Clustering

CS4780 – Machine Learning
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Reading: Manning/Schuetze Chapter 14 (not 14.1.3, 14.1.4)

Based on slides from Prof. Claire Cardie, Prof. Ray Mooney, Prof. Yiming Yang

Outline

- **Supervised vs. Unsupervised Learning**
- **Hierarchical Clustering**
  - Hierarchical Agglomerative Clustering (HAC)
- **Non-Hierarchical Clustering**
  - K-means
  - EM-Algorithm

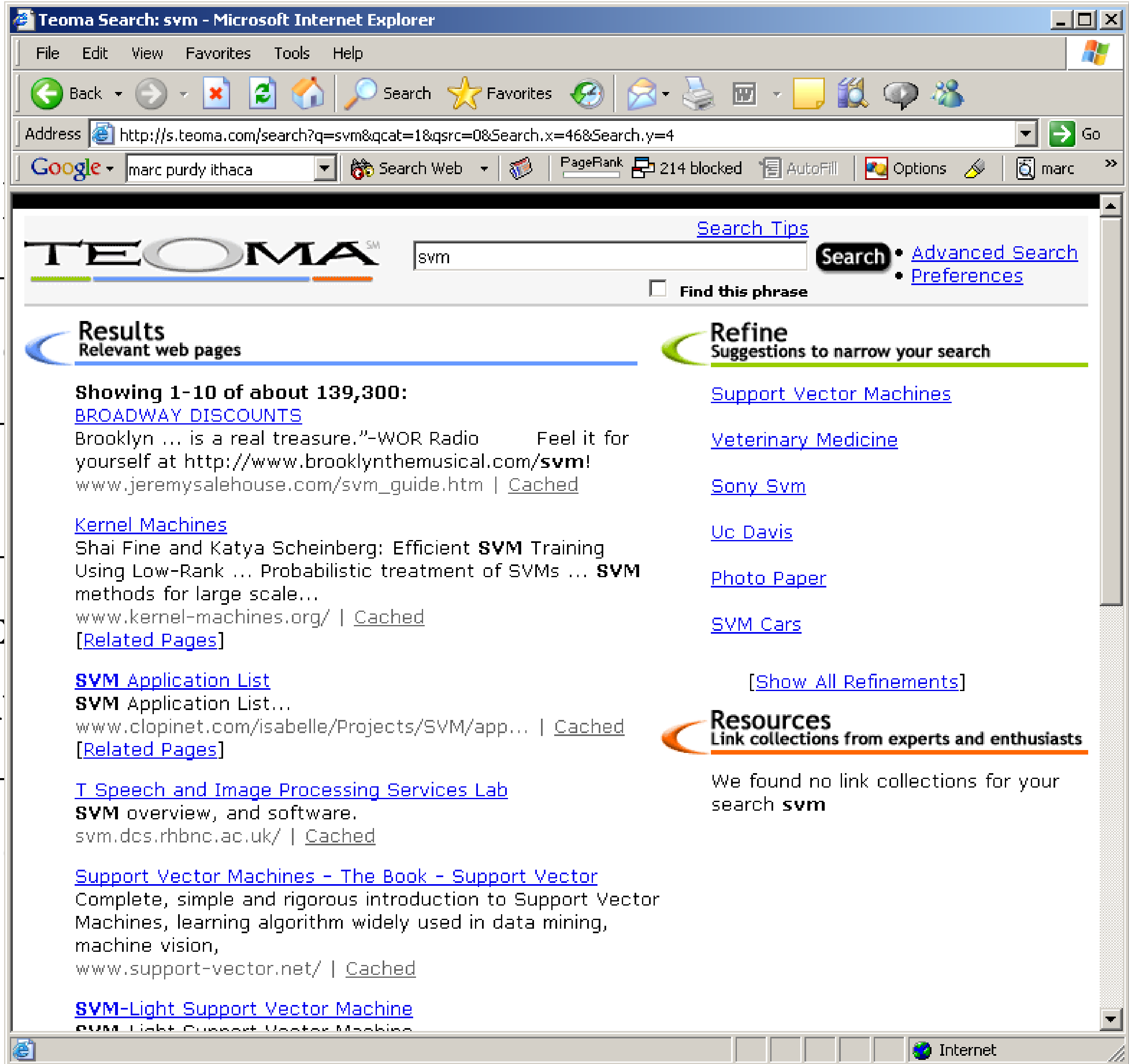
Supervised vs. Unsupervised Learning

- **Supervised Learning**
  - *Classification:* partition examples into groups according to pre-defined categories
  - *Regression:* assign value to feature vectors
  - Requires labeled data for training
- **Unsupervised Learning**
  - *Clustering:* partition examples into groups when no pre-defined categories/classes are available
  - *Novelty detection:* find changes in data
  - *Outlier detection:* find unusual events (e.g. hackers)
  - Only instances required, but no labels

