Course. Introduction to Machine Learning
Lecture 2. Introduction to unsupervised learning and Cluster Analysis (Part I)

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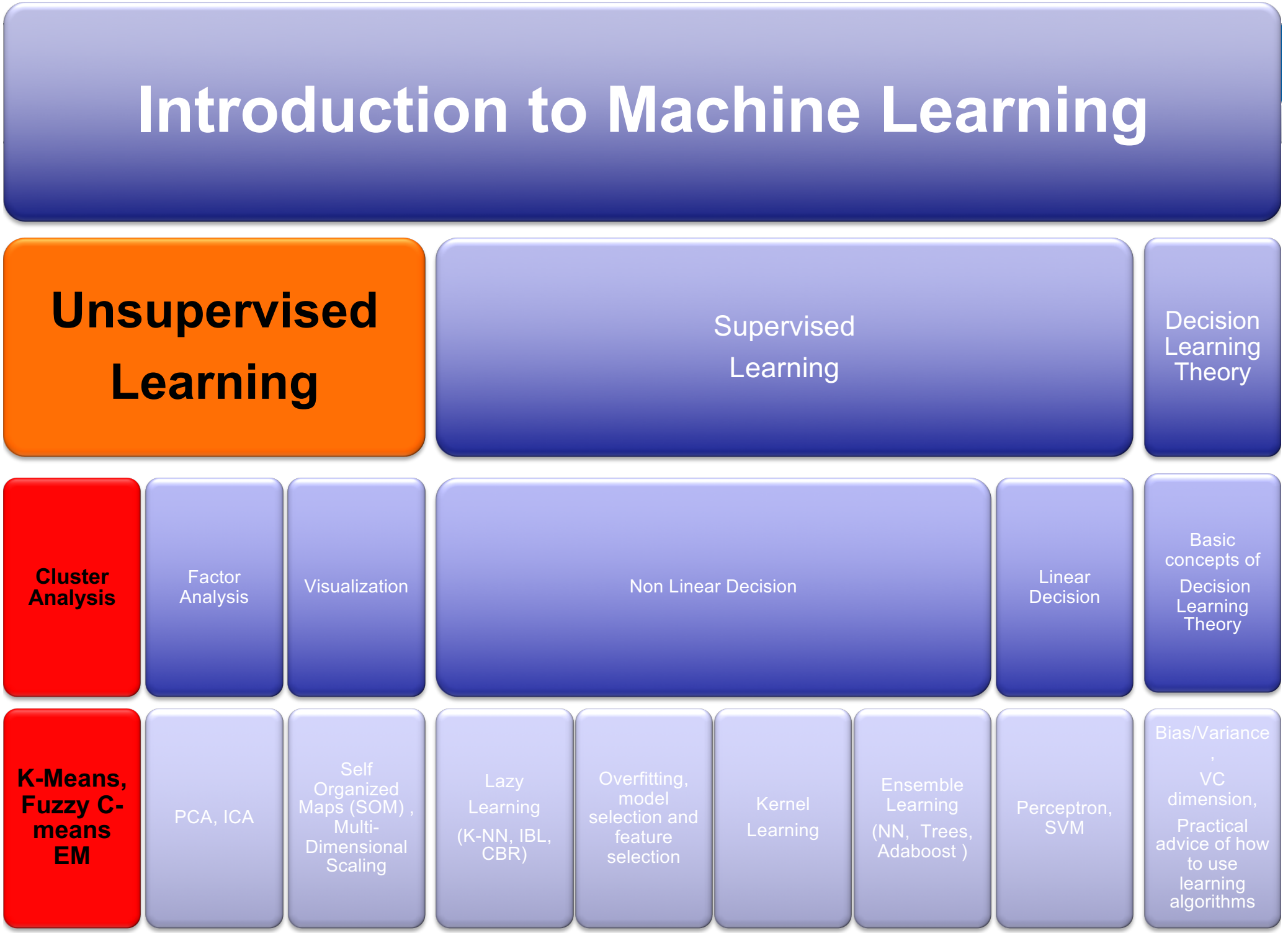
Introduction to Machine Learning



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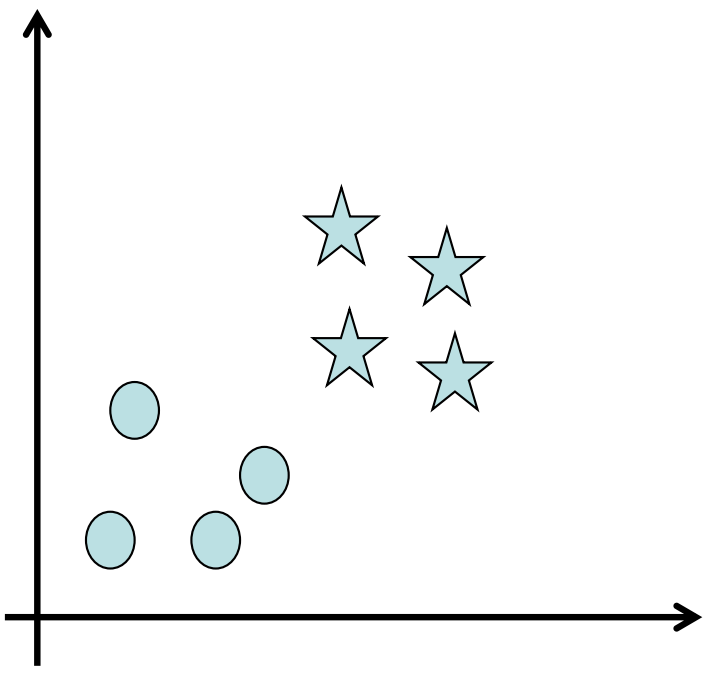
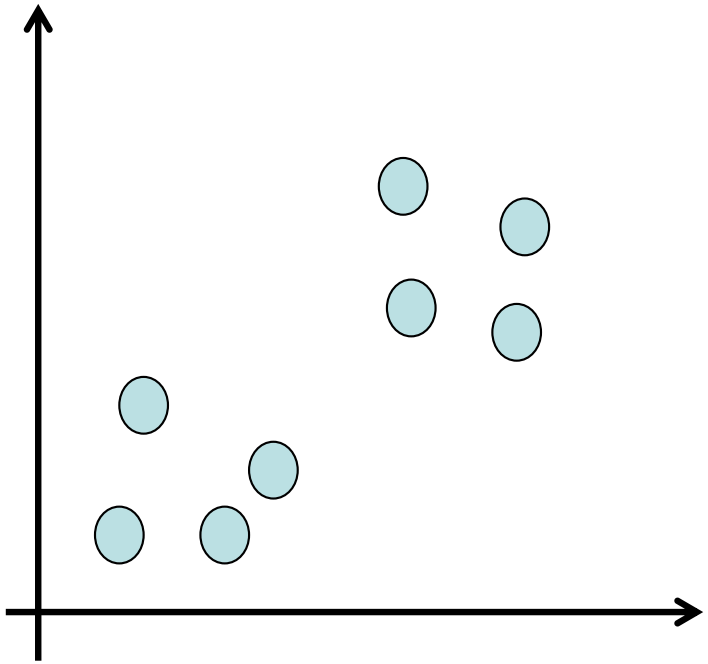
Introduction to Unsupervised learning

