Week 2

Course. Introduction to Machine Learning

Theory 2. Introduction to unsupervised learning and Cluster Analysis (Part I)

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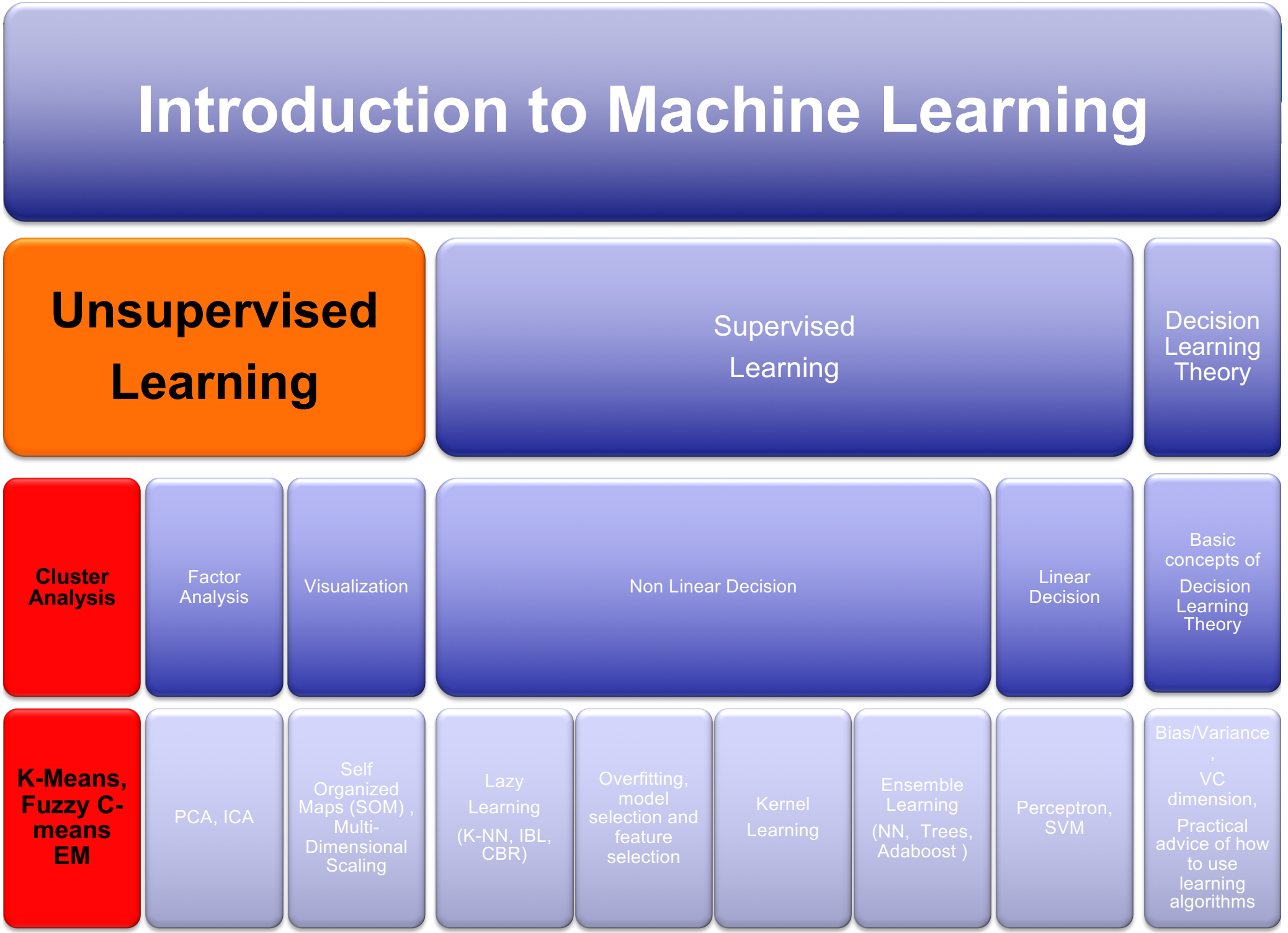
Introduction to Machine Learning



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   3. Definition of unsupervised learning
   4. Unsupervised learning approaches
2. **Introduction to Cluster analysis (Theory 2)**
   1. Defining clustering analysis
   2. Areas that apply clustering
   3. Classification of clustering algorithms
3. **Hierarchical clustering (Theory 2)**
4. **Partitional clustering (Theory 3)**
   1. K-Means algorithm,
   2. Bisecting K-Means,
   3. Fuzzy C-Means
   4. EM (expectation maximization algorithm)

Introduction to unsupervised learning

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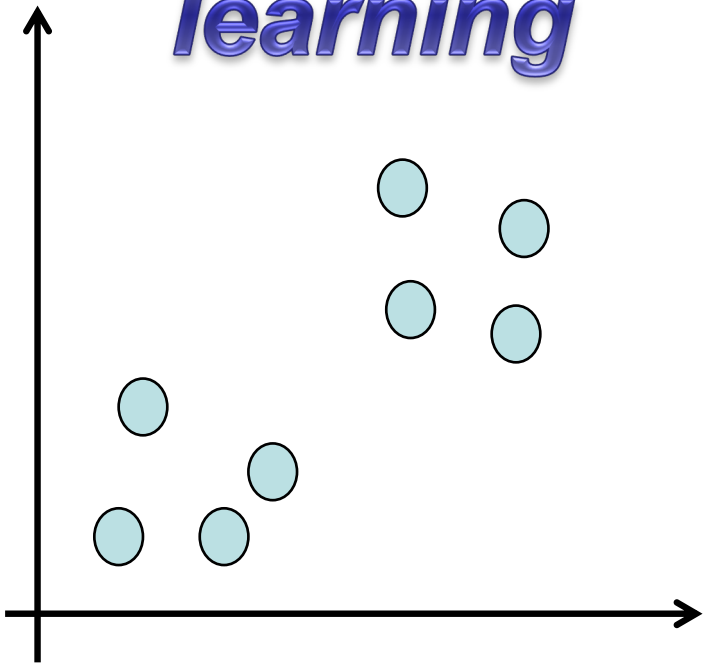
Introduction to Unsupervised learning

Supervised learning

Inferring a function from labelled training data

Unsupervised learning



Try to find hidden structure in unlabeled data

https://youtu.be/ukzFI9rgwfU

Unsupervised learning

There are two main goals in unsupervised learning

1. **Summarization**: To obtain representations that describe an unlabeled dataset
2. **Understanding**: To discover the key concepts inside the data

- These tasks are difficult because the discovery process is biased by context
  - Different answers can be valid depending of the discovery goal or the domain
  - There are few criterion to validate the results
- Representation of the clusters:
  - Relational (hierarchies)
  - Unstructured (partitions)

Examples of unsupervised learning

- Bioinformatics
- Medicine
- Market research
- Social network analysis
- NLP: document clustering, text mining, concept extraction
- Image segmentation
- Educational data mining
- Climatology
- …

https://theappsolutions.com/blog/development/unsupervised-machine-learning/

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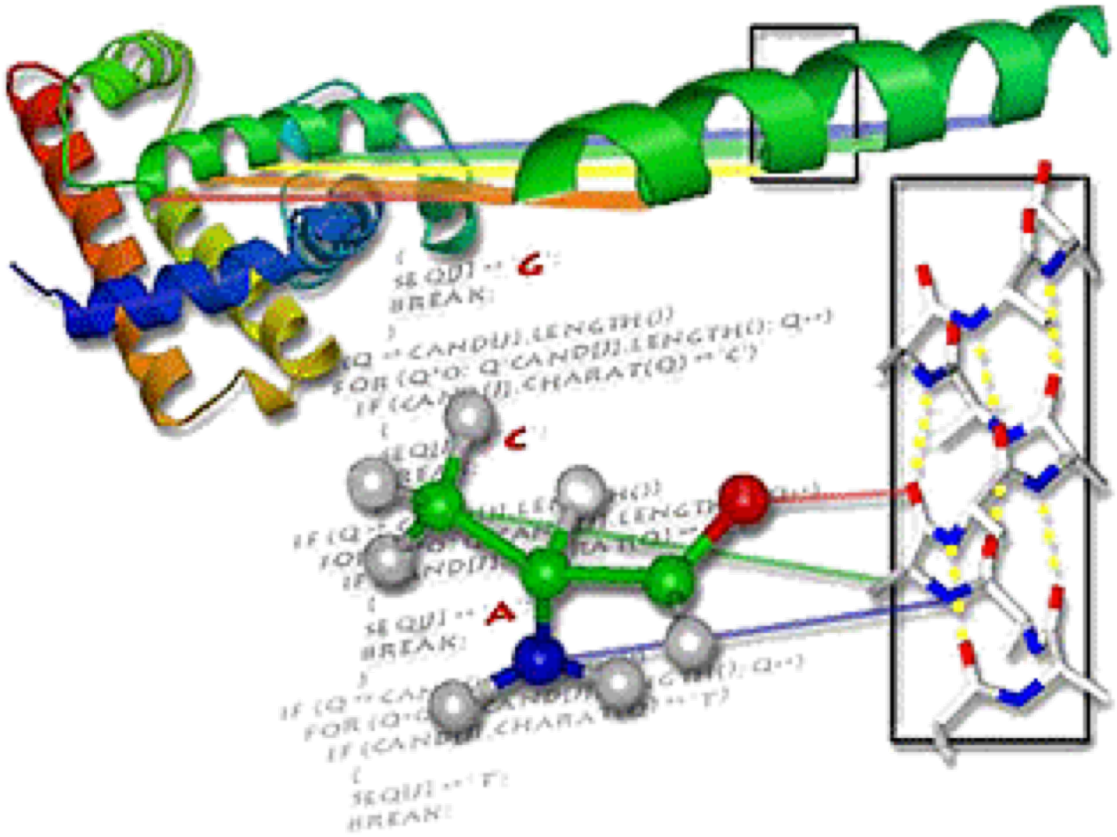
Bioinformatics



