Machine Learning

Lecture 19: Unsupervised Clustering (I): Hierarchical

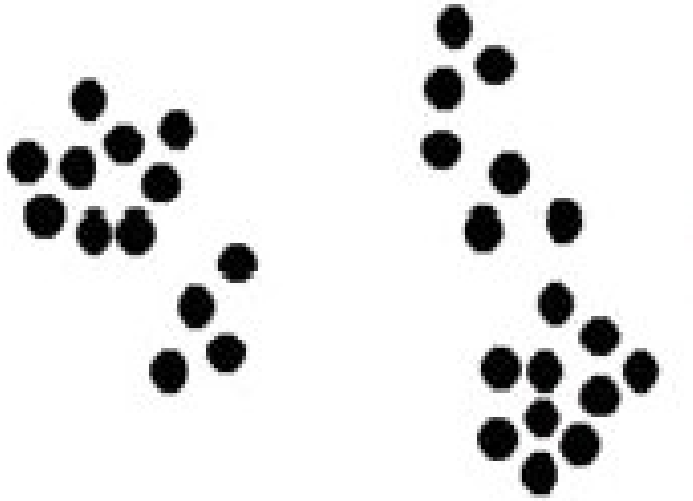
Dr. Beilun Wang

Southeast University
School of Computer Science
and Engineering

Course Content Plan

- Regression (supervised) — Y is a continuous
- Classification (supervised) — Y is a discrete
- Unsupervised models — NO Y
  - Dimension Reduction (PCA)
  - Clustering (K-means, GMM/EM, Hierarchical)
- Learning theory — About f()
- Graphical models — About interactions among X1,… Xp
- Reinforcement Learning — Learn program to Interact with its environment

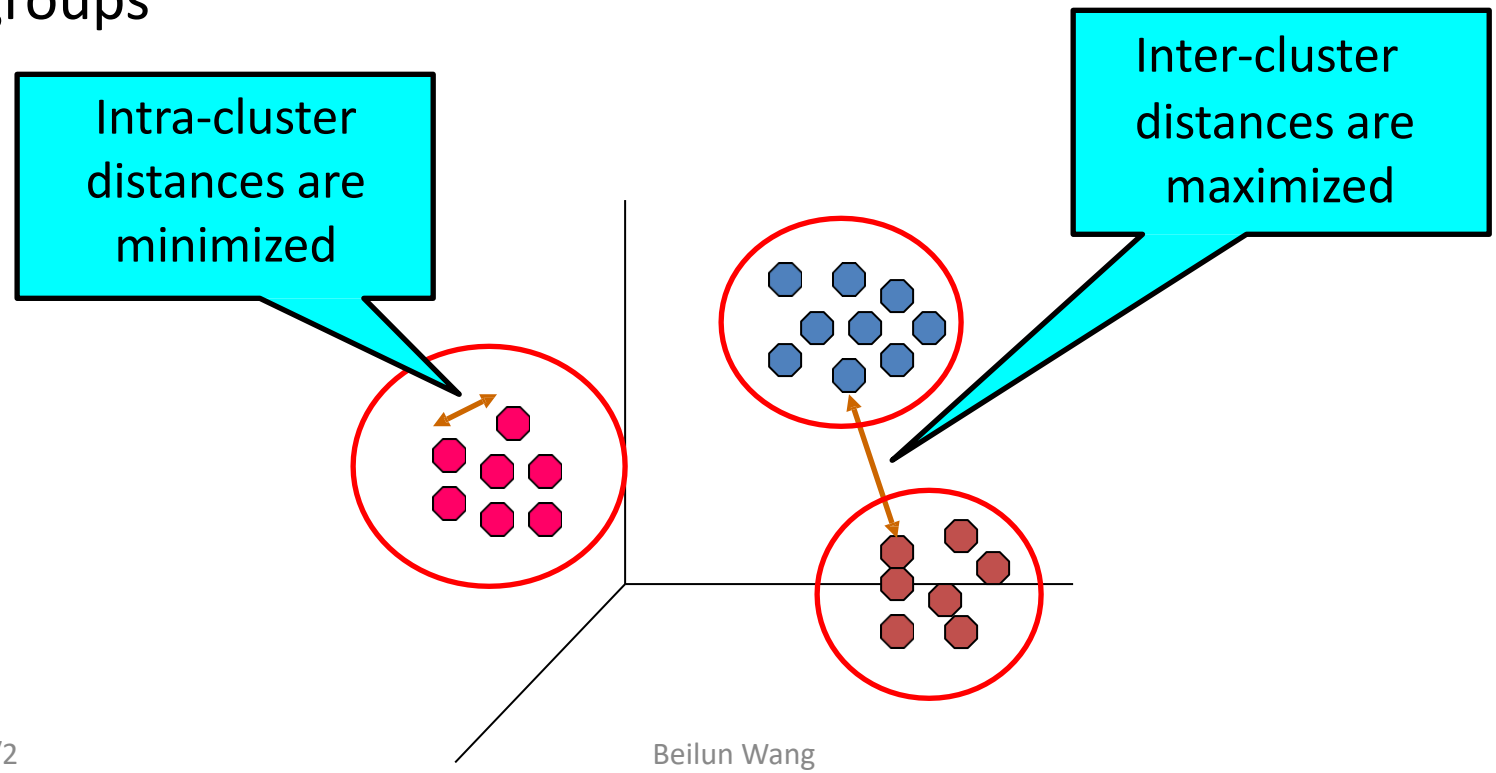
What is clustering?



- Are there any “groups”?
- What is each group?
- How many?
- How to identify them?

What is clustering?

- Find groups (clusters) of data points such that data points in a group will be similar (or related) to one another and different from (or unrelated to) the data points in other groups



What is clustering?

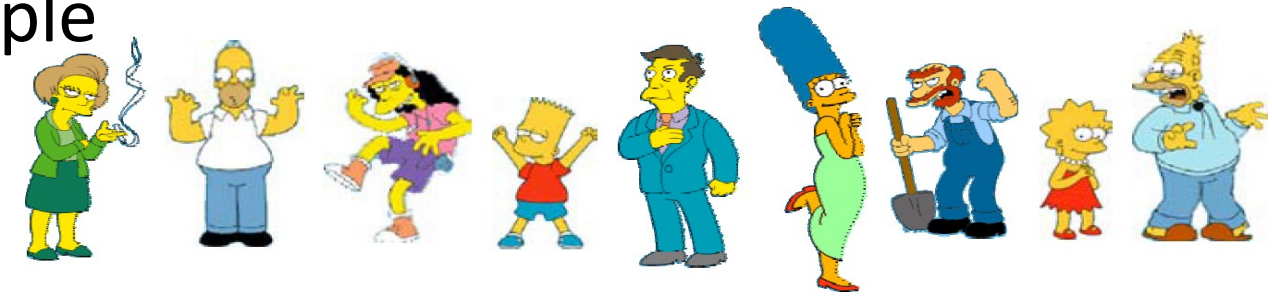
- Clustering: the process of grouping a set of objects into classes of similar objects
  - high intra-class similarity
  - low inter-class similarity
  - It is the commonest form of unsupervised learning

What is clustering?

