

UVA CS 4774: Machine Learning

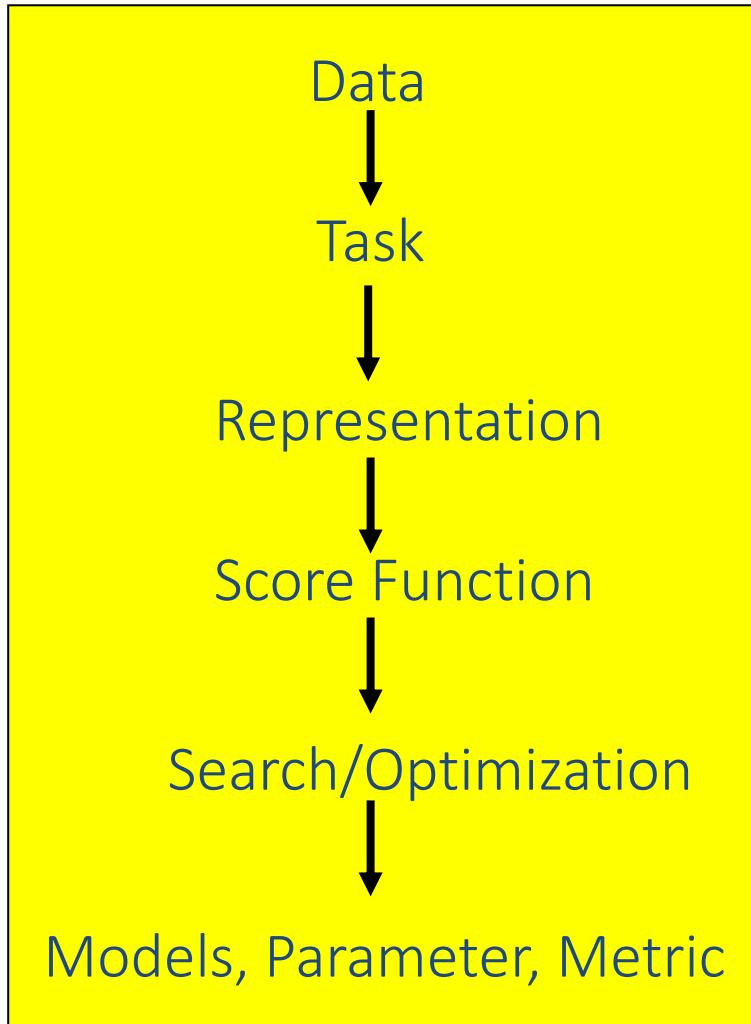
S5: Lecture 24: Unsupervised Clustering (I): Hierarchical

Dr. Yanjun Qi

Module I

University of Virginia
Department of Computer Science

Machine Learning in a Nutshell



ML grew out of work in AI

Optimize a performance criterion using example data or past experience,

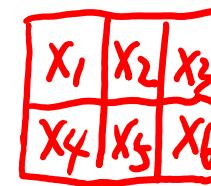
Aiming to generalize to unseen data

Course Content Plan → Regarding

Data

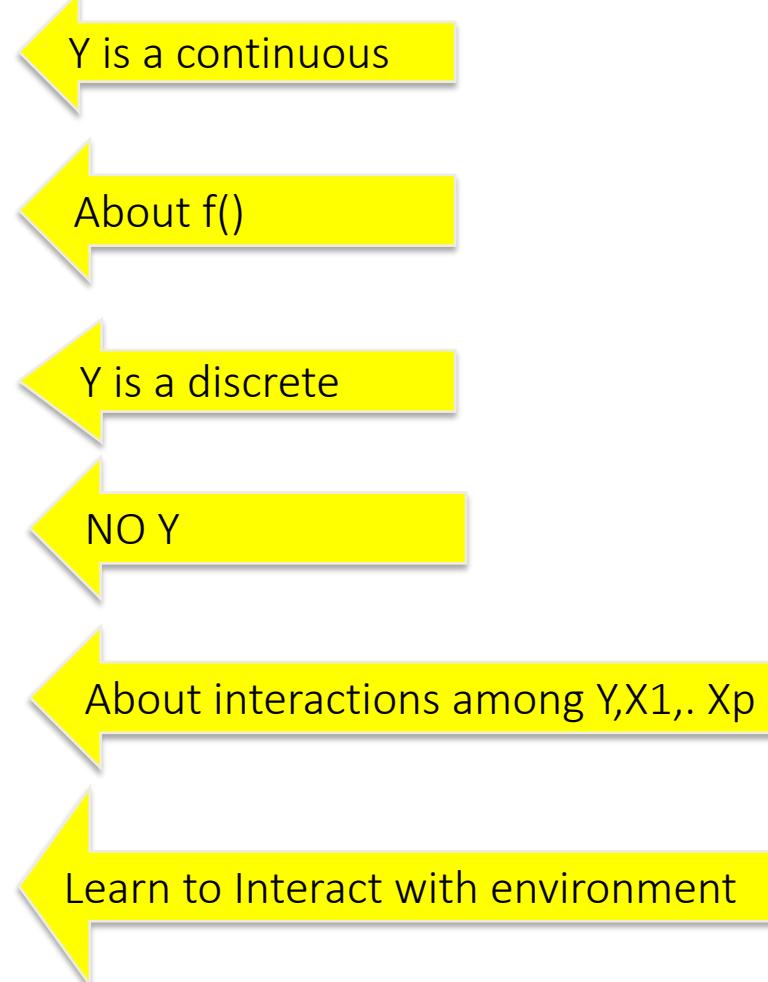


- Tabular / Matrix
- 2D Grid Structured: Imaging
- 1D Sequential Structured: Text
- Graph Structured (Relational)
- Set Structured / 3D /



Course Content Plan → Regarding Tasks

- ~~Regression (supervised)~~
- ~~Learning theory~~
- ~~Classification (supervised)~~
- Unsupervised models
- ~~Graphical models~~
- Reinforcement Learning



	X_1	X_2	X_3
S_1			
S_2			
S_3			
S_4			
S_5			
S_6			

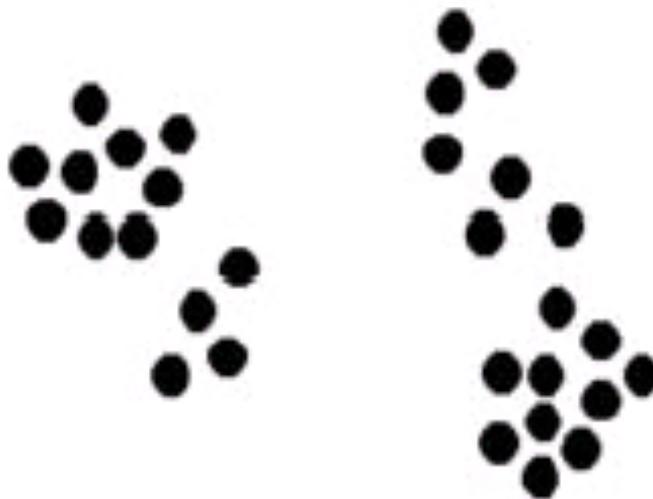
An unlabeled Dataset X

a data matrix of n observations on p variables x_1, x_2, \dots, 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]

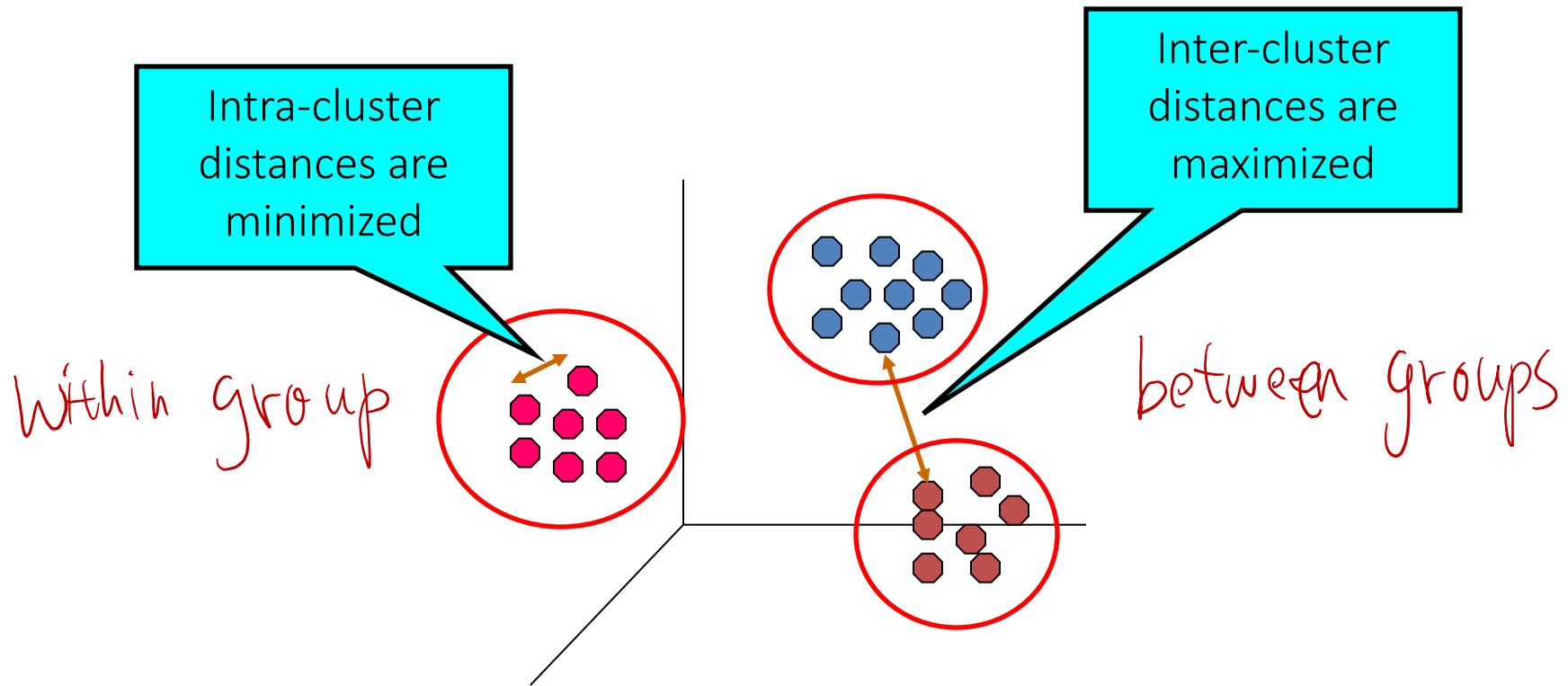
Today: What is clustering?