Supervised



Unsupervised



Unsupervised learning

- **Main Goals**:
  - **Summarization**: To obtain representations that describe an unlabeled dataset
  - **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:
  - Unstructured (partitions)
  - Relational (hierarchies)

Examples of unsupervised learning

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

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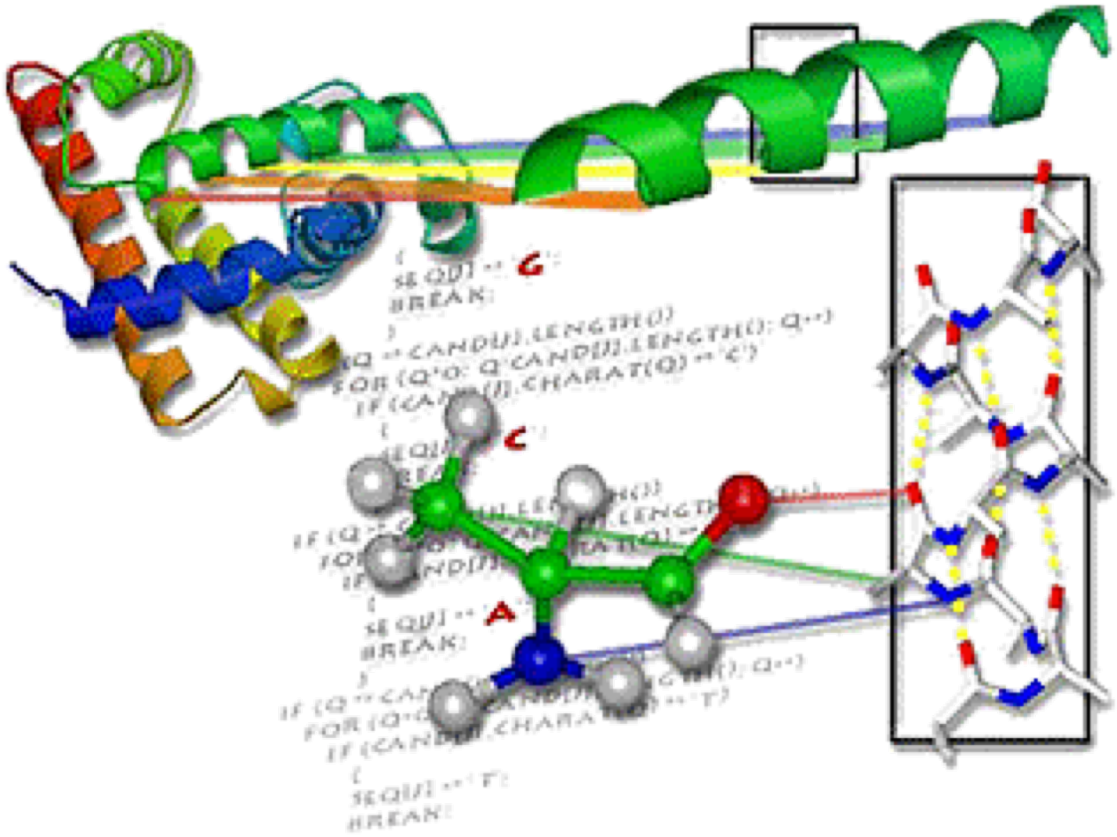
Bioinformatics



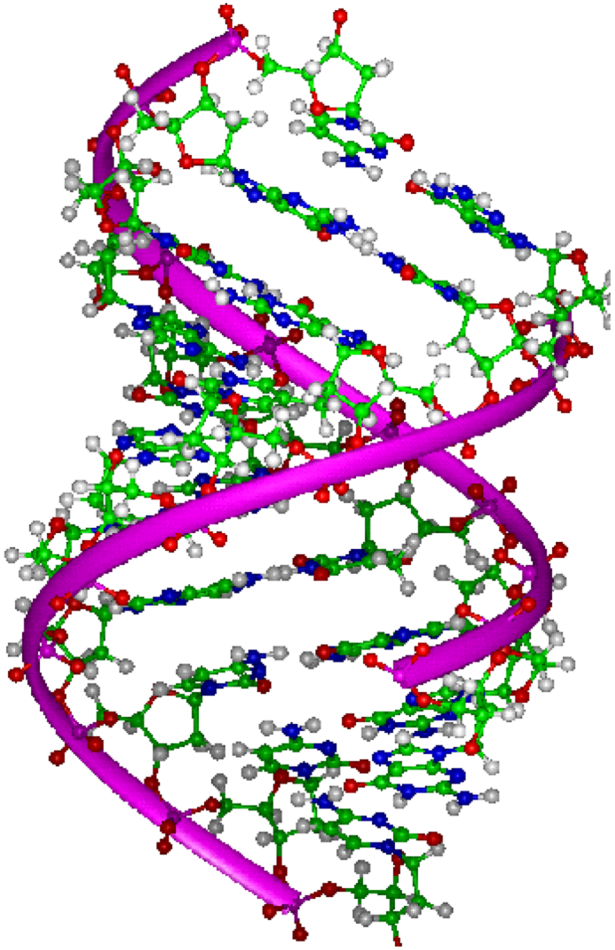
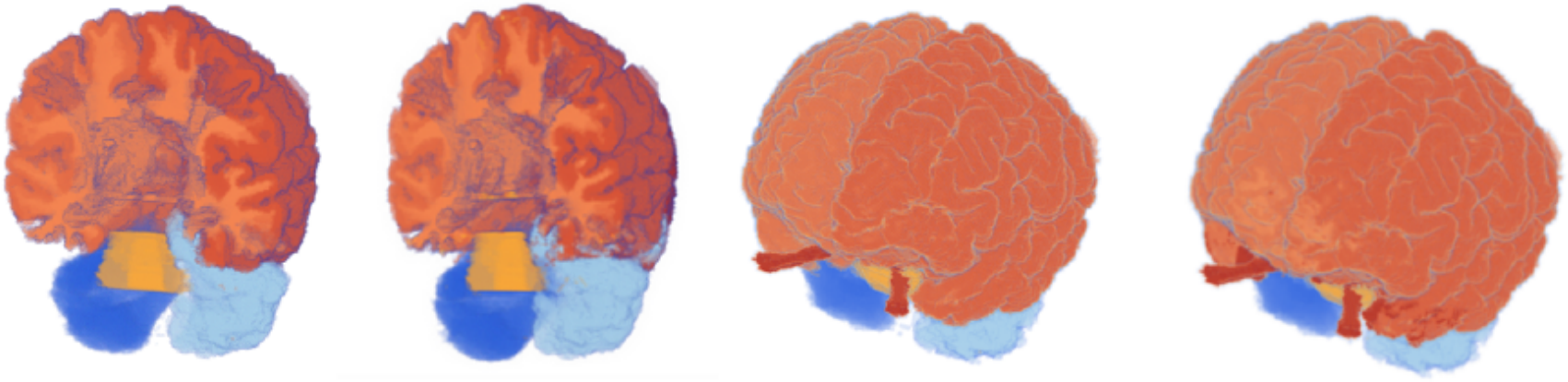