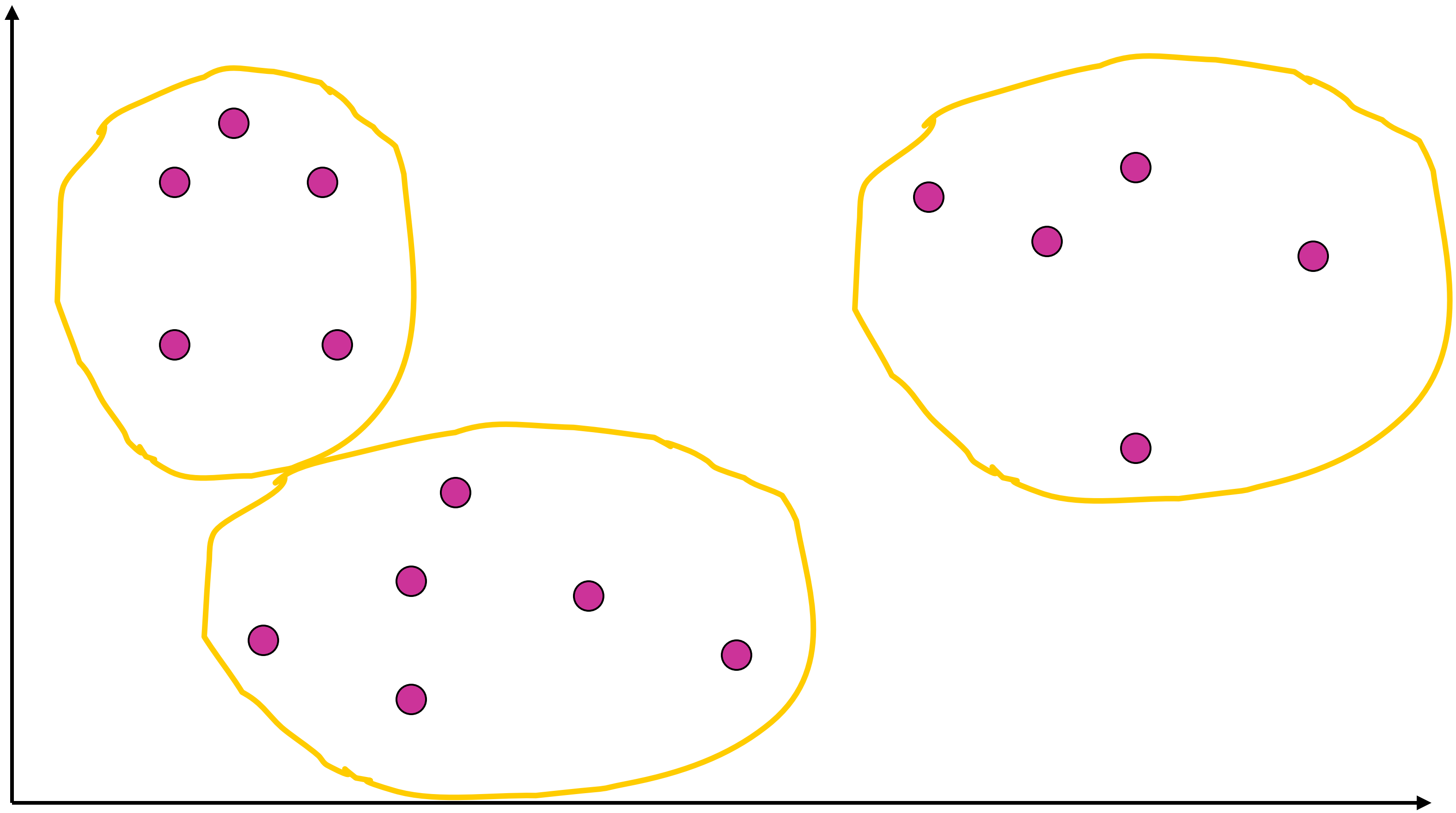
Clustering

- **Partition unlabeled examples into disjoint subsets of *clusters*, such that:**
  - Examples within a cluster are similar
  - Examples in different clusters are different
- **Discover new categories in an *unsupervised* manner (no sample category labels provided).**