- 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
 - Identify similar objects from pictures

Toy Examples

- People



- Images



- Language

Piotr *Pyotr* *Petros* *Pietro* *Pedro* *Pierre* *Piero* *Peter* *Peder* *Peka* *Peadar*

- species



About 37,200,000 results (0.43 seconds)

partition

Application (I): Search Result Clustering

JaguarUSA.com - Jaguar® Convertible Car

ⓘ

Ad www.jaguarusa.com/ ▾

Real Comfort Comes From Control. Schedule Your Test Drive Today.

Jaguar USA has 1,261,482 followers on Google+.

Build & Price

Design A Jaguar Car To Your Driving Style and Personal Tastes.

Locate A Retailer

Find Your New Dream Car At Your Closest Jaguar Retailer Today.

Naughty Car. Nice Price.

Unwrap A Jaguar® Vehicle During Our Winter Sales Event On November 3rd.

Request A Quote

Get A Quote On Your Favorite Model From Your Local Jaguar Retailer.

Jaguar: Luxury Cars & Sports Cars | Jaguar USA

www.jaguarusa.com/ ▾ Jaguar Cars ▾

The official home of Jaguar USA. Our luxury cars feature innovative designs along with legendary performance to deliver one of the top sports cars in the ...

Models - F-Type - XF - XJ

Jaguar - Wikipedia, the free encyclopedia

en.wikipedia.org/wiki/Jaguar ▾ Wikipedia ▾

The **jaguar** *Panthera onca*, is a big cat, a feline in the *Panthera* genus, and is the only *Panthera* species found in the Americas. The **jaguar** is the third-largest ...

Jaguar Cars - Jaguar (disambiguation) - Tapir - List of solitary animals

Jaguar Cars - Wikipedia, the free encyclopedia

en.wikipedia.org/wiki/Jaguar_Cars ▾ Wikipedia ▾

Jaguar Cars is a brand of Jaguar Land Rover, a British multinational car manufacturer headquartered in Whitley, Coventry, England, owned by Tata Motors since ...

Images for jaguar

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[More images for jaguar](#)

Application (II): Navigation

Hierarchy

Entertainment in the Yahoo! Directory - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://dir.yahoo.com/Entertainment/ Google

Getting Started Latest Headlines

Yahoo! My Yahoo! Mail Welcome, Guest [Sign In]

YAHOO! DIRECTORY

Search: the Web | the Directory | this category

Entertainment

Value City Furniture www.vcf.com Quality Home Entertainment Packages Browse Today and Find a Store.

CATEGORIES (What's This?)

Top Categories

- Music (76772) NEW!
- Actors (19211) NEW!
- Movies and Film (40031) NEW!
- Television Shows (17085) NEW!
- Humor (3927)
- Comics and Animation (5778) NEW!

Additional Categories

- Amusement and Theme Parks (449)
- Awards (698)
- Blogs@
- Books and Literature@
- Chats and Forums (47)
- Comedy (1730)
- Consumer Electronics (1355) NEW!
- Contests, Sweepstakes and Polls (27) NEW!
- Magic (353)
- News and Media (443)
- Organizations (33)
- Performing Arts@
- Radio@
- Randomized Things (57)
- Reviews (32)
- Shopping and Services@

SPONSOR RESULTS

Entertainment Center Furniture Save 30-60% On A Variety Of Furniture For Any Room Thru 11/13. JCPenney.com

Studiotech Official Site StudioTech Entertainment Furniture. Factory Direct... www.StudioTech.com

Bush Entertainment Furniture Save up to 50% factory-direct. www.bushfurniturecollection.com

Done

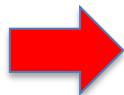
start

10/19/2008 11:46 AM

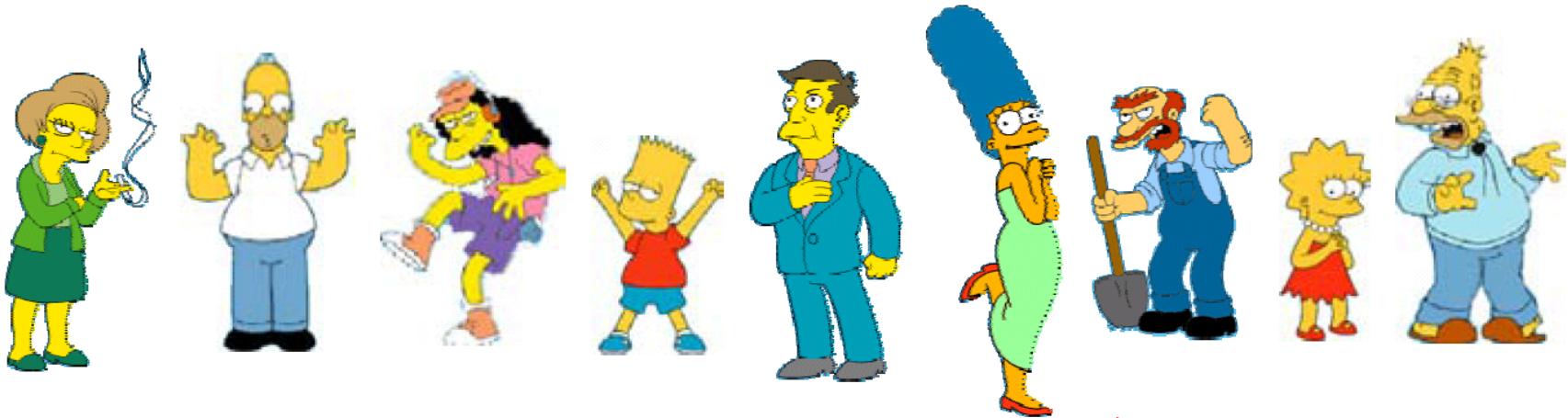
Issues for clustering

- 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

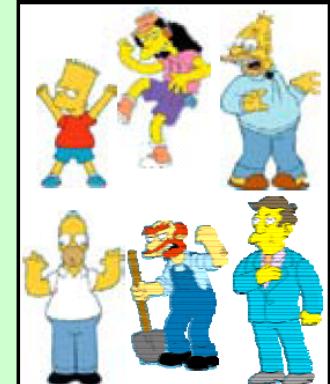
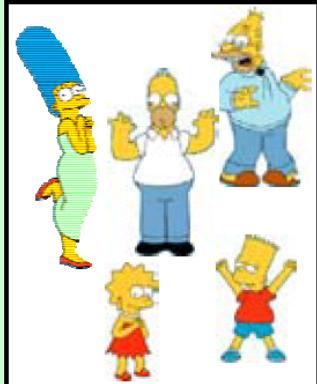
Today Roadmap: clustering

- 
- Definition of "groupness"
 - Definition of "similarity/distance"
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What is a natural grouping among these objects?



Clustering is subjective



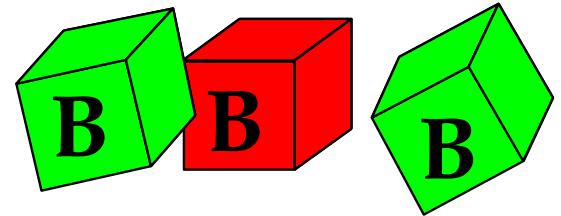
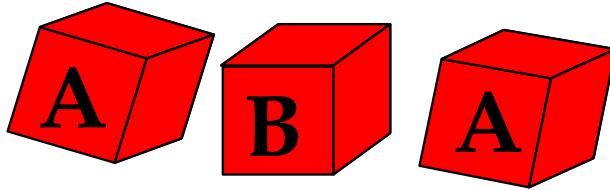
1 Simpson's Family

School Employees

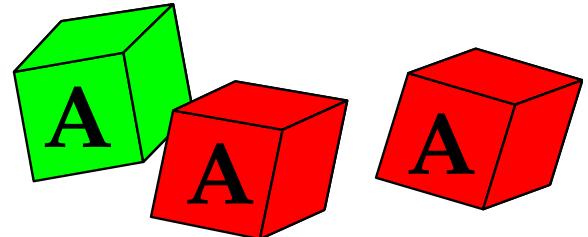
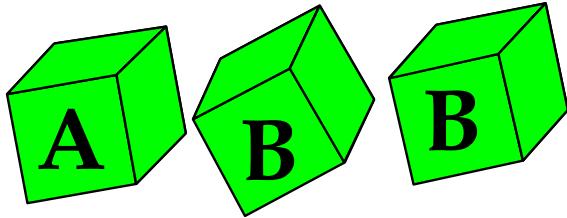
Females

Males

Another example: clustering is subjective



Two possible Solutions...





