UVA CS 6316: Machine Learning

Lecture 19: Unsupervised Clustering (I): Hierarchical

Dr. Yanjun Qi

University of Virginia
Department of Computer Science

Course Content Plan → Six major sections of this course

- ~~Regression (supervised)~~
- ~~Classification (supervised)~~
  - ~~Feature Selection~~
- Unsupervised models
  - ~~Dimension Reduction (PCA)~~
  - Clustering (K-means, GMM/EM, Hierarchical)
- Learning theory
- Graphical models
- Reinforcement Learning

Y is a continuous

Y is a discrete

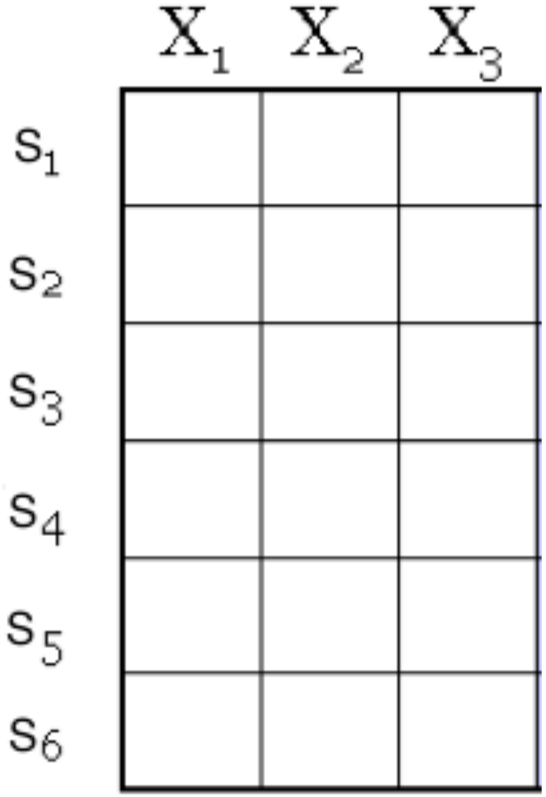
NO Y

About f()

About interactions among X1,... Xp

Learn program to Interact with its environment

An unlabeled Dataset X



a data matrix of n observations on p variables $x_1, x_2, \ldots x_p$

Unsupervised learning = learning from raw (unlabeled, unannotated, etc) data, as opposed to supervised data where label of examples is given

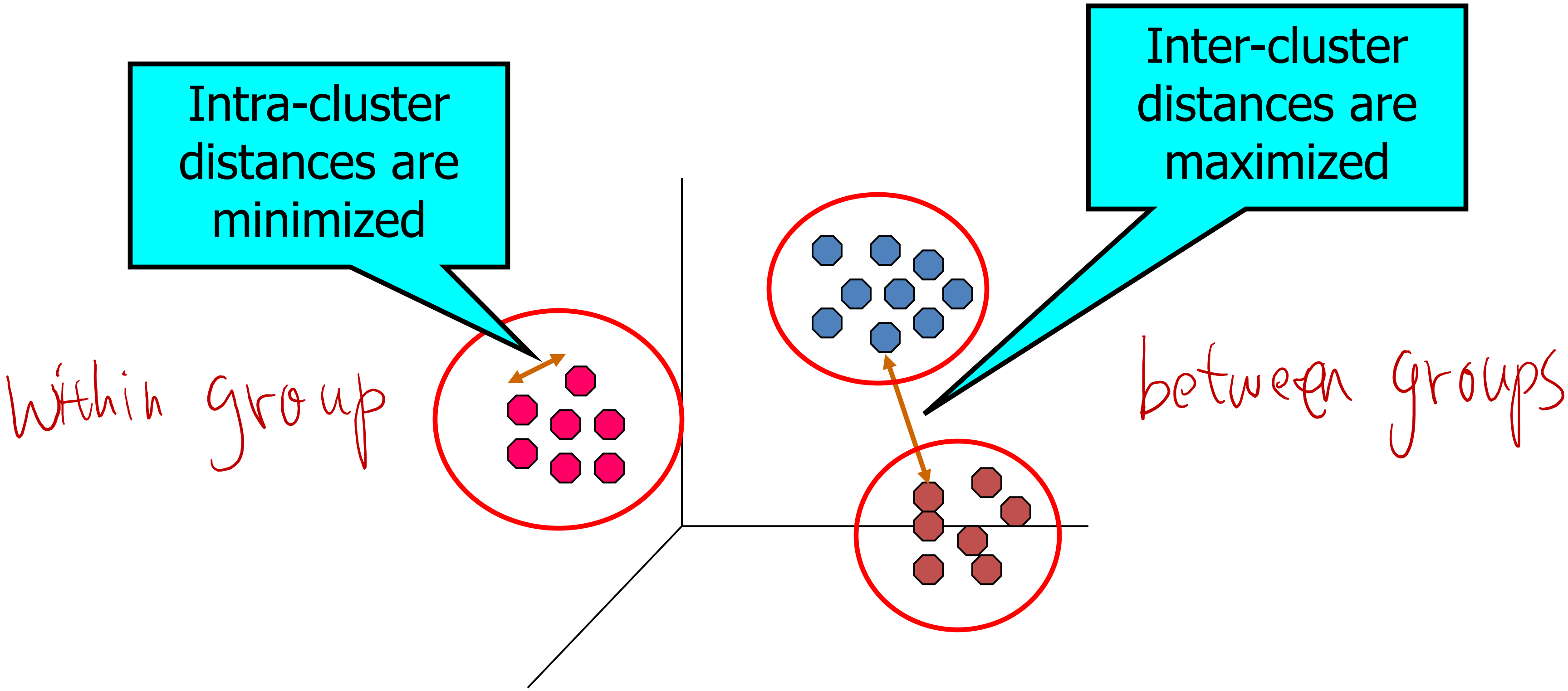
- **Data**/*points/instances/examples/samples/records*: [rows]
- **Features**/*attributes/dimensions/independent variables/covariates/predictors/regressors*: [columns]

Today: 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

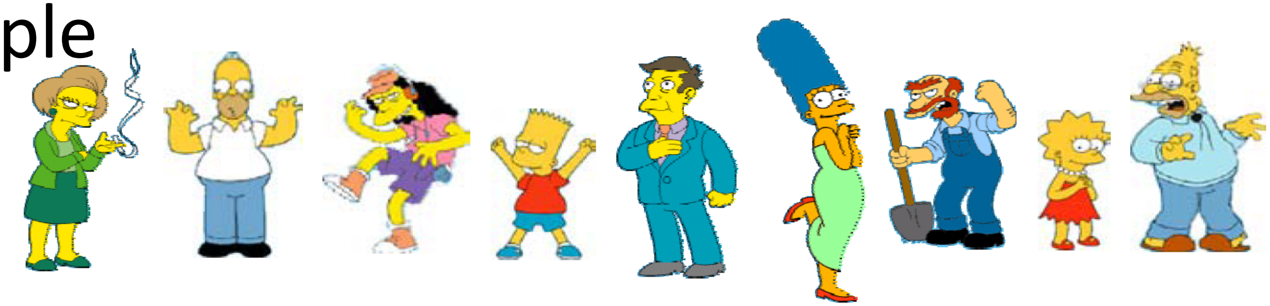
What is clustering?