- Clustering: the process of grouping a set of objects into classes of similar objects
  - high intra-class similarity
  - low inter-class similarity
  - It is the commonest form of unsupervised learning
- A common and important task that finds many applications in Science, Engineering, information Science, and other places, e.g.
  - Group genes that perform the same function
  - Group individuals that has similar political view
  - Categorize documents of similar topics
  - Ideality similar objects from pictures

Toy Examples

- People



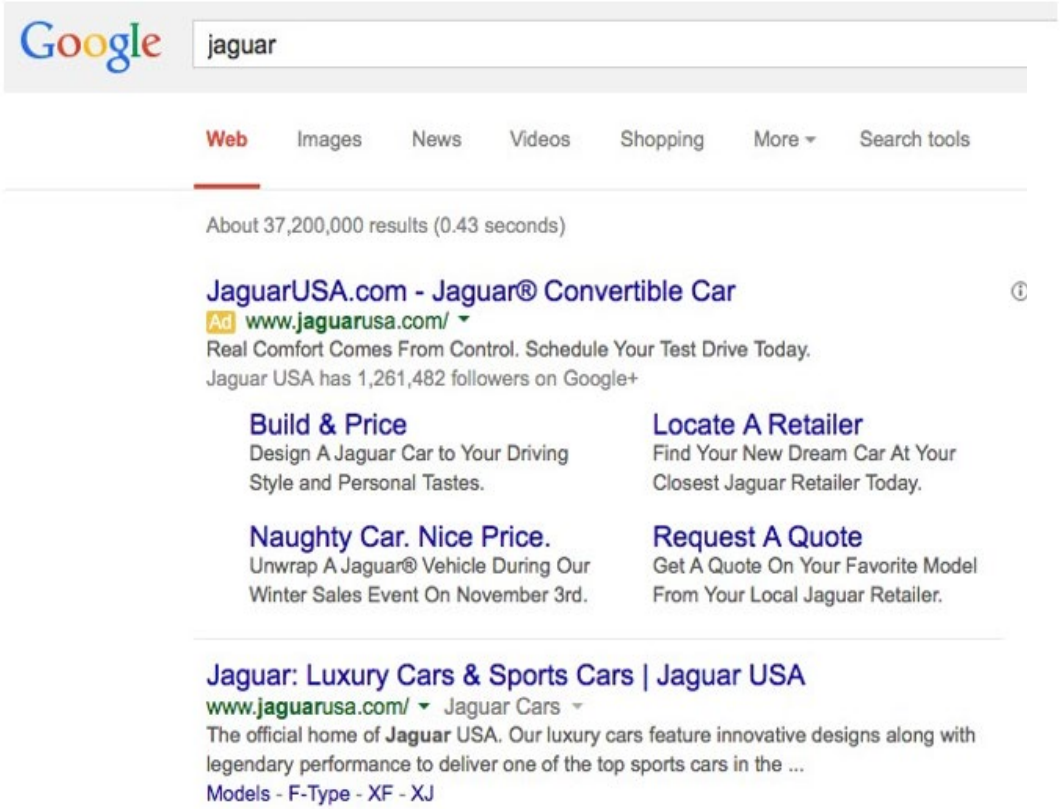
- Images

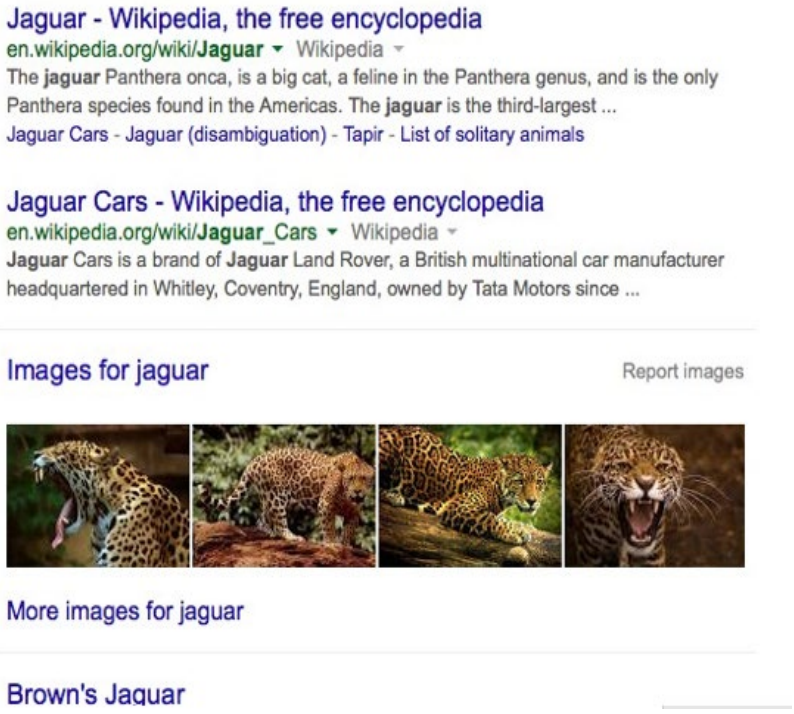
- Language

Piotr Pyotr Petros Pietro Pedro Pierre Piero Peter Peder Peka Peadar

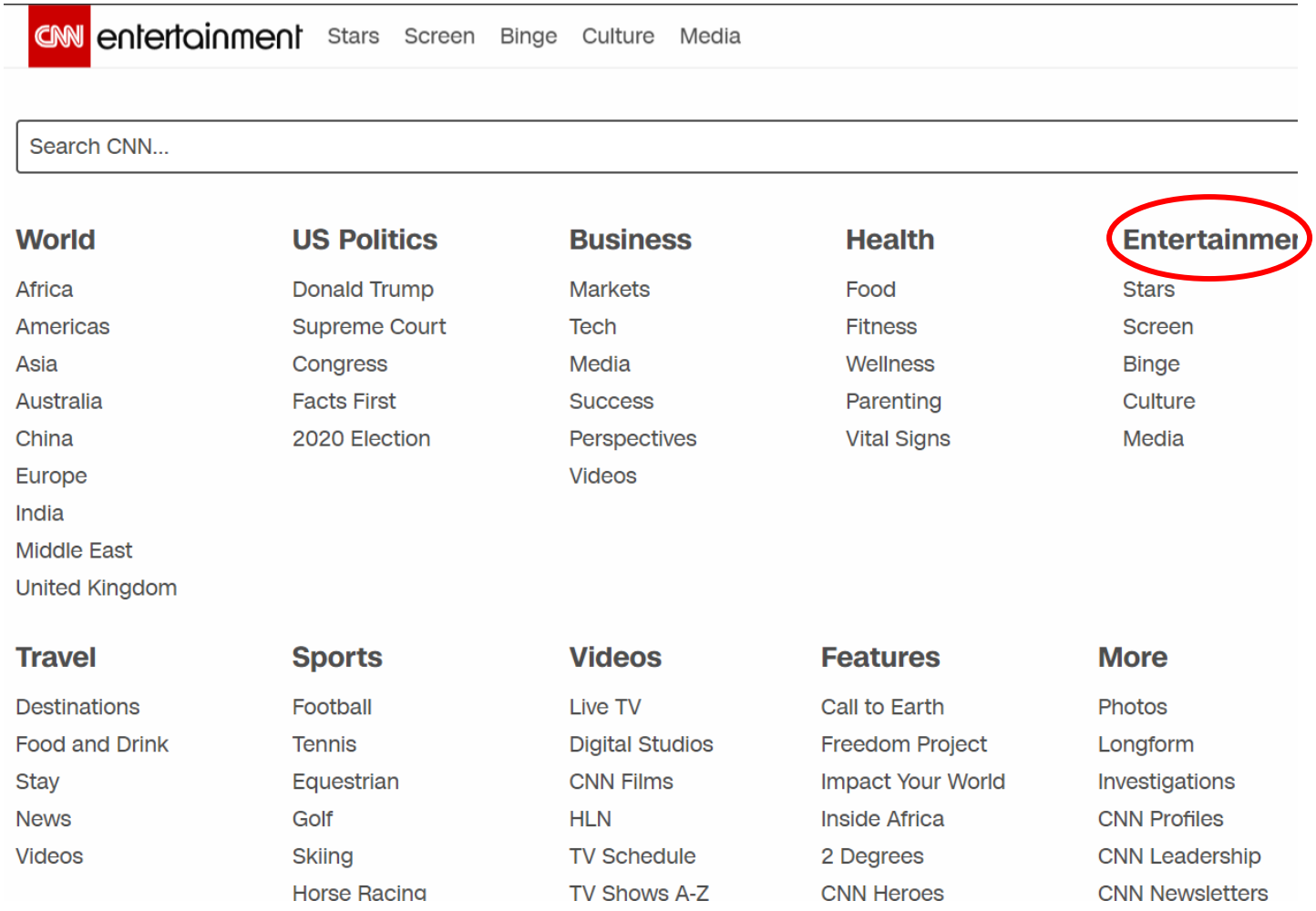
- species

Application (I): Search Result Clustering





Application (II): Navigation



Hierachy

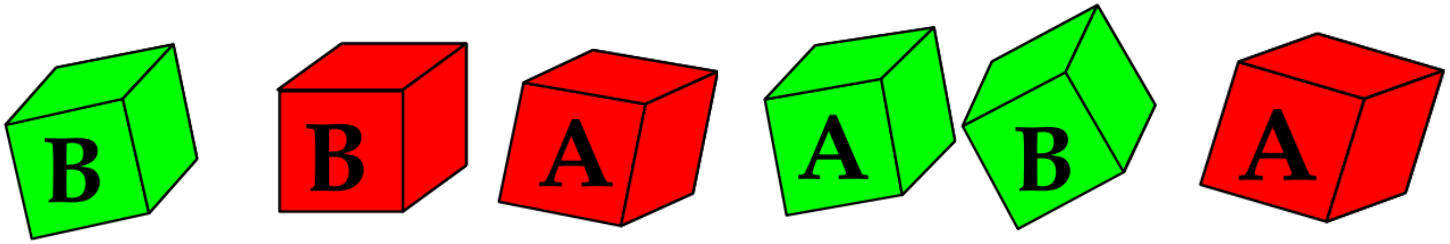
Issues for clustering

- What is a natural grouping among these objects?
- What makes objects “related”?
- Representation for objects
- How many clusters?
- Clustering Algorithms
- Formal foundation and convergence

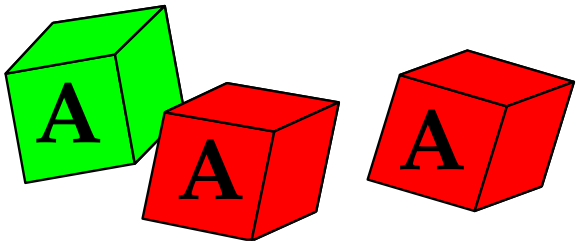
Today

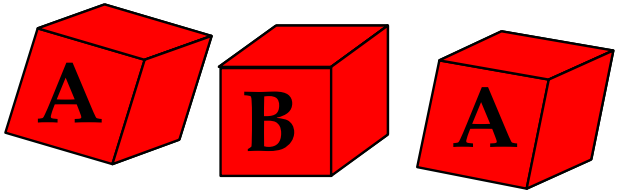
- Definition of "groupness"
- Definition of "similarity/distance“
- Clustering Algorithms
  - Hierarchical algorithms
  - Partitional algorithms
- Formal foundation and convergence
- How many clusters?

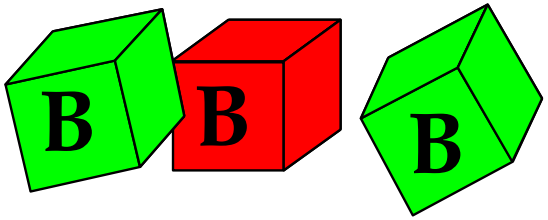
What is a natural grouping among them?