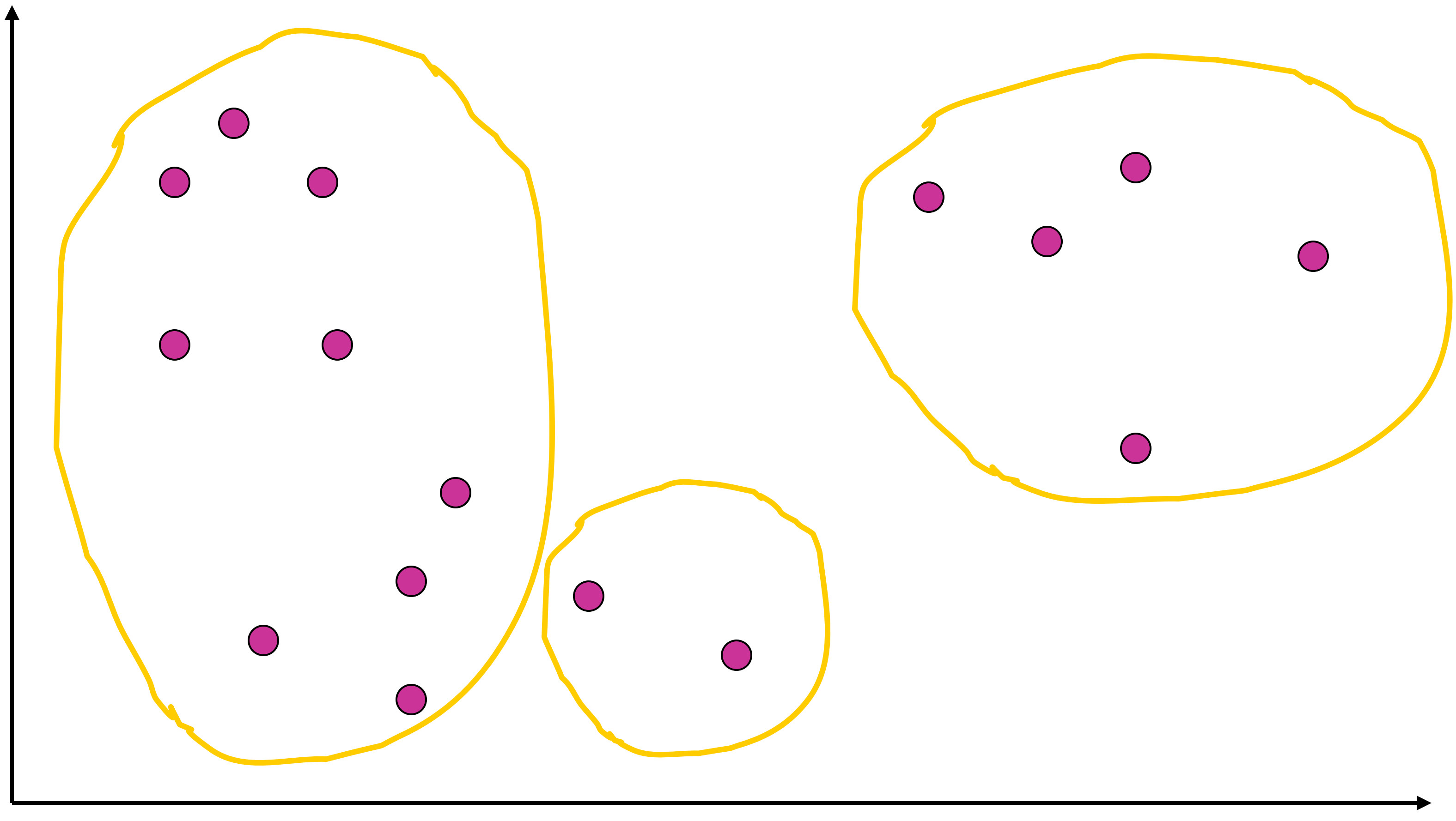
- C
  - user
- D
- E
- A nies
- C



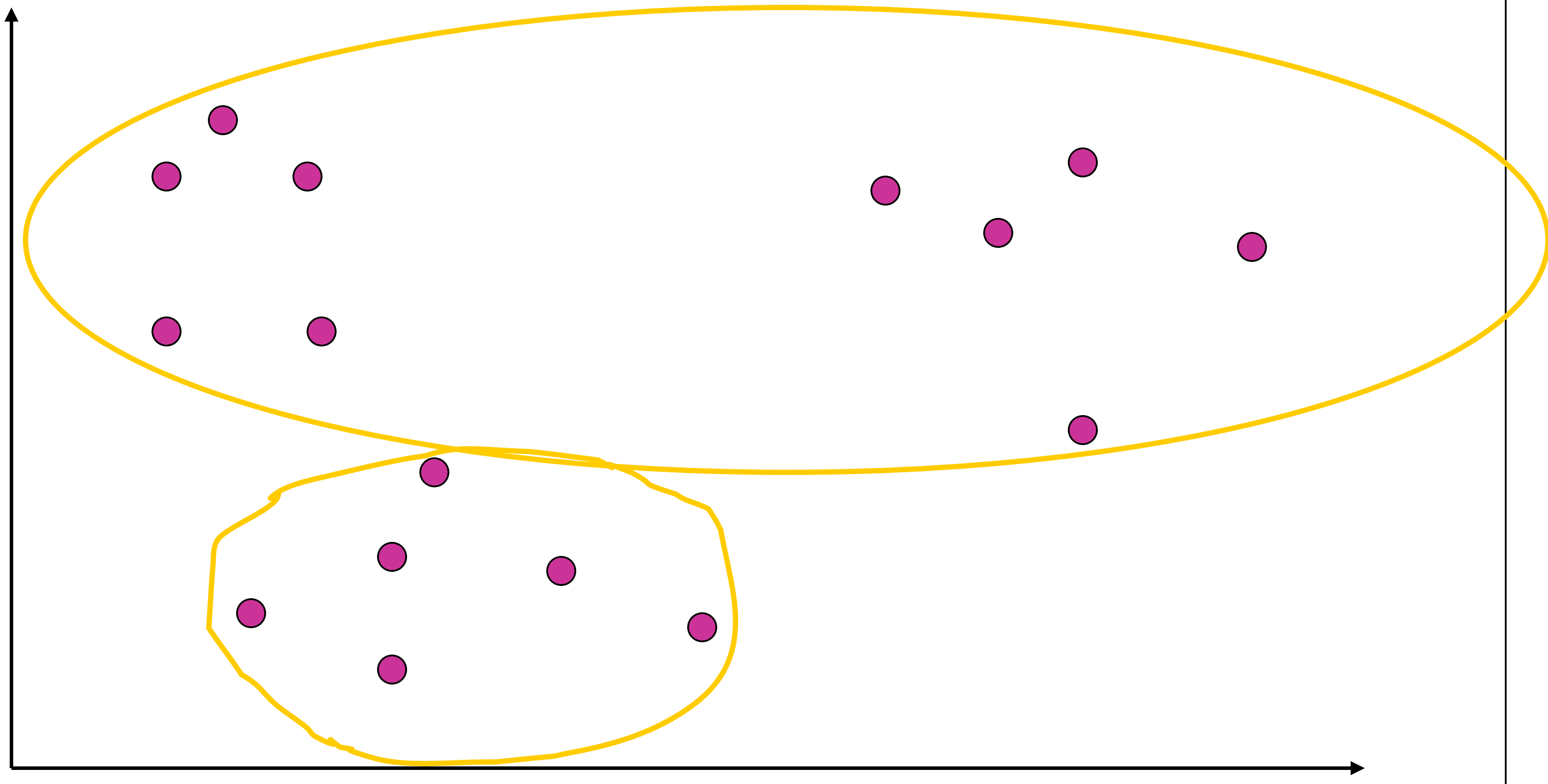
Clustering Example



Clustering Example



Clustering Example