- 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

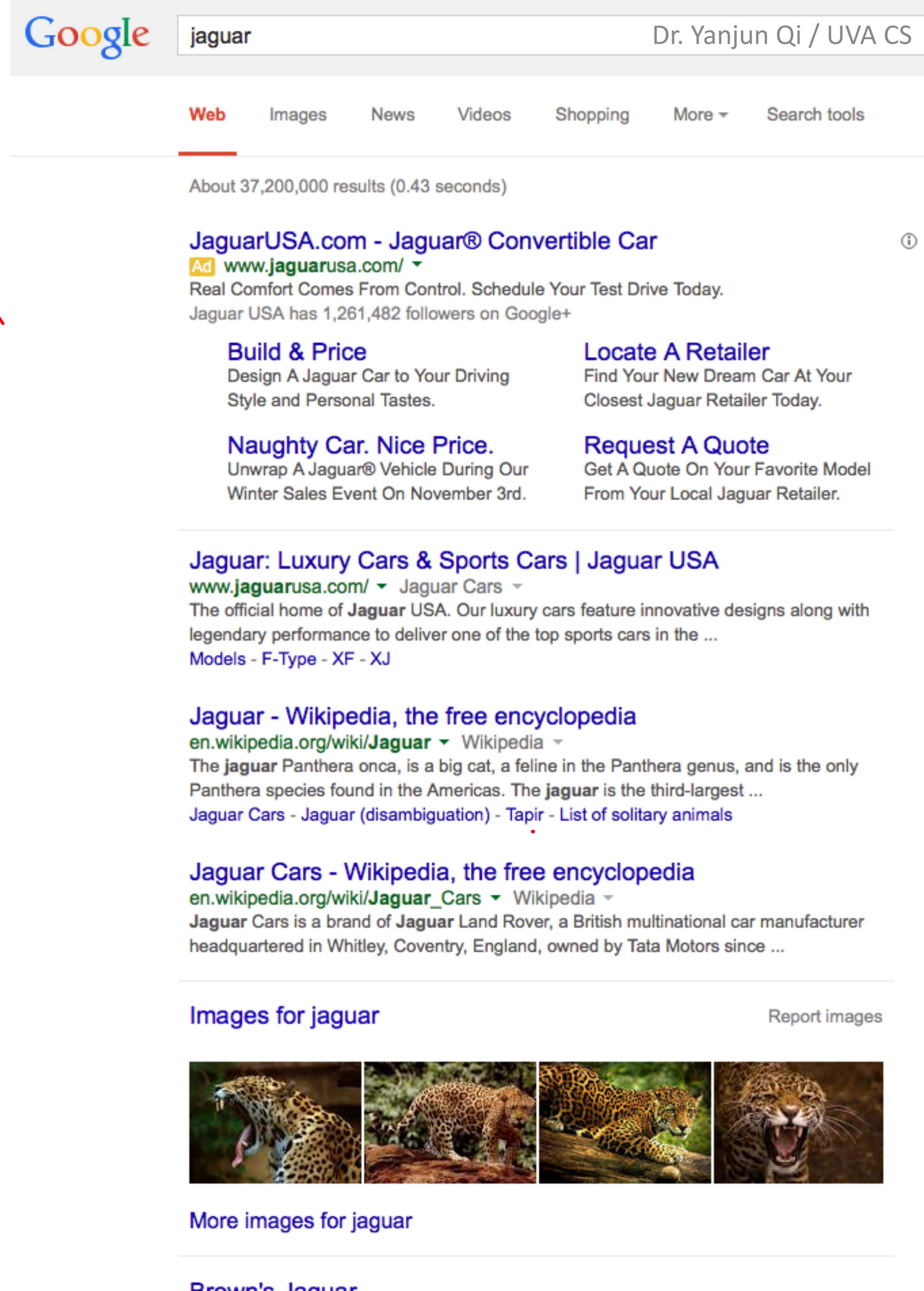
- Language

Piotr Pyotr Petros Pietro Pedro Pierre Piero Peter Peder Peka Peadar

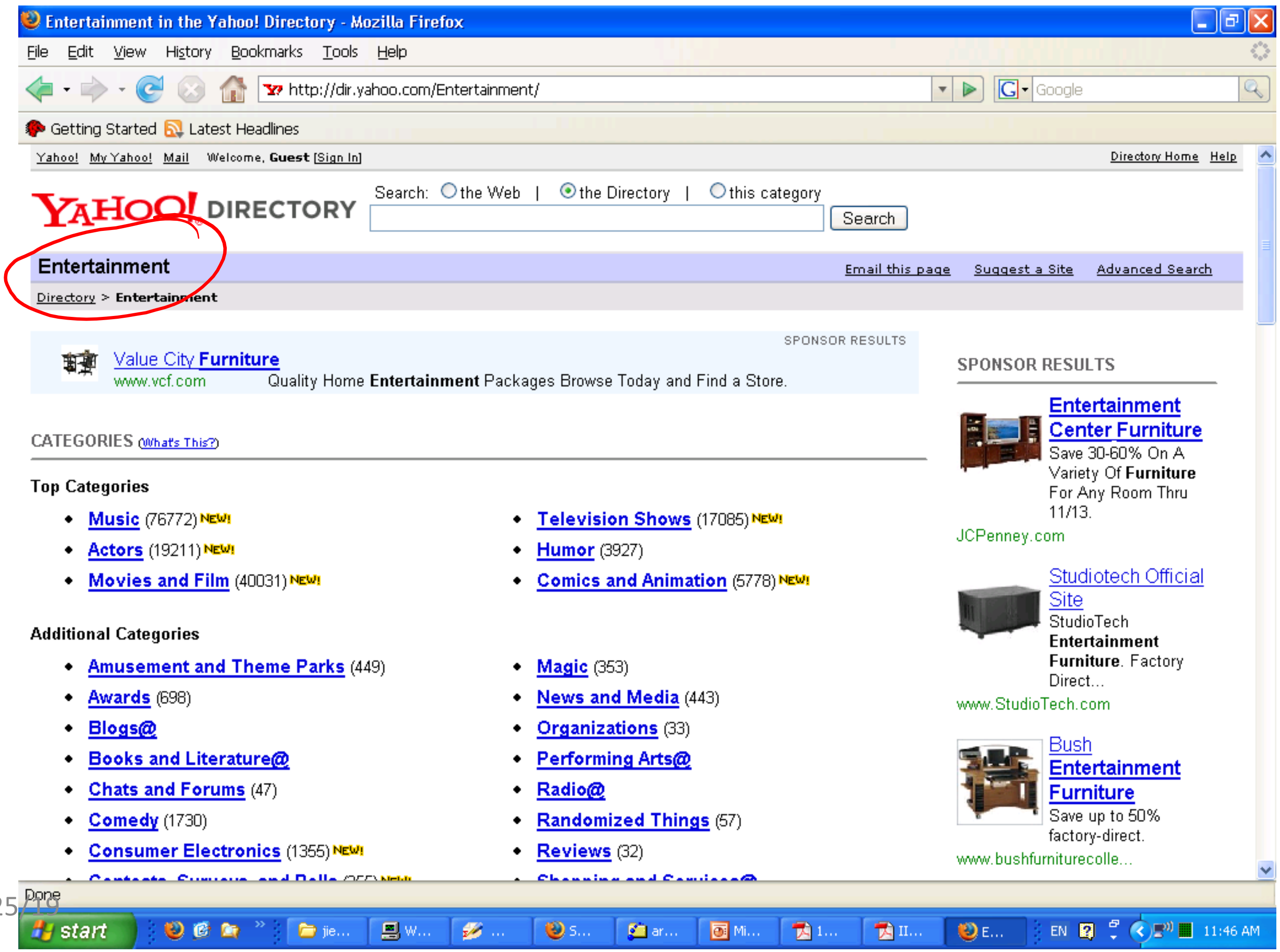
- species

Partition

Application (I): Search Result Clustering



Application (II): Navigation



Hierachy

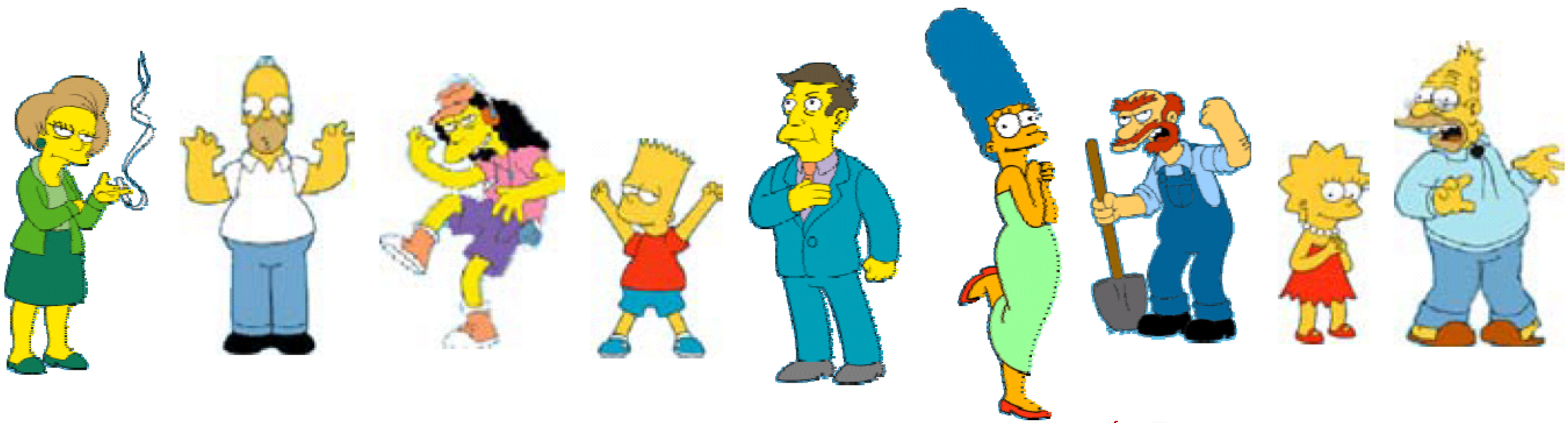
Issues for clustering

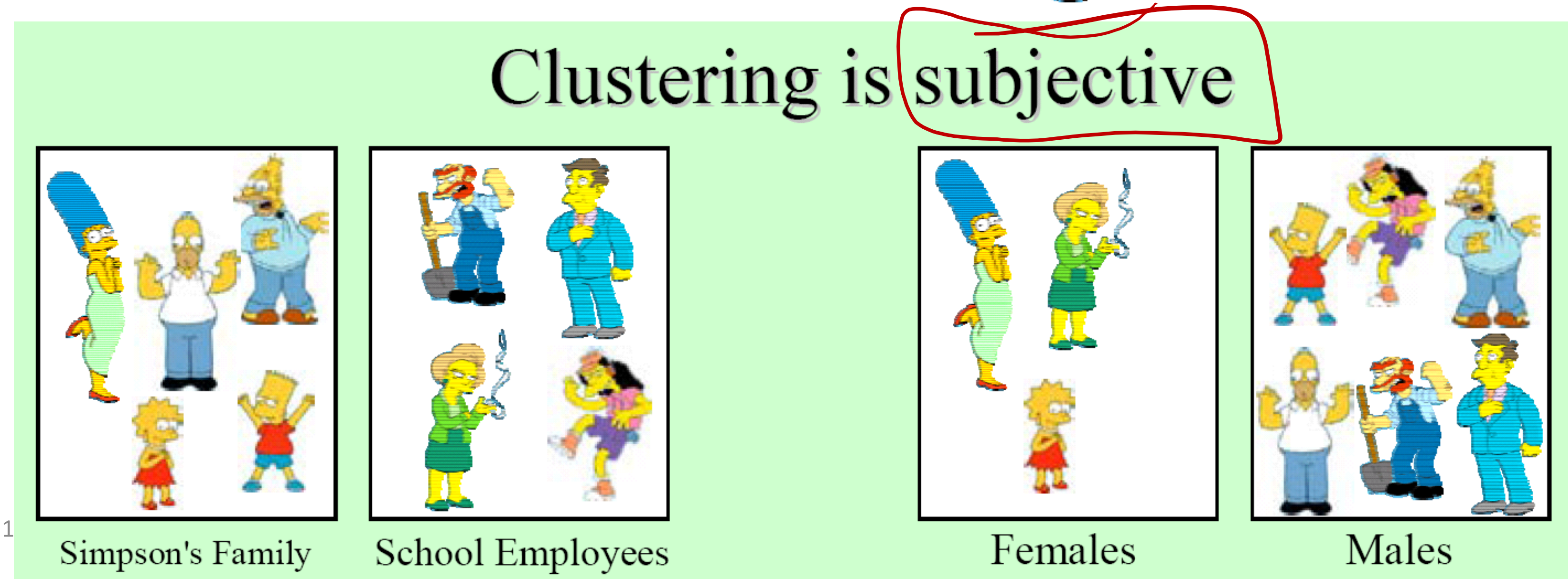
- What is a natural grouping among these objects?
  - Definition of "groupness"
- What makes objects “related”?
  - Definition of "similarity/distance"
- Representation for objects
  - Vector space? Normalization?
- How many clusters?
  - Fixed a priori?
  - Completely data driven?
    - Avoid “trivial” clusters - too large or small
- Clustering Algorithms
  - Partitional algorithms
  - Hierarchical algorithms
- Formal foundation and convergence

Today Roadmap: clustering

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

What is a natural grouping among these objects?





Another example: clustering is subjective

Two possible Solutions…

Today Roadmap: clustering

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

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.

What properties should a distance measure have?

- 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*

Intuitions behind desirable properties of distance measure

- $D(A,B) = D(B,A)$ *Symmetry*
  - *Otherwise you could claim "Alex looks like Bob, but Bob looks nothing like Alex"*
- $D(A,A) = 0$ *Constancy of Self-Similarity*
  - *Otherwise you could claim "Alex looks more like Bob, than Bob does"*
- $D(A,B) = 0$ IIf A= B *Positivity Separation*
  - *Otherwise there are objects in your world that are different, but you cannot tell apart.*
- $D(A,B) <= D(A,C) + D(B,C)$ *Triangular Inequality*
  - *Otherwise you could claim "Alex is very like Bob, and Alex is very like Carl, but Bob is very unlike Carl"*

Distance Measures: Minkowski Metric