Thank You

Thank you

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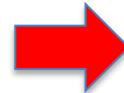
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II

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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*
- $D(A,B) = 0 \text{ IIf } A= B$ *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"
- $D(A,B) = 0 \text{ IIf } A = B$ *Positivity Separation*
 - Otherwise there are objects in your world that are different, but you cannot tell apart.
- $D(A,B) \leq D(A,C) + D(B,C)$ *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 objects 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

1, $r = 2$ (Euclidean distance)

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

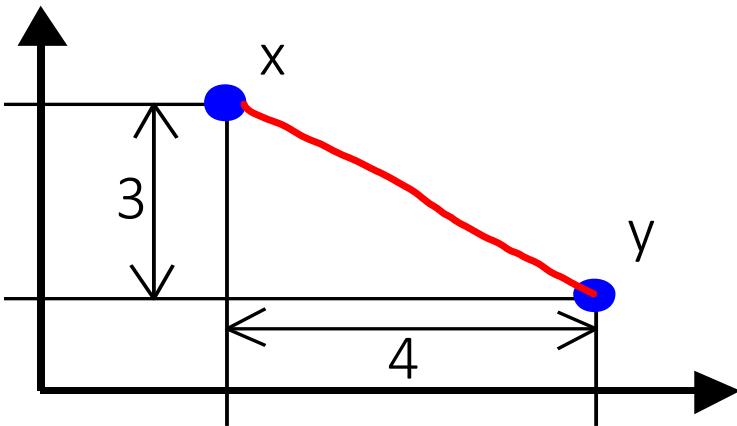
2, $r = 1$ (Manhattan distance)

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

3, $r = +\infty$ ("sup" distance)

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

An Example

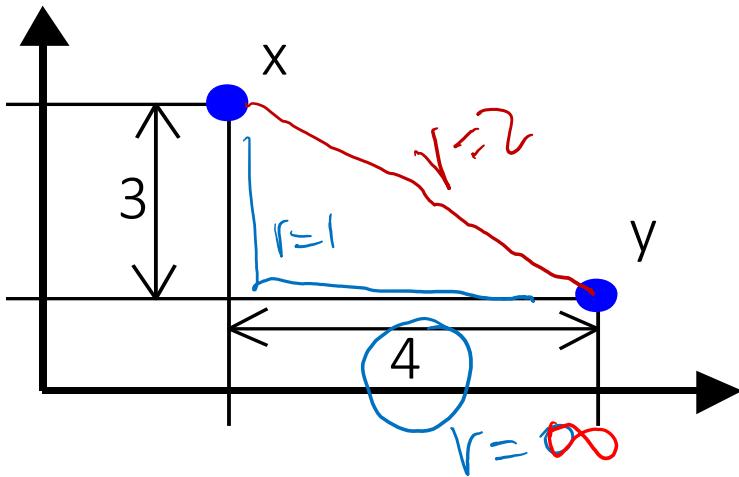


1: Euclidean distance: $\sqrt{4^2 + 3^2} = 5.$

2: Manhattan distance: $4 + 3 = 7.$

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

An Example



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

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	1	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 $\bar{y} = \frac{1}{p} \sum_{i=1}^p y_i$.

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

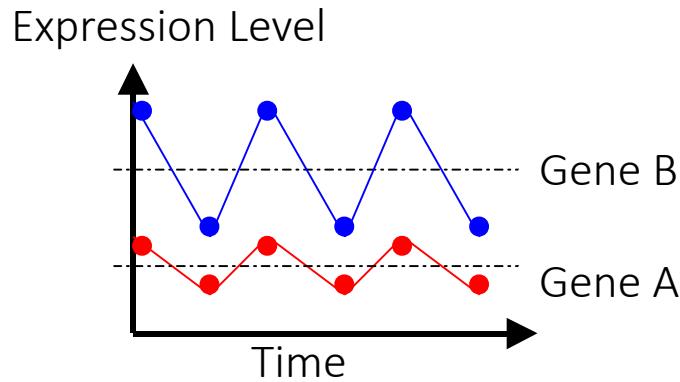
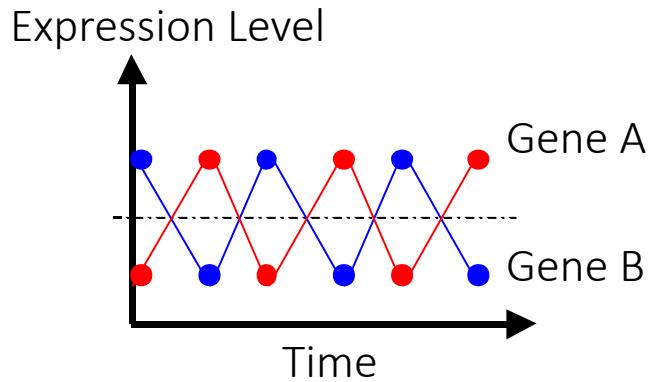
Correlation is unit independent

- Special case: cosine distance

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

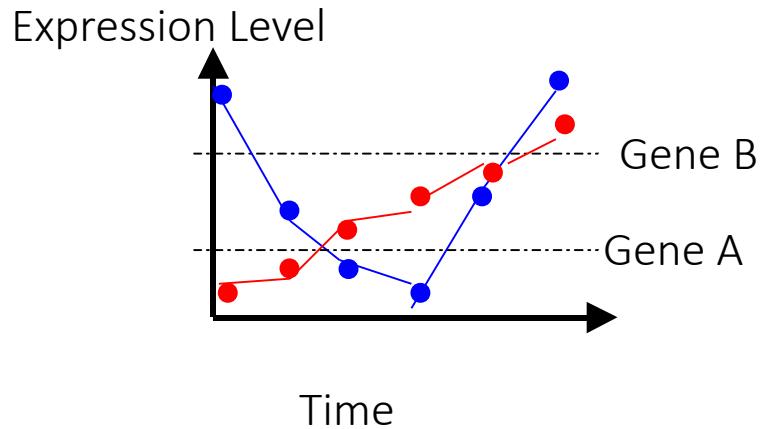
- Measuring the **linear correlation** between two sequences, x and y,
- giving a value between +1 and -1 inclusive, where 1 is total positive **correlation**, 0 is no **correlation**, and -1 is total negative **correlation**.

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.

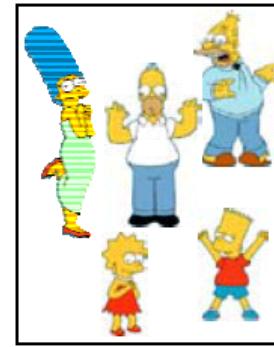


Today Roadmap: clustering

- Definition of "groupness"
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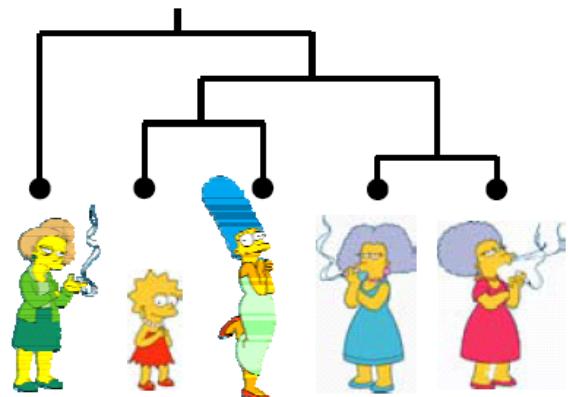
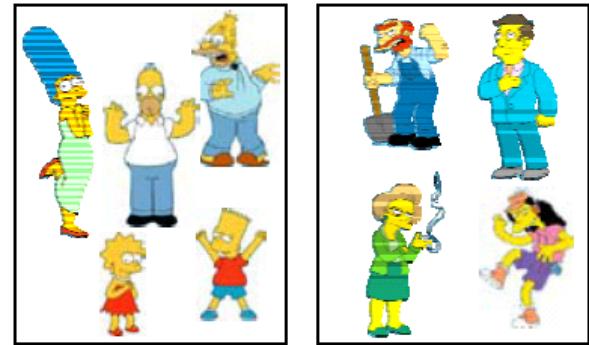
Clustering Algorithms

- 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

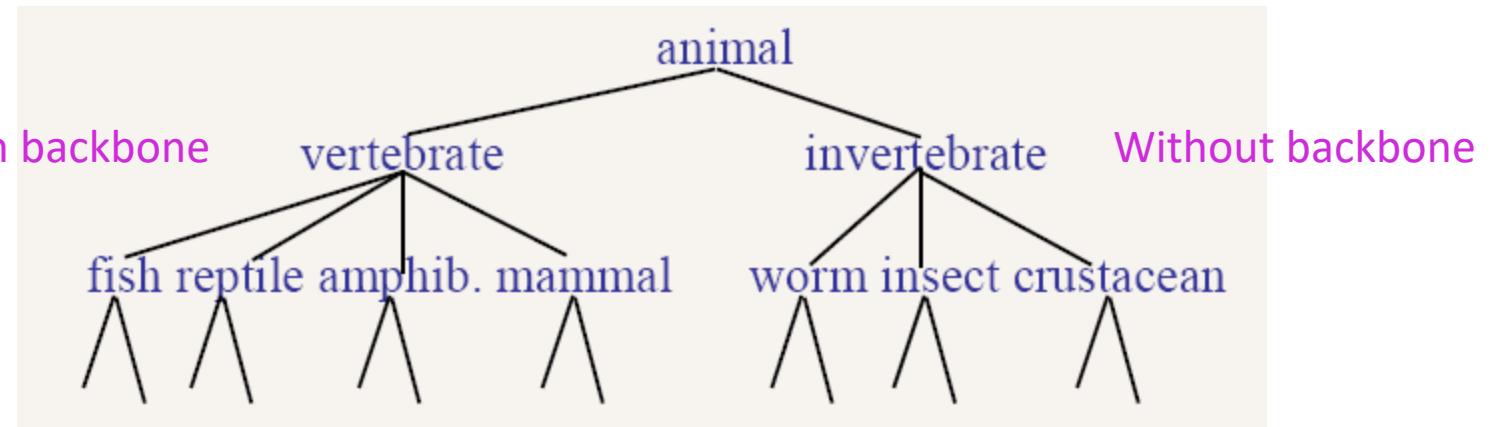


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Hierarchical Clustering

- 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.
 - 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:



