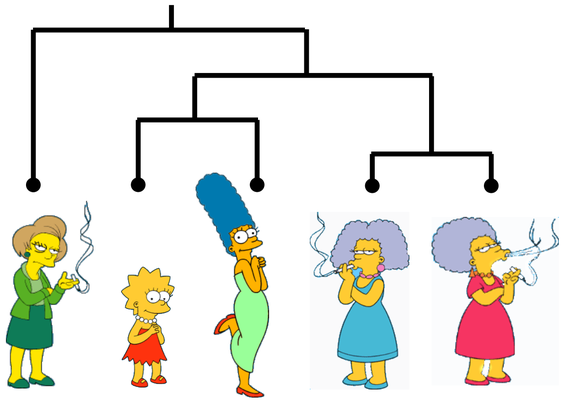

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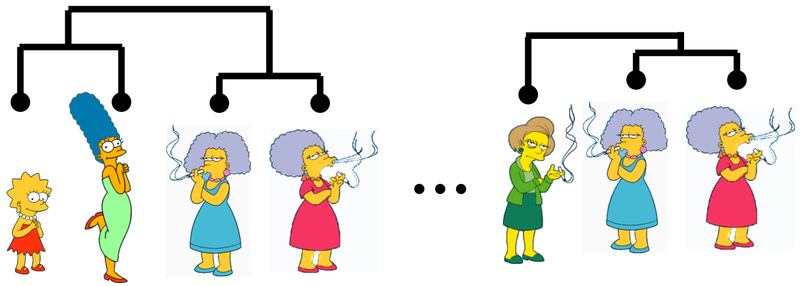
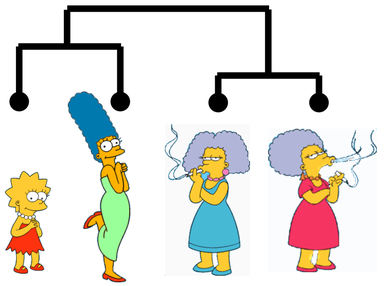


Choose the best



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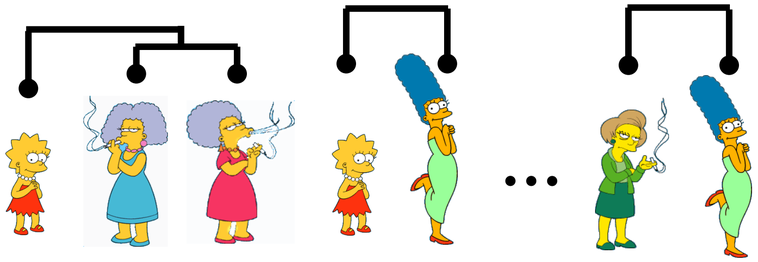
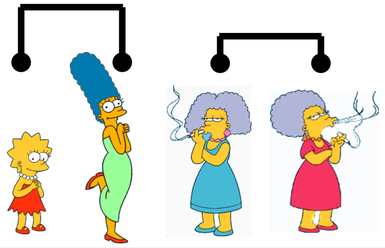


Choose the best



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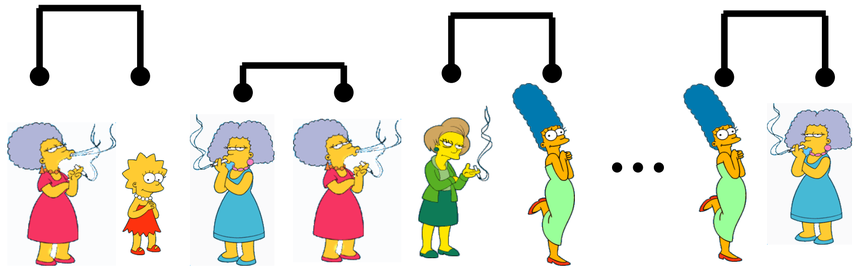
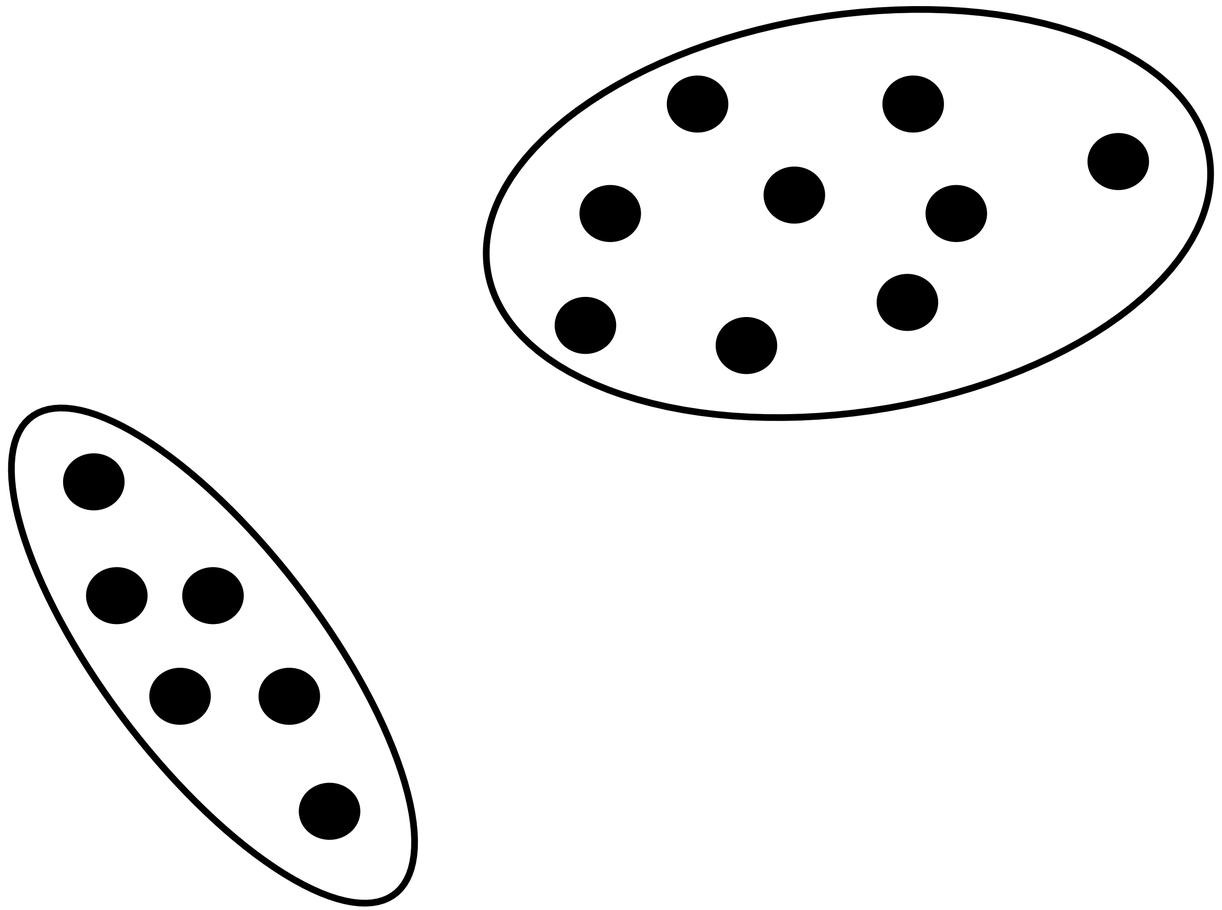