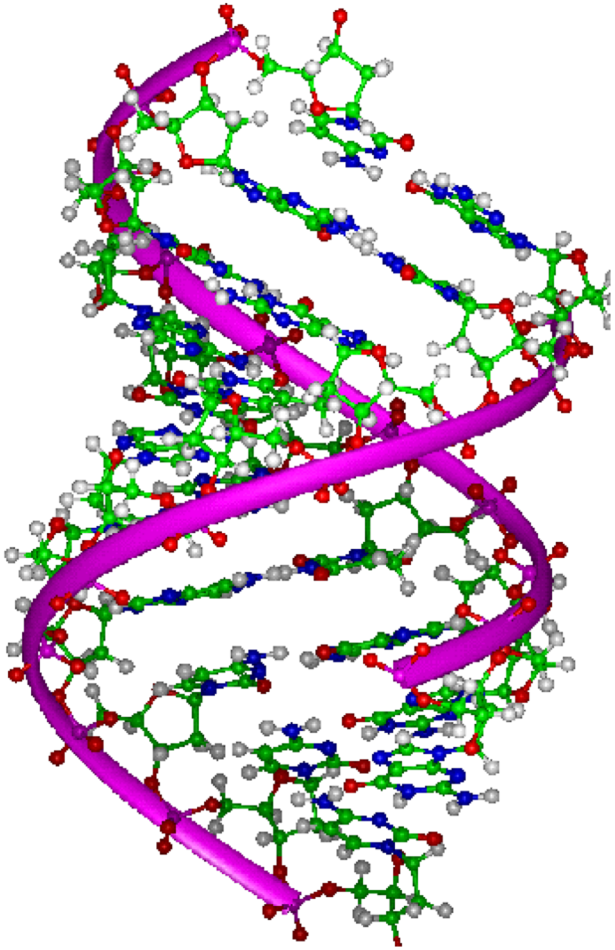


Illustration by Brian Haas, Phillips lab

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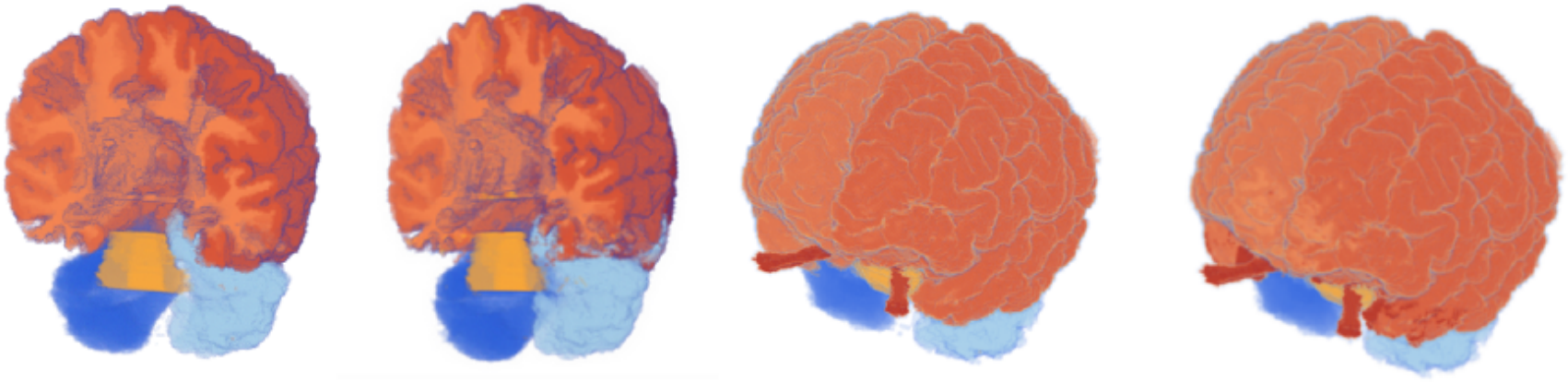
Bioinformatics

- Objective
  - To extract or recognize patterns that share common characteristics

- It could be:
  - **Sequence analysis** (also known as sequence alignment)
    - Clustering is used to group homologous sequences into gene families
  - **Genome annotation** (i.e., gene finding)

Medicine



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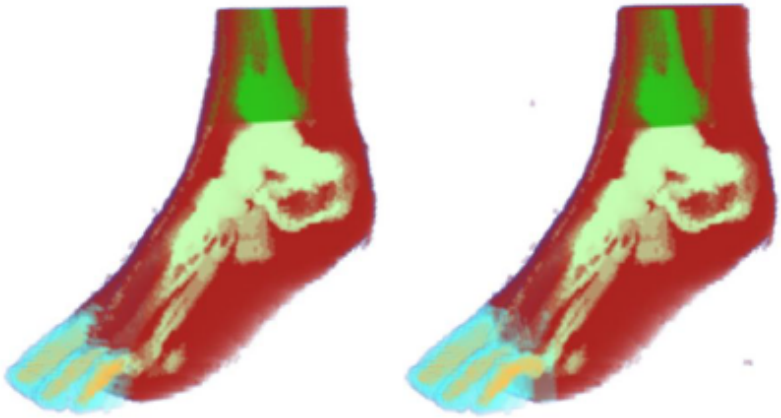

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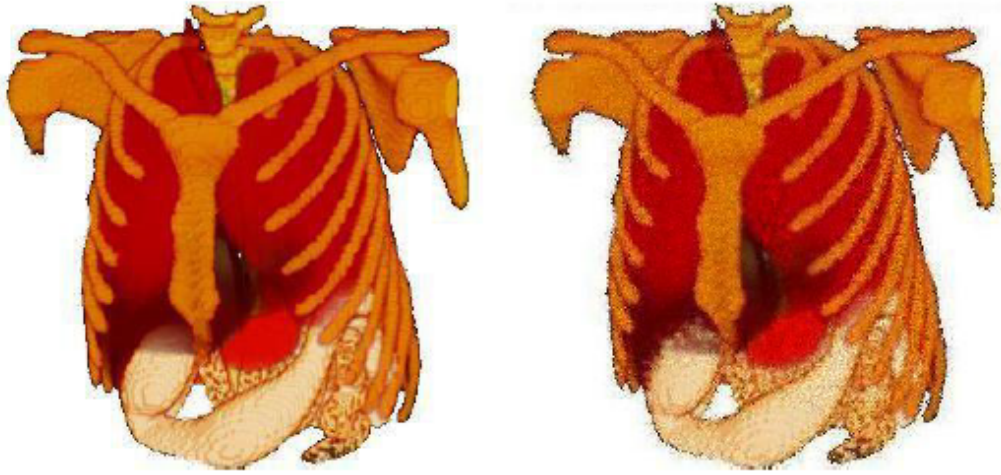

(c)

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Medicine

- Objective
  - On PET scans, cluster analysis can be used to differentiate between different types of tissue and blood in a three dimensional image

- Note that in this application, actual position does not matter, but the voxel intensity is considered as a vector, with a dimension for each image that was taken over time.
- This technique allows, for example, accurate measurement of the rate a radioactive tracer is delivered to the area of interest, without a separate sampling of arterial blood, an intrusive technique that is most common today.