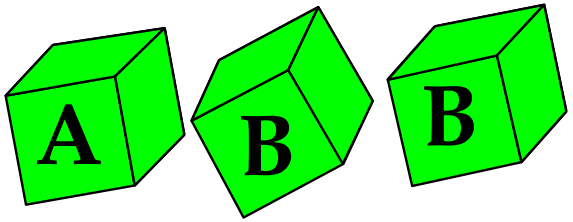


Two possible Solutions:

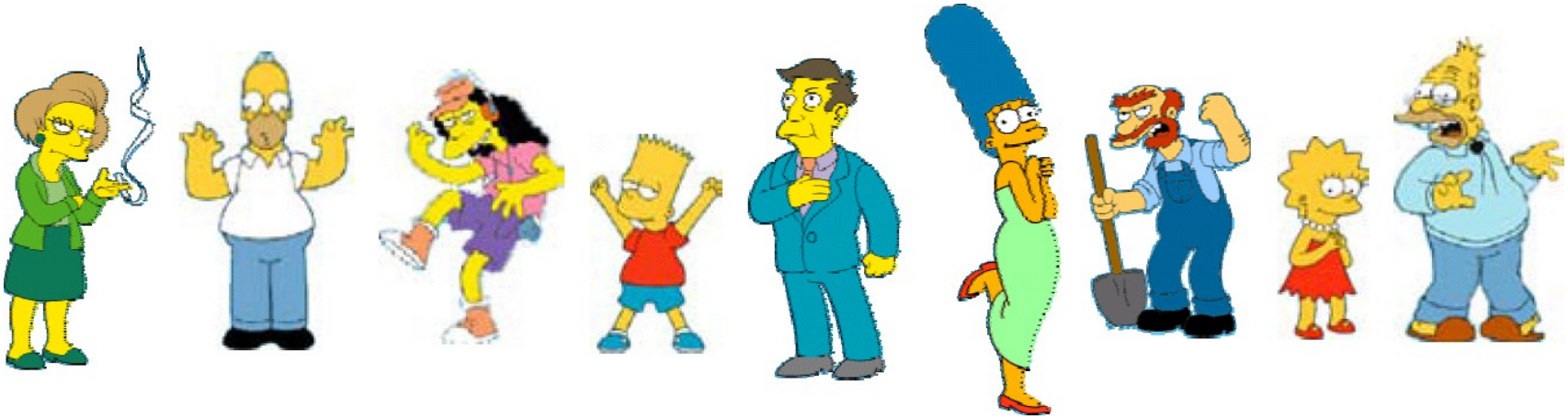




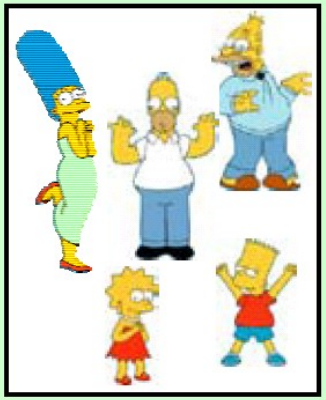




What is a natural grouping among them?

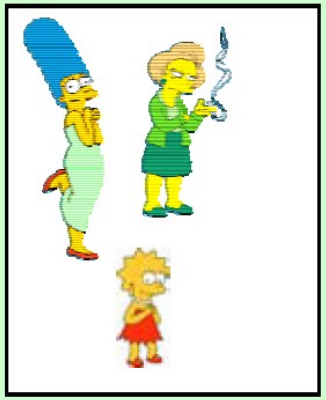


Clustering is subjective



Simpson's Family

School Employees



Females

Males

Today

- Definition of "groupness"
- Definition of "similarity/distance"
- Clustering Algorithms
  - Hierarchical algorithms
  - Partitional algorithms
- Formal foundation and convergence
- How many clusters?

What is Similarity?

Hard to define.
But we know it
when we see it.

- The real meaning of similarity is a philosophical question. We will take a more pragmatic approach.
- Depends on representation and algorithm. For many rep./alg., easier to think in terms of a distance (rather than similarity) between vectors.

Properties of distance measure

- $D(A,B) = D(B,A)$ *Symmetry*
- $D(A,A) = 0$ *Constancy of Self-Similarity*
- $D(A,B) = 0$ IIf A= B *Positivity Separation*
- $D(A,B) <= D(A,C) + D(B,C)$ *Triangular Inequality*

Distance Measures: Minkowski Metric

- Suppose two object *x* and *y* both have *p* features

$$x = (x_1, x_2, \dots, x_p)$$

$$y = (y_1, y_2, \dots, y_p)$$

- The Minkowski metric is defined by

$$d(x,y) = \sqrt[r]{\sum_{i=1}^{p} |x_i - y_i|^r}$$

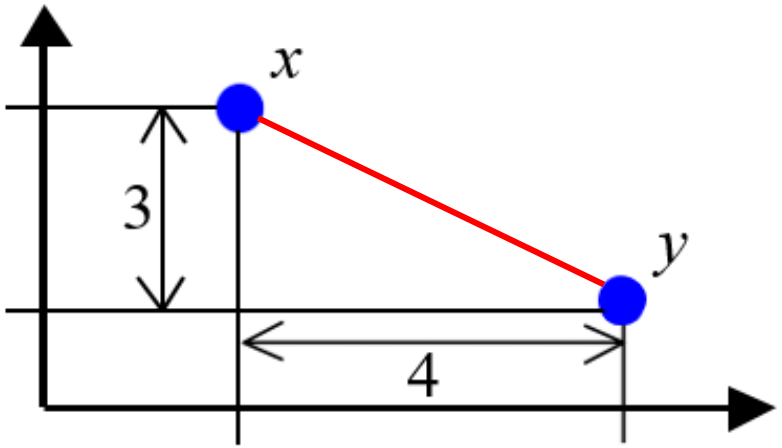
- Most Common Minkowski Metrics

$r = 2$ (Euclidean distance) $\quad d(x,y) = \sqrt[2]{\sum_{i=1}^{p} |x_i - y_i|^2}$