Illustration by Brian Haas, Phillips lab

Medicine



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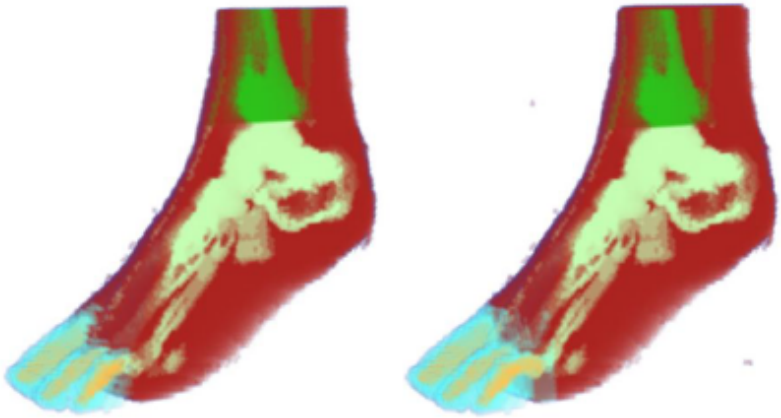

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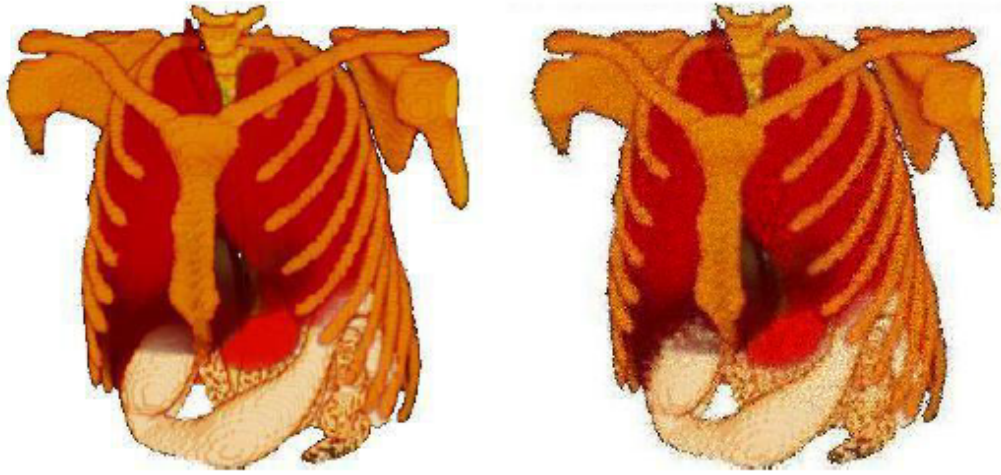

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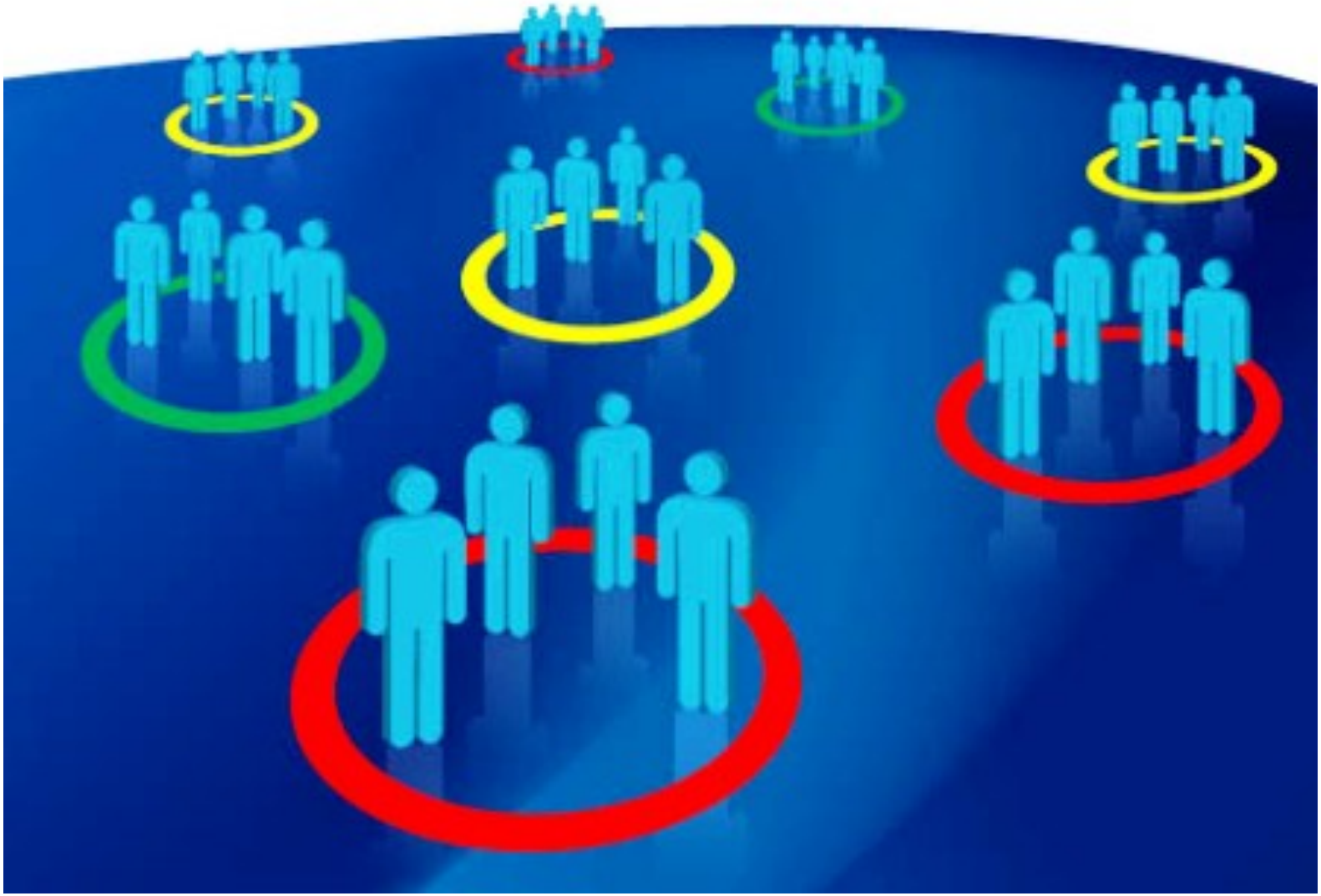
Market research