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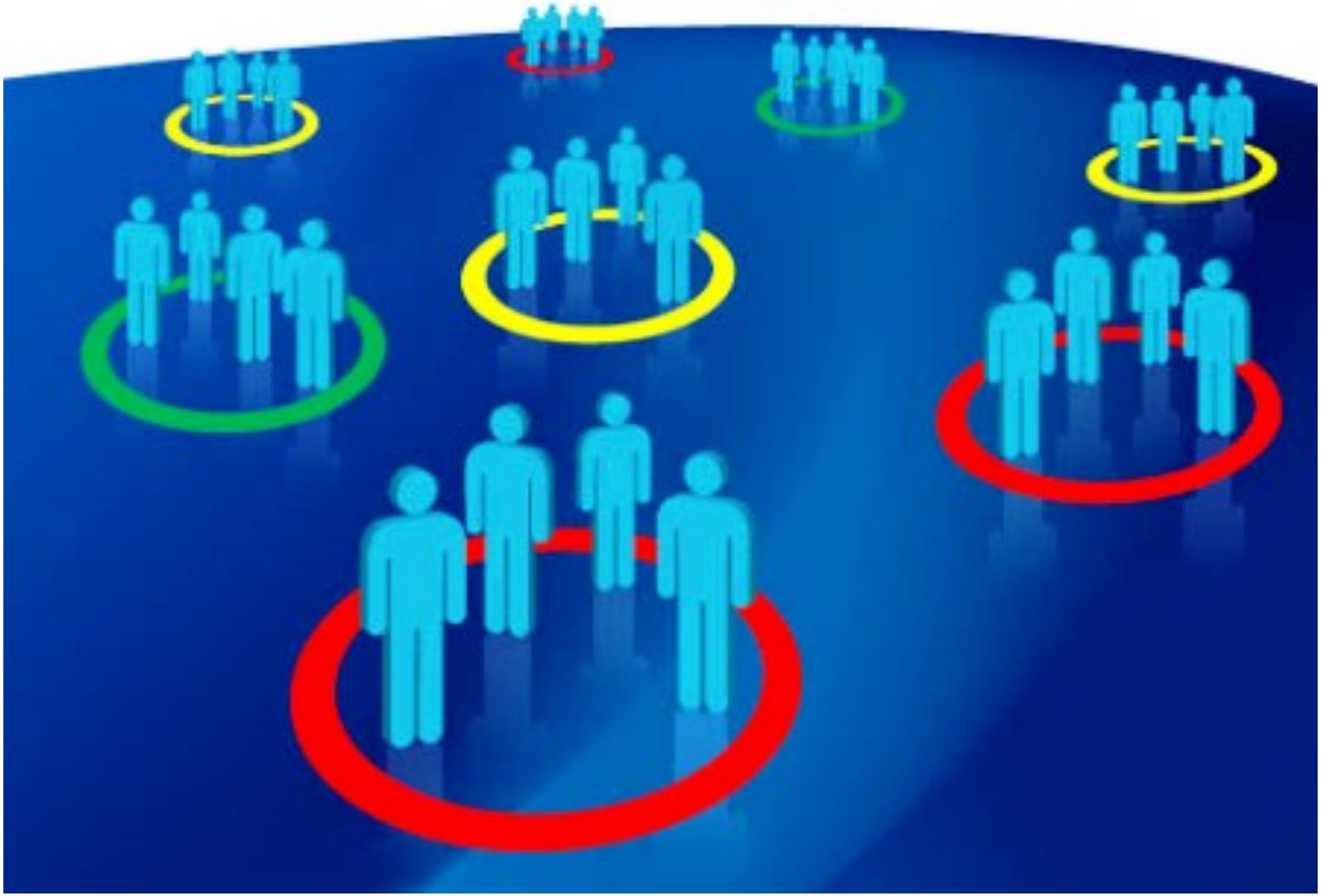
Market research



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Market research

- Objective
  - Obtain valuable information about your customers and potential customers because it is essential to the success of any business

- Market research data can be used
  - Before starting any new business
  - When expanding an existing one
- The idea is to perform an extensive market research to establish whether there is a need for your product or service

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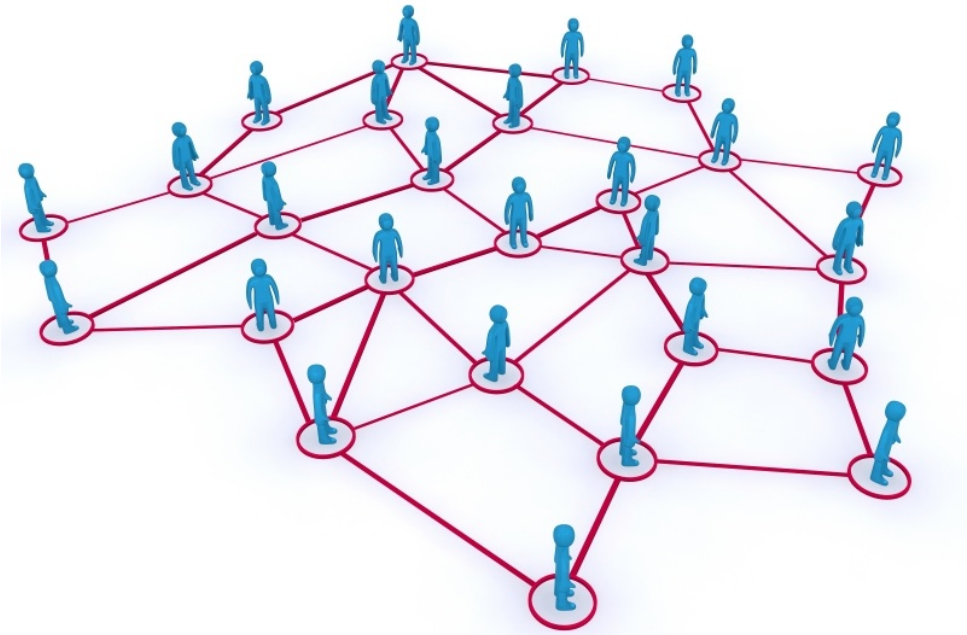
Social network analysis



In the study of social networks, clustering may be used to recognize communities within large groups of people.

Unsupervised learning approaches

- **Clustering**
  - It is the task of grouping a set of objects in such a way that objects in the same group (called a **cluster**) are more similar (in some sense or another) to each other than to those in other groups (clusters)
- **Factor Analysis**
  - Statistical methods used to describe variability among observed, correlated variables in terms of a potentially lower number of unobserved variables called factors.
- **Visualization**
  - Study of (interactive) visual representations of abstract data to reinforce human cognition.

Unsupervised learning approaches

- **Clustering**: method by which large sets of data is grouped into clusters of smaller sets of similar data
  - **Based on connectivity**: Hierarchical clustering
  - **Based on centroids**: K-means
  - **Distribution-based models**: Mixture models, Expectation-Maximization
  - Density models: DBScan, Optics
  - Subspace models: Biclustering
  - Group models
  - Graph-based models

Unsupervised learning approaches

- **Factor analysis**: blind signal separation using *feature extraction* techniques for *dimensionality reduction*

  - **Principal components analysis (PCA)**
  - **Independent component analysis (ICA)**
  - Non-negative matrix factorization
  - Singular value decomposition (SVD)
  - ...

Unsupervised learning approaches

- **Visualization**: a set of techniques often used in information visualization for exploring similarities and dissimilarities in data
  - **Neural network models**:
    - **Self-organized maps (SOM)**
    - Adaptive resonance theory (ART)
  - **Multi-dimensional scaling (MDS)**
    - **Classical multidimensional scaling**
    - Metric multidimensional scaling
    - Non metric multidimensional scaling
    - Generalized multidimensional scaling