$r = 1$ (Manhattan distance) $\quad d(x,y) = \sum_{i=1}^{p} |x_i - y_i|$

$r = +\infty$ ("sup" distance) $\quad d(x,y) = \max_{1 \le i \le p} |x_i - y_i|$

An Example



1. Euclidean distance: $\sqrt[2]{4^2+3^2}=5.$
2. Manhattan distance: $4+3=7.$
3. "sup" distance: $\max\{4,3\}=4.$

Hamming distance: discrete features

- Manhattan distance is called *Hamming distance* when all features are binary or discrete.

$$d(x,y)=\sum_{i=1}^{p}|x_i-y_i|$$

– E.g., Gene Expression Levels Under 17 Conditions (1-High,0-Low)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
GeneA	0	1	1	0	0	1	0	0	1	0	0	1	1	1	0	0	1
GeneB	0	1	1	1	0	0	0	0	1	1	1	1	1	1	0	1	1

Hamming Distance: $\#(01)+\#(10)=4+1=5$.

Similarity Measures: Correlation Coefficient

- Pearson correlation coefficient

$$s(x,y)=\frac{\sum_{i=1}^{p}(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_{i=1}^{p}(x_i-\bar{x})^2\times\sum_{i=1}^{p}(y_i-\bar{y})^2}}$$

where $\bar{x}=\frac{1}{p}\sum_{i=1}^{p}x_i$ and $\bar{y}=\frac{1}{p}\sum_{i=1}^{p}y_i$.

$$|s(x,y)|\le 1$$

Correlation is unit independent

- Measuring the linear **correlation** between two sequences, x and y,
- giving a value between +1 and −1 inclusive, where 1 is total positive **correlation**, 0 is no **correlation**, and −1 is total negative **correlation**.

- Special case: cosine distance

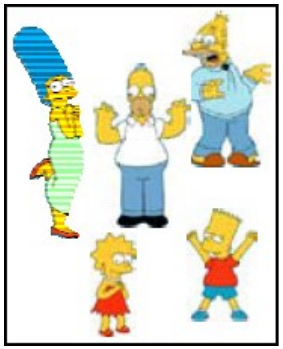
$$s(x,y)=\frac{\vec{x}\cdot\vec{y}}{|\vec{x}|\cdot|\vec{y}|}$$

Today

- Definition of "groupness"
- Definition of "similarity/distance"
- Clustering Algorithms
  - Hierarchical algorithms
  - Partitional algorithms
- Formal foundation and convergence
- How many clusters?

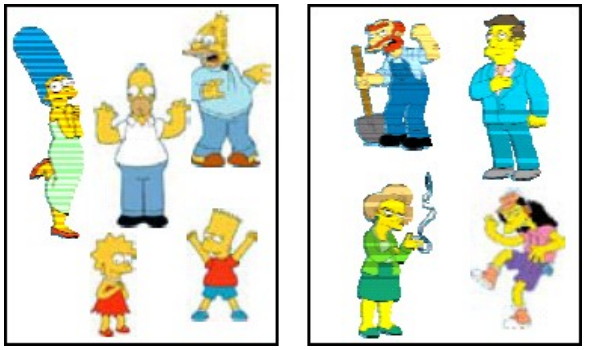
Clustering Algorithms

- Partitional algorithms
  - Usually start with a random (partial) partitioning
  - Refine it iteratively
    - K means clustering
    - Mixture-Model based clustering

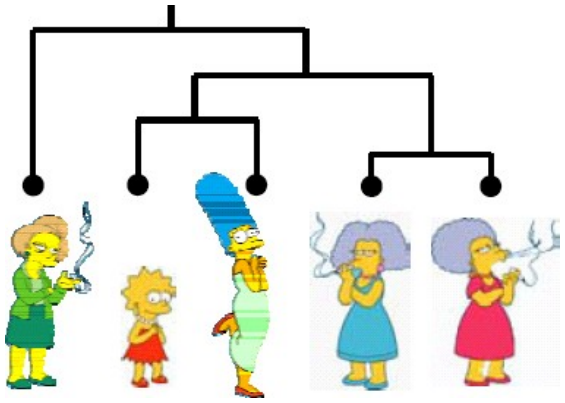


Clustering Algorithms

- Partitional algorithms
  - Usually start with a random (partial) partitioning
  - Refine it iteratively
    - K means clustering
    - Mixture-Model based clustering



- Hierarchical algorithms
  - Bottom-up, agglomerative
  - Top-down, divisive

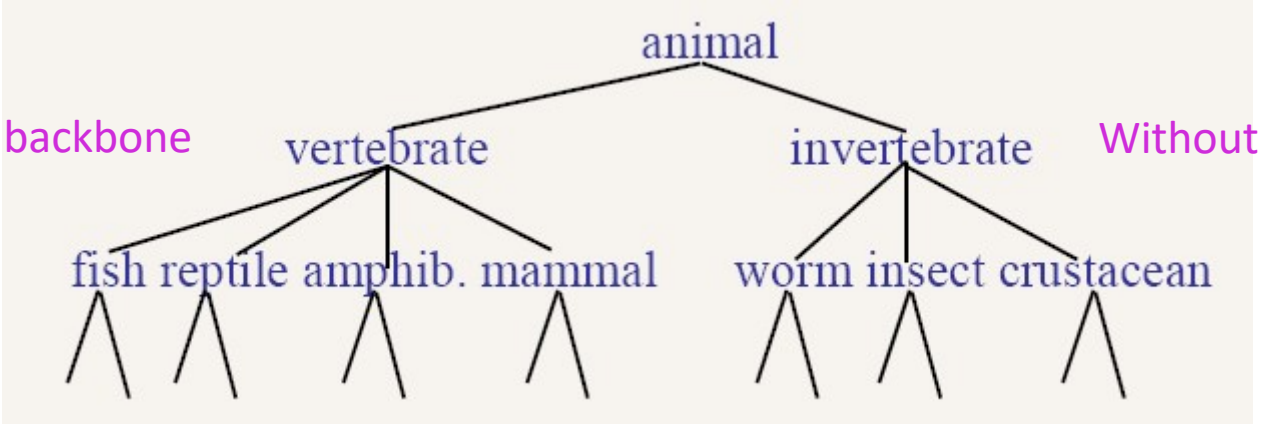


Today

- Definition of "groupness"
- Definition of "similarity/distance"
- Clustering Algorithms
  - Hierarchical algorithms
  - Partitional algorithms
- Formal foundation and convergence
- How many clusters?

Hierarchical Clustering

- Build a tree-based hierarchical taxonomy (dendrogram) from a set of objects, e.g. organisms, documents.