Thank You

Thank you

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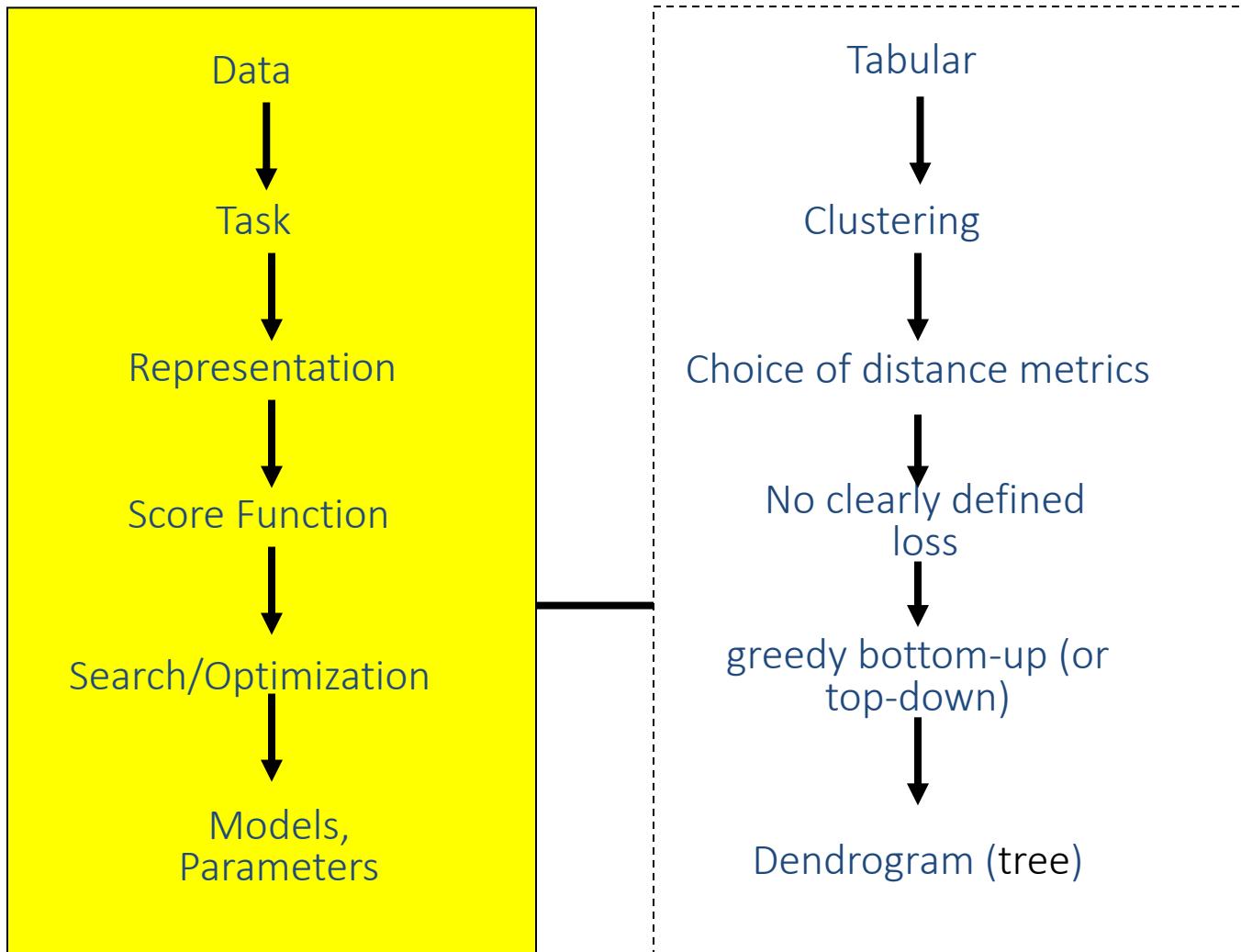
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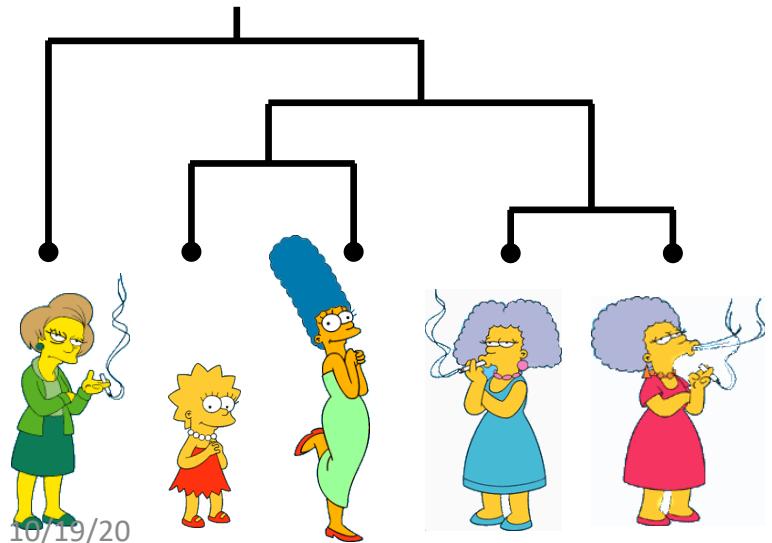
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Hierarchical Clustering



(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.

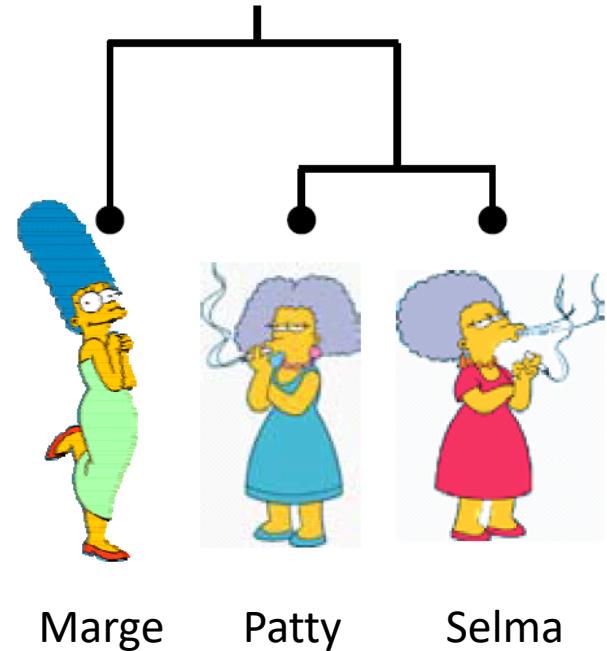
Change dress color, 1 point
 Change earring shape, 1 point
 Change hair part, 1 point

$$D(\text{Patty}, \text{Selma}) = 3$$

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

$$D(\text{Marge}, \text{Selma}) = 5$$



This is called the Edit distance or the Transformation distance¹⁹

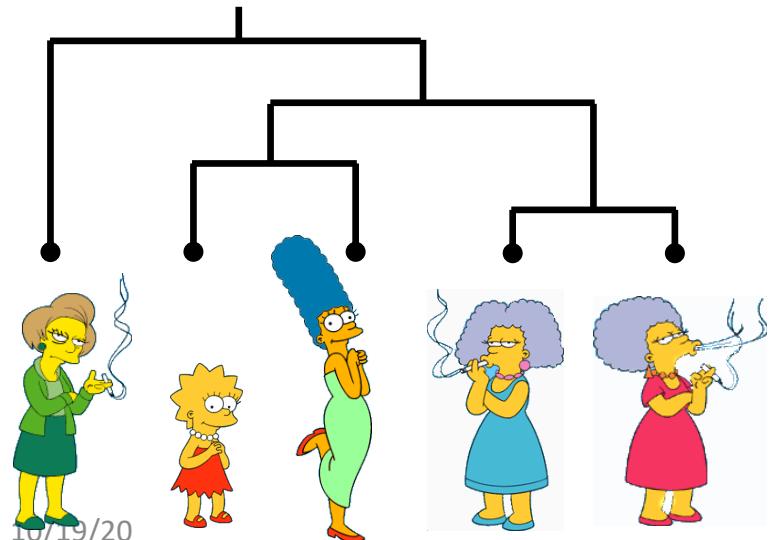
(How-to) Hierarchical Clustering

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

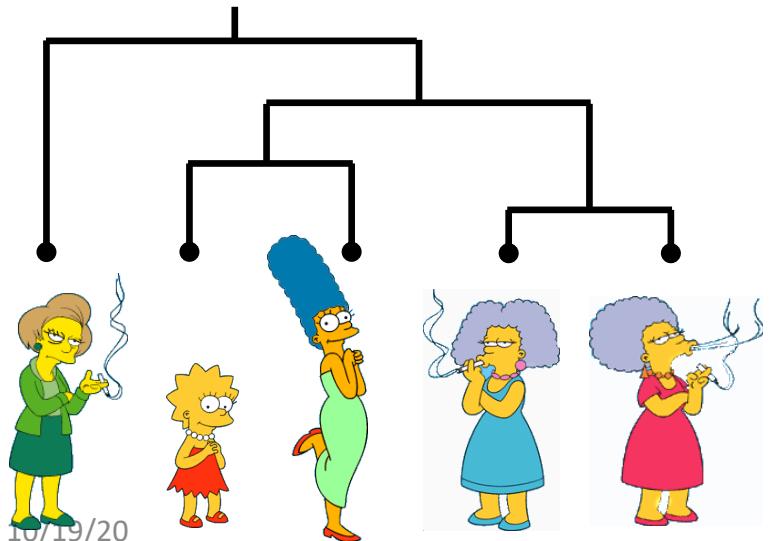
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Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.



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.

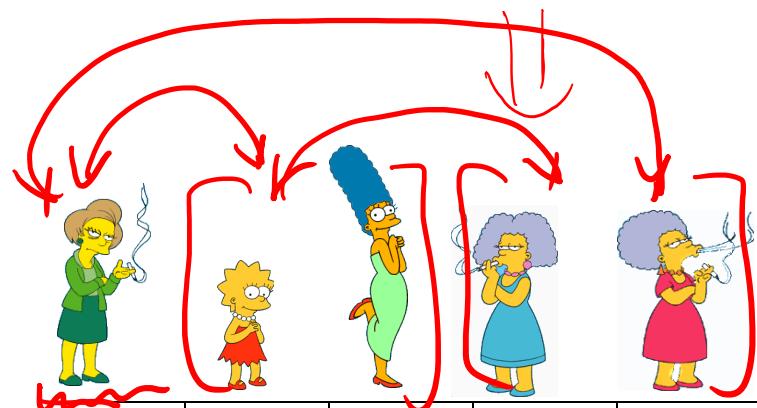
\Rightarrow min. Within cluster distance

$$D(\text{Marge, Lisa}) = 8$$

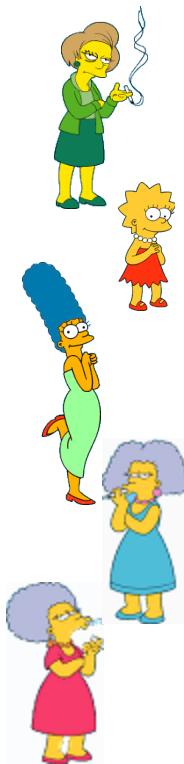
$$D(\text{Edna, Marge}) = 1$$

10/19/20

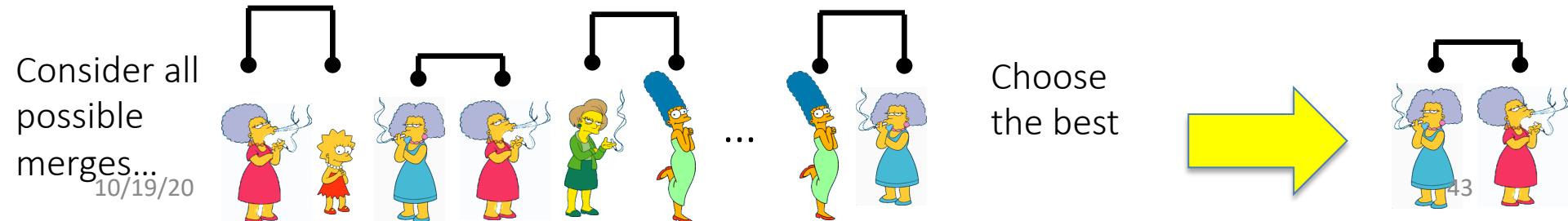
$$\begin{cases} D(A, A) = 0 \\ D(A, B) = D(B, A) \end{cases}$$



