Hierarchical clustering

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Today's lecture

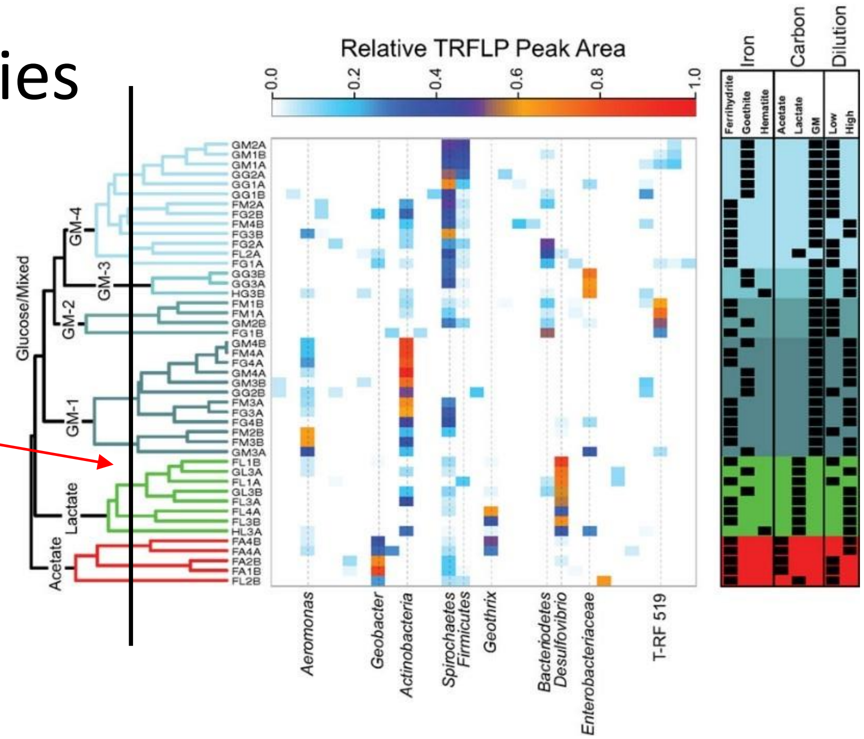
- Hierarchical clustering algorithm
  - Bottom-up: agglomerative
  - Distance between clusters
  - Complexity analysis

Hierarchical clustering

- Build a tree-based hierarchical taxonomy from a set of instances
  - Dendrogram – a useful tool to summarize

similarities

After cutting, each connected component will be a cluster



Agglomerative hierarchical clustering

- Pairwise distance metric between instances

	Captain America	Superman	Spiderman	Ironman	Supergirl	Invisible Woman	Elektra
Captain America	0	1	2	2	3	3	4
Superman		0	2	2	3	3	4
Spiderman			0	2	3	3	4
Ironman				0	3	4	4
Supergirl					0	2	3
Invisible Woman						0	2
Elektra							0

Agglomerative hierarchical clustering

1. Every instance is in its own cluster when initialized
2. Repeat until one cluster left ***Enumerate all the possibilities!***
   1. Find the best pair of clusters to merge and break the tie arbitrarily

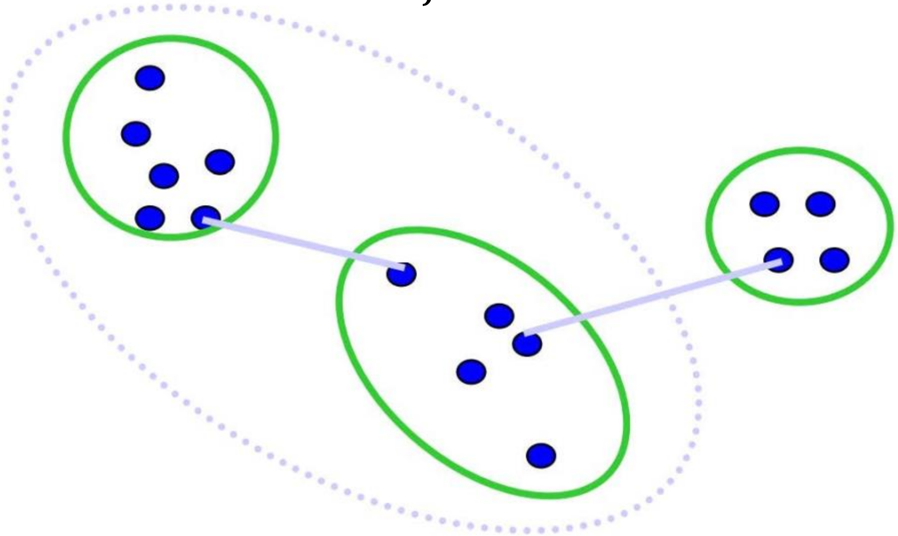
How to compare distance between an ? instance and a cluster of instances?