Introduction to cluster analysis

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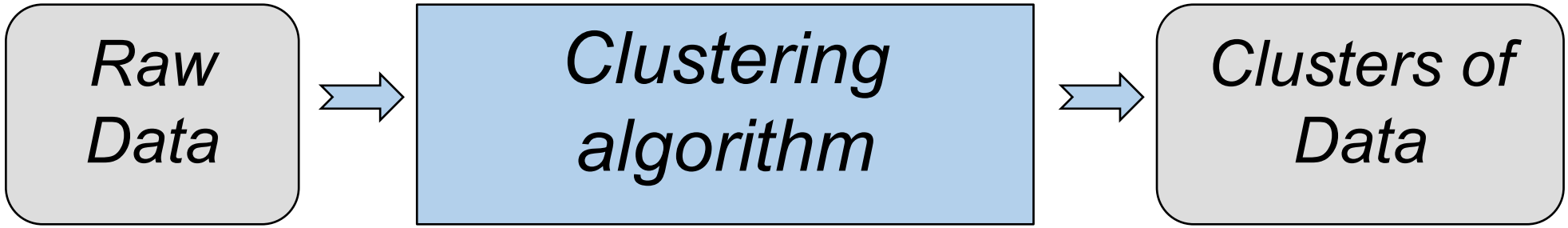
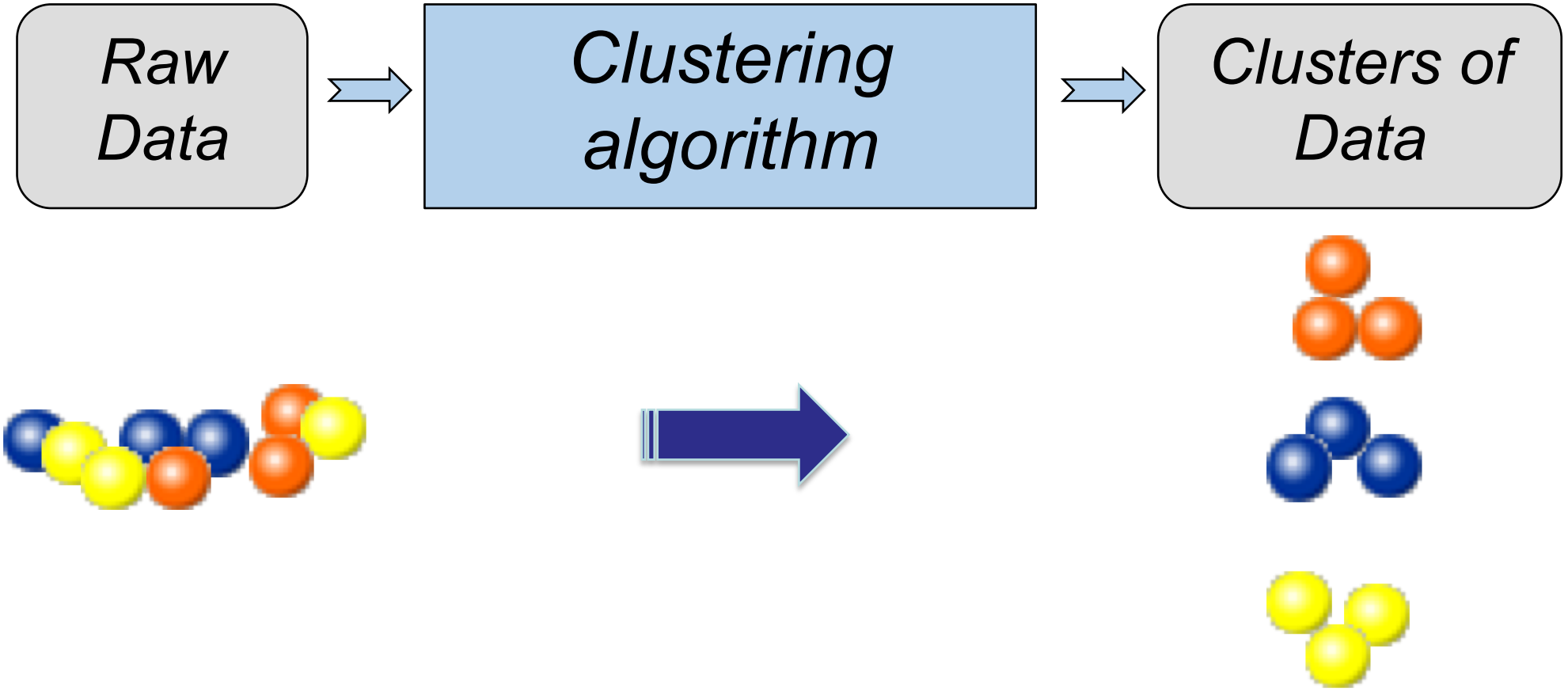
Defining clustering analysis

- **Cluster analysis** or **clustering** is the task of assigning a set of unlabelled objects into groups (**clusters**) so that the objects in the same cluster are very similar (in some sense or another) to each other than those of the other clusters.
- Cluster analysis discover new categories in an **unsupervised** manner



Defining clustering analysis

- A clustering algorithm attempts to find natural groups of components (or data) based on some similarity (in the example below, based on the colour)



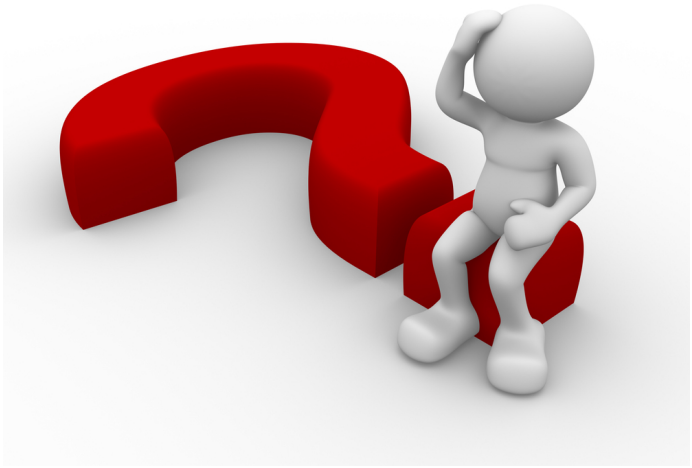
Areas that apply clustering

Clustering is ...

- Main task of explorative **data mining**
- Common technique for **statistical data** analysis used in many fields:
  - Machine learning
  - Pattern recognition
  - Information retrieval
  - Bioinformatics
  - Natural language processing
  - Recommender systems
  - Data mining
  - ...

Clustering Example

How many clusters?



Take a moment to think about it

….

think a bit about the number of clusters
you see in the example

(You will have the answer in the online session)

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Issues for clustering

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

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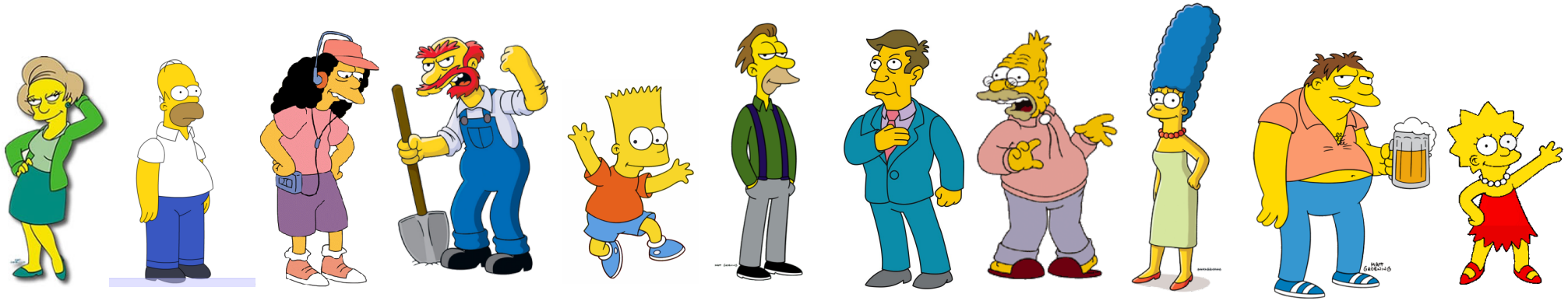
What is a natural grouping?

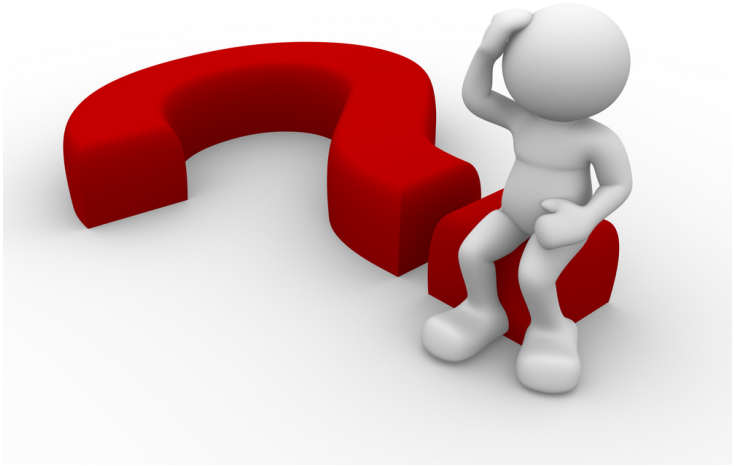


Decide how to group them !!!

Take a moment to think about it

….

Think in a way to group them and make a note about it



(You will have the answer in the online session)

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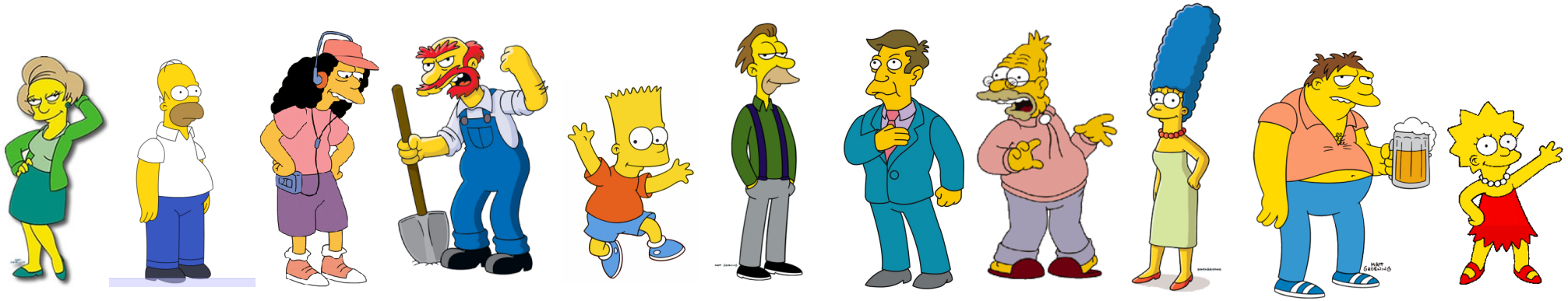
What is a natural grouping?