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

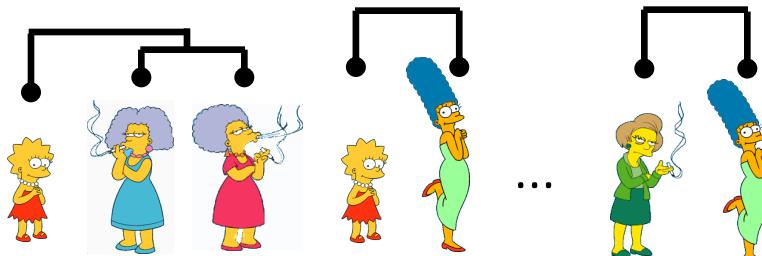


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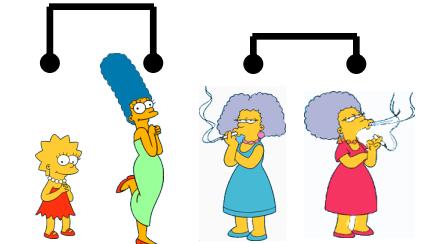


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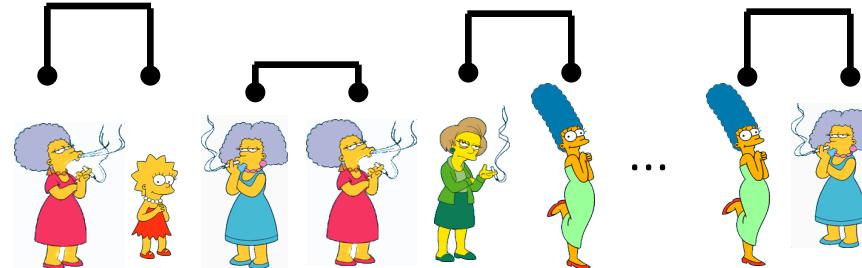
Consider all possible merges...



Choose the best



Consider all possible merges...
10/19/20



Choose the best



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

$$D(\text{Marge, Lisa}) = 8$$

$$D(\text{Marge, Marge}) = 1$$

10/19/20

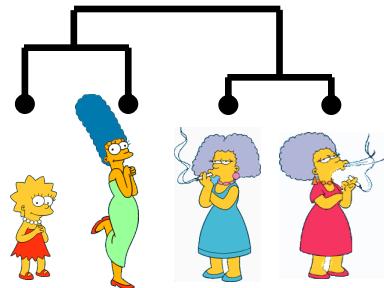
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0	8	8	7	7
	0	2	4	4
		0	3	3
			0	1
				0

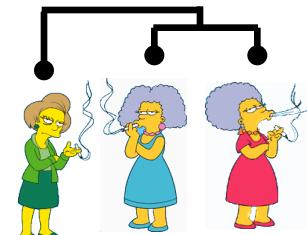
45

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.

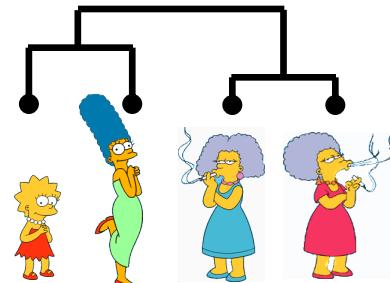
Consider all possible merges...



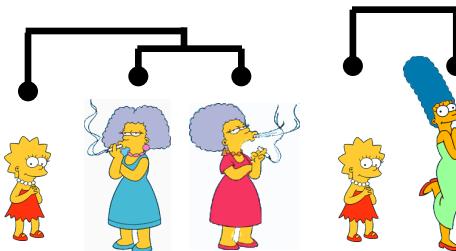
...



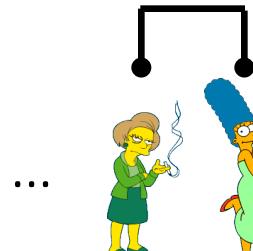
Choose the best



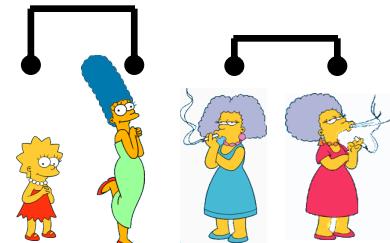
Consider all possible merges...



...



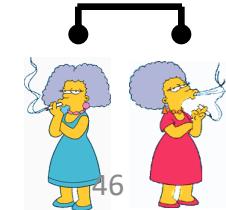
Choose the best



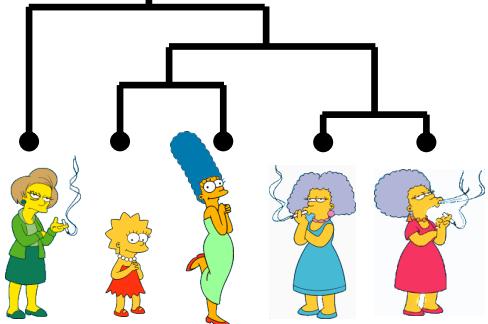
Consider all possible merges...



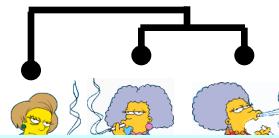
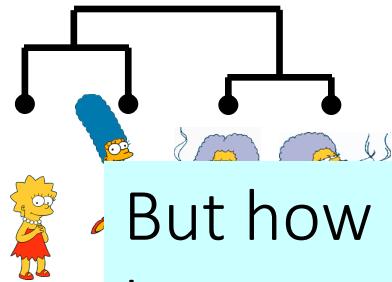
Choose the best



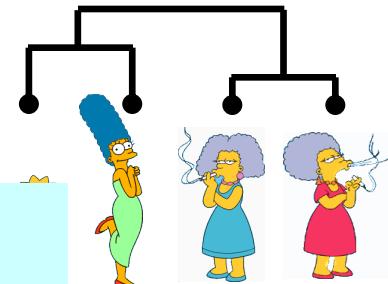
Bottom-Up (agglomerative): Starting with each item in its own cluster, find the best pair to merge into a new cluster. Repeat until all clusters are fused together.



Consider all possible merges...

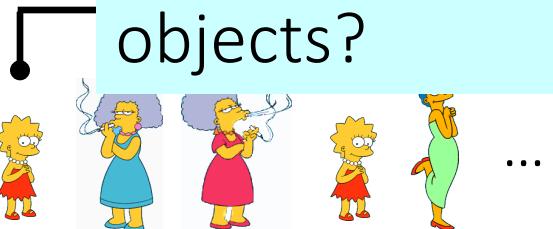


Choose the best

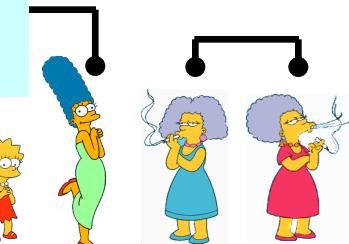


But how do we compute distances between clusters rather than objects?

Consider all possible merges...



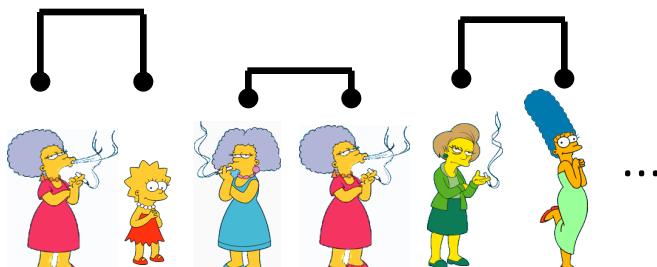
the best



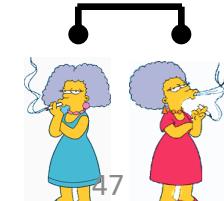
Consider all possible merges...