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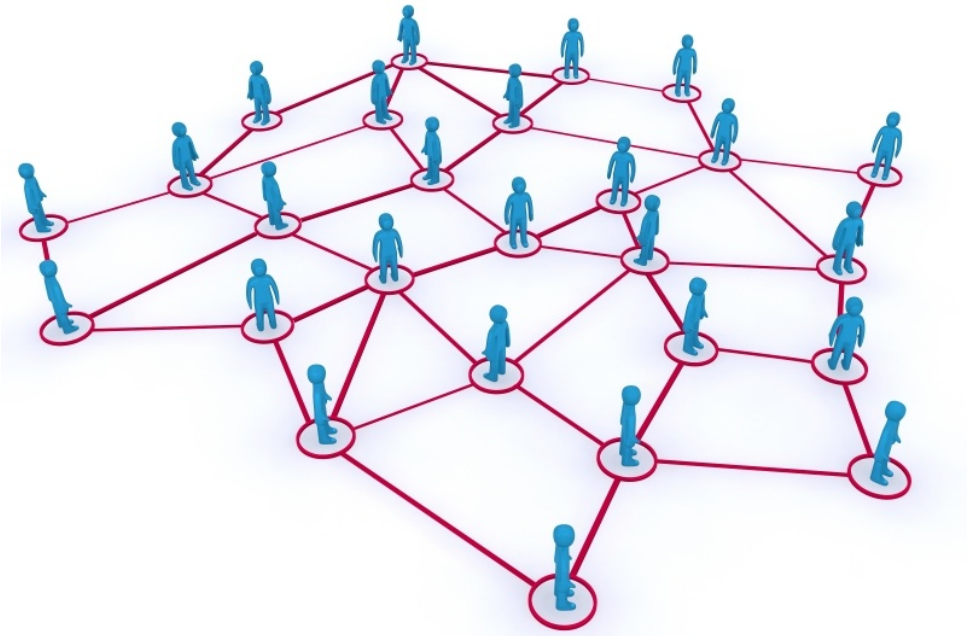
Social network analysis



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

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2. **Cluster analysis**
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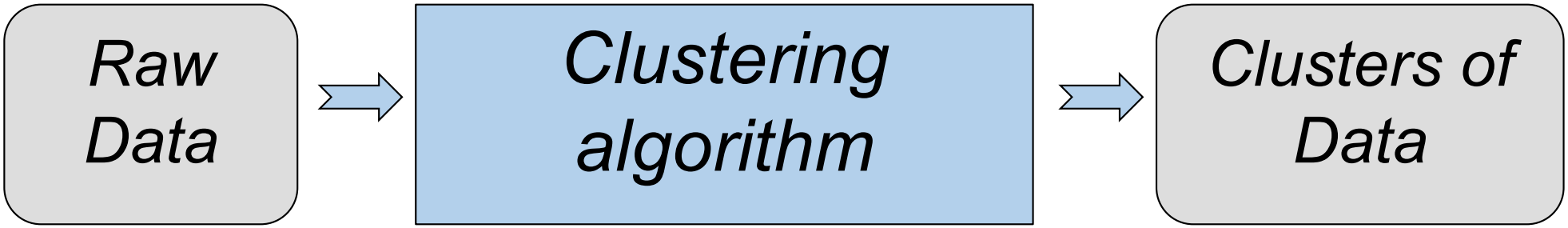
    3. Classification of clustering algorithms
    4. K-Means
    5. EM
    6. Other algorithms
    7. Applications