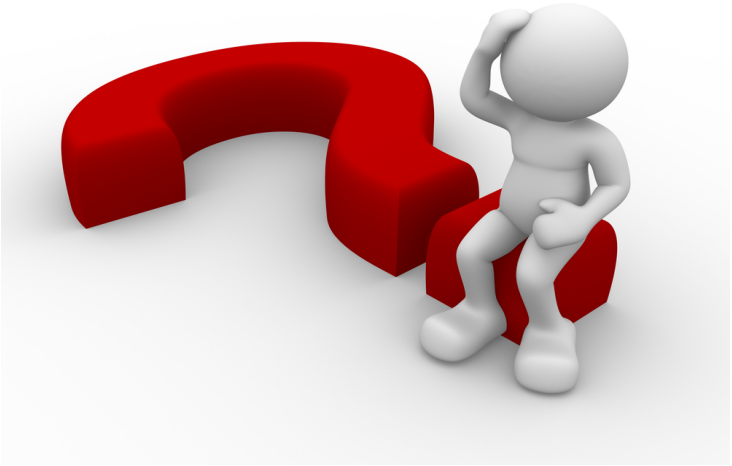
Decide how to group them, in a diferent way !!!

Take a moment to think about it

....

Do not look at the next slide yet,
Think in another way to group them and make an additional note about it

(You will have the answer in the online session)



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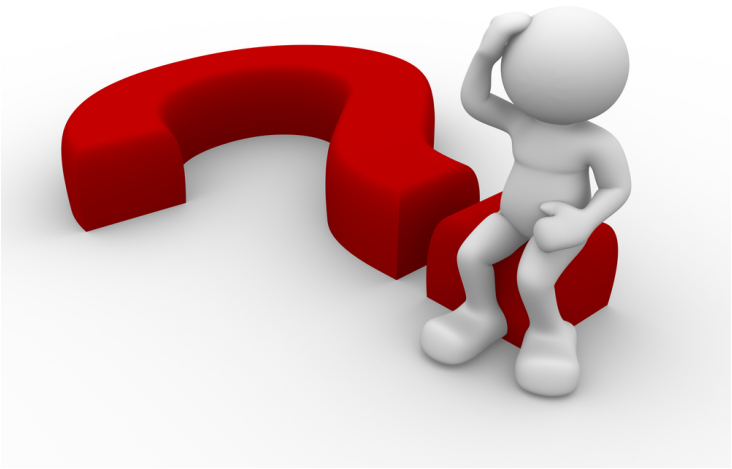
What is similarity?

Take a moment to think about it

….

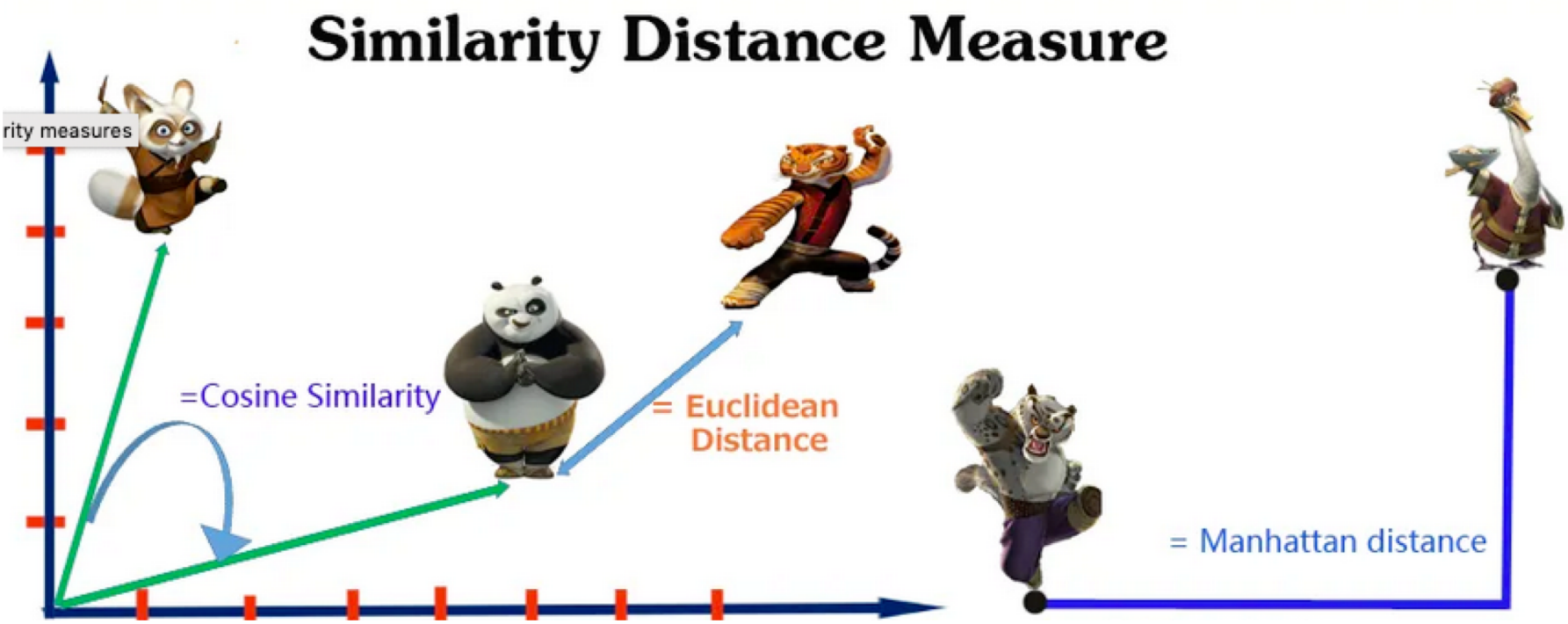
How do you consider there is great similarity between two objects

(You will have the answer in the online session)



Similarity measures in ML

Similarity in ML is computed using distance measures



There are many in ML, here you will find some examples

https://dataaspirant.com/five-most-popular-similarity-measures-implementation-in-python/

Desirable distance measure properties

- D(A, B) = D(B,A) **Symmetry**
  - Otherwise you could claim “Alex looks like bob but bob looks like 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 | if A=B **Positivity Separation**
  - Otherwise there are objects in your world that are diferent 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

Ontañón, S. (2020) “An overview of distance and similarity functions for structured data”, Artificial Intelligence Review

Read page 1, 2, 3 and the beginning of 4 (until Section 2.2.1 included, no more)

Distance measure: 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

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

Distance measure: Minkowski

- Most Common Minkowski Metrics

$1, r = 2$ (Euclidean distance)

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

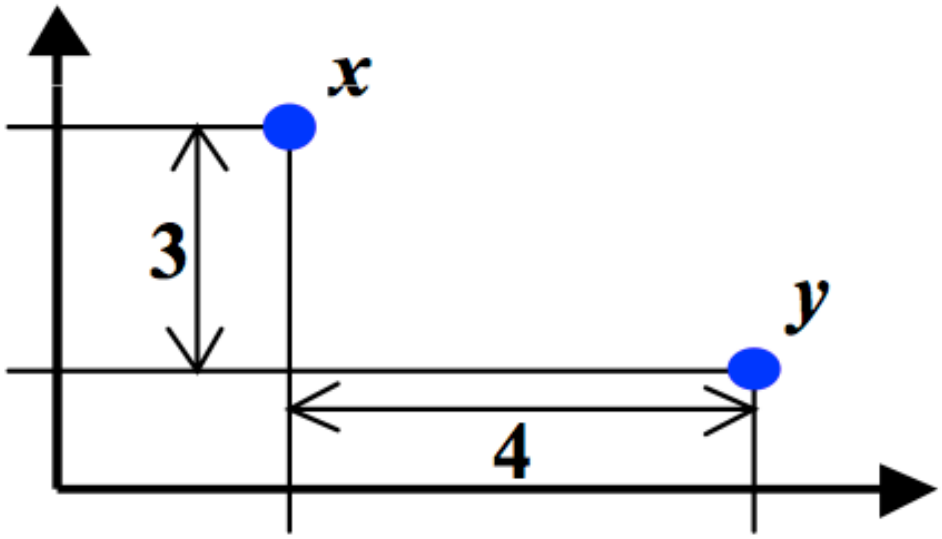
$2, r = 1$ (Manhattan distance)

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

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

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

An example



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

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

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

Distance measure: Pearson correlation

- Pearson correlation coefficient:

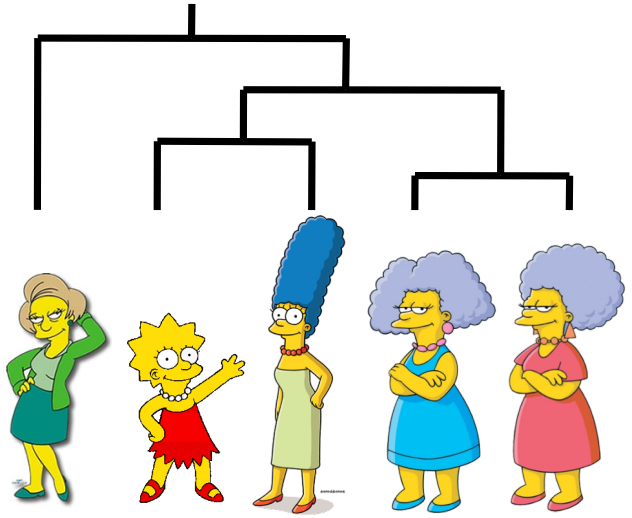
$$s(x,y) = \frac{\sum_{i=1}^{p}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{p}(x_i - \bar{x})^2 \times \sum_{i=1}^{p}(y_i - \bar{y})^2}}$$