Choose the best



10/19/20



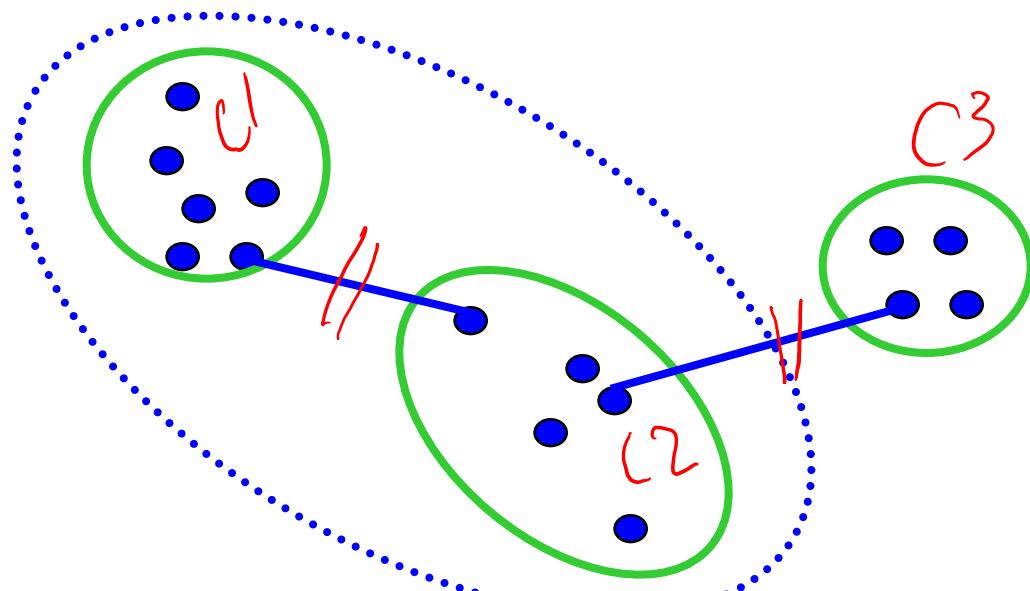
47

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

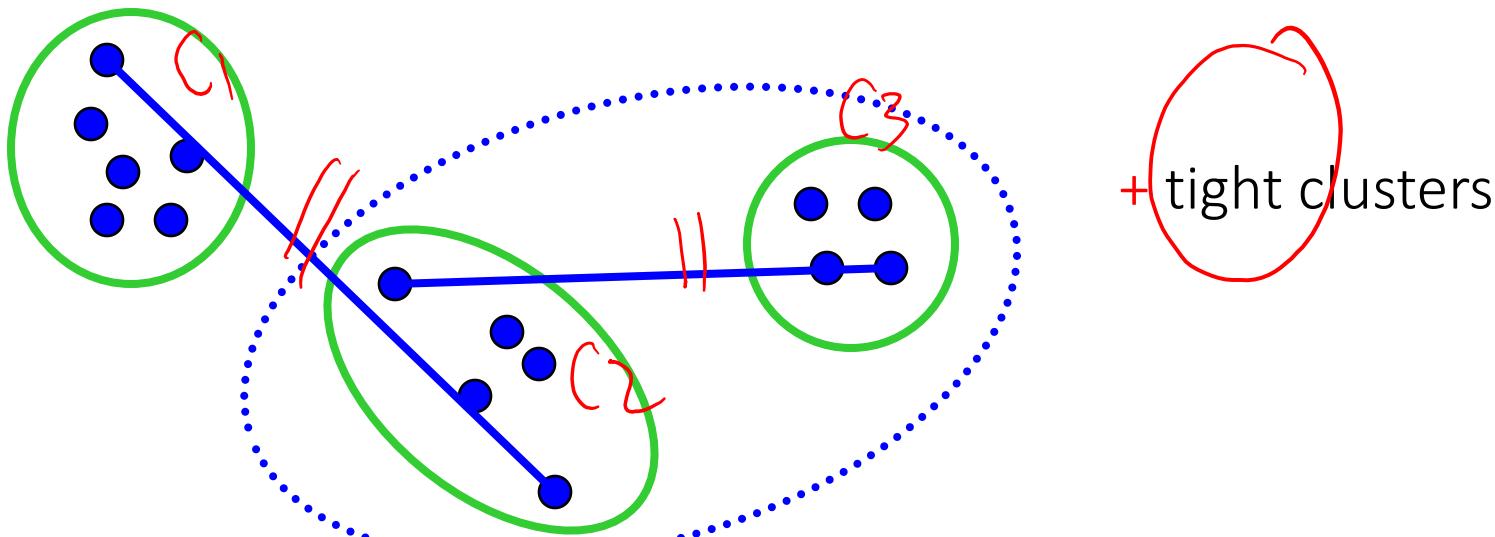
- cluster distance = distance of two **closest** members in each class



- Potentially long
and skinny clusters

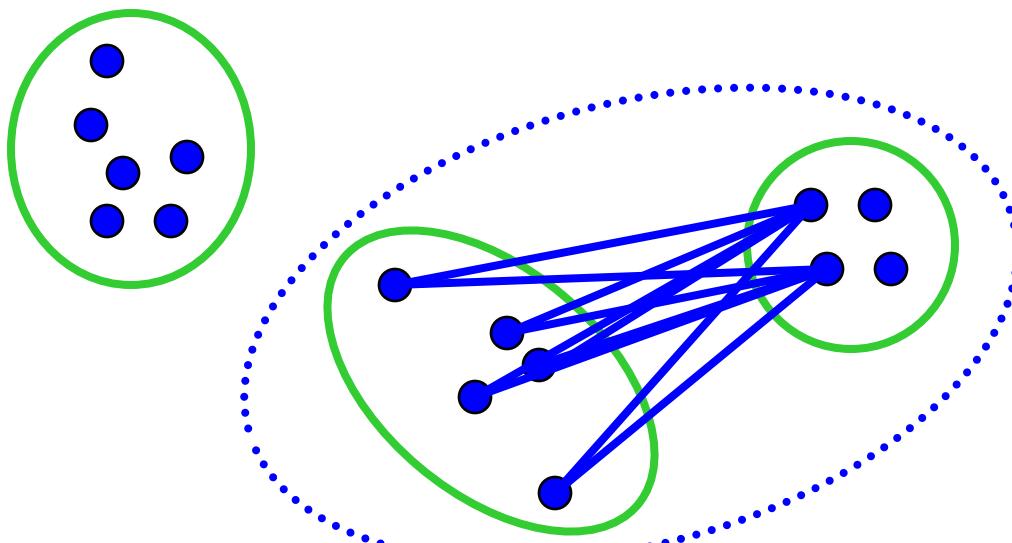
Computing distance between clusters: : Complete Link

- cluster distance = distance of two farthest members



Computing distance between clusters: Average Link

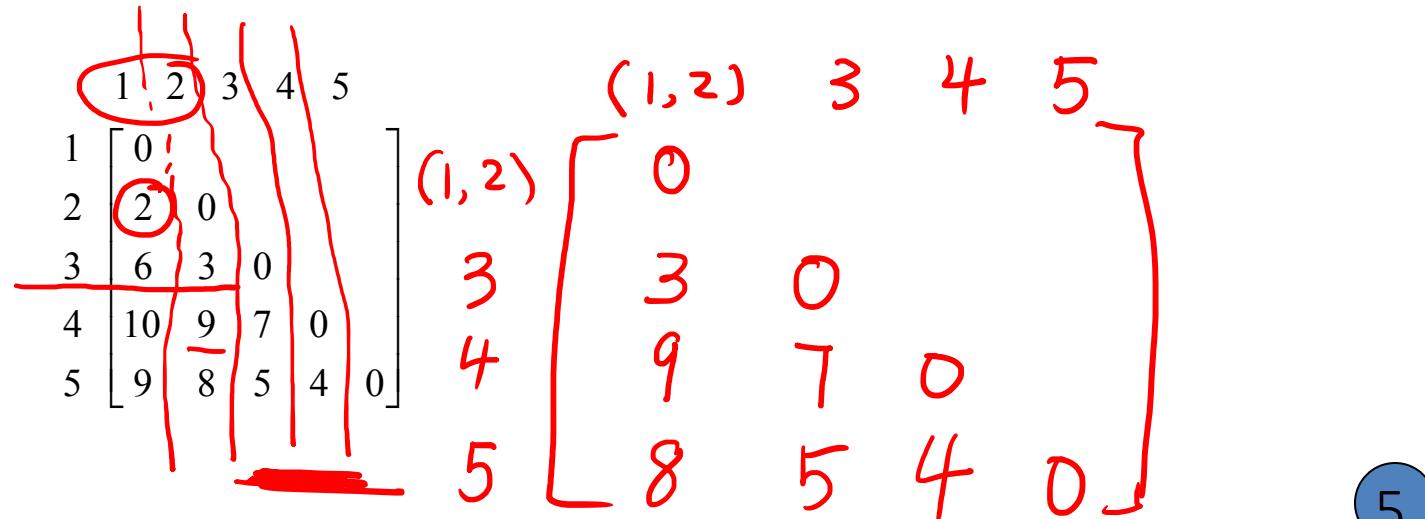
- cluster distance = **average distance** of all pairs



the most widely used measure

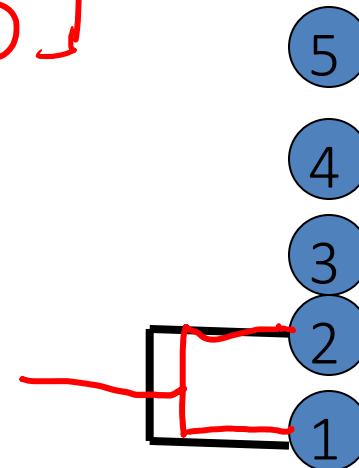
Robust against noise

Example: single link



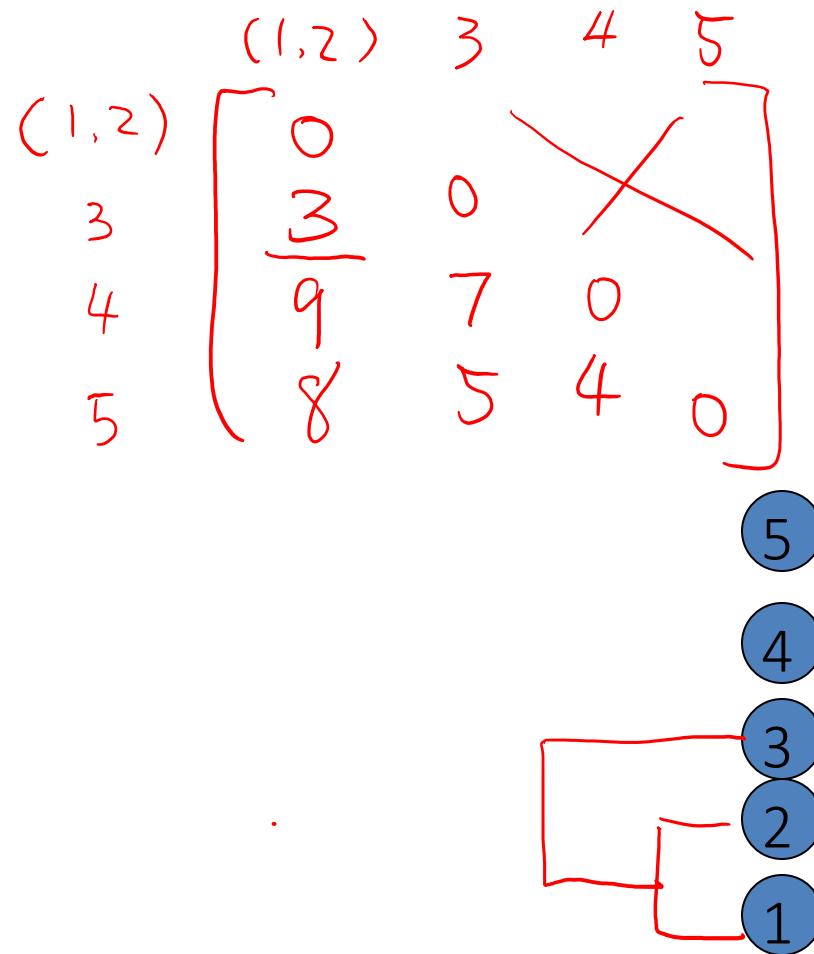
① Best ② re-matrix

$$\begin{array}{c}
 (1,2) \\
 3 \\
 4 \\
 5
 \end{array}
 \left[\begin{array}{cccc}
 0 & & & \\
 6 & 0 & & \\
 10 & 7 & 0 & \\
 9 & 5 & 4 & 0
 \end{array} \right]
 \text{Complete}$$