Similarity (Distance) Measures

- **Euclidian distance (L_2 norm):**

$$L_2(\vec{x}, \vec{x}') = \sum_{i=1}^{m} (x_i - x_i')^2$$

- **L_1 norm:**

$$L_1(\vec{x}, \vec{x}') = \sum_{i=1}^{m} \left| x_i - x_i' \right|$$

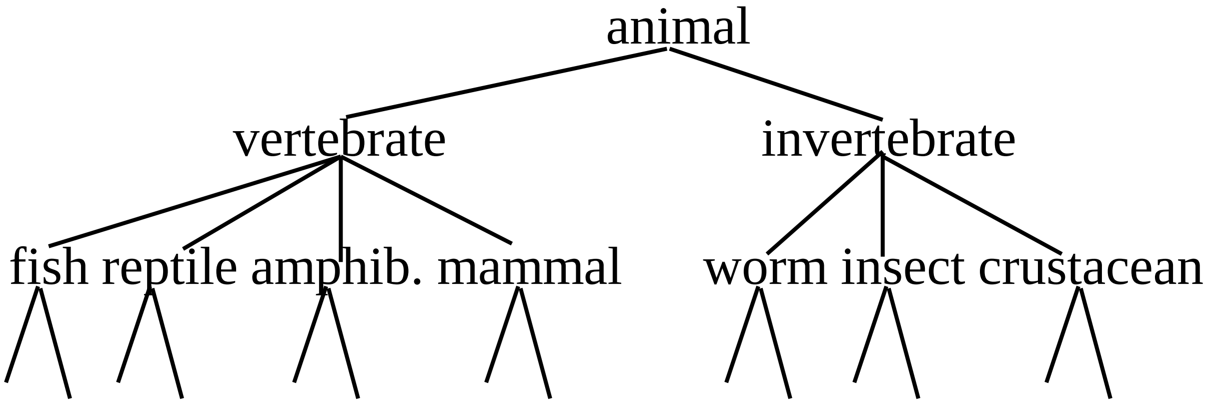
- **Cosine similarity:**

$$\cos(\vec{x}, \vec{x}') = \frac{\vec{x} \bullet \vec{x}'}{\left|\vec{x}\right| \cdot \left|\vec{x}'\right|}$$