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

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

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

- The Minkowski metric is defined by

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

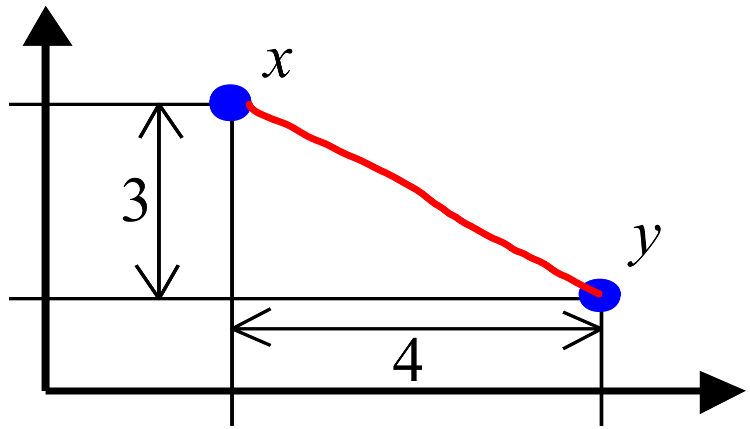
- Most Common Minkowski Metrics

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

$$2, r = 1 \text{ (Manhattan distance)} \qquad d(x, y) = \sum_{i=1}^{p} |x_i - y_i|$$

$$3, r = +\infty \text{ ("sup" distance)} \qquad d(x, y) = \max_{1 \le i \le p} |x_i - y_i|$$

An Example

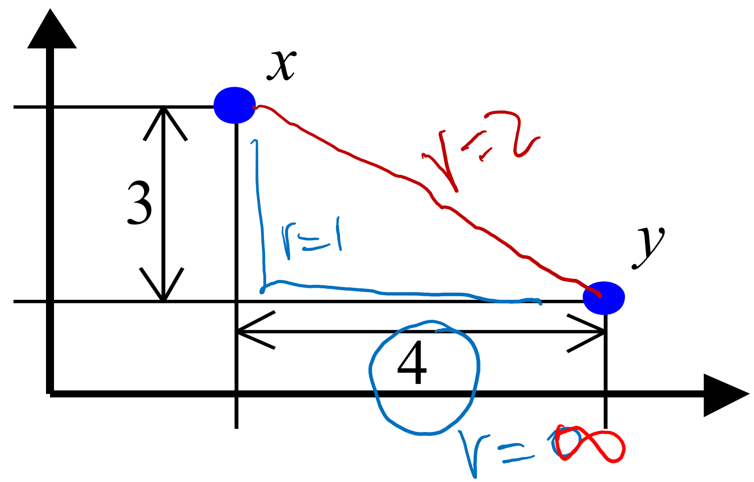


$$1:\ \text{Euclidean distance}: \quad \sqrt[2]{4^2+3^2}=5.$$

$$2:\ \text{Manhattan distance}: \quad 4+3=7.$$

$$3:\ \text{"sup" distance}: \quad \max\{4,3\}=4.$$

An Example



$$1:\ \text{Euclidean distance}:\quad \sqrt[2]{4^2+3^2}=5.$$

$$2:\ \text{Manhattan distance}:\quad 4+3=7.$$

$$3:\ \text{"sup" distance}:\quad \max\{4,3\}=4.$$

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

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

Similarity Measures: Correlation Coefficient

- Pearson correlation coefficient

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

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

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

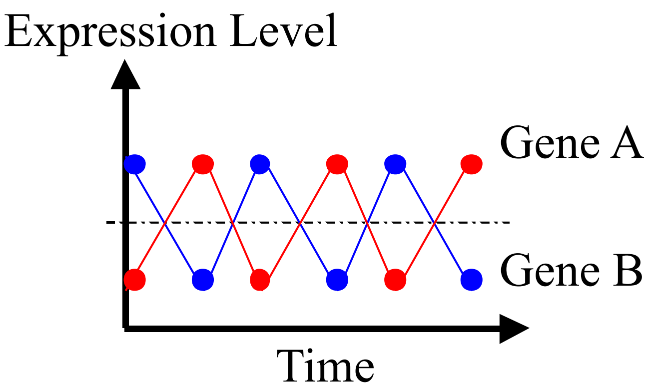
Correlation is unit independent

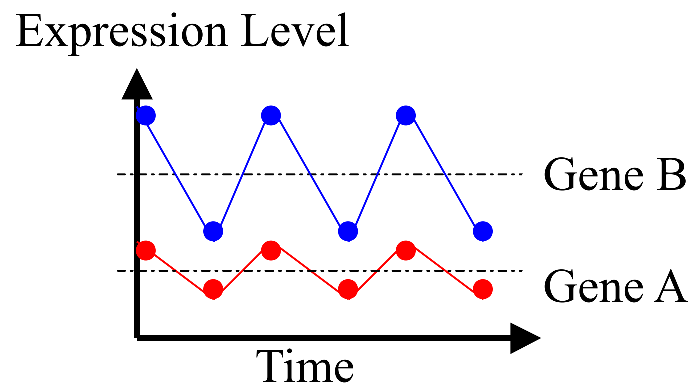
- Measuring the linear **correlation** between two sequences, x and y,
- giving a value between +1 and −1 inclusive, where 1 is total positive **correlation**, 0 is no **correlation**, and −1 is total negative **correlation**.

- Special case: cosine distance

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

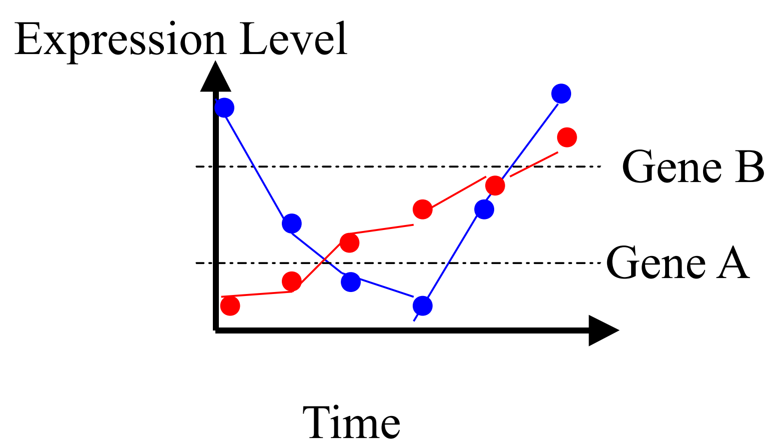
Similarity Measures: e.g., Correlation Coefficient on time series samples





Correlation is unit independent;

If you scale one of the objects ten times, you will get different euclidean distances and same correlation distances.