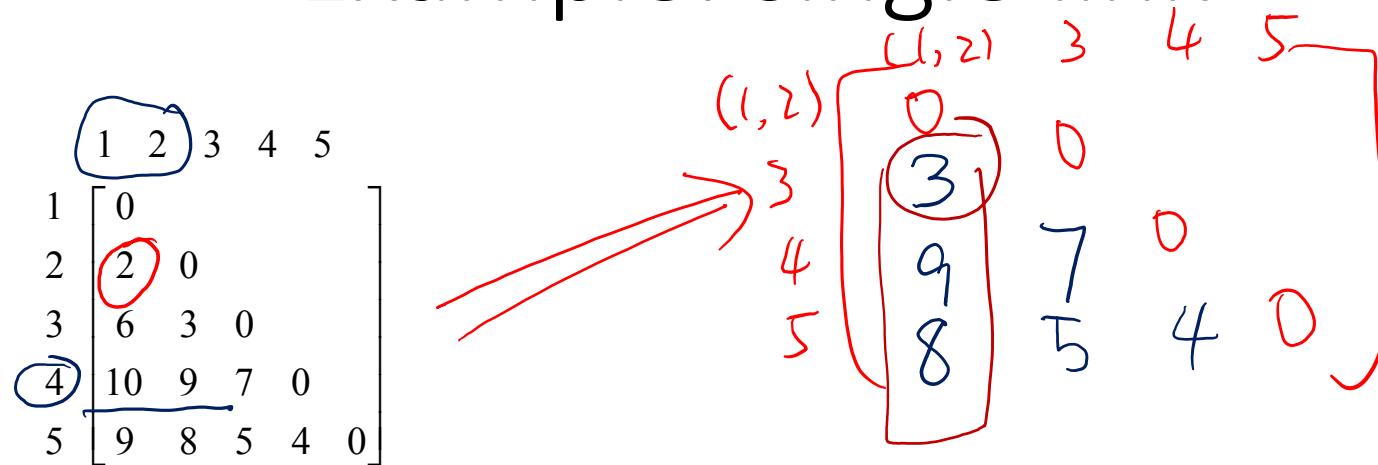


Example: single link

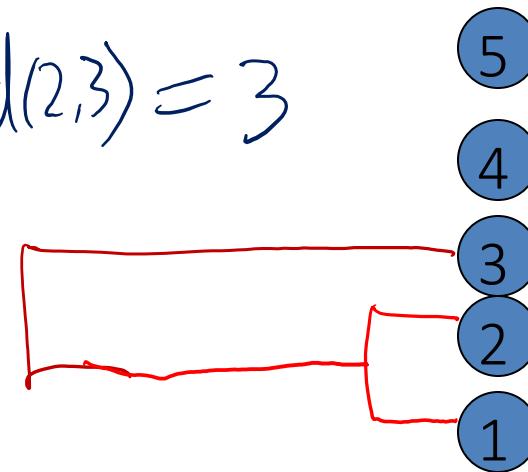
	1	2	3	4	5
1	0				
2	2	0			
3	6	3	0		
4	10	9	7	0	
5	9	8	5	4	0



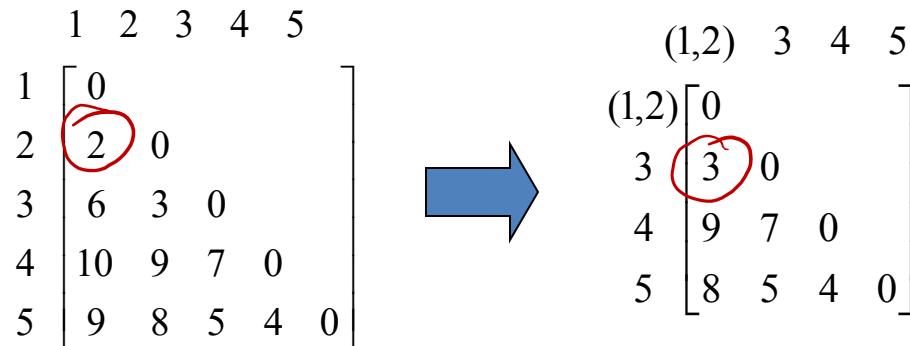
Example: single link



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



Example: single link



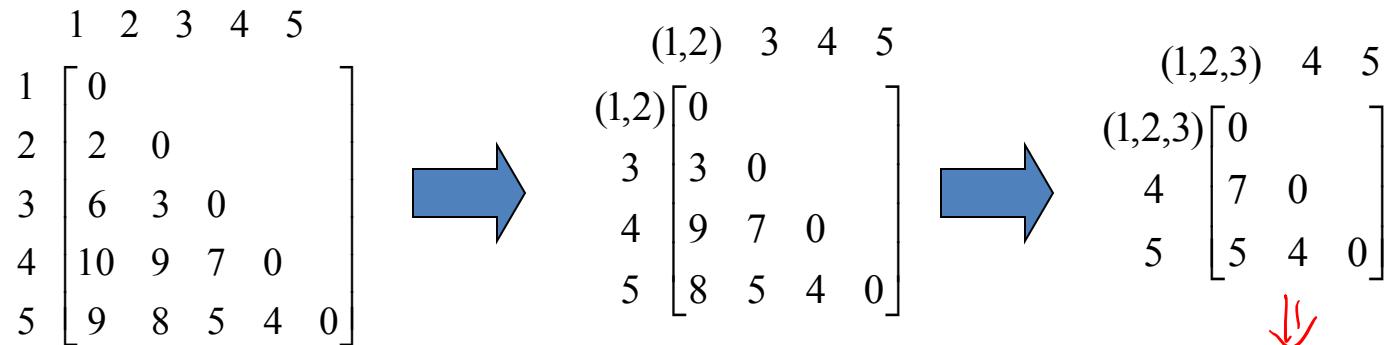
$$d_{(1,2),3} = \min\{ d_{1,3}, d_{2,3} \} = \min\{ 6, 3 \} = 3$$

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

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

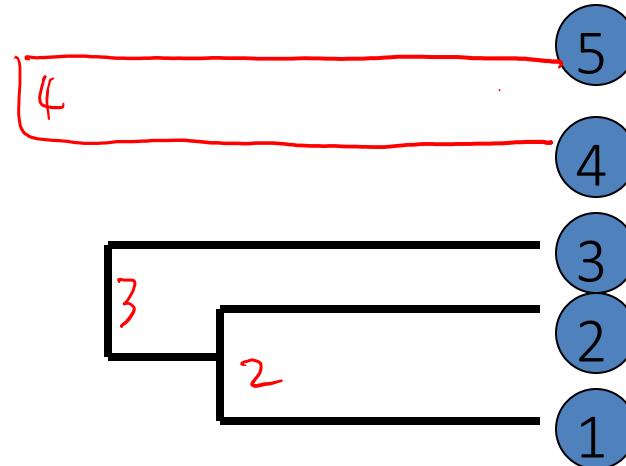
5
4
3
2
1

Example: single link



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

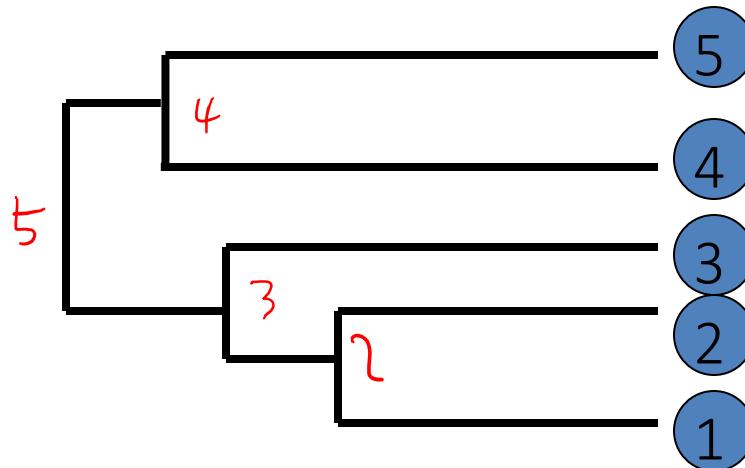
$$d_{(1,2,3),5} = \min\{ d_{(1,2),5}, d_{3,5} \} = \min\{ 8, 5 \} = 5$$