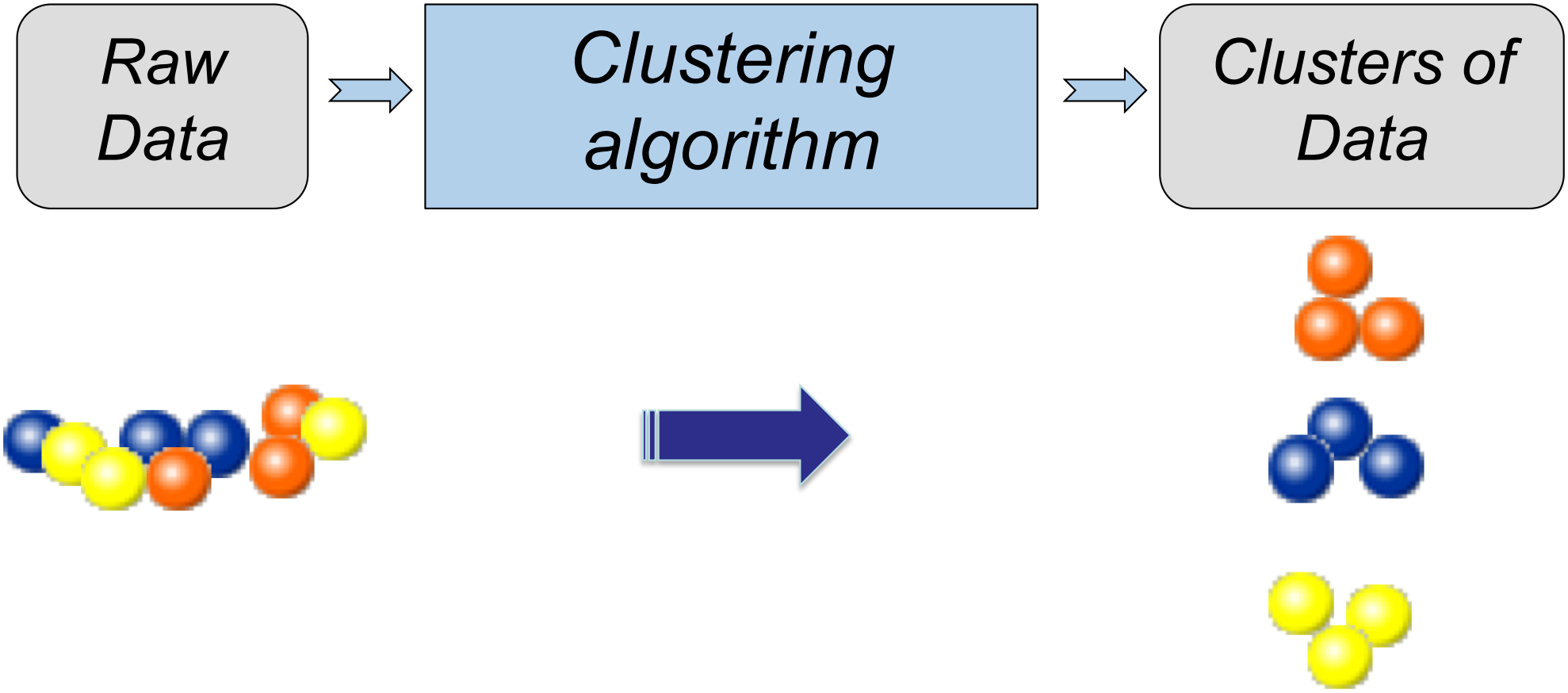
Defining clustering analysis

- **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.



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?

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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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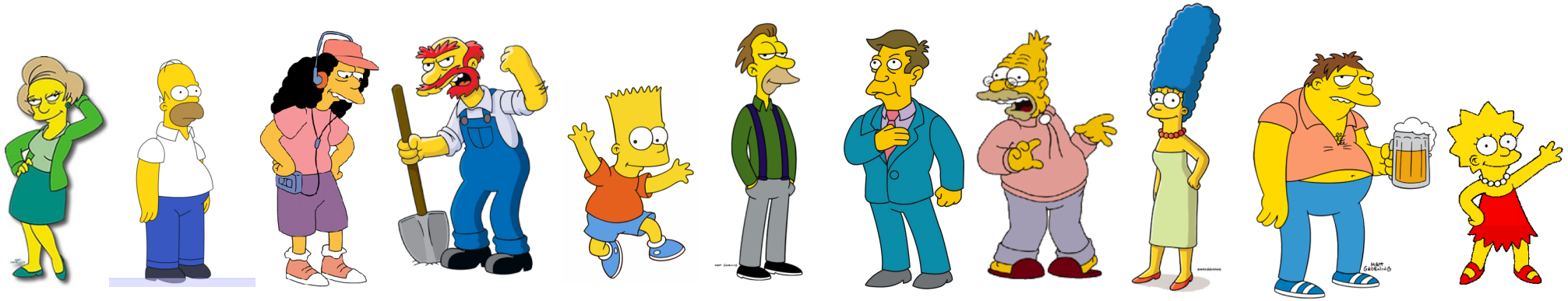
What is a natural grouping?



Decide how to group them !!!

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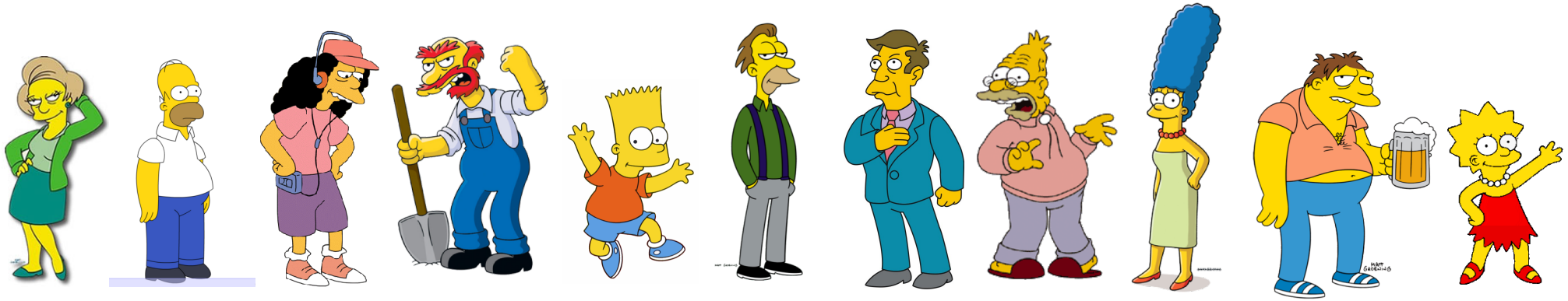
What is a natural grouping?



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

What is similarity?

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Desirable distance measure properties

- $D(A, B) = D(B,A)$ Symmetry
- $D(A,A)= 0$ Constancy of Self-Similarity
- $D(A,B) = 0$ | if $A=B$ Positivity Separation
- $D(A,B) \leq D(A,C)+ D(B,C)$ Triangular Inequality

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 measures:

Pearson correlation

- Pearson correlation coefficient:

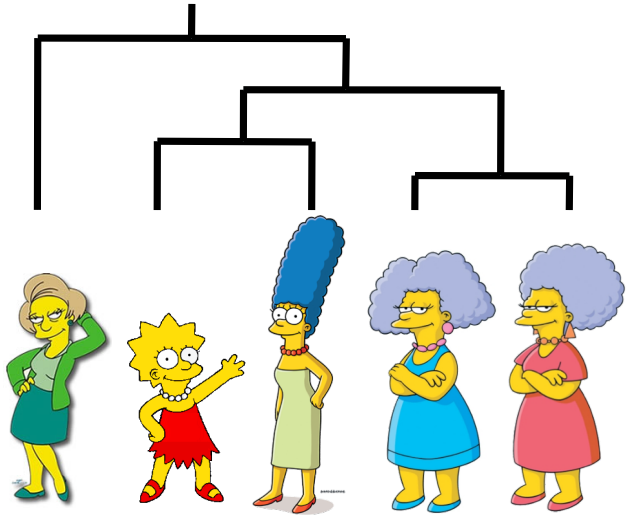
$$s(x,y) = \frac{\sum_{i=1}^{p}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{p}(x_i - \bar{x})^2 \times \sum_{i=1}^{p}(y_i - \bar{y})^2}}$$