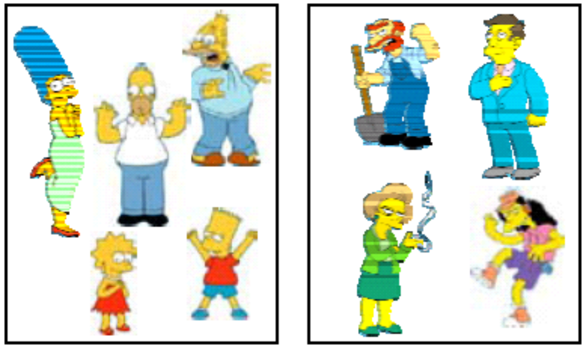


Today Roadmap: clustering

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

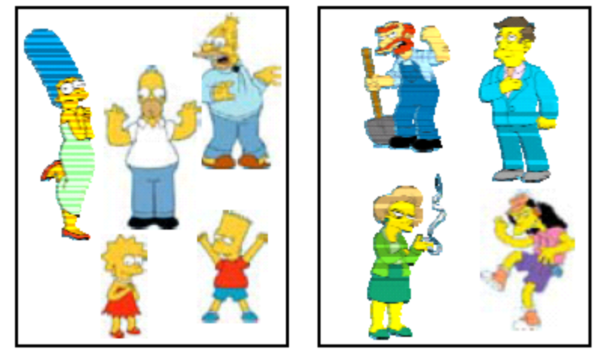
Clustering Algorithms

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

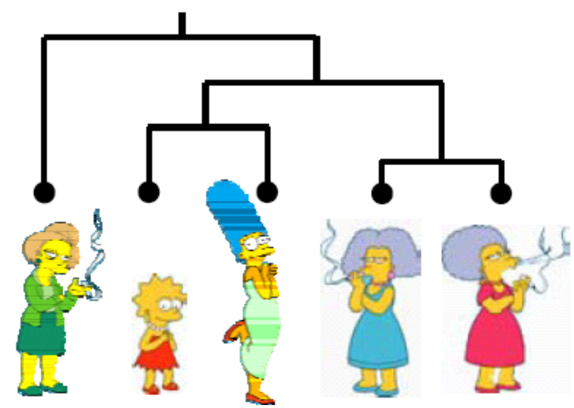


Clustering Algorithms

- 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



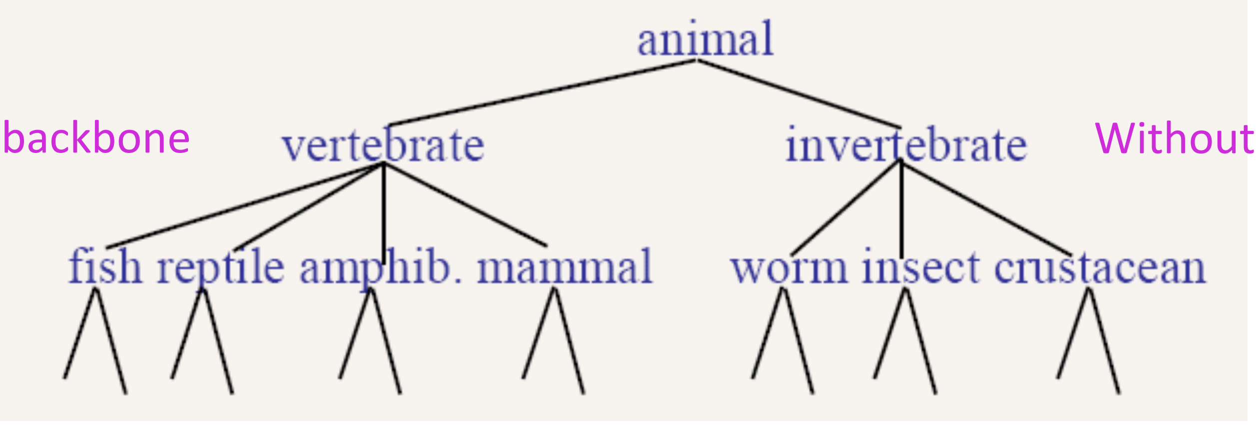
Today Roadmap: clustering

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

Hierarchical Clustering

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

With backbone



Without backbone

- Note that hierarchies are commonly used to organize information, for example in a web portal.
  - Yahoo! hierarchy is manually created, we will focus on automatic creation of hierarchies

(How-to) Hierarchical Clustering

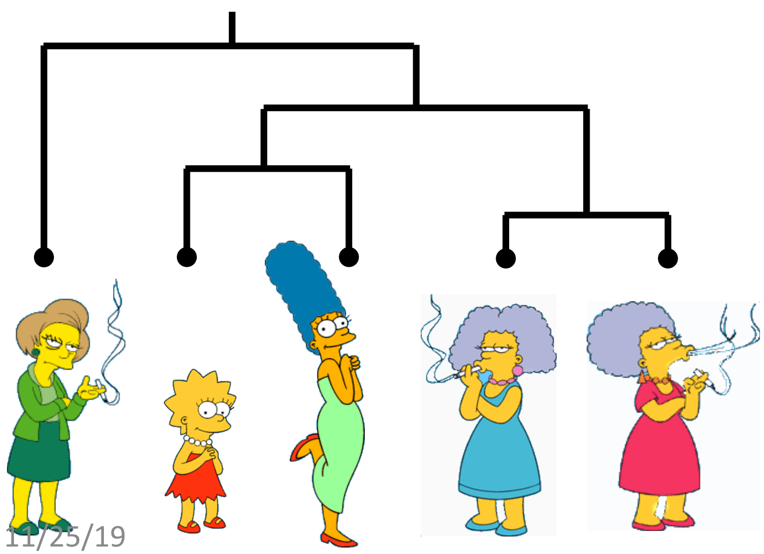
- Given: a set of objects and the pairwise distance matrix

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

Hierarchical Clustering

Task	Clustering
↓	↓
Representation	Choice of distance metrics
↓	↓
Score Function	No clearly defined loss
↓	↓
Search/Optimization	greedy bottom-up (or top-down)
↓	↓
Models, Parameters	Dendrogram (tree)

(How-to) Hierarchical Clustering



Clustering: the process of grouping a set of objects into classes of similar objects ➔
- high intra-class similarity
- low inter-class similarity

(Domain-Specific Edit) Distance:

A generic 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.

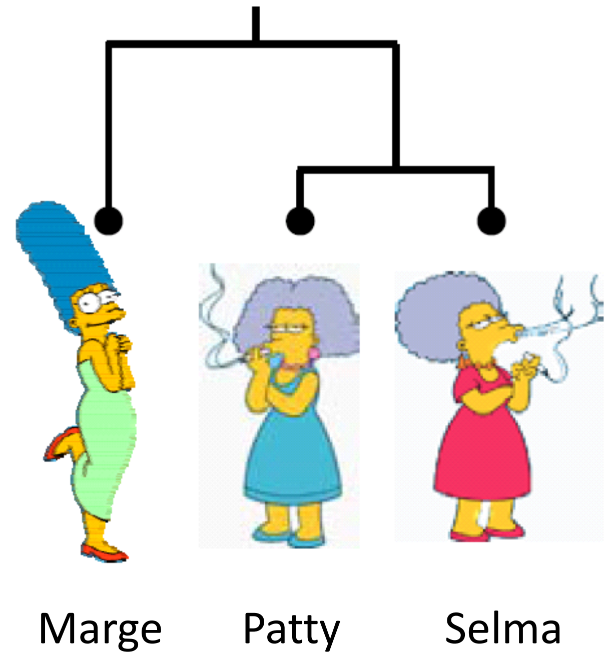
Change dress color, 1 point
Change earring shape, 1 point
Change hair part, 1 point

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**



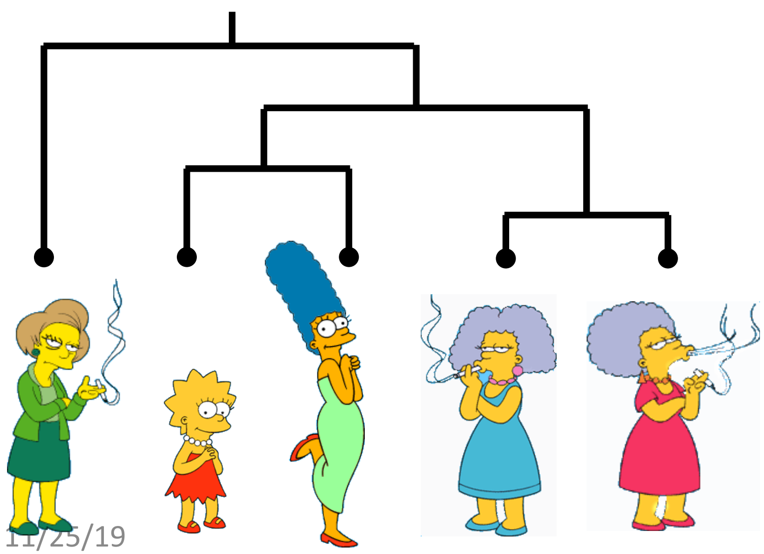
This is called the Edit distance or the Transformation distance