- **Kernels**

Hierarchical Clustering

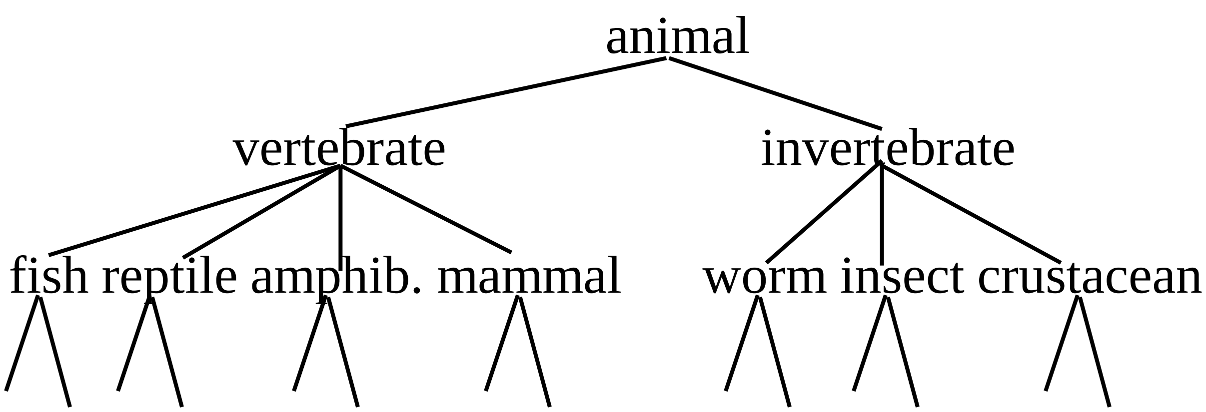
- **Build a tree-based hierarchical taxonomy from a set of unlabeled examples.**



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

Agglomerative vs. Divisive Clustering

- ***Agglomerative*** **(*bottom-up*) methods start with each example in its own cluster and iteratively combine them to form larger and larger clusters.**
- ***Divisive*** **(*top-down*) separate all examples immediately into clusters.**



Hierarchical Agglomerative Clustering (HAC)

- **Assumes a *similarity function* for determining the similarity of two clusters.**
- **Starts with all instances in a separate cluster and then repeatedly joins the two clusters that are most similar until there is only one cluster.**
- **The history of merging forms a binary tree or hierarchy.**
- **Basic algorithm:**
  - Start with all instances in their own cluster.
  - Until there is only one cluster:
    - Among the current clusters, determine the two clusters, c_i and c_j, that are most similar.
    - Replace c_i and c_j with a single cluster $c_i \cup c_j$

Cluster Similarity

- **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.