0	1	2	2	3	3	4
	0	2	2	3	3	4
		0	2	3	3	4
			0	3	4	4
				0	2	3
					0	2
						0

- Single link – Cluster distance = distance of two closest members between the clusters

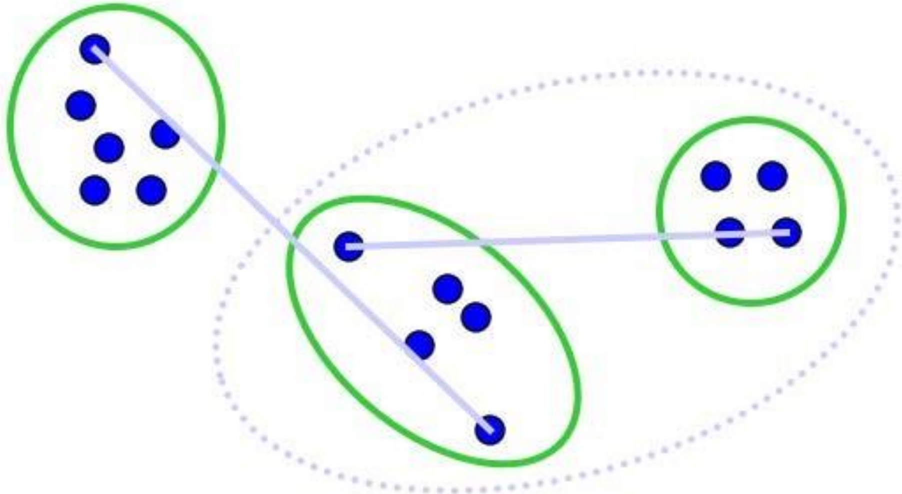
  - $d(c_i, c_j) = \min_{x_n \in c_i, x_m \in c_j} d(x_n, x_m)$

Tend to generate scattered clusters



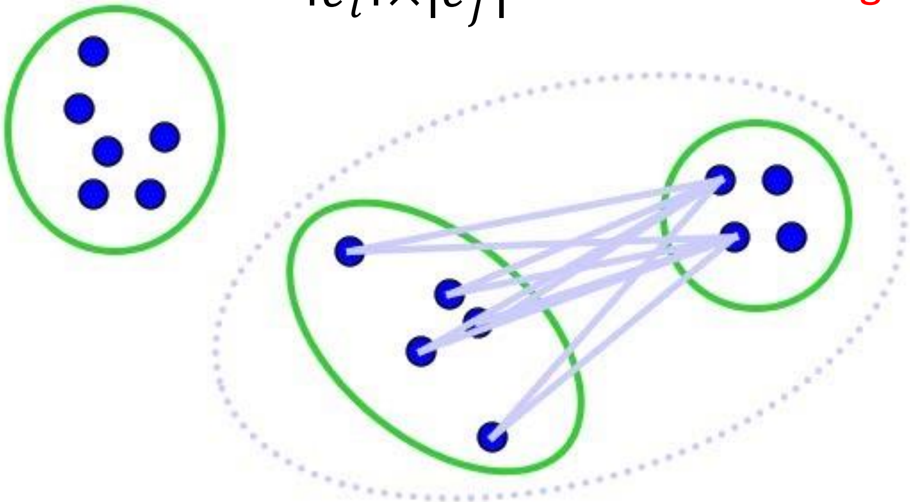
- Complete link
  - Cluster distance = distance of two farthest members between the clusters
  - $d(c_i, c_j) = \max_{x_n \in c_i, x_m \in c_j} d(x_n, x_m)$

Tend to generate tight clusters



- Average link
  - Cluster distance = average distance of all pairs of members between the clusters
  - $d(c_i, c_j) = \frac{\sum_{x_n \in c_i, x_m \in c_j} d(x_n, x_m)}{|c_i| \times |c_j|}$

Mostly popularly used measure, robust against noise



Agglomerative hierarchical clustering

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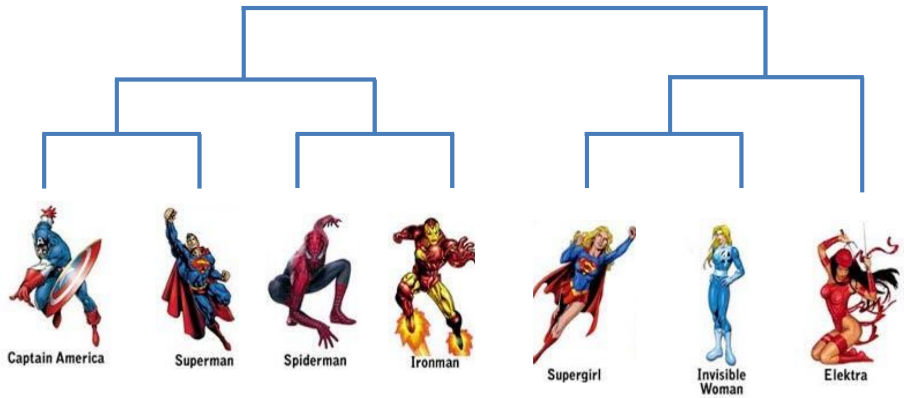

0	1	2	2	3	3	4
	0	2	2	3	3	4
		0	2	3	3	4
			0	3	4	4
				0	2	3
					0	2
						0

Complexity analysis

- In step one, compute similarity between all pairs of nn individual instances - $OO(nn^2)$

- In the following $nn-2$ steps
  - It could be $OO(nn^2 \log nn)$ or even $OO(nn^3)$ (naïve implementation)

In k-means, we have $OO(kknnkk)$, a much faster algorithm

Comparisons

- Hierarchical clustering
  - Efficiency: $OO(nn^3)$, slow

- Assumptions – No assumption – Only need distance metric
- Output
  - Dendrogram, a tree
- k-means clustering
  - Efficiency: $OO(kknnkk)$, fast
- Assumptions
  - Strong assumption –

    centroid, latent cluster membership

- Need to specify kk

- Output
  - kk clusters

How to get final clusters?

- If kk is specified, find a cut that generates kk clusters
  - Since every time we only merge 2 clusters, such cut must exist

- If kk is not specified, use the same strategy as in k-means – Cross validation with internal or external validation

What you should know

- Agglomerative hierarchical clustering
  – Three types of linkage function • Single link, complete link and average link

- – Comparison with *k*-means
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