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

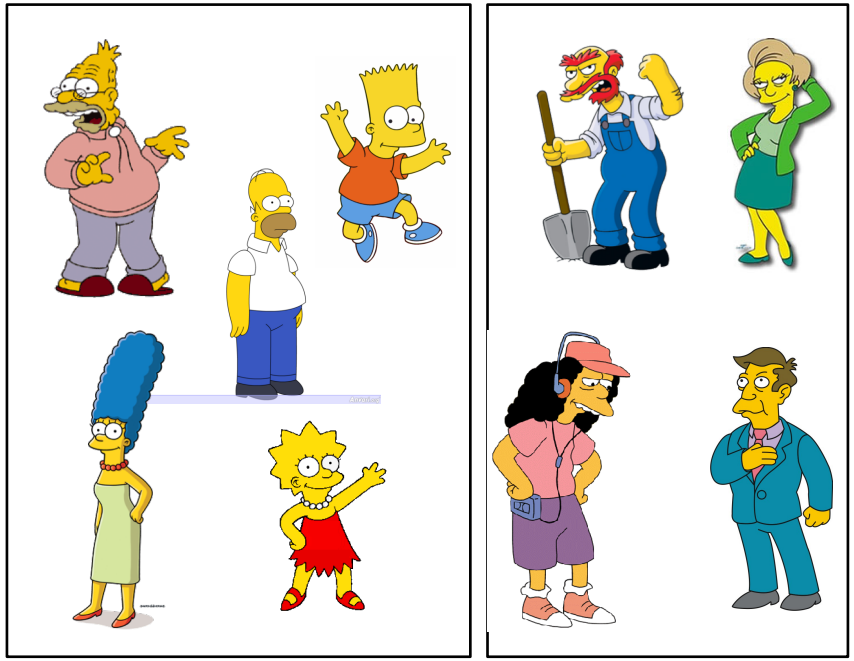
$$\left| s(x,y) \right| \leq 1$$

Taxonomy

- **Hierarchical algorithms**
  - Examples are organized as a binary tree
  - No explicit division in groups
    - **Bottom-up**
    - Top-down



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



Hierarchical clustering

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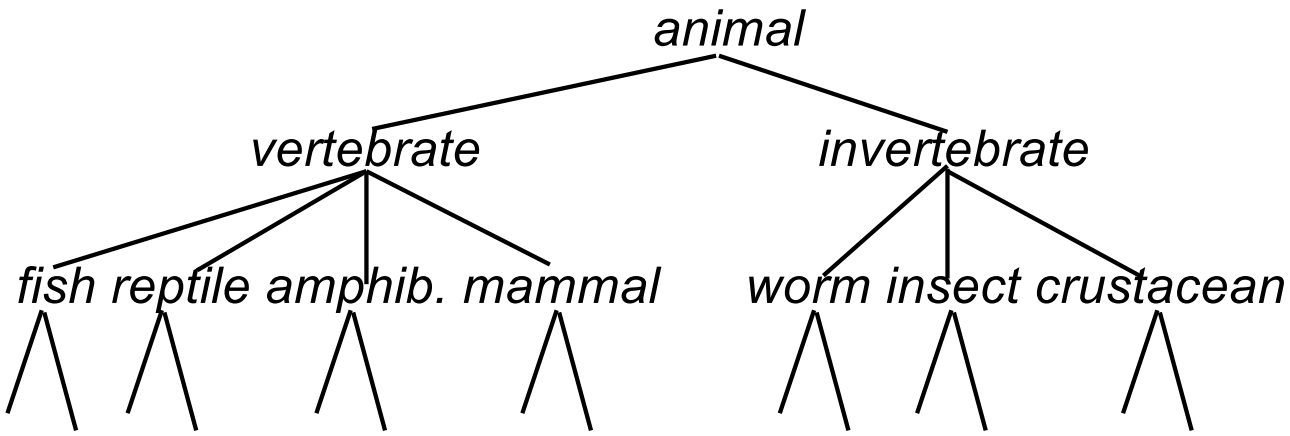
Hierarchical Clustering algorithms

- Build a tree-based hierarchical taxonomy (***dendrogram***) from a set of unlabeled examples

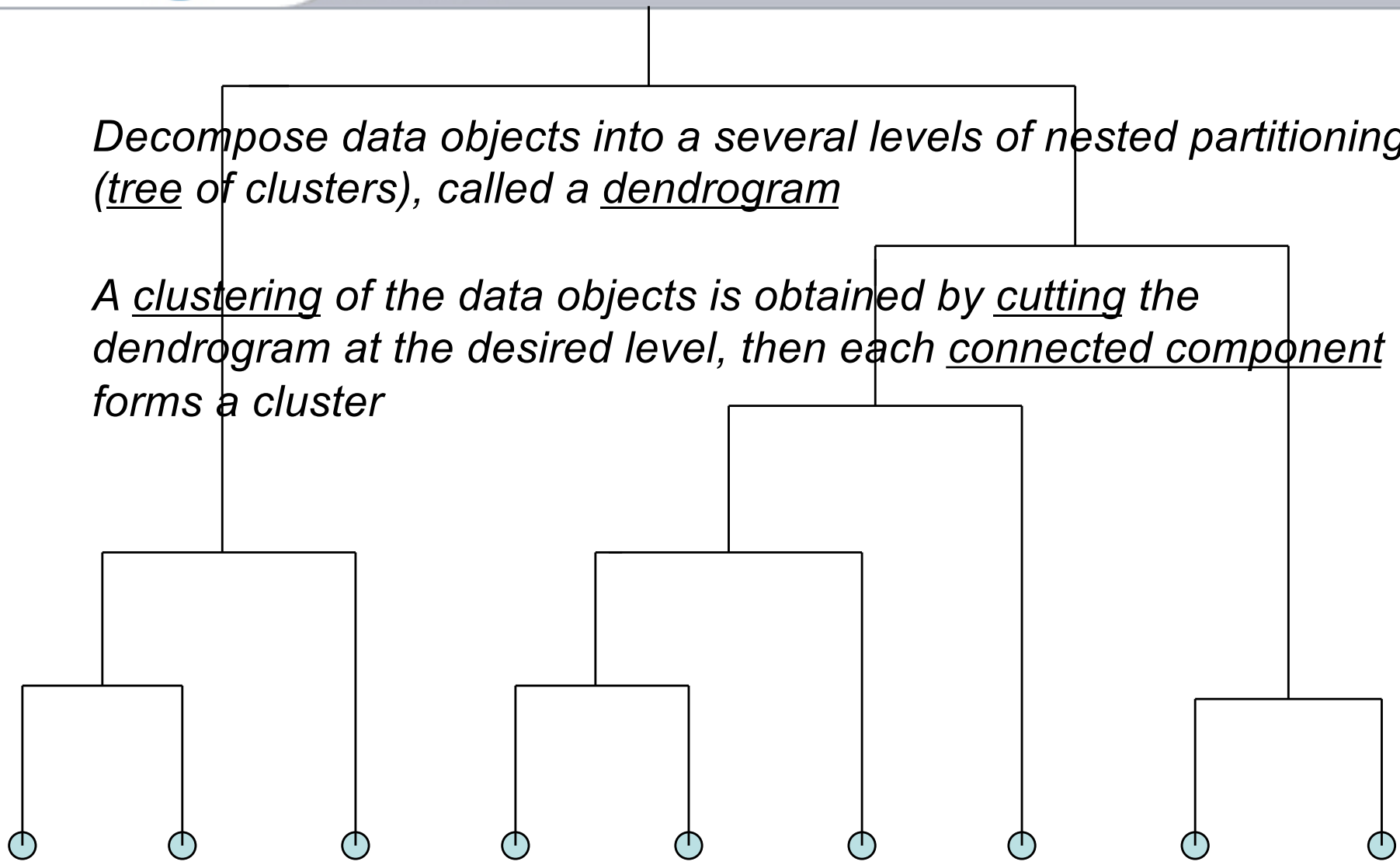


- Recursive application of a standard clustering algorithm can produce a hierarchical clustering

Dendrogram: Shows How Clusters are Merged

Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram

A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster



Hierarchical Clustering Algorithms

Basic approaches for generating a hierarchical clustering

- ***Agglomerative*** (*bottom-up*)
  - Methods start with each example in its own cluster
  - Iteratively combine them to form larger and larger clusters

- ***Divisive*** (*partitional, top-down*)
  - Methods start with all the examples in a single cluster
  - Consider all the possible way to divide the cluster into two. Choose the best division
  - Recursively operate on both sides

https://youtu.be/EUQY3hL38cw

Hierarchical Agglomerative Clustering

(HAC algorithm)

Basic HAC algorithm:

1. Compute the similarity matrix between the input data points
2. Start with all instances in their own cluster
3. **Repeat**
4. Among the current clusters, determine the two clusters, c_i and c_j, that are most similar
5. Merge them and replace c_i and c_j with a single cluster $c_i \cup c_j$
6. Update the similarity matrix
7. **until** there is only one single cluster