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

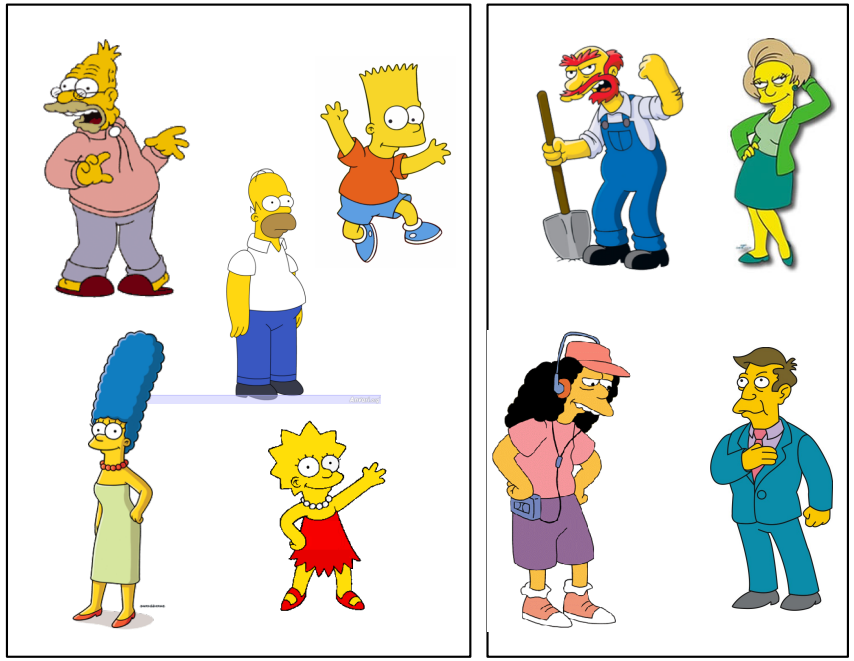
$$\left| s(x,y) \right| \leq 1$$

Taxonomy

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

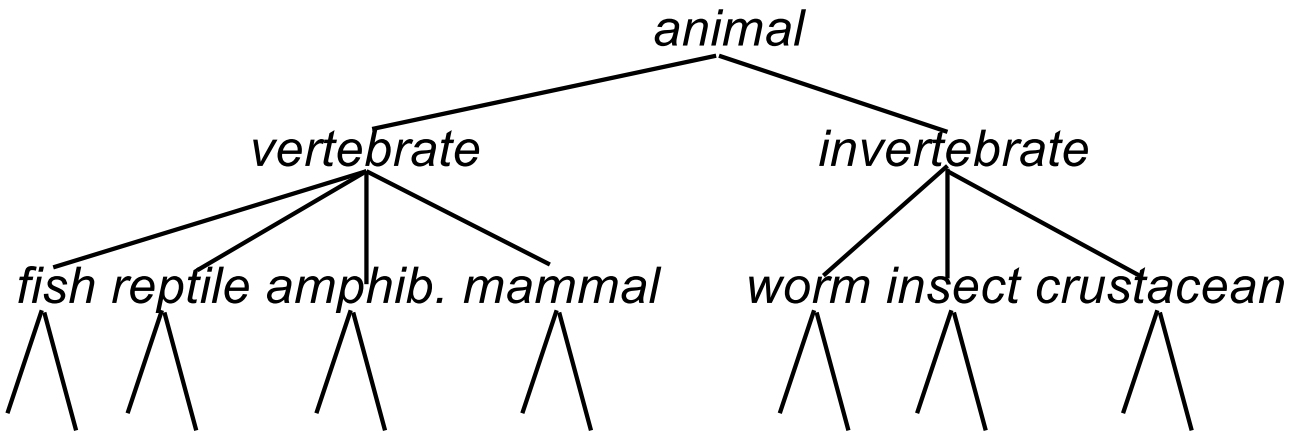


- **Partitional algorithms**
  - Usually start with a random (partial) partitioning
  - Refine it iteratively:
    - **K-means clustering**
    - **Mixture-model based clustering**



Hierarchical Clustering

- 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

Hierarchical Clustering Algorithms

- *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

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

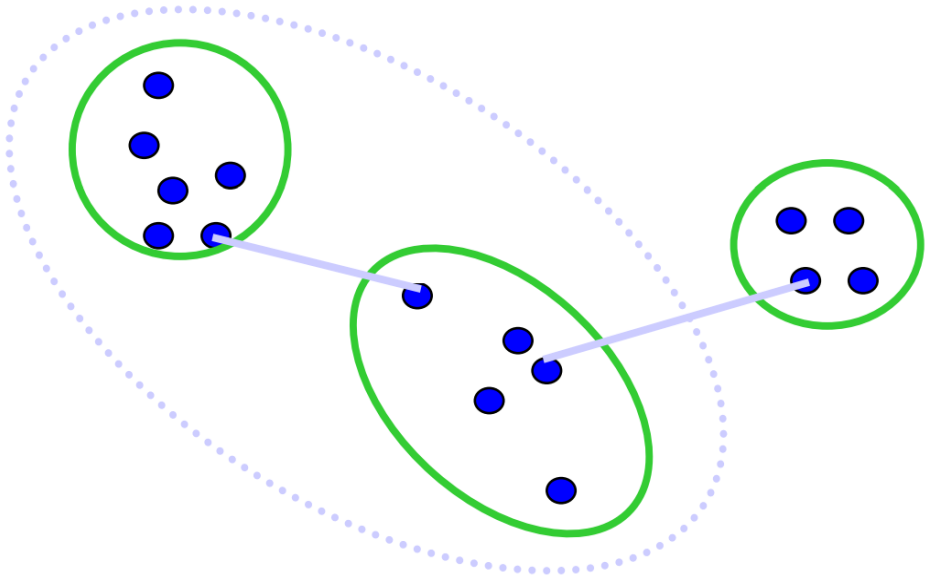
- Assume a similarity function that determines the similarity of two instances: ***sim*(*x*,*y*)**
  - For example, Cosine similarity of document vectors
- How to compute similarity of two clusters each possibly containing multiple instances?
  - **Single Link**: Similarity of two most similar members
  - **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