(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

NP



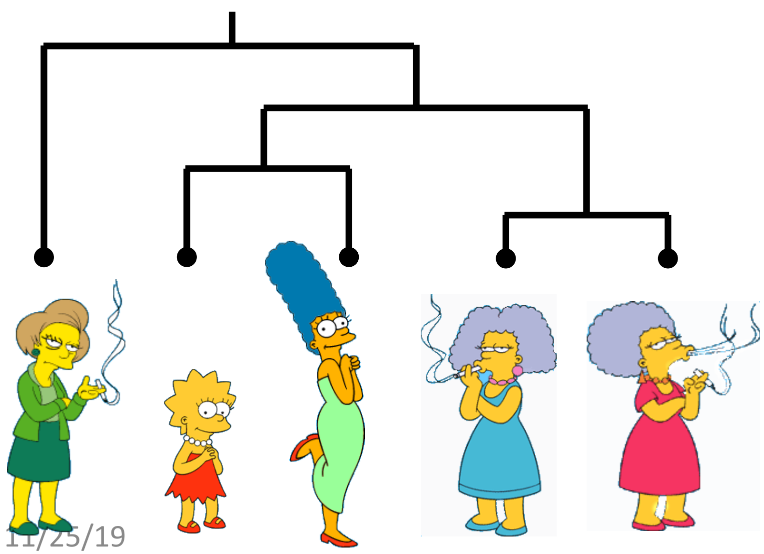
Clustering: the process of grouping a set of objects into classes of similar objects ➔
high intra-class similarity
low inter-class similarity

(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

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 ➔

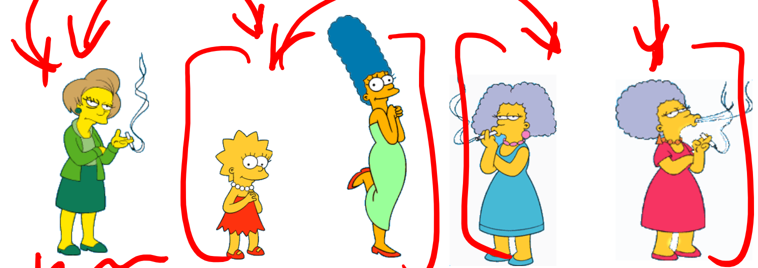
high intra-class similarity

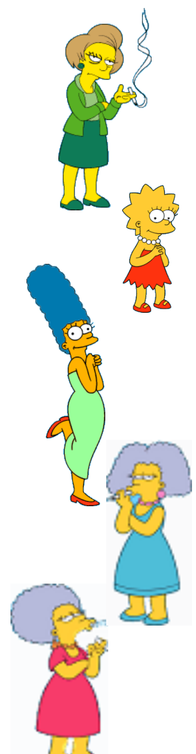
low inter-class similarity

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

$$\begin{cases} D(A,A) = 0 \\ D(A,B) = D(B,A) \end{cases}$$

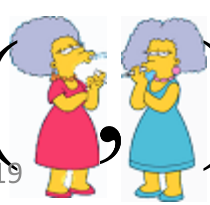
$\Rightarrow$ min. within cluster distance





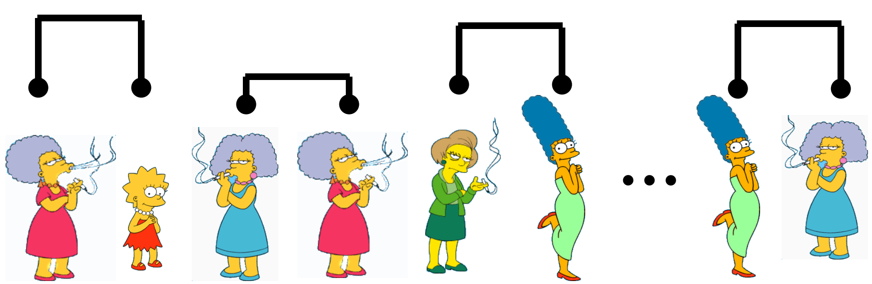
0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
				0

D() = 8

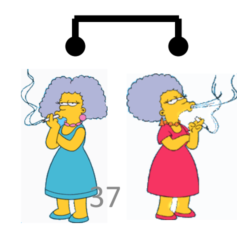
D() = 1

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.

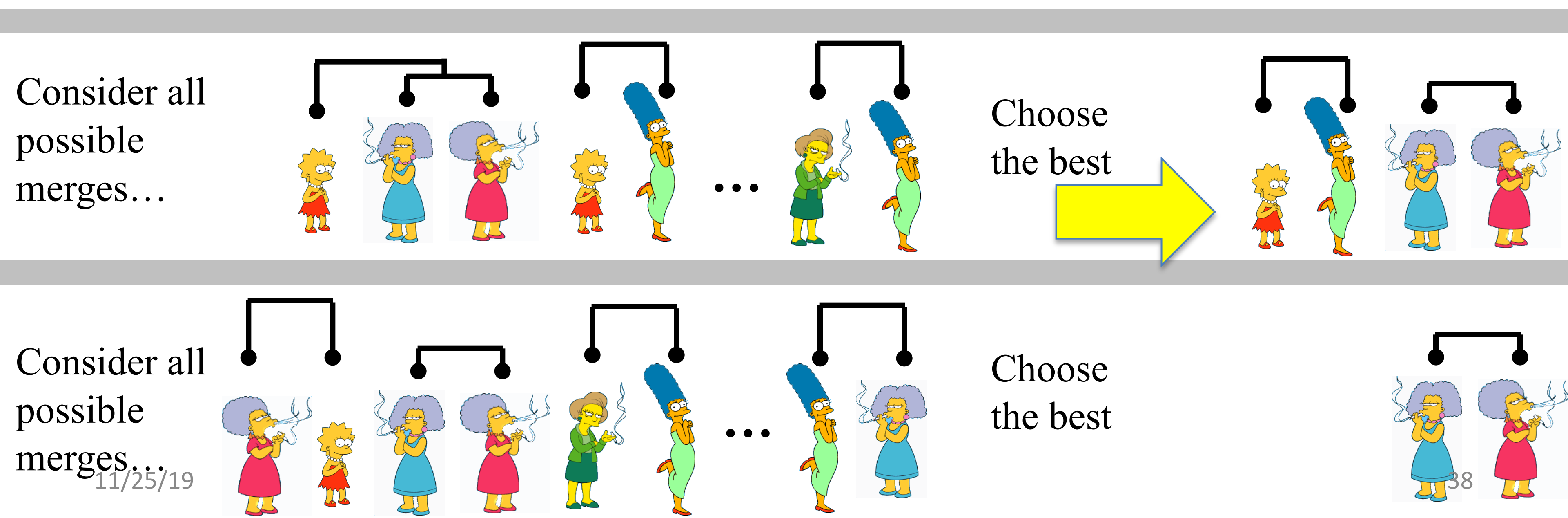
Consider all possible merges…



Choose the best

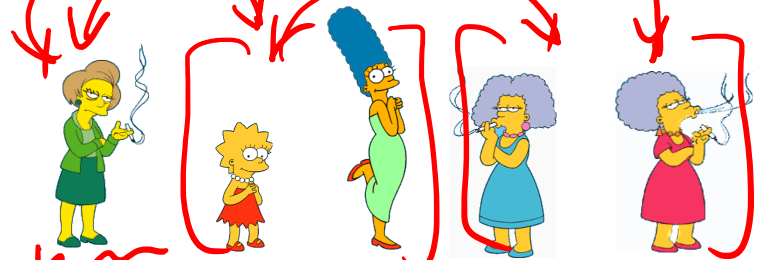


Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.



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

$$\begin{cases} D(A,A) = 0 \\ D(A,B) = D(B,A) \end{cases}$$



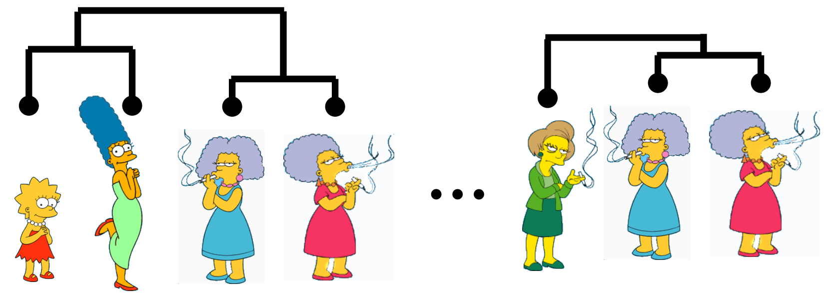
0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
				0

D() = 8

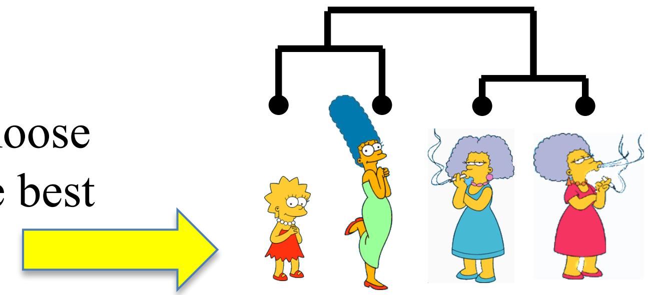
D() = 1

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.