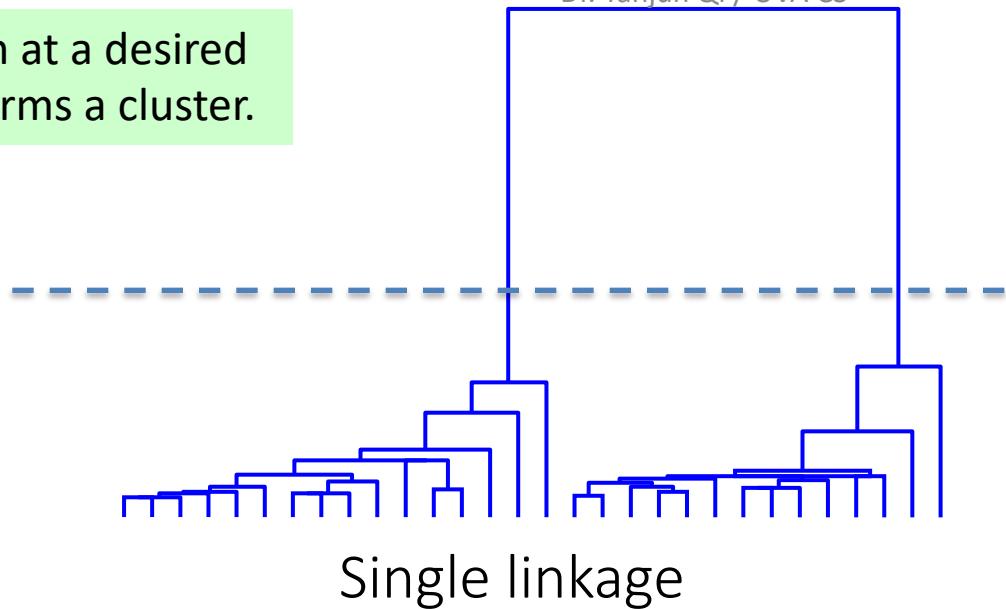
Example: single link

$$\begin{array}{c}
 \begin{matrix} & 1 & 2 & 3 & 4 & 5 \\ 1 & \left[\begin{matrix} 0 & & & & \\ 2 & 0 & & & \\ 3 & 6 & 3 & 0 & \\ 4 & 10 & 9 & 7 & 0 \\ 5 & 9 & 8 & 5 & 4 & 0 \end{matrix} \right] \end{matrix} \rightarrow \begin{matrix} (1,2) & 3 & 4 & 5 \\ (1,2) \left[\begin{matrix} 0 & & & \\ 3 & 3 & 0 & \\ 4 & 9 & 7 & 0 \\ 5 & 8 & 5 & 4 & 0 \end{matrix} \right] \end{matrix} \rightarrow \begin{matrix} (1,2,3) & 4 & 5 \\ (1,2,3) \left[\begin{matrix} 0 & & \\ 4 & 7 & 0 \\ 5 & 5 & 4 & 0 \end{matrix} \right] \end{matrix}
 \end{array}$$

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

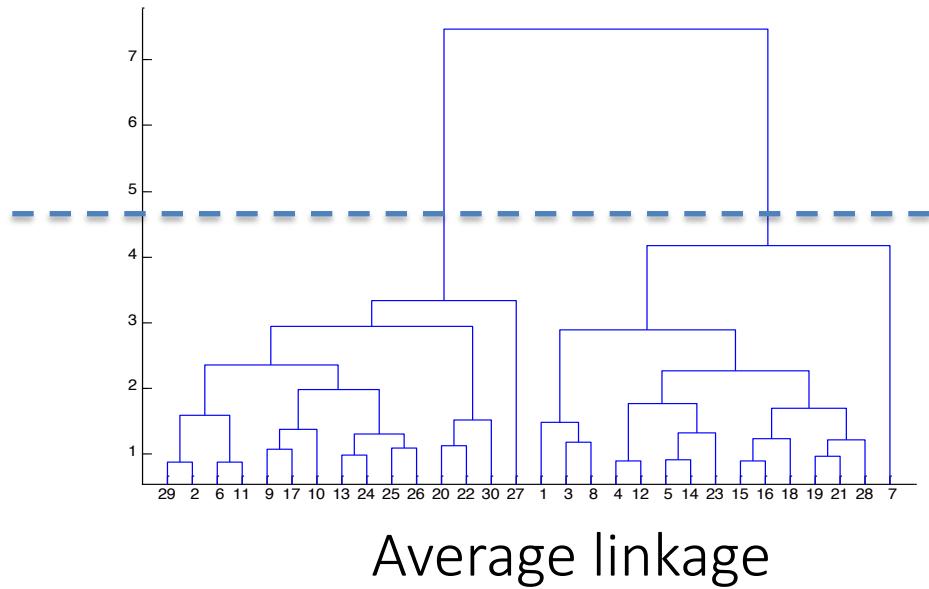


Partitions by cutting the dendrogram at a desired level: each connected component forms a cluster.



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

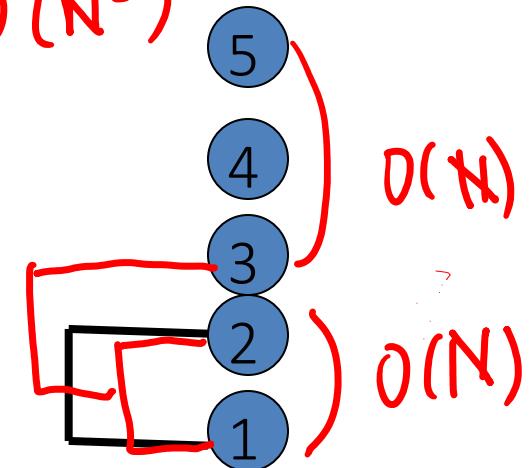
	1	2	3	4	5
1	0				
2	2	0			
3	6	3	0		
4	10	9	7	0	
5	9	8	5	4	0

$N \times N$

$\vec{x}_i \in \mathbb{R}^P, (\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N)$
 time: $O(\text{dist}(\vec{x}_i, \vec{x}_j)) \sim O(P)$
 $O(\text{pairse Matrix}) \sim O(PN^2)$
 $\text{BestCluster} \sim O(N^2)$

	(1,2)	3	4.	5
(1,2)	0	.	.	.
3	.	0	.	.
4	.	.	0	.
5	.	.	.	0

$\Rightarrow O(N)$



A total of $n-1$ merging iterations

Hierarchical Clustering

Time Complexity

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

A total of $n-1$ merging iterations

$$O(n^3 p)$$

Computational Complexity

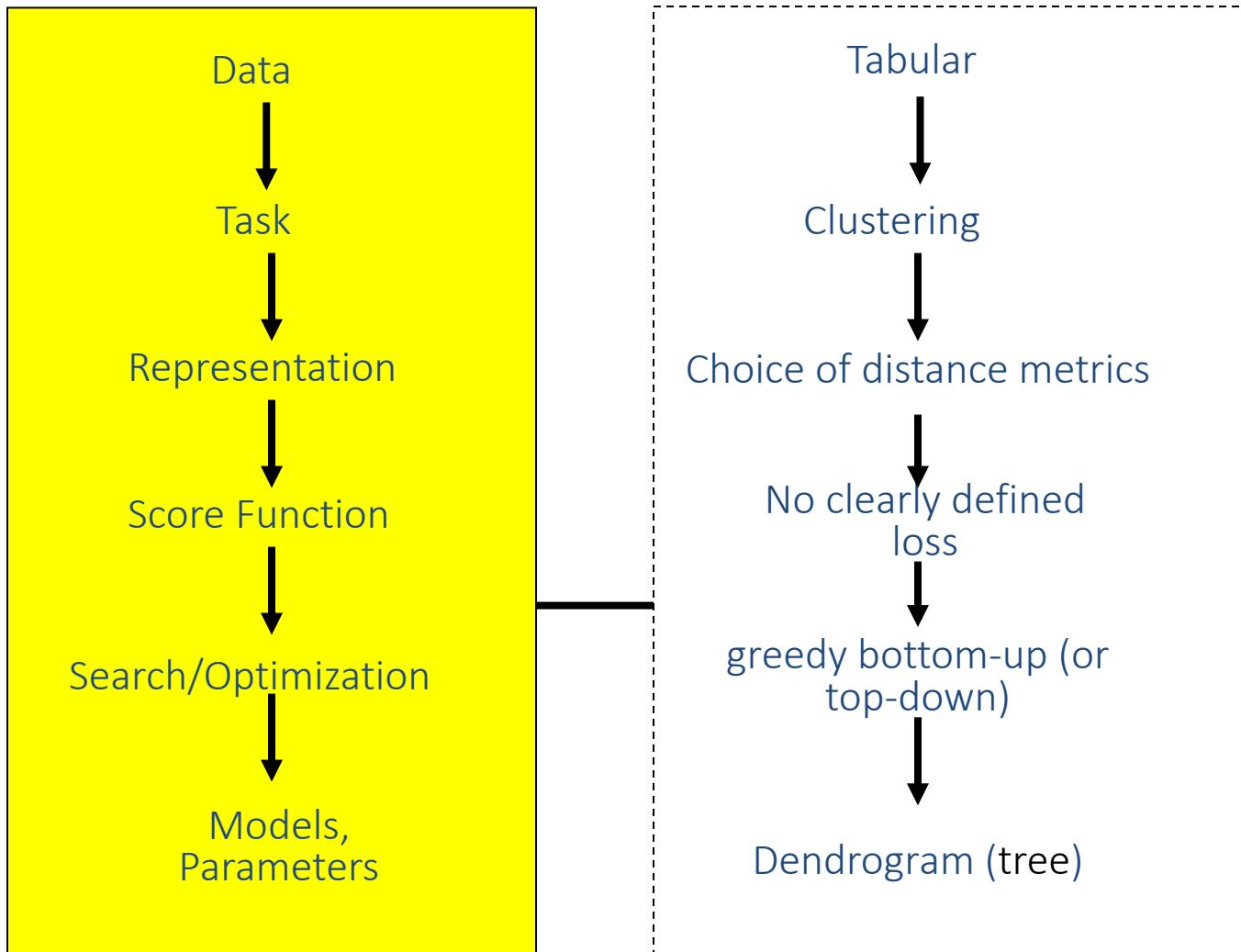
$$\sum_{i=1}^p (x_i - y_i)^2 \Rightarrow O(p)$$

- In the first iteration, all HAC methods need to compute similarity of all pairs of n individual instances which is $O(n^2 p)$.
[Matrix]
- In each of the subsequent 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. $O(n^3)$ if done naively

Summary of Hierarchical 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





Thank You

Thank you

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