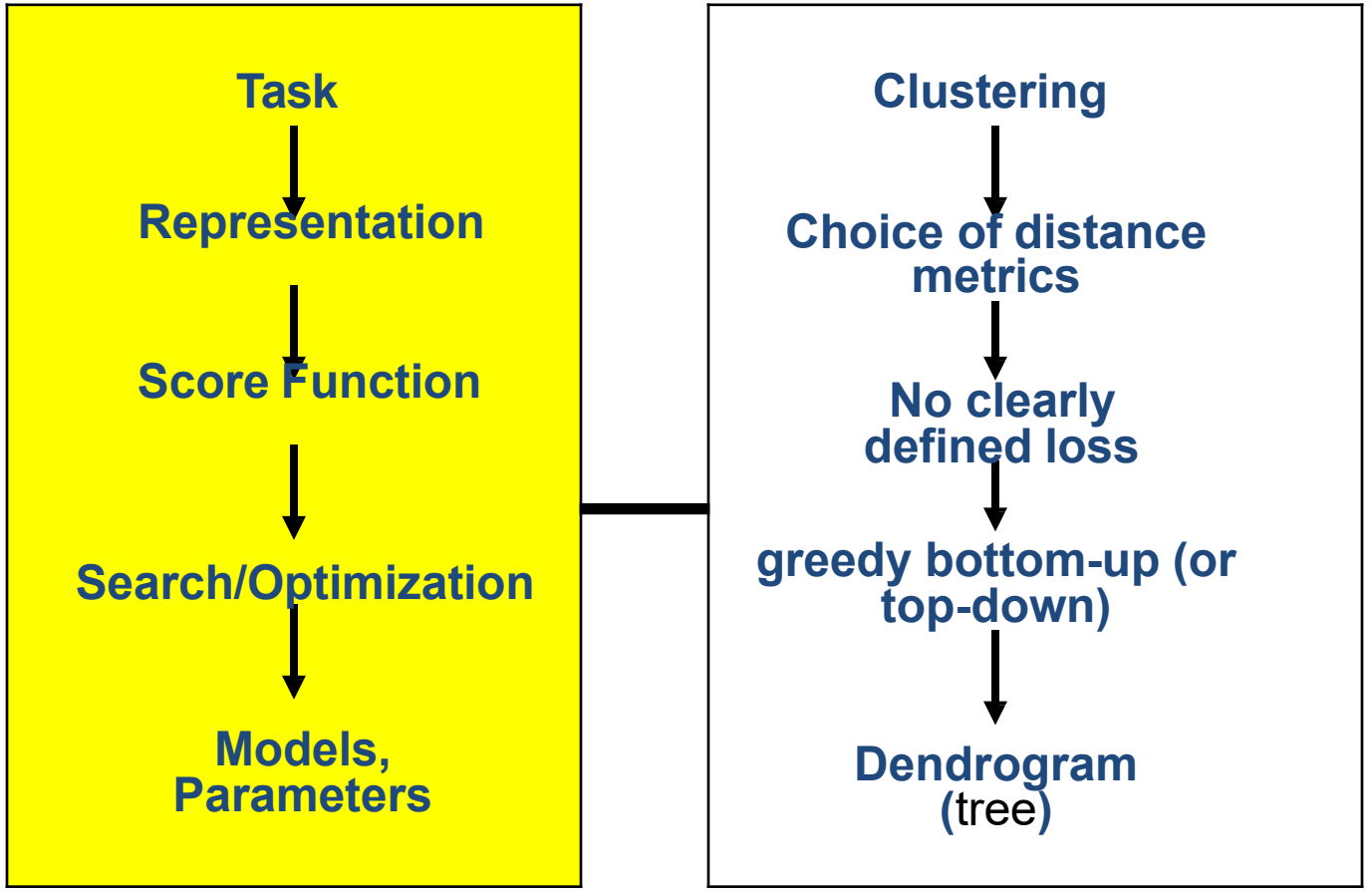
- Note that hierarchies are commonly used to organize information, for example in a web portal.

Hierarchical Clustering

- Given: a set of objects and the pairwise distance matrix

- Find: a tree that optimally hierarchical clustering objects
  - Globally optimal: exhaustively enumerate all tree
  - Effective heuristic methods

Hierarchical Clustering



Distance: A technique for measuring similarity

- To measure the similarity between two objects, transform one of the objects into the other, and measure how much effort it took. The measure of effort becomes the distance measure.

The distance between Patty and Selma.

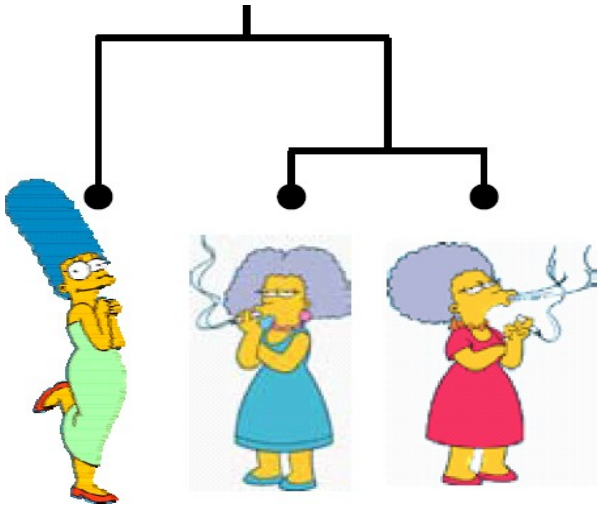
Change dress color, 1 point
Change earring shape, 1 point
Change hair part, 1 point

D(Patty,Selma) = **3**

The distance between Marge and Selma.

Change dress color, 1 point
Add earrings, 1 point
Decrease height, 1 point
Take up smoking, 1 point
Lose weight, 1 point

D(Marge,Selma) = **5**



Marge Patty Selma

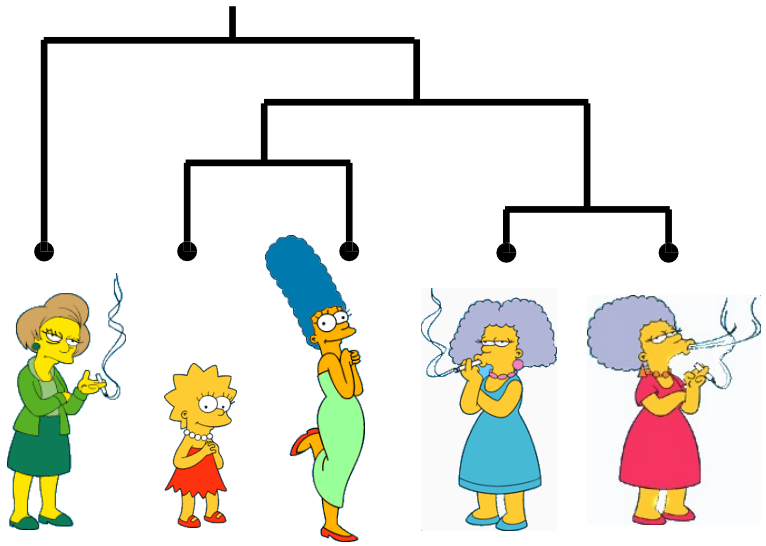
This is called the Edit distance or the Transformation distance

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

np



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.

A greedy local optimal solution

Clustering: the process of grouping a set of objects into classes of similar objects ➔

high intra-class similarity
low inter-class similarity

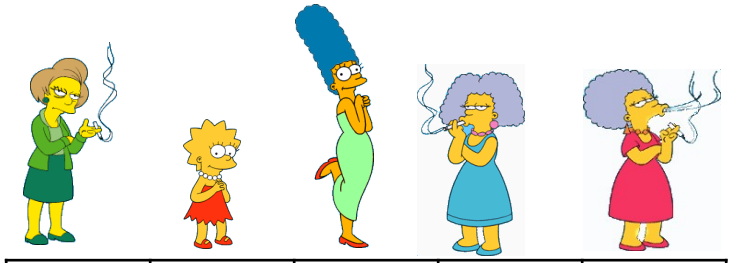
Hierarchical Clustering

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

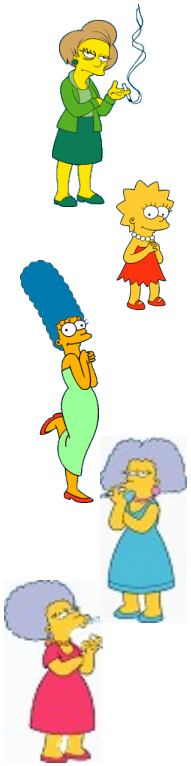
⇒min within cluster distance

$D($  $) = 8$

$D($  $) = 1$

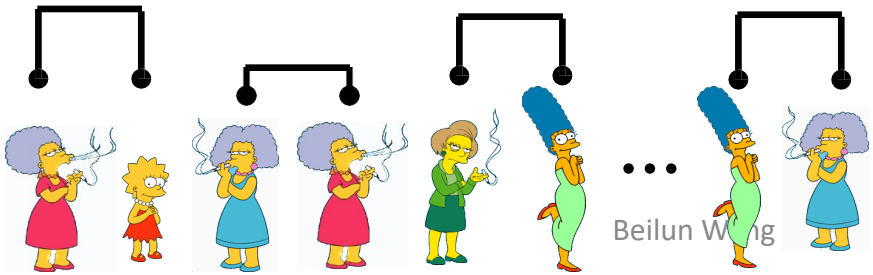


0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
				0

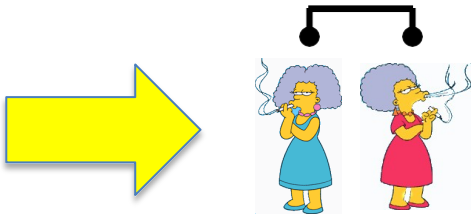


Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.