- **Key operation is the computation of the similarity between two clusters**
  - Different definitions of the **similarity** between clusters lead to different algorithms

Cluster Similarity

- Assume a similarity function that determines the similarity of two instances: ***sim*(*x*,*y*)**
  - For example, Cosine similarity of document vectors

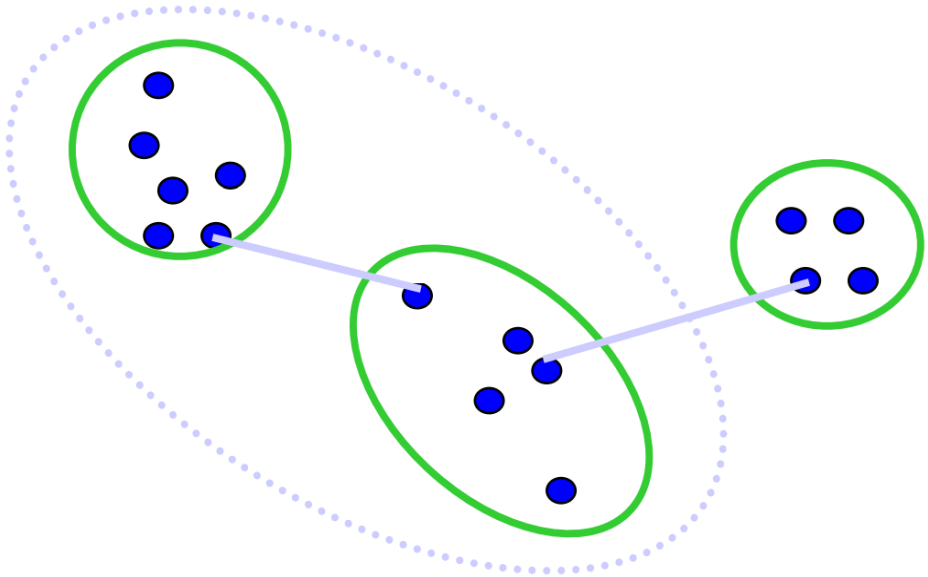
- How to compute similarity of two clusters each possibly containing multiple instances?
  - **Single Link**: Similarity of two most similar members
  - **Complete Link**: Similarity of two least similar members
  - **Group Average**: Average similarity between members
  - **Centroid**: clusters whose centroids are the most cosine similar

Single-Link Agglomerative Clustering

- Use maximum similarity of pairs:

$$sim(c_i, c_j) = \max_{x \in c_i, y \in c_j} sim(x, y)$$

- Can result in "straggly" (long and thin) clusters due to *chaining effect*.
  - Appropriate in some domains, such as clustering islands

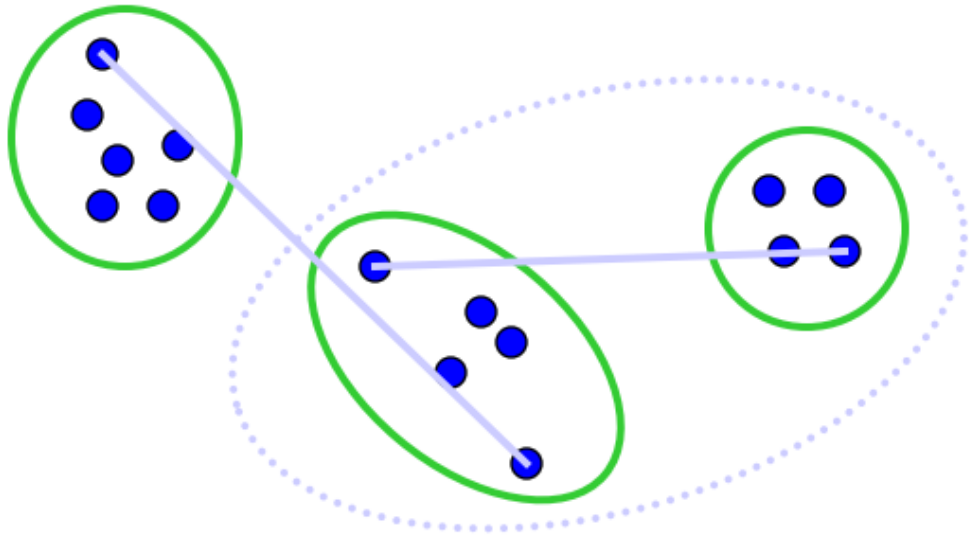


Complete-Link Agglomerative Clustering

- Use minimum similarity of pairs:

$$sim(c_i, c_j) = \min_{x \in c_i, y \in c_j} sim(x, y)$$

- Makes more "tight," spherical clusters that are typically preferable



Computational Complexity

- In the first iteration, all HAC methods need to compute similarity of all pairs of ***n*** individual instances which is **O(n^2)**.
- In each of the subsequent $n-2$ merging iterations, it must compute the distance between the most recently created cluster and all other existing clusters.
- 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

Computing Cluster Similarity

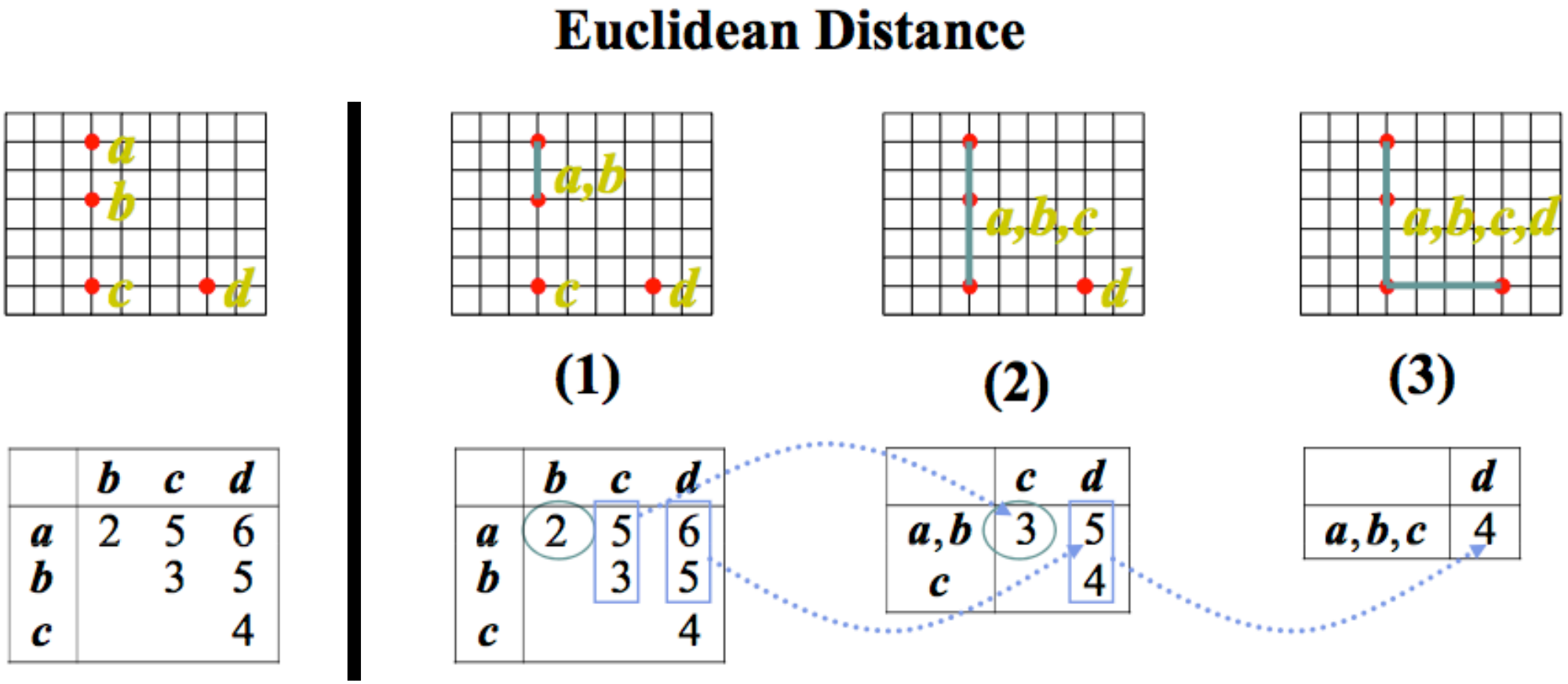
- After merging c_i and c_j, the similarity of the resulting cluster to any other cluster, c_k, can be computed by:
  - **Single-Link**:

$$sim((c_i \cup c_j), c_k) = \max(sim(c_i, c_k), sim(c_j, c_k))$$

  - **Complete-Link**:

$$sim((c_i \cup c_j), c_k) = \min(sim(c_i, c_k), sim(c_j, c_k))$$

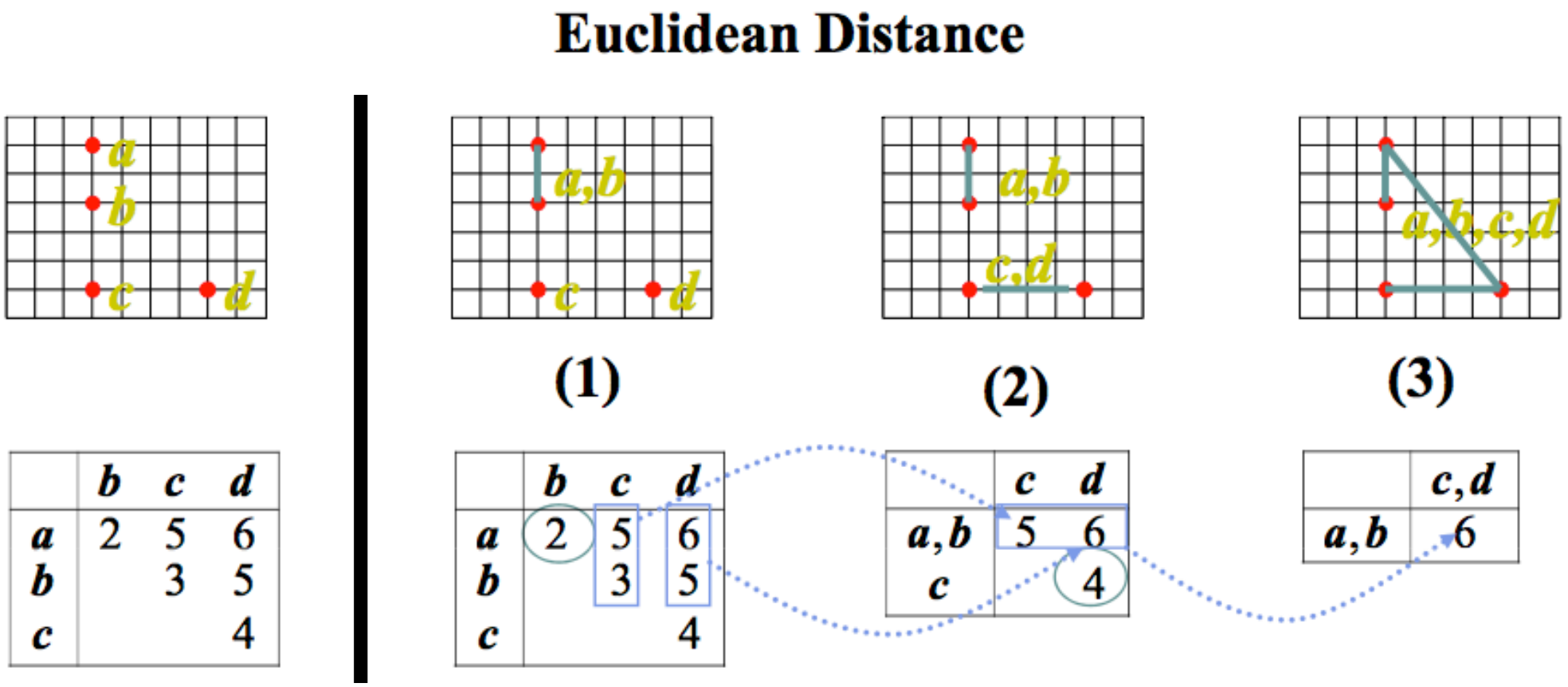
Single-Link Example



Distance Matrix

Illustration by Eric Xing @ CMU

Complete-Link Example

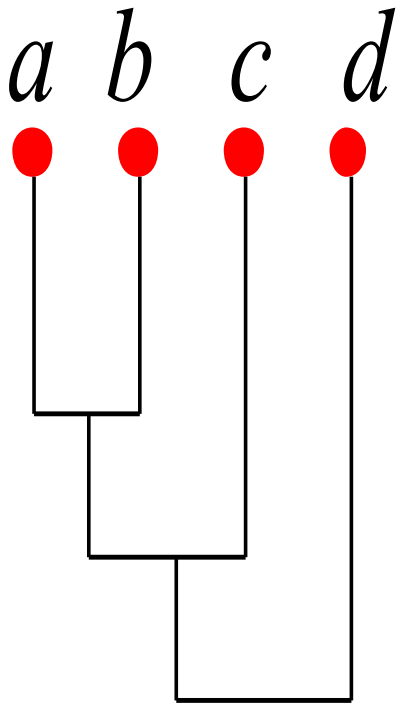


Distance Matrix

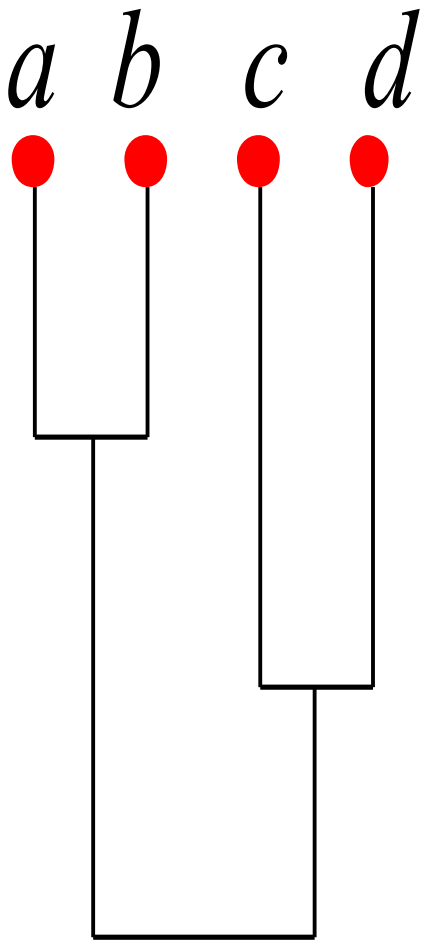
Illustration by Eric Xing @ CMU

Dendrograms Comparison

Single-Link



Complete-Link

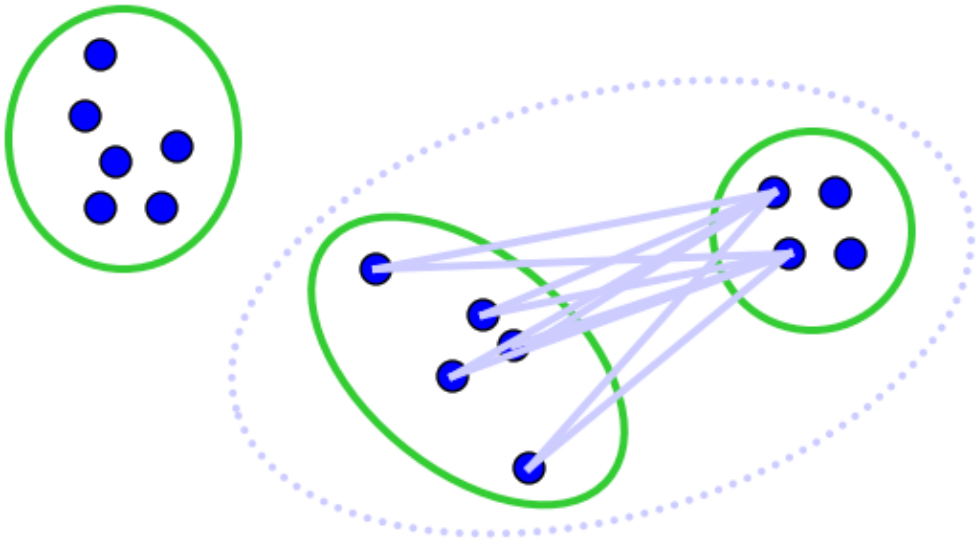


Group Average Agglomerative Clustering

- Use average similarity across all pairs within the merged cluster to measure the similarity of two clusters.

$$sim(c_i, c_j) = \frac{1}{\left|c_i \cup c_j\right|\left(\left|c_i \cup c_j\right| - 1\right)} \sum_{\vec{x} \in (c_i \cup c_j)} \sum_{\vec{y} \in (c_i \cup c_j): \vec{y} \neq \vec{x}} sim(\vec{x}, \vec{y})$$

- Compromise between Single and Complete link.



Computing Group Average Similarity

- Assume cosine similarity and normalized vectors with unit length.
- Always maintain sum of vectors in each cluster.

$$\vec{s}(c_j) = \sum_{\vec{x} \in c_j} \vec{x}$$

- Compute similarity of clusters in constant time:

$$sim(c_i, c_j) = \frac{(\vec{s}(c_i) + \vec{s}(c_j)) \bullet (\vec{s}(c_i) + \vec{s}(c_j)) - (|c_i| + |c_j|)}{(|c_i| + |c_j|)(|c_i| + |c_j| - 1)}$$

What else?

Arriving at this point:

TO READ

Chapter 8 - Cluster Analysis: Basic concepts and algorithms

- Pages 487, 488, 489, 490
- Section 8.1: Overview
  - Section 8.1.1
  - Section 8.1.2
  - Section 8.1.3 (optional)
- Section 8.3: Agglomerative Hierarchical Clustering
  - Read all the subsections