Choose the best

Distance between two clusters

What does it even mean to measure this?

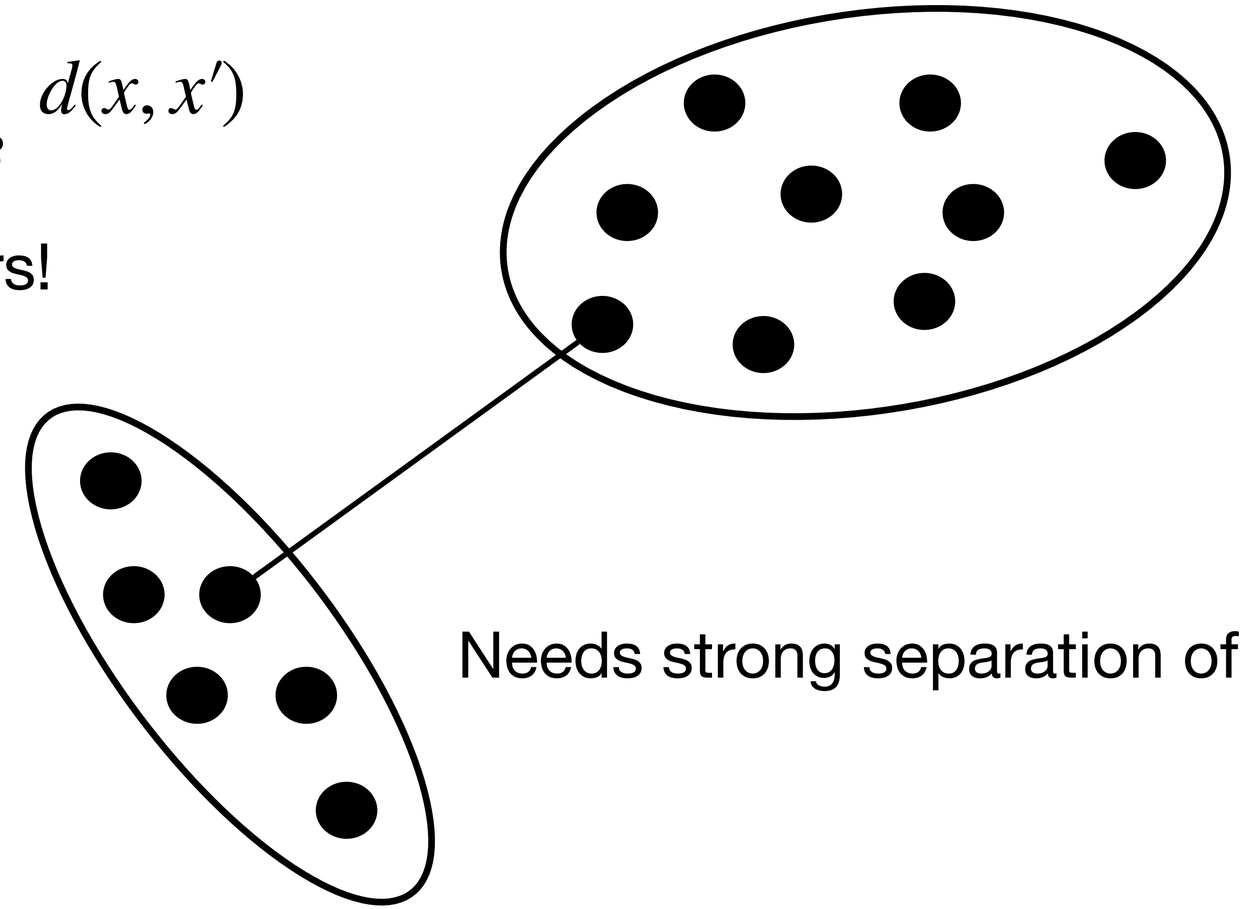


What is the distance between two clusters?