Consider all Possible merges

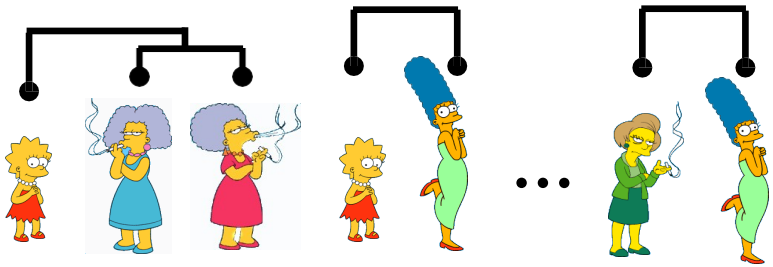


Choose the best

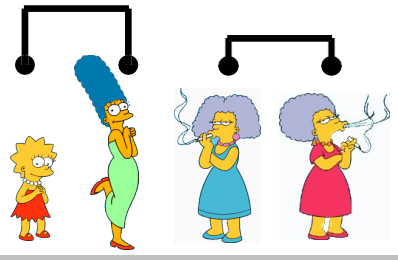


Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.

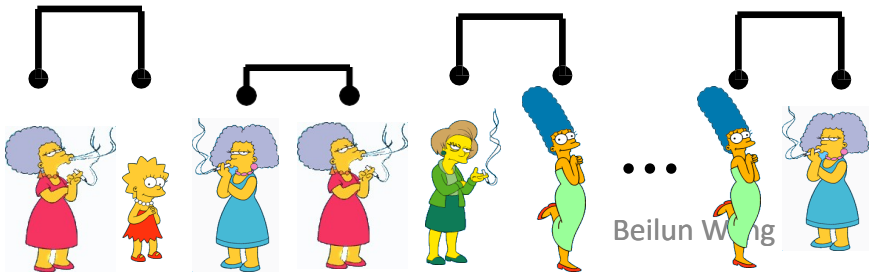
Consider all possible merges…



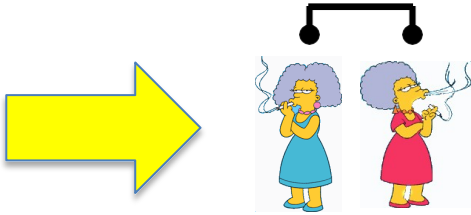
Choose the best



Consider all Possible merges

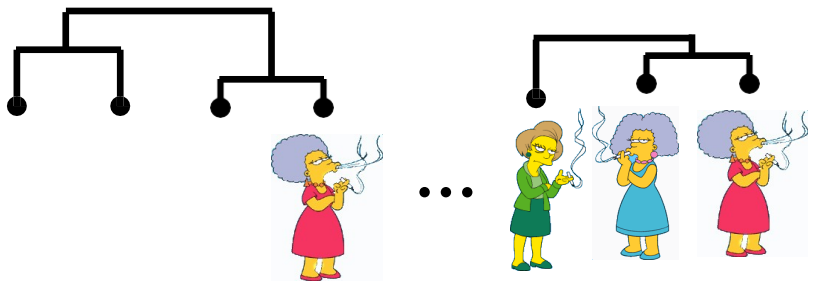


Choose the best

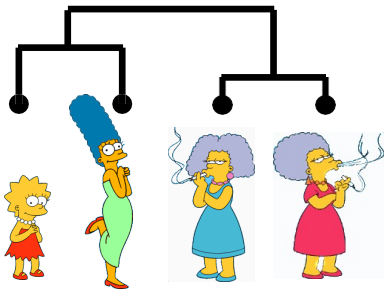


Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.

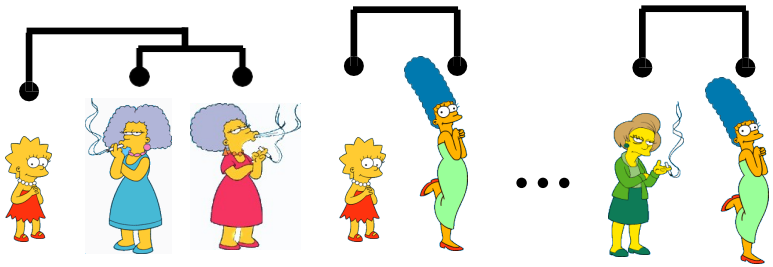
Consider all possible merges…



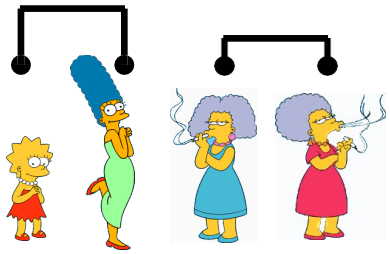
Choose the best



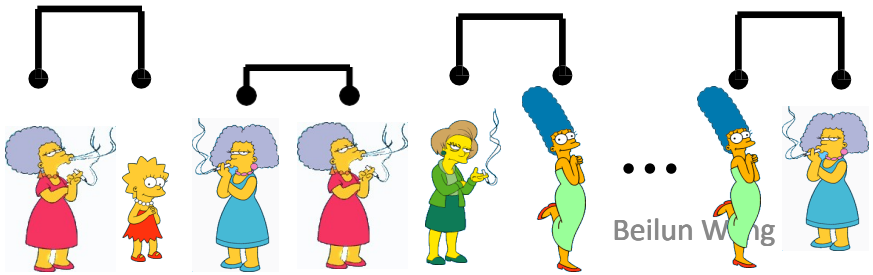
Consider all possible merges…



Choose the best

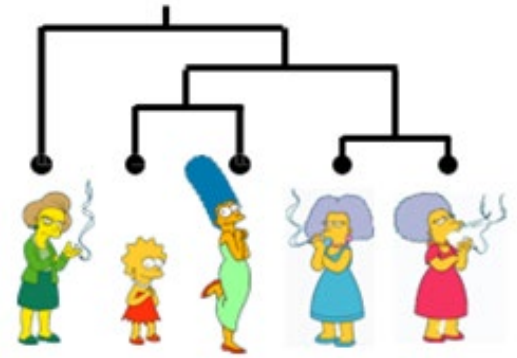


Consider all Possible merges



Choose the best

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

But how do we compute distances between clusters rather than objects?