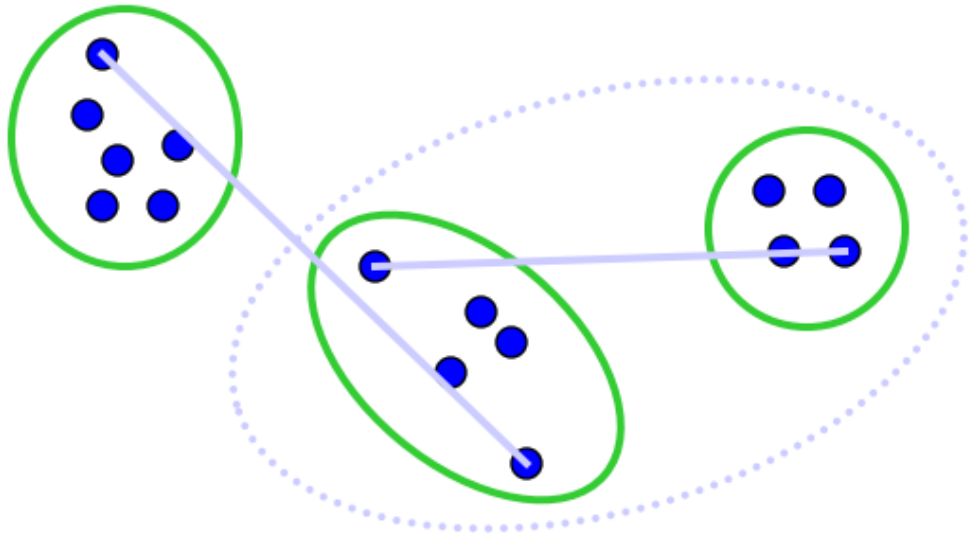


Complete-Link Agglomerative Clustering

- 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

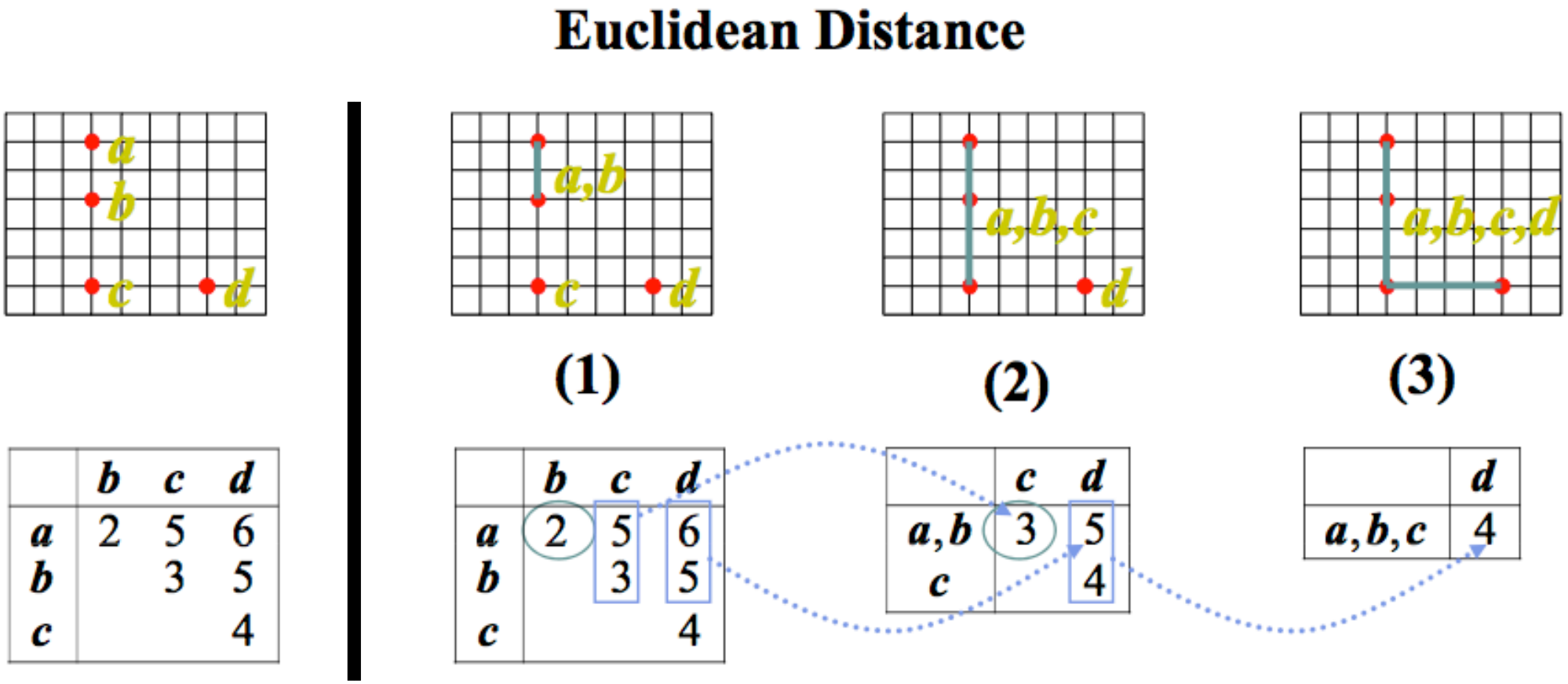
- After merging c_i and c_j, the similarity of the resulting cluster to any other cluster, c_k, can be computed by:
  - **Single-Link**:

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

  - **Complete-Link**:

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

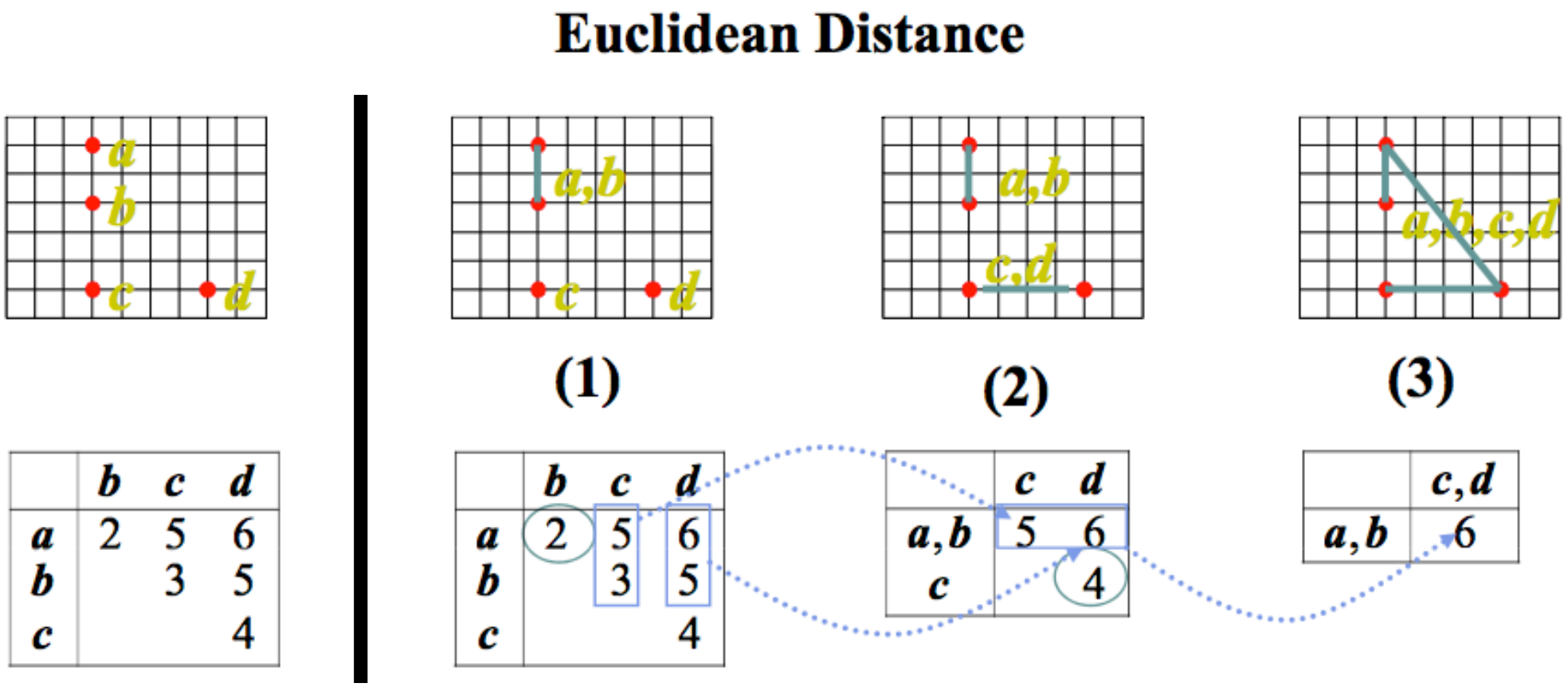
Single-Link Example



Distance Matrix

Illustration by Eric Xing @ CMU

Complete-Link Example

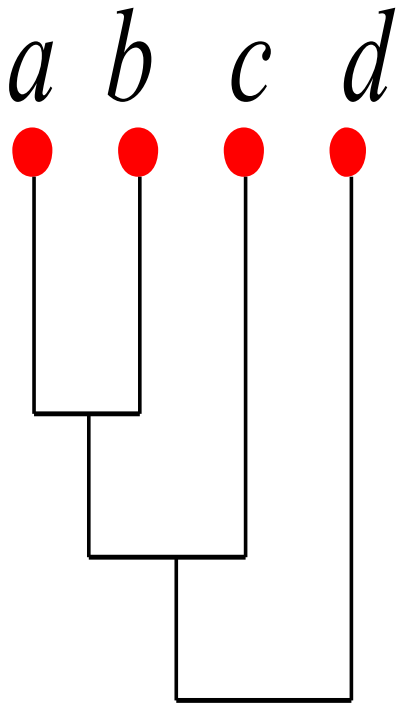


Distance Matrix

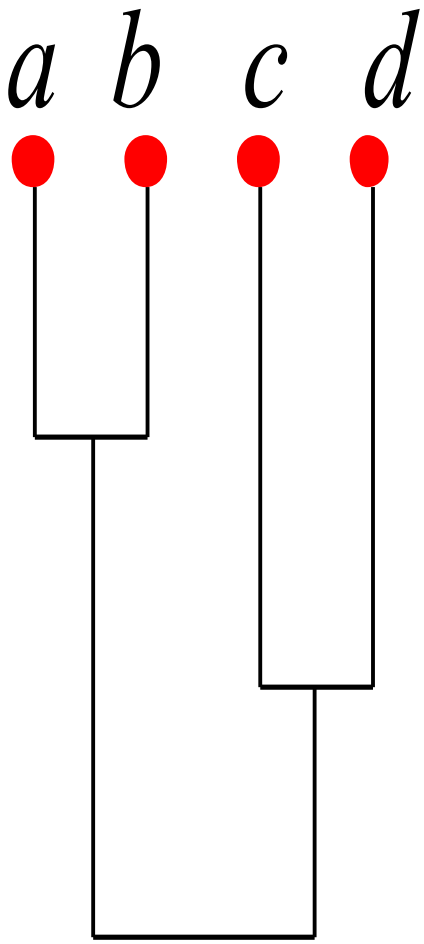
Illustration by Eric Xing @ CMU

Dendrograms Comparison

Single-Link



Complete-Link

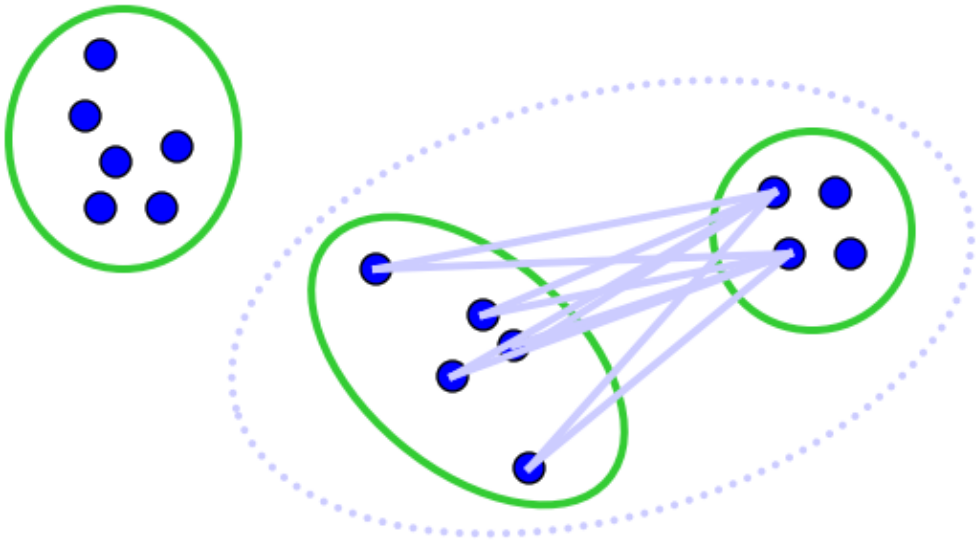


Group Average Agglomerative Clustering

- 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:

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