Single linkage

$$d(A, B) = \min_{x \in A, x' \in B} d(x, x')$$

Sensitive to outliers!



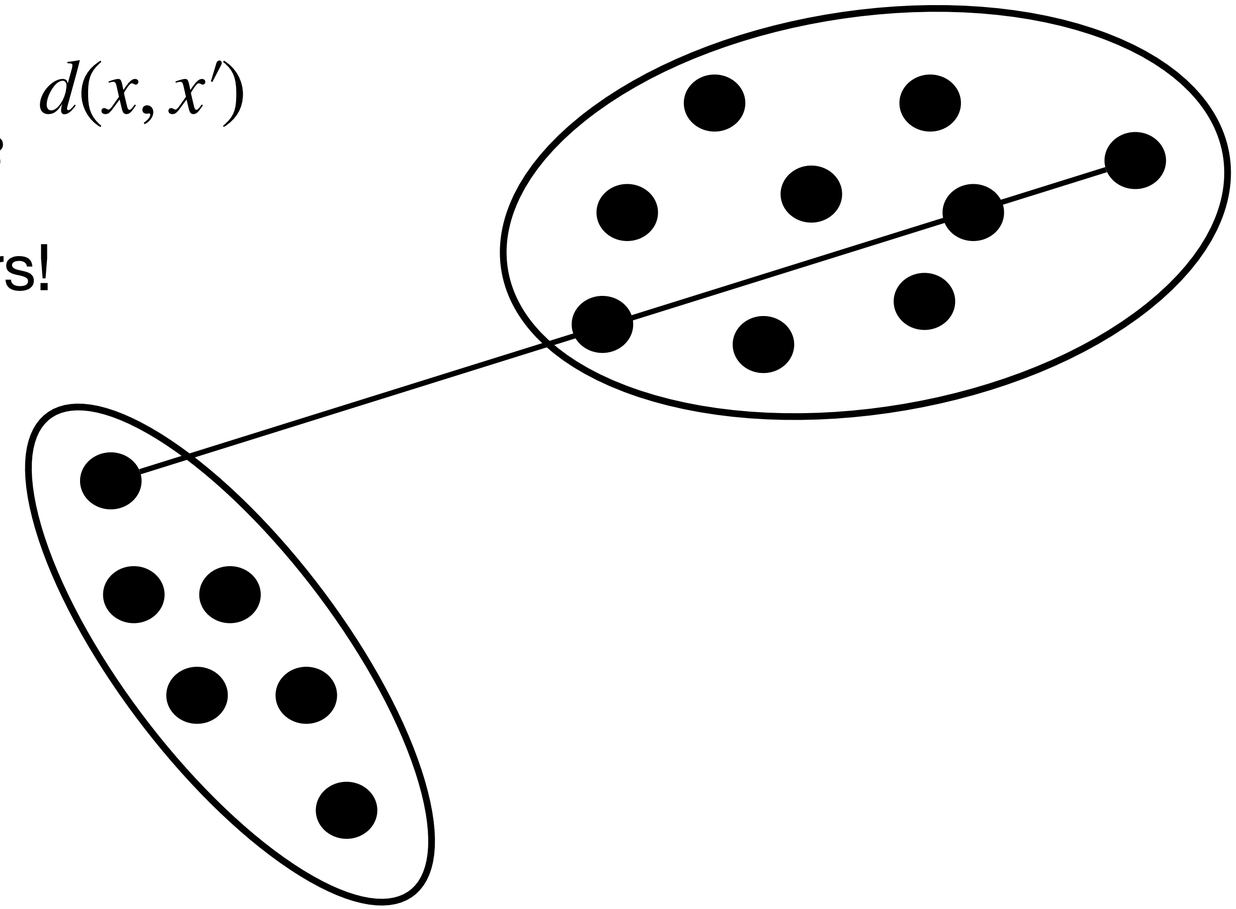
Needs strong separation of compact clusters

What is the distance between two clusters?