Consider all possible merges…

Choose the best

Consider all Possible merges

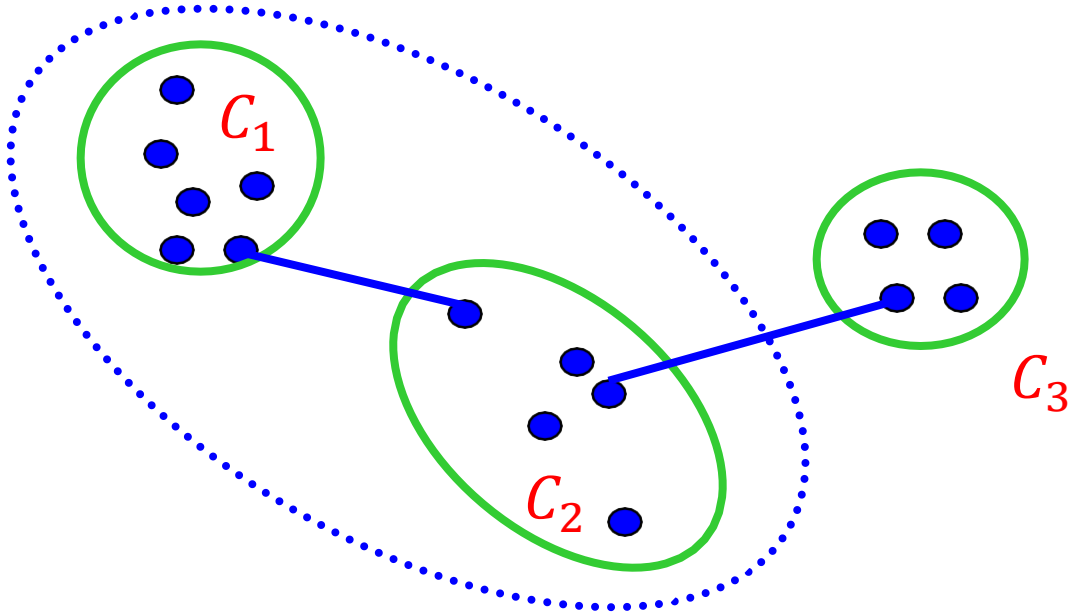
Choose the best

How to decide the distances between clusters?

- Single-Link
  - Nearest Neighbor: their closest members.
- Complete-Link
  - Furthest Neighbor: their furthest members.
- Average:
  - average of all cross-cluster pairs.

Single Link

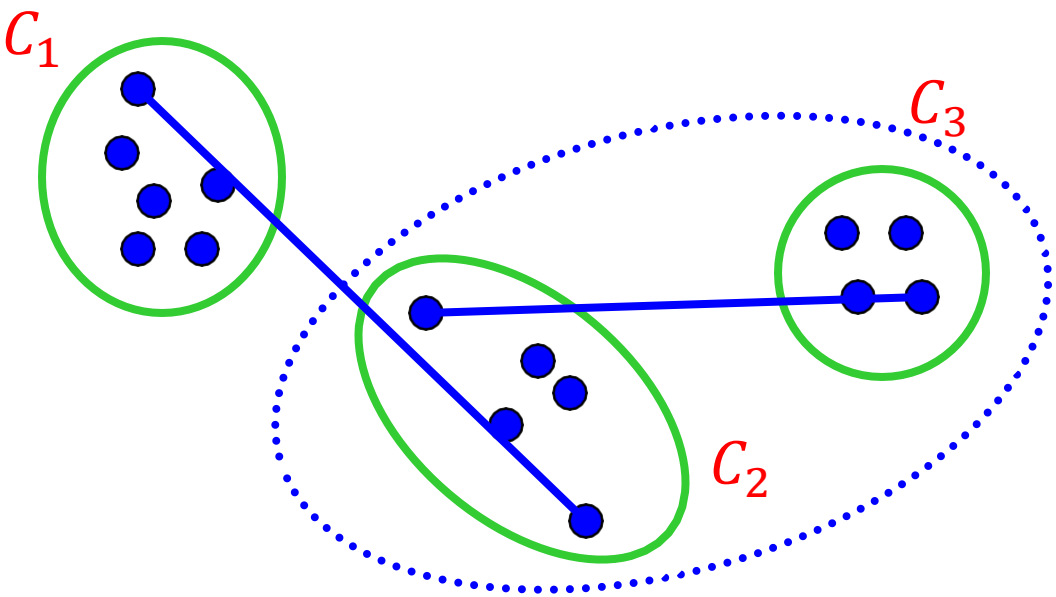
- cluster distance = distance of two closest members in each class



Potentially long and skinny clusters

Complete Link

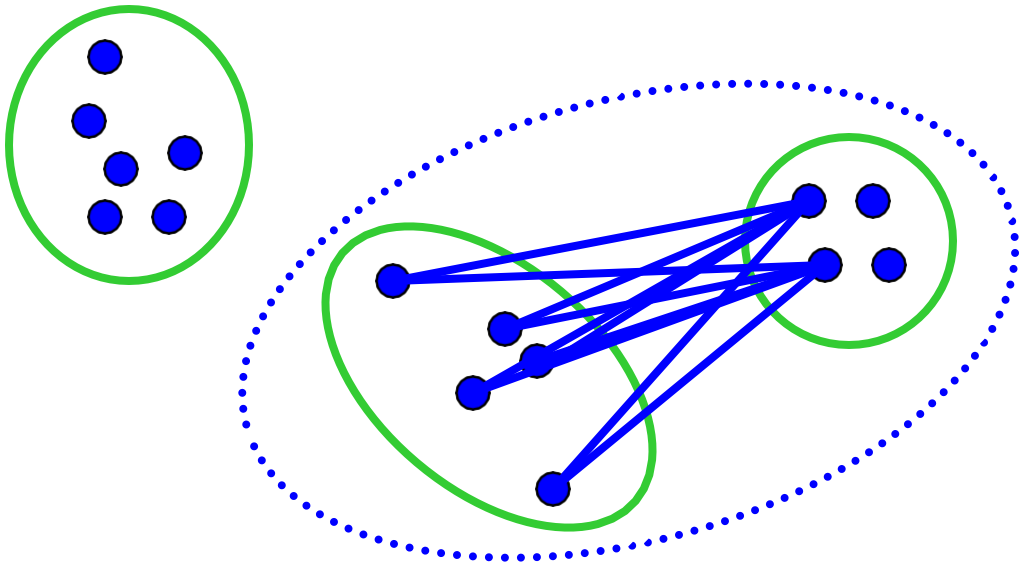
- cluster distance = distance of two farthest members



tight clusters

Average Link

- cluster distance = average distance of all pairs



the most widely used measure

Robust against noise

Example: single link

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

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

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

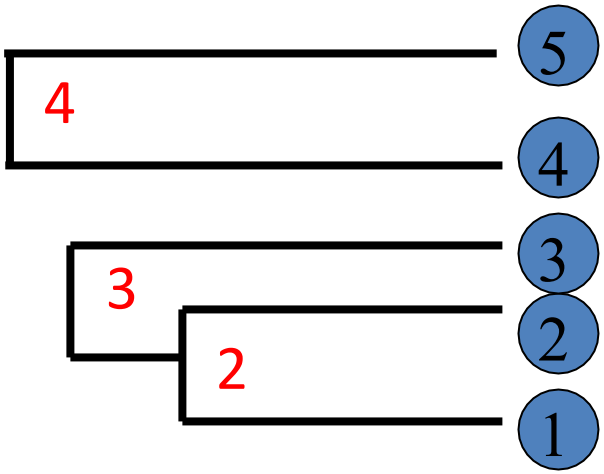
$$d_{(1,2),5} = \min\{ d_{1,5}, d_{2,5} \} = \min\{ 9,8 \} = 8$$

Example: single link

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

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

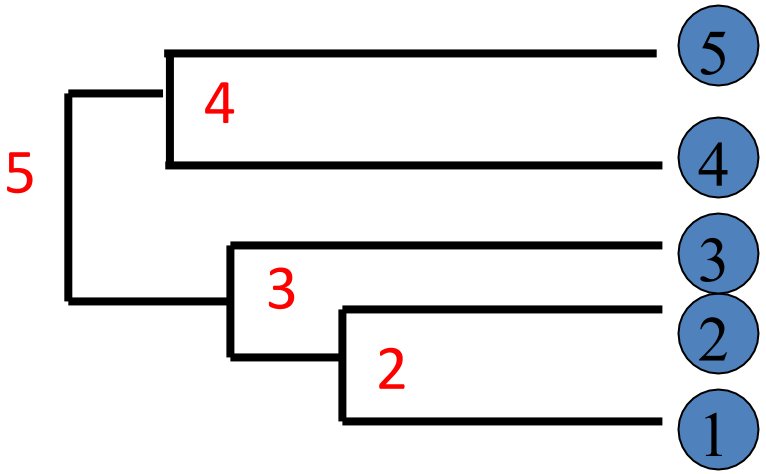
$$d_{(1,2,3),5} = \min\{ d_{(1,2),5}, d_{3,5} \} = \min\{ 8,5 \} = 5$$