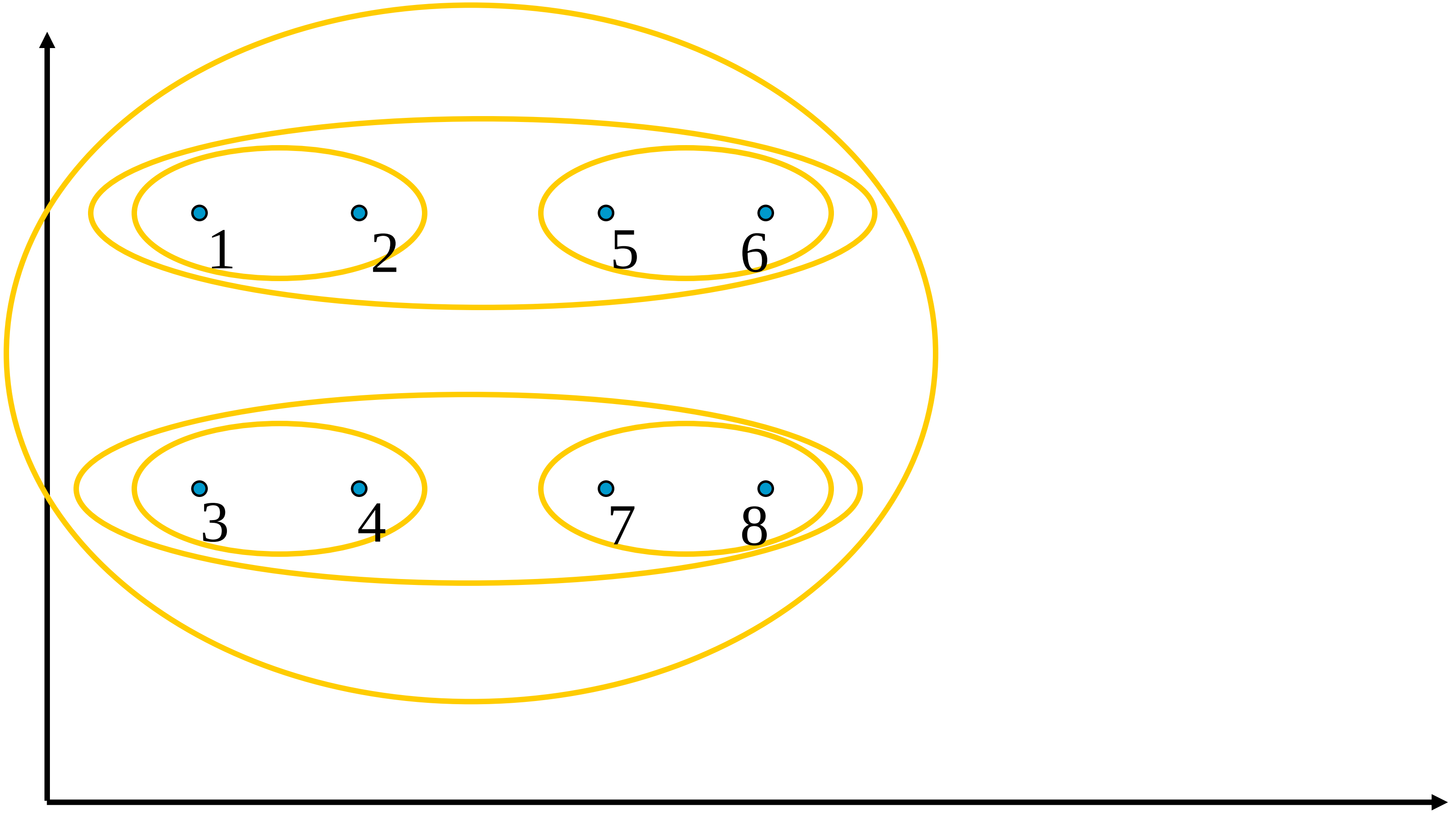
Single-Link Agglomerative Clustering

- **When computing cluster similarity, 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.**