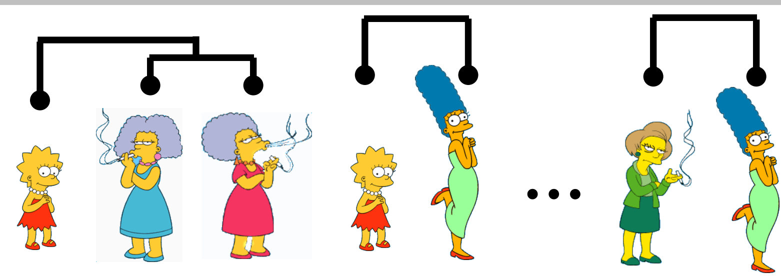
Consider all possible merges…



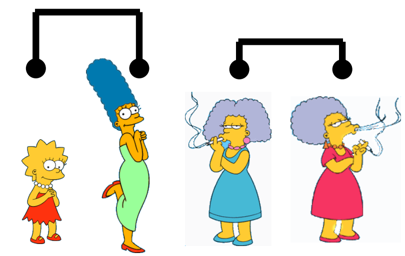
Choose the best



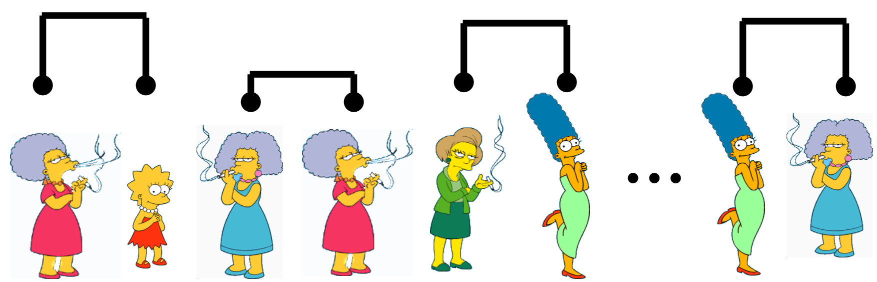
Consider all possible merges…



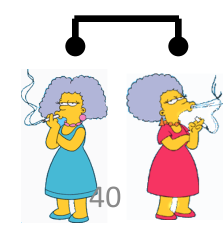
Choose the best



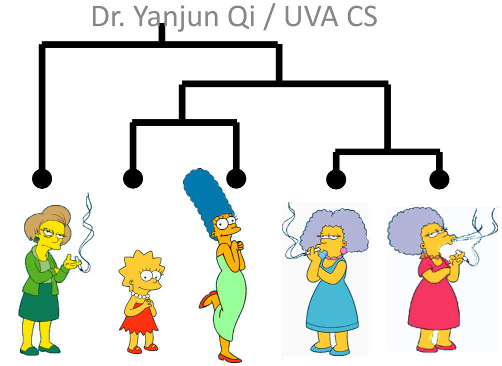
Consider all possible merges…



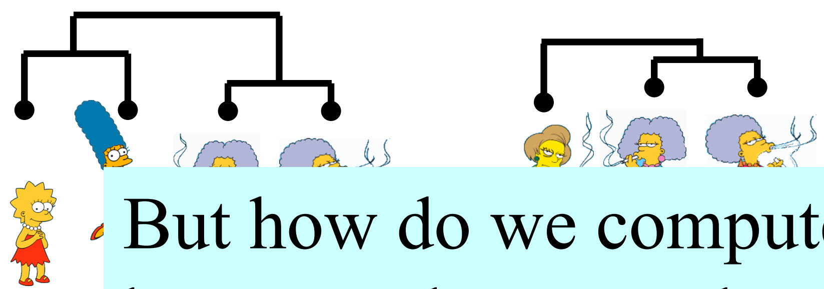
Choose the best



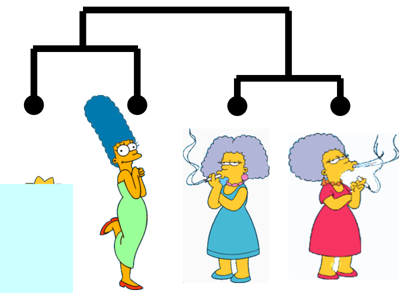
Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.



Consider all possible merges…

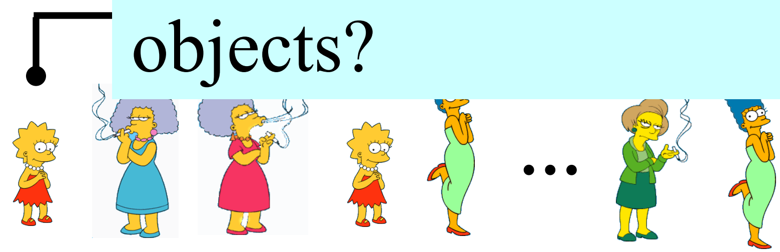


Choose

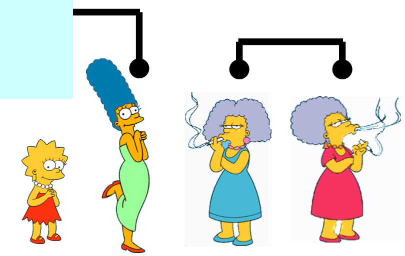


But how do we compute distances between clusters rather than objects?

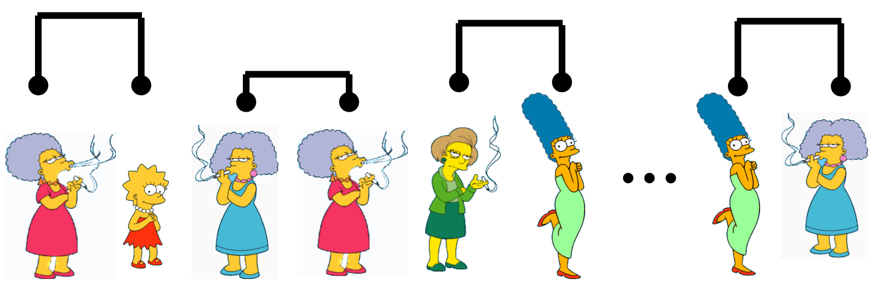
Consider all possible merges…



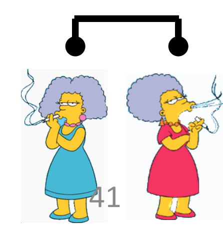
the best



Consider all possible merges…



Choose the best

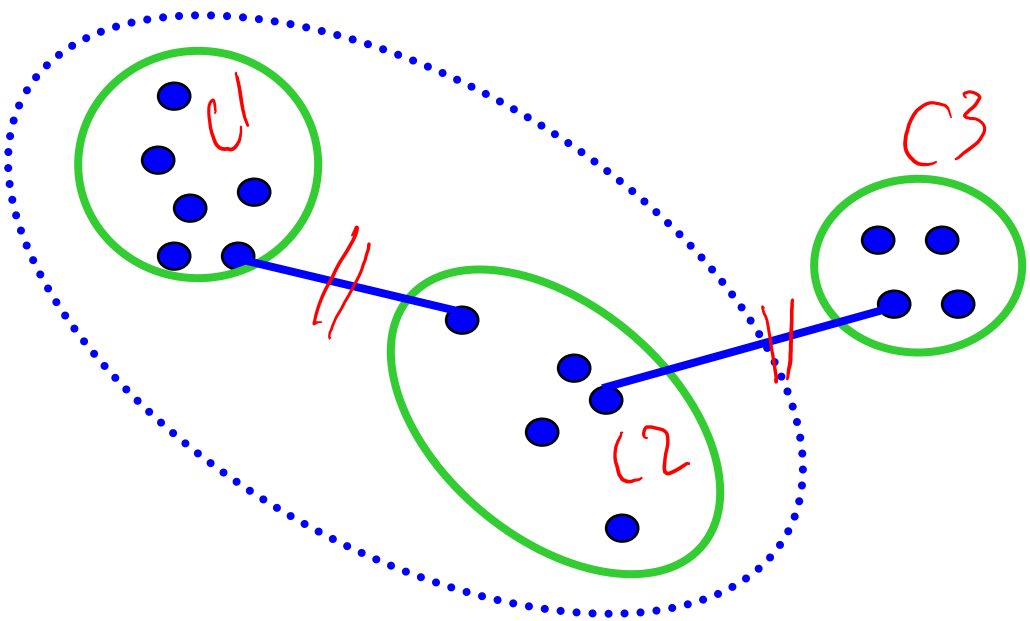


How to decide the distances between clusters ?