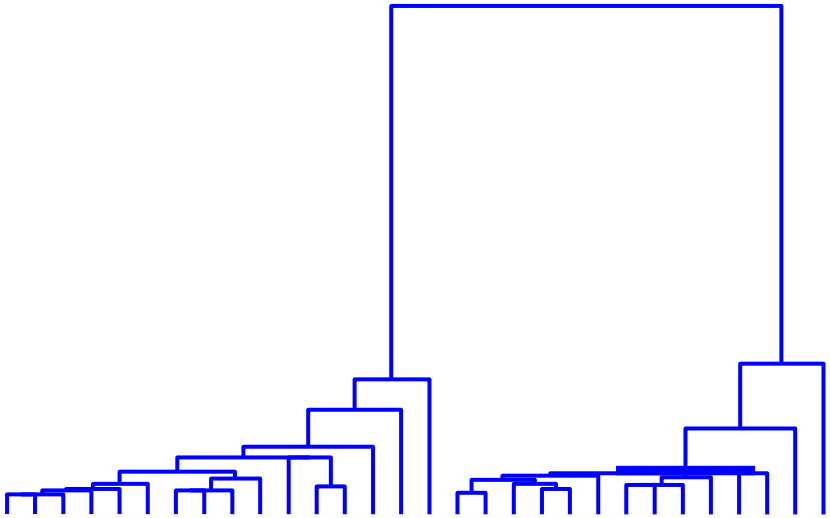
Example: single link

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

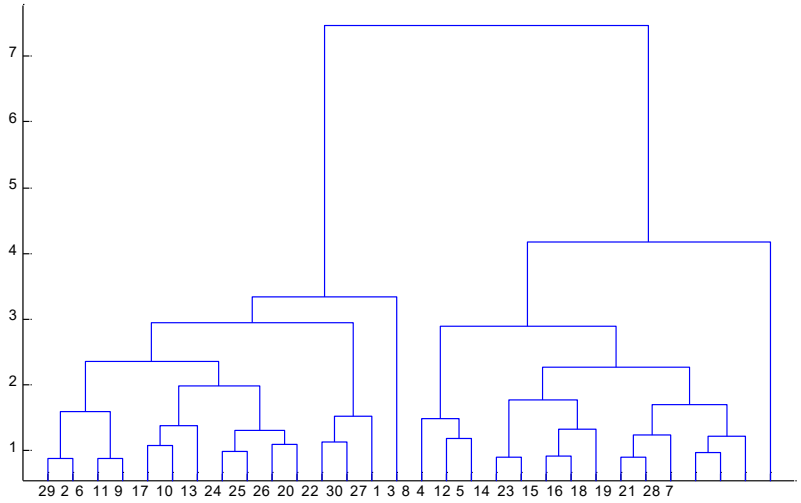
$$d_{(1,2,3),(4,5)} = \min\{ d_{(1,2,3),4}, d_{(1,2,3),5} \} = 5$$



Single link & Average link



Single linkage



Average linkage

Hierarchical Clustering

- Bottom-Up Agglomerative Clustering
  - Starts with each object in a separate cluster
  - repeatedly joins the closest pair of clusters
  - Until there is only one cluster
- Top-Down divisive
  - Start with all the data in a single cluster
  - Consider every possible way to divide the cluster into two. Choose the best division.
  - Recursively operate on both sides

Time Complexity

- Computing distance between two objs is $O(p)$ where p is the dimensionality of the vectors.
- (Re-) calculating pairwise distance distance $O(n^2p)$ computations,
- Computing current best cluster: $O(n^2)$

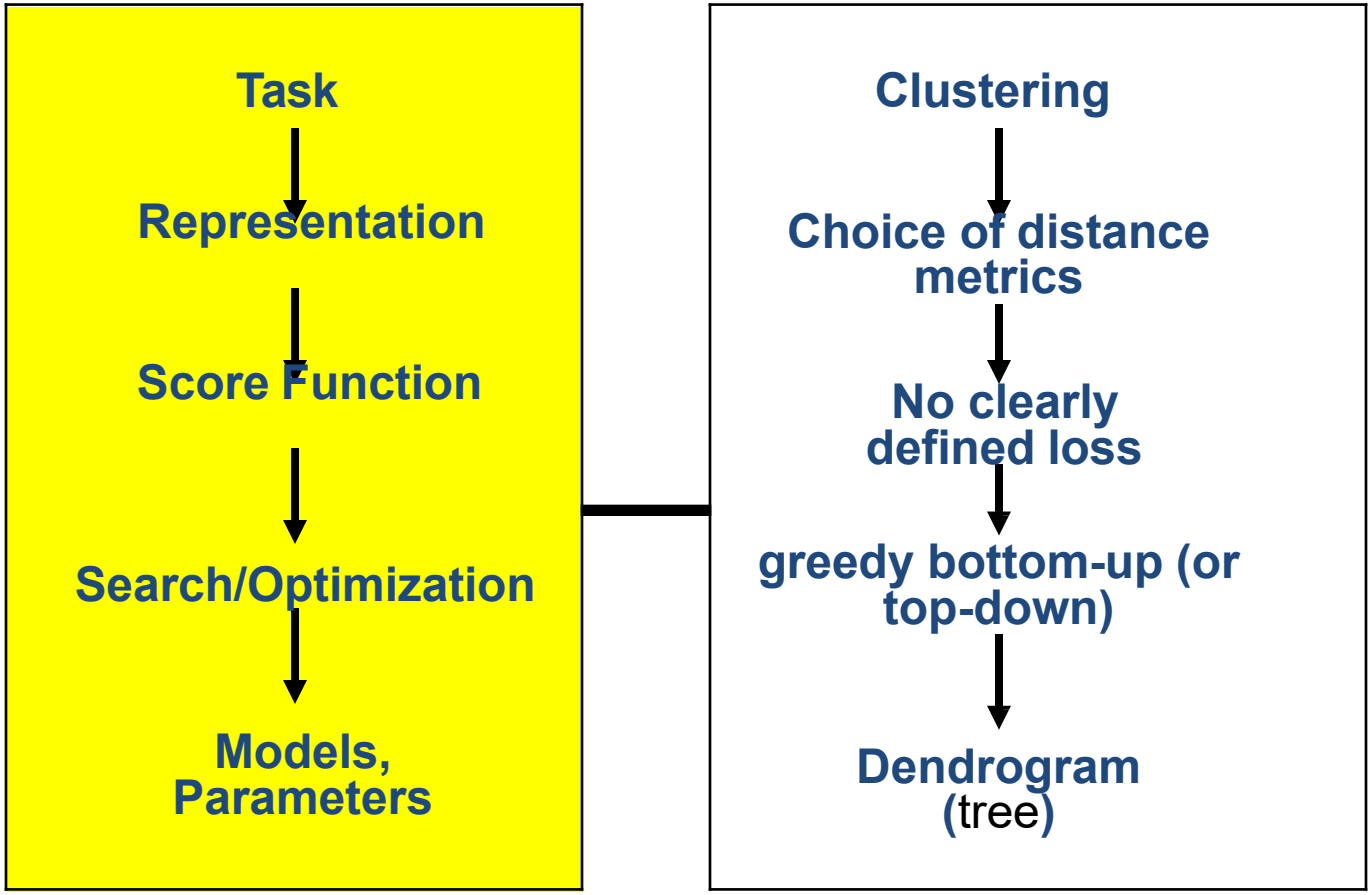
A total of n−1
merging iterations

$O(n^3p)$

Summary of Hierarchal Clustering

- No need to specify the number of clusters in advance.
- Hierarchical structure maps nicely onto human intuition for some domains.
- They do not scale well: time complexity of at least $O(n^2)$, where n is the number of total objects.
- Like any heuristic search algorithms, local optima is a problem.
- Interpretation of results is (very) subjective.

Recap: Hierarchical Clustering



References

- https://qiyanjun.github.io/2019f-UVA-CS6316-MachineLearning/
- Hastie, Trevor, et al. The elements of statistical learning. Vol. 2. No. 1. New York: Springer, 2009.

- Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
- Big thanks to Prof. Ziv Bar-Joseph @ CMU for allowing me to reuse some of his slides

Thanks for listening