Single Link Example



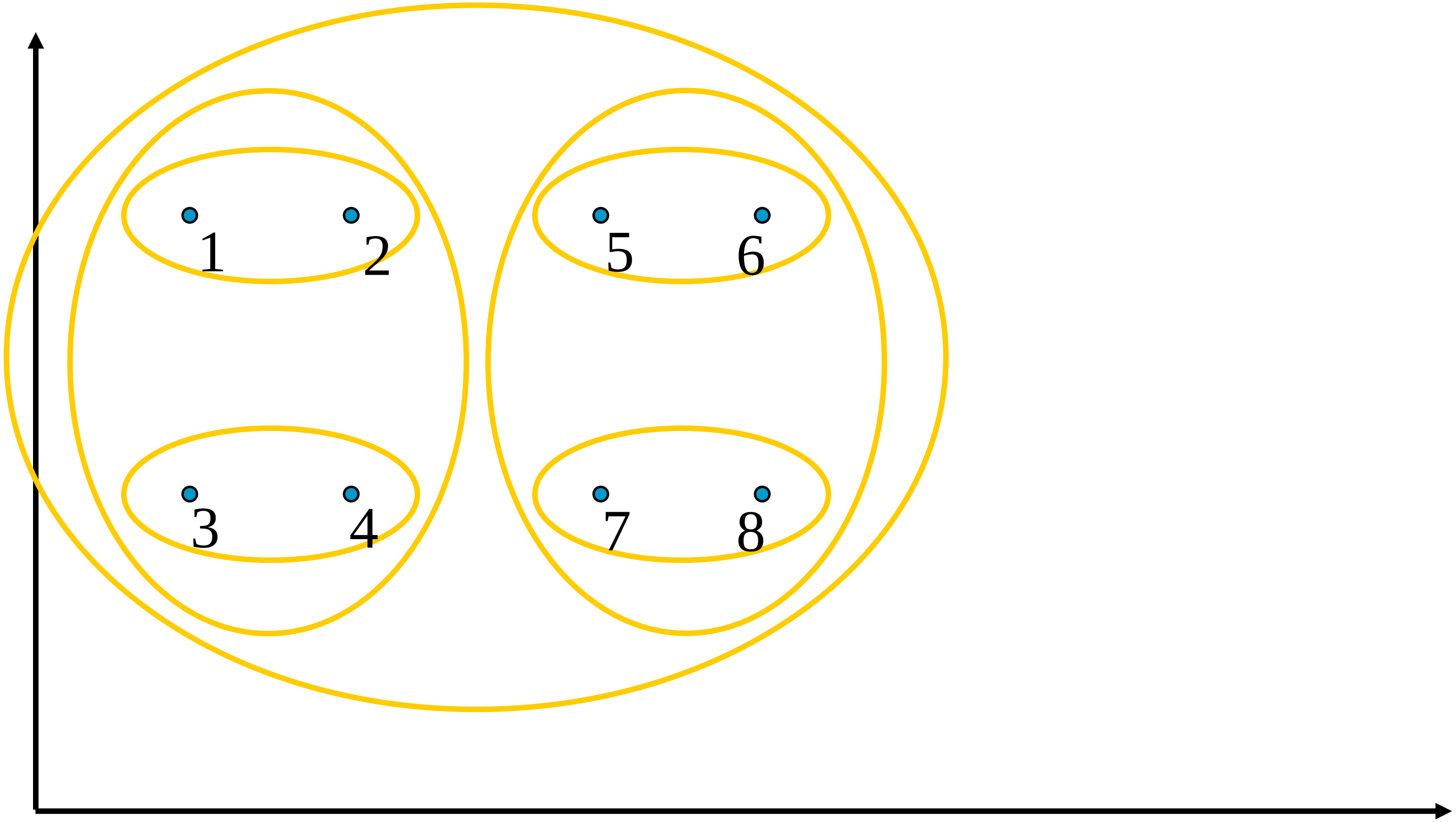
Complete Link Agglomerative Clustering

- **When computing cluster similarity, 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.**

Complete Link Example



Computational Complexity of HAC

- **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 the similarity matrix in $O(n^2)$ overall, computing the similarity to any other cluster must each be done in constant time.**
- **Maintain e.g. Heap to find smallest pair**

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:

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

Group Average Agglomerative Clustering

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

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

- **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:**

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

Non-Hierarchical Clustering

- **Single-pass clustering**
- **K-means clustering (“hard”)**
- **Expectation maximization (“soft”)**

Clustering Criterion

- **Evaluation function that assigns a (usually real-valued) value to a clustering**
  - Clustering criterion typically function of
    - within-cluster similarity and
    - between-cluster dissimilarity
- **Optimization**
  - Find clustering that maximizes the criterion
    - Global optimization (often intractable)
    - Greedy search
    - Approximation algorithms

Centroid-Based Clustering

- **Assumes instances are real-valued vectors.**
- **Clusters represented via *centroids* (i.e. mean of points in a cluster) *c*:**