Complete linkage

$$d(A, B) = \max_{x \in A, x' \in B} d(x, x')$$

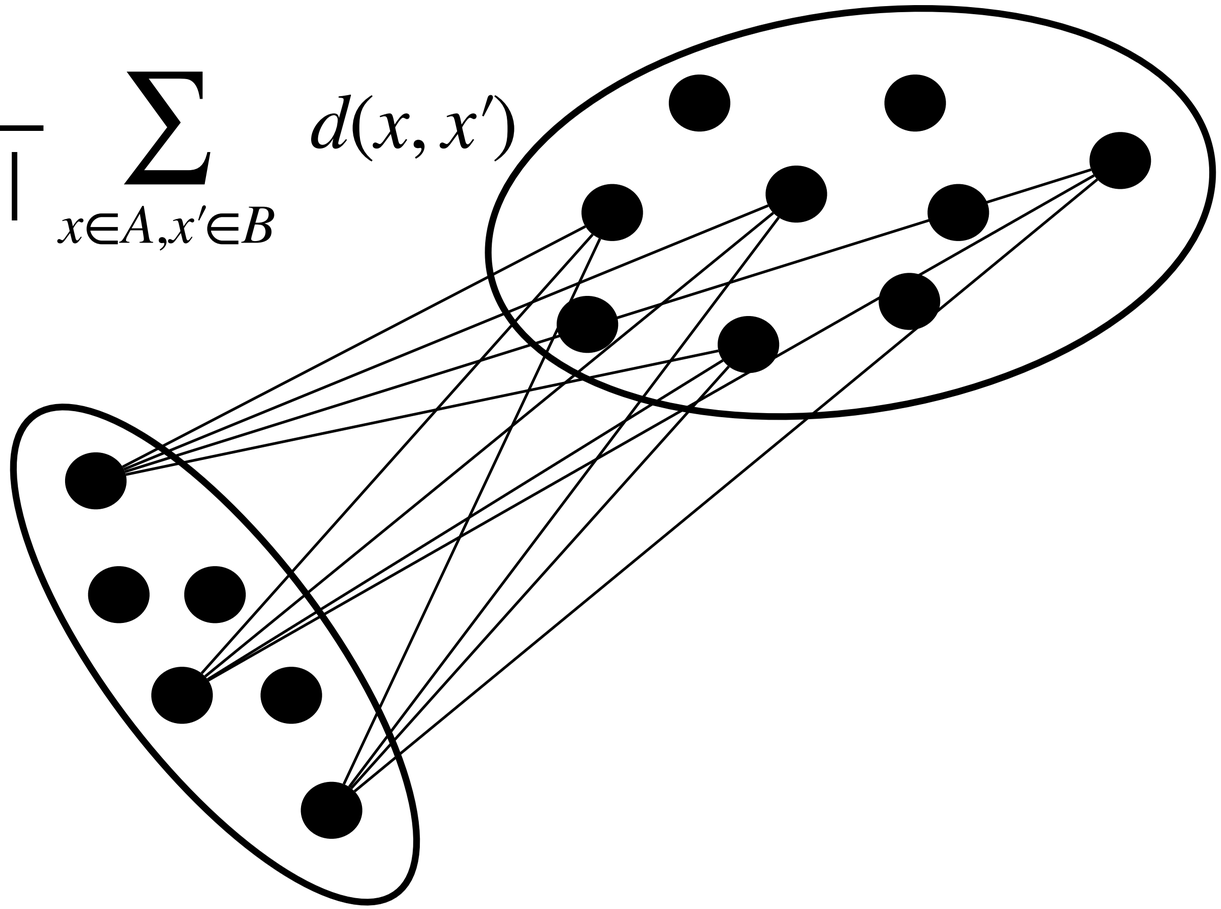
Sensitive to outliers!



What is the distance between two clusters?