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

Computing distance between clusters: Single Link

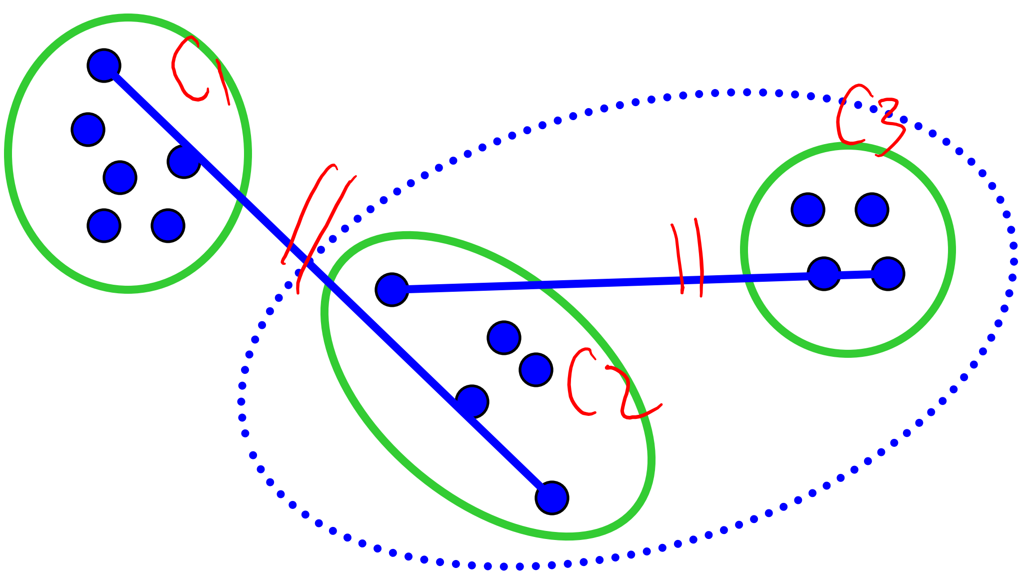
- cluster distance = distance of two closest members in each class



- Potentially long and skinny clusters

Computing distance between clusters: : Complete Link

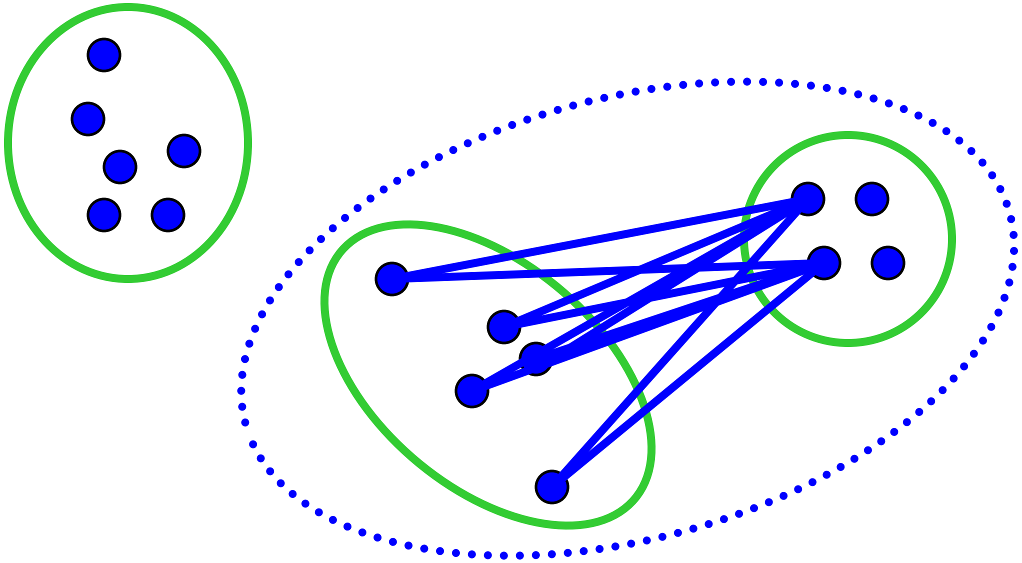
- cluster distance = distance of two farthest members



+ tight clusters

Computing distance between clusters: Average Link

- cluster distance = average distance of all pairs



the most widely used measure

Robust against noise

Example: single link

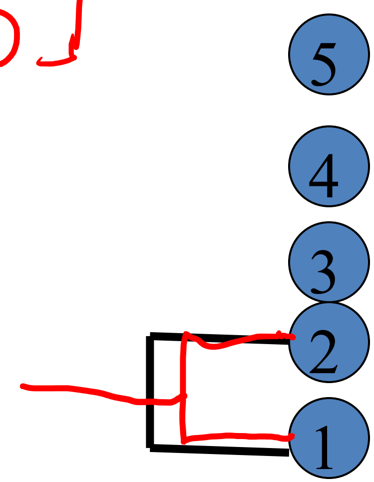
$$
\begin{array}{c c}
 & \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\
\begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} &
\begin{bmatrix}
0 & & & & \\
2 & 0 & & & \\
6 & 3 & 0 & & \\
10 & 9 & 7 & 0 & \\
9 & 8 & 5 & 4 & 0
\end{bmatrix}
\end{array}
\qquad
\begin{array}{c c}
 & \begin{array}{cccc}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

① Best

② re-matrix

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

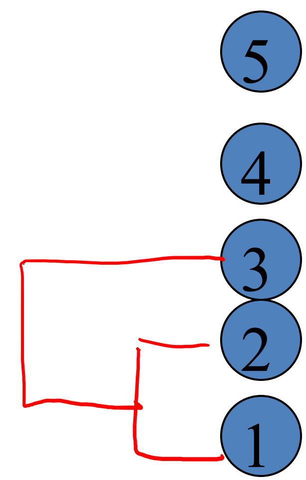
⇐ Complete



Example: single link

$$
\begin{array}{c|ccccc}
 & 1 & 2 & 3 & 4 & 5 \\
\hline
1 & 0 & & & & \\
2 & 2 & 0 & & & \\
3 & 6 & 3 & 0 & & \\
4 & 10 & 9 & 7 & 0 & \\
5 & 9 & 8 & 5 & 4 & 0
\end{array}
$$

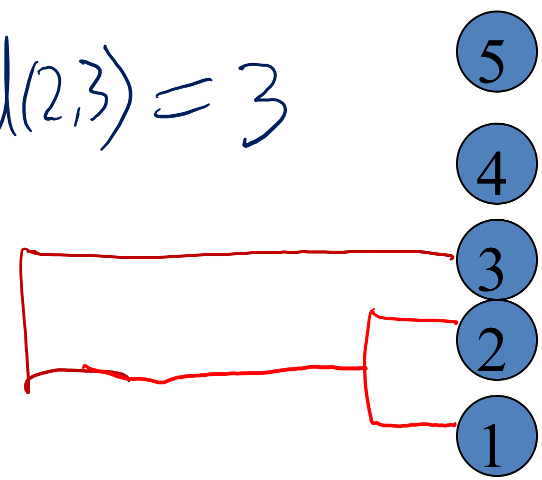
$$
\begin{array}{c|cccc}
 & (1,2) & 3 & 4 & 5 \\
\hline
(1,2) & 0 & & & \\
3 & 3 & 0 & & \\
4 & 9 & 7 & 0 & \\
5 & 8 & 5 & 4 & 0
\end{array}
$$



Example: single link

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

$$d((1,2),3) = \min(d(1,3), d(2,3)) = 3$$



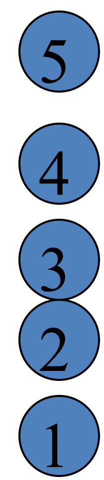
Example: single link

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

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

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

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

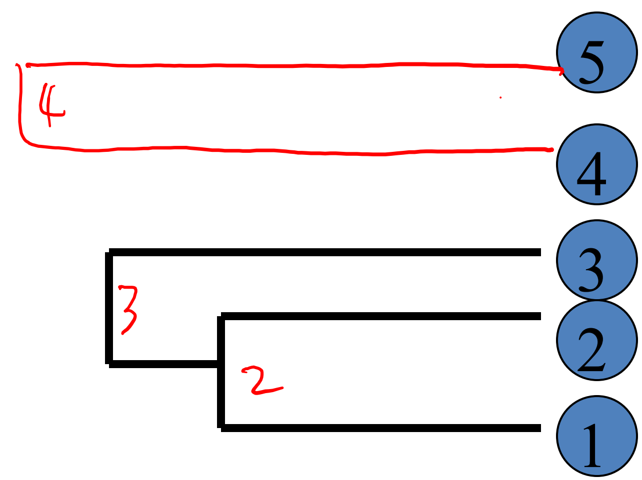


Example: single link

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

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

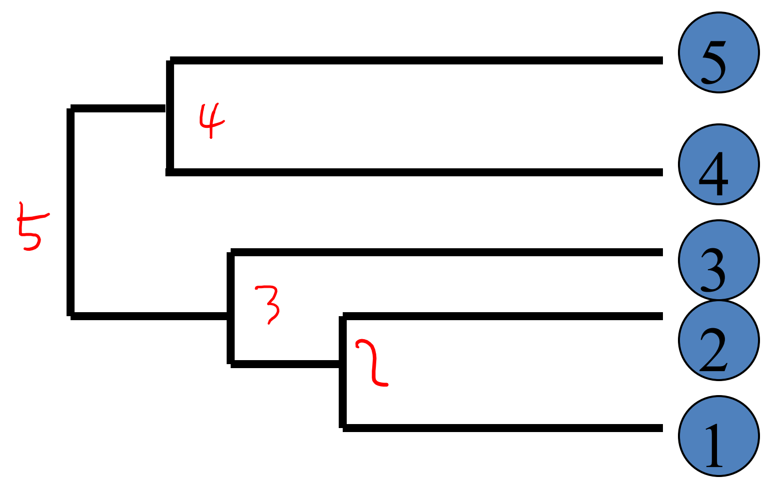
$$d_{(1,2,3),5} = \min\{ d_{(1,2),5}, d_{3,5} \} = \min\{ 8,5 \} = 5$$