Average linkage

$$d(A, B) = \frac{1}{|A||B|} \sum_{x \in A, x' \in B} d(x, x')$$

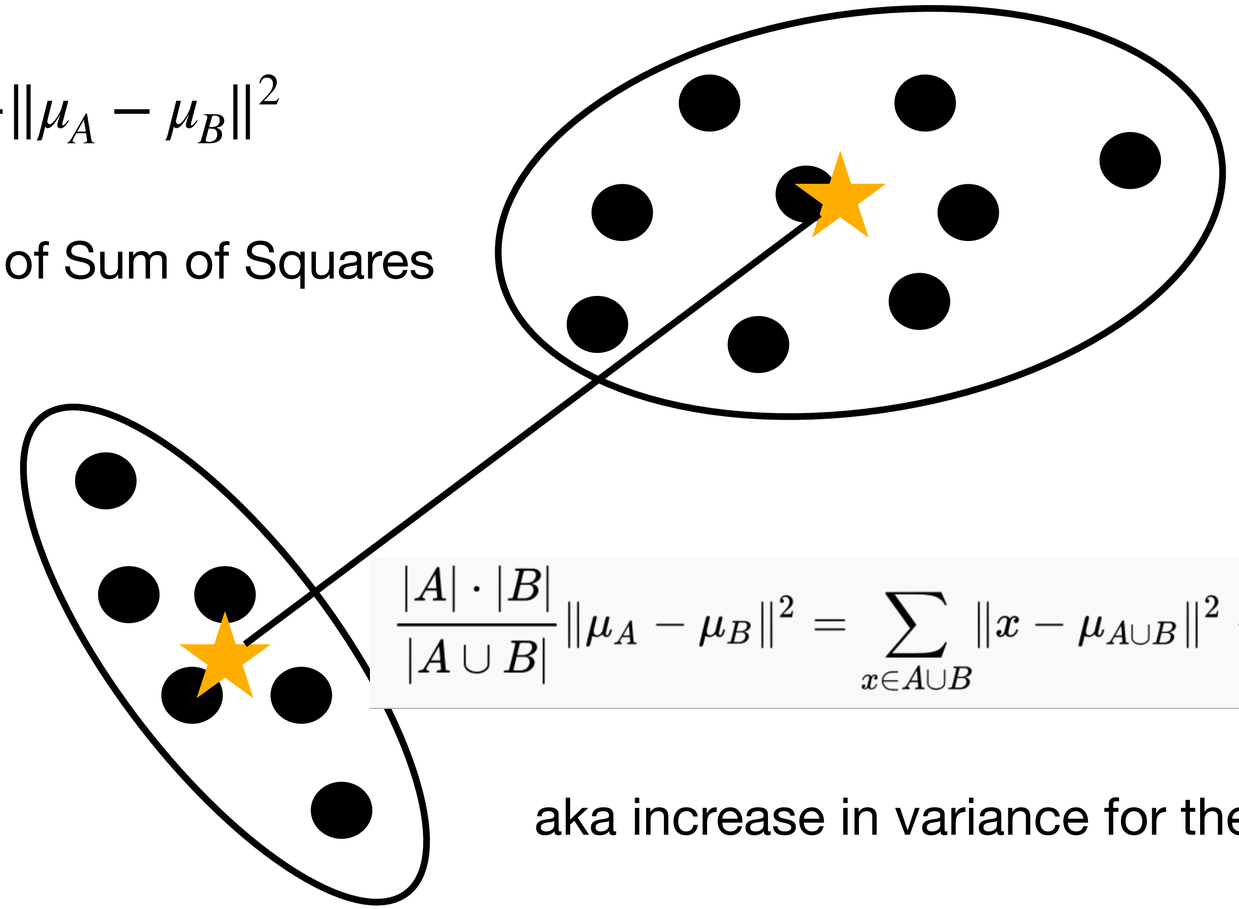


What is the distance between two clusters?

Ward linkage

$$d(A,B) = \frac{|A||B|}{|A|+|B|}\|\mu_A - \mu_B\|^2$$

aka Minimum Increase of Sum of Squares

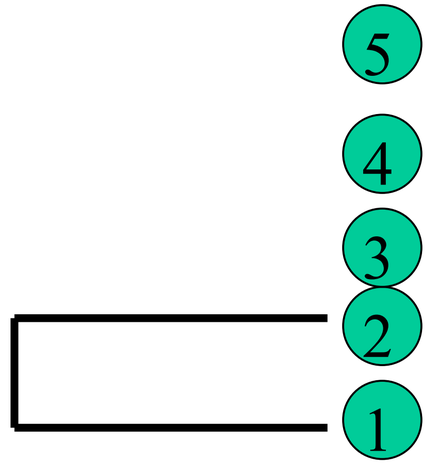


$$\frac{|A|\cdot|B|}{|A\cup B|}\|\mu_A-\mu_B\|^2 = \sum_{x\in A\cup B}\|x-\mu_{A\cup B}\|^2 - \sum_{x\in A}\|x-\mu_A\|^2 - \sum_{x\in B}\|x-\mu_B\|^2$$

aka increase in variance for the cluster being merged

Example: single link

	1	2	3	4	5
1	0				
2	2	0			
3	6	3	0		
4	10	9	7	0	
5	9	8	5	4	0



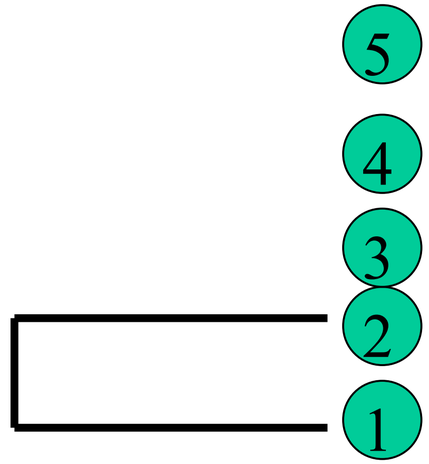
Example: single link

$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}\begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & & & & \\ 2 & 0 & & & \\ 6 & 3 & 0 & & \\ 10 & 9 & 7 & 0 & \\ 9 & 8 & 5 & 4 & 0 \end{bmatrix} \end{array} \Rightarrow \begin{array}{c} \\ (1,2) \\ 3 \\ 4 \\ 5 \end{array}\begin{array}{c} \begin{array}{cccc} (1,2) & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & & & \\ 3 & 0 & & \\ 9 & 7 & 0 & \\ 8 & 5 & 4 & 0 \end{bmatrix} \end{array}$$

$$d_{(1,2),3} = \min\{d_{1,3}, d_{2,3}\} = \min\{6,3\} = 3$$

$$d_{(1,2),4} = \min\{d_{1,4}, d_{2,4}\} = \min\{10,9\} = 9$$

$$d_{(1,2),5} = \min\{d_{1,5}, d_{2,5}\} = \min\{9,8\} = 8$$

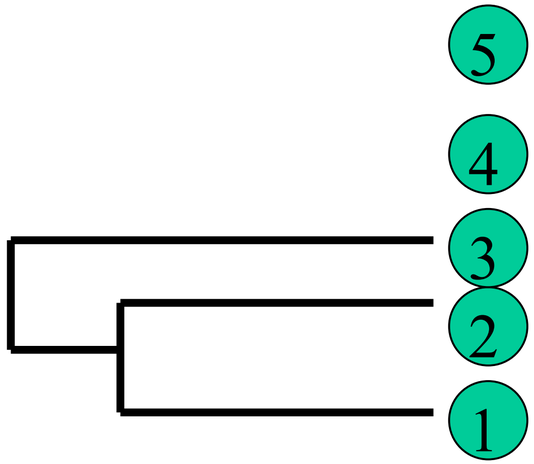


Example: single link

$$\begin{array}{c|ccccc} & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & & & & \\ 2 & 2 & 0 & & & \\ 3 & 6 & 3 & 0 & & \\ 4 & 10 & 9 & 7 & 0 & \\ 5 & 9 & 8 & 5 & 4 & 0 \end{array} \Rightarrow \begin{array}{c|cccc} & (1,2) & 3 & 4 & 5 \\ (1,2) & 0 & & & \\ 3 & 3 & 0 & & \\ 4 & 9 & 7 & 0 & \\ 5 & 8 & 5 & 4 & 0 \end{array} \Rightarrow \begin{array}{c|ccc} & (1,2,3) & 4 & 5 \\ (1,2,3) & 0 & & \\ 4 & 7 & 0 & \\ 5 & 5 & 4 & 0 \end{array}$$

$$d_{(1,2,3),4} = \min\{d_{(1,2),4}, d_{3,4}\} = \min\{9,7\} = 7$$

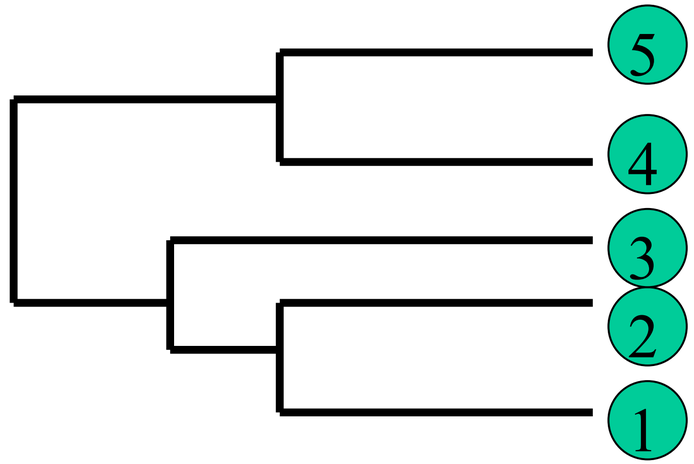
$$d_{(1,2,3),5} = \min\{d_{(1,2),5}, d_{3,5}\} = \min\{8,5\} = 5$$



Example: single link

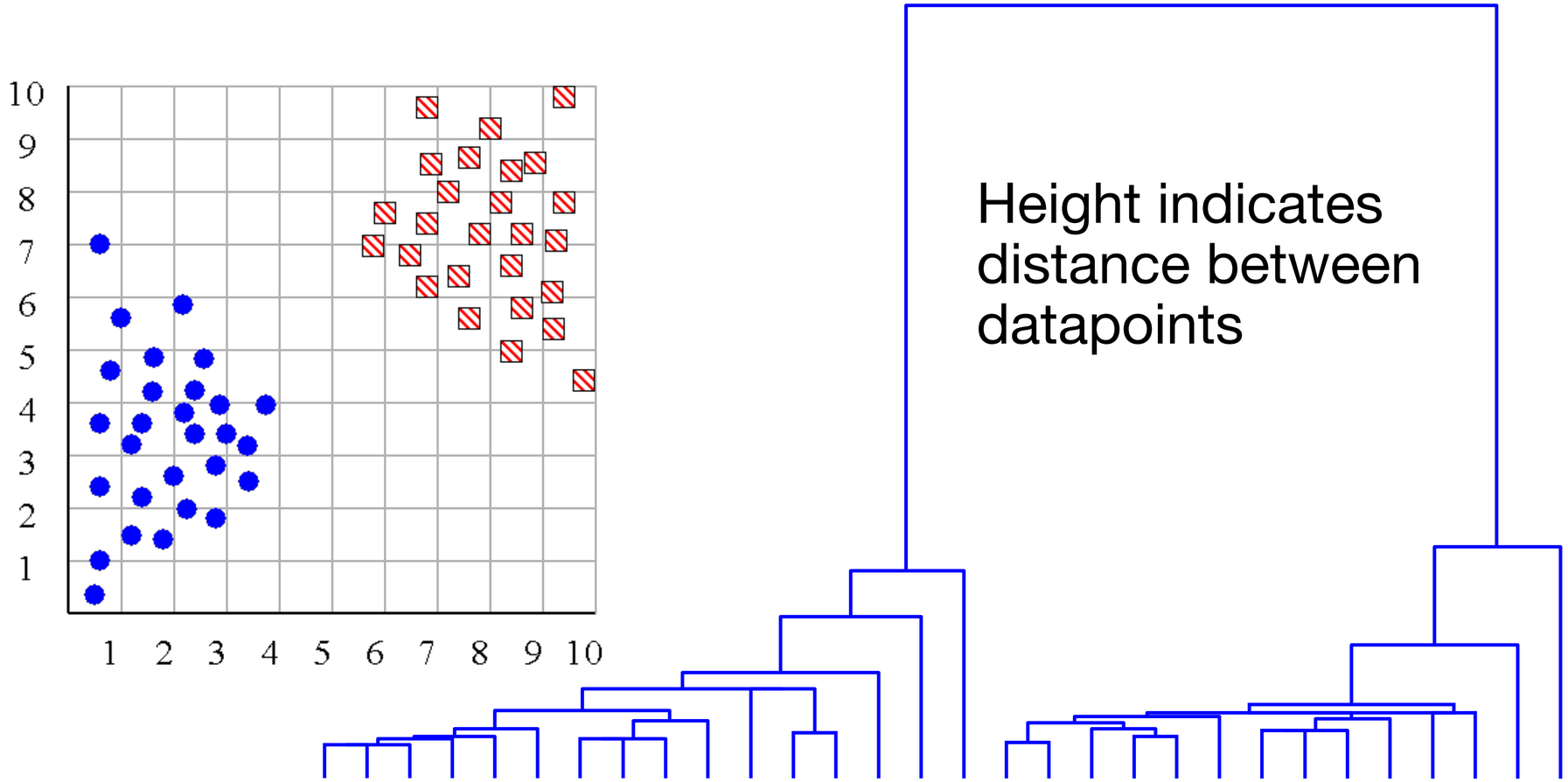
$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}\begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & & & & \\ 2 & 0 & & & \\ 6 & 3 & 0 & & \\ 10 & 9 & 7 & 0 & \\ 9 & 8 & 5 & 4 & 0 \end{bmatrix} \end{array} \Rightarrow \begin{array}{c} \\ (1,2) \\ 3 \\ 4 \\ 5 \end{array}\begin{array}{c} \begin{array}{cccc} (1,2) & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & & & \\ 3 & 0 & & \\ 9 & 7 & 0 & \\ 8 & 5 & 4 & 0 \end{bmatrix} \end{array} \Rightarrow \begin{array}{c} \\ (1,2,3) \\ 4 \\ 5 \end{array}\begin{array}{c} \begin{array}{ccc} (1,2,3) & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & & \\ 7 & 0 & \\ 5 & 4 & 0 \end{bmatrix} \end{array}$$

$$d_{(1,2,3),(4,5)} = \min\{d_{(1,2,3),4}, d_{(1,2,3),5}\} = 5$$



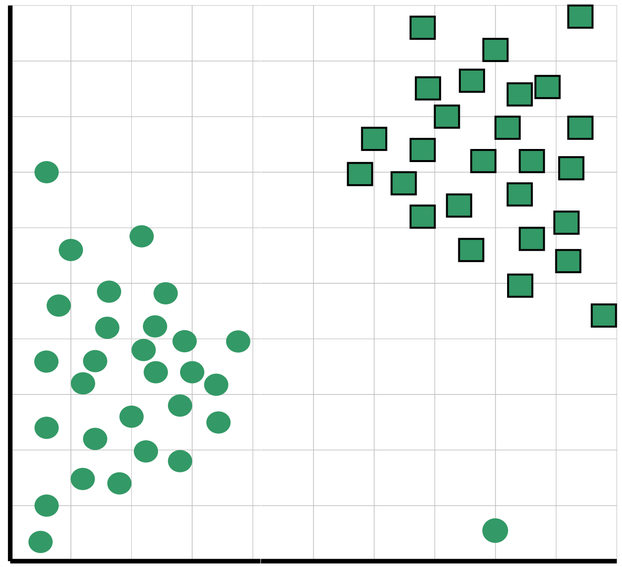
But what are the clusters?

In some cases we can determine the “correct” number of clusters.
However, things are rarely this clear cut, unfortunately.



One potential use of a dendrogram is to detect outliers

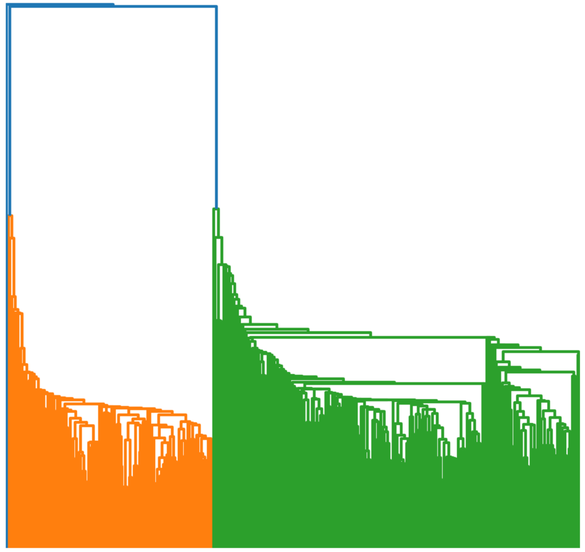
The single isolated branch is suggestive of a data point that is very different to all others



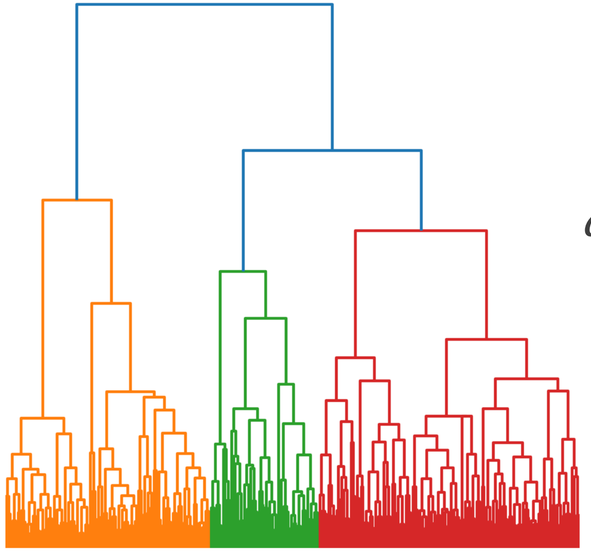
Outlier

$$d(A,B) = \min_{x \in A, x' \in B} d(x,x')$$

Single linkage



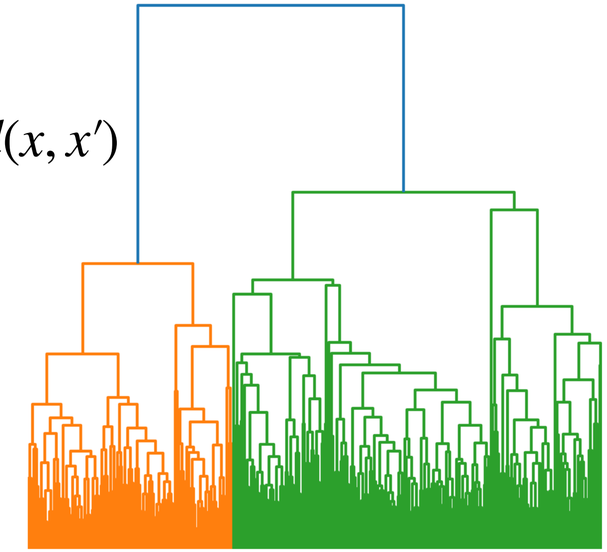
Complete linkage



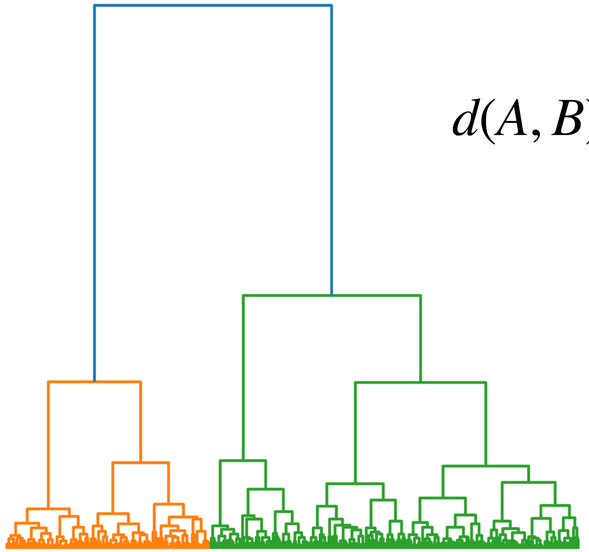
$$d(A,B) = \max_{x \in A, x' \in B} d(x,x')$$

$$d(A,B) = \frac{1}{|A|\,|B|} \sum_{x \in A, x' \in B} d(x,x')$$

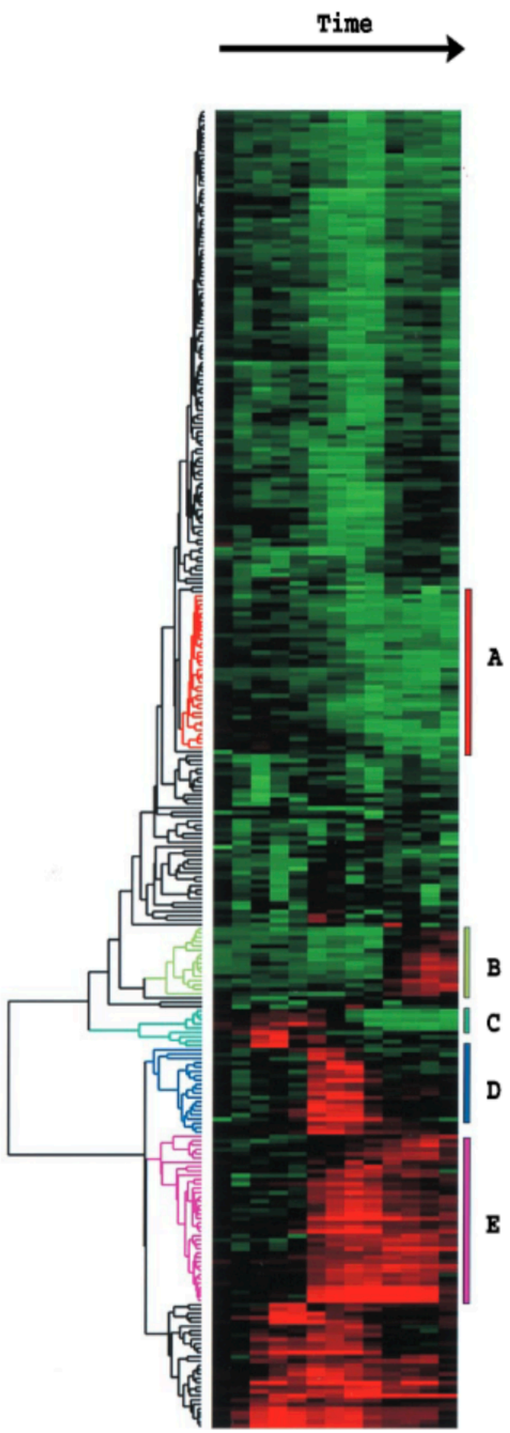
Average linkage



Ward linkage



$$d(A,B) = \frac{|A|\,|B|}{|A| + |B|} \|\mu_A - \mu_B\|^2$$



Hierarchical clustering is frequently used in science, esp genomics

MB Eisen et al, PNAS (1998) >20k citations shows that you can use these techniques to

- Demonstrate gene networks that co-express over time
- Infer function of a gene you didn't know about based on its co-expression partners in the cluster
- (A) cholesterol biosynthesis, (B) the cell cycle, (C) the immediate–early response, (D) angiogenesis, and (E) wound healing and tissue remodeling.