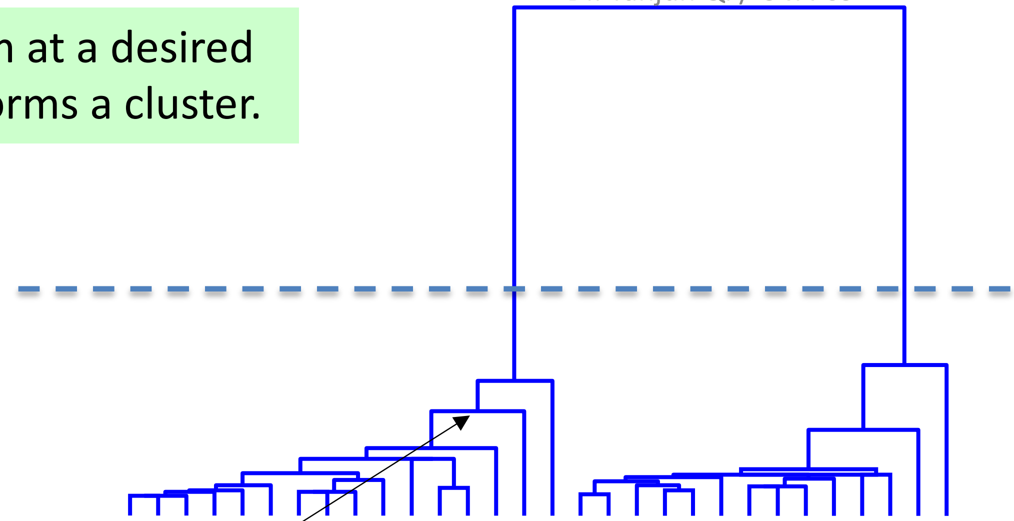
Example: single link

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

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

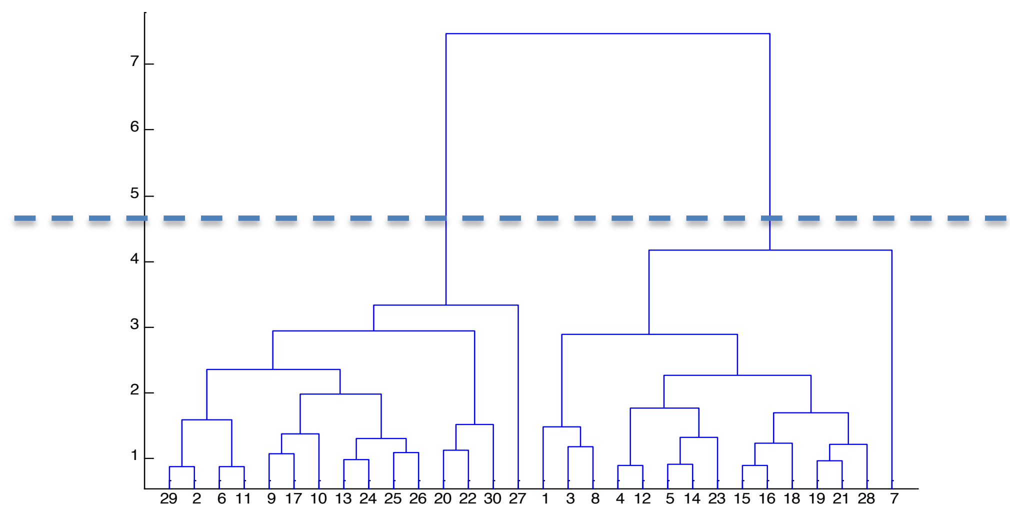


Partitions by cutting the dendrogram at a desired level: each connected component forms a cluster.



Single linkage

Height represents distance between objects / clusters



Average linkage

Hierarchical Clustering

- Bottom-Up Agglomerative Clustering
  - Starts with each object 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 (dendrogram)

- 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.

Example: Cost analysis

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

N×N

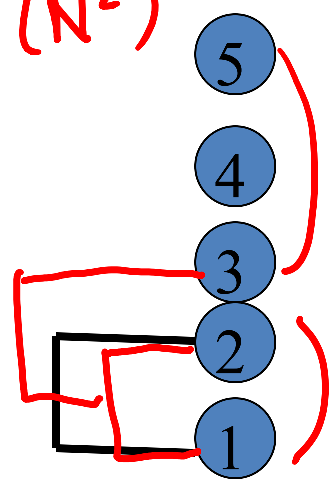
$$\begin{array}{c|c}
 & \begin{array}{cccc} (1,2) & 3 & 4 & 5 \end{array} \\
\begin{array}{c} (1,2) \\ 3 \\ 4 \\ 5 \end{array} &
\begin{bmatrix} 0 & & & \\ 3 & 0 & & \\ 9 & 7 & 0 & \\ 8 & 5 & 4 & 0 \end{bmatrix}
\end{array} \Rightarrow O(N)$$

$\vec{x}_i \in R^p$, $(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N)$

time: $O(dist(\vec{x}_i, \vec{x}_j)) \sim O(p)$

$O(\text{pairse Matrix}) \sim O(pN^2)$

$\text{BestCluster} \sim O(N^2)$



O(N)

O(N)

Computational Complexity

$$\sqrt{\sum_{i=1}^{p}(x_i-y_i)^2} \Rightarrow O(p)$$

- In the first iteration, all HAC methods need to compute similarity of all pairs of *n* individual instances which is $O(n^2p)$.

(Matrix)

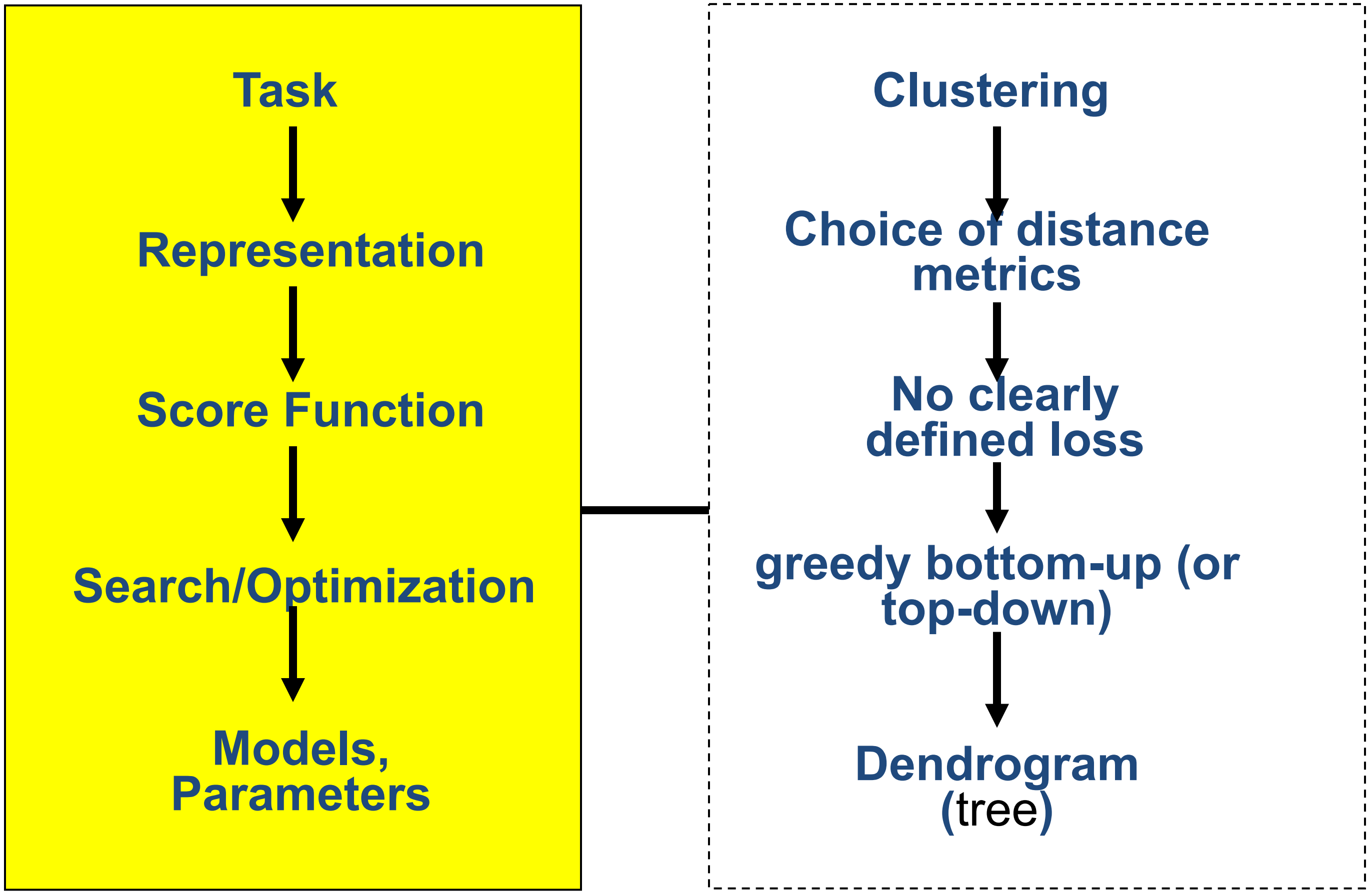
- In each of the subsequent *n*−*2* merging iterations, compute the distance between the most recently created cluster and all other existing clusters.

- For the subsequent steps, in order to maintain an overall $O(n^2)$ performance, computing similarity to each other cluster must be done in constant time. Else $O(n^2 \log n)$ or $O(n^3)$ if done naively

Summary of Hierarchal Clustering Methods

- 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 are a problem.
- Interpretation of results is (very) subjective.

Recap: Hierarchical Clustering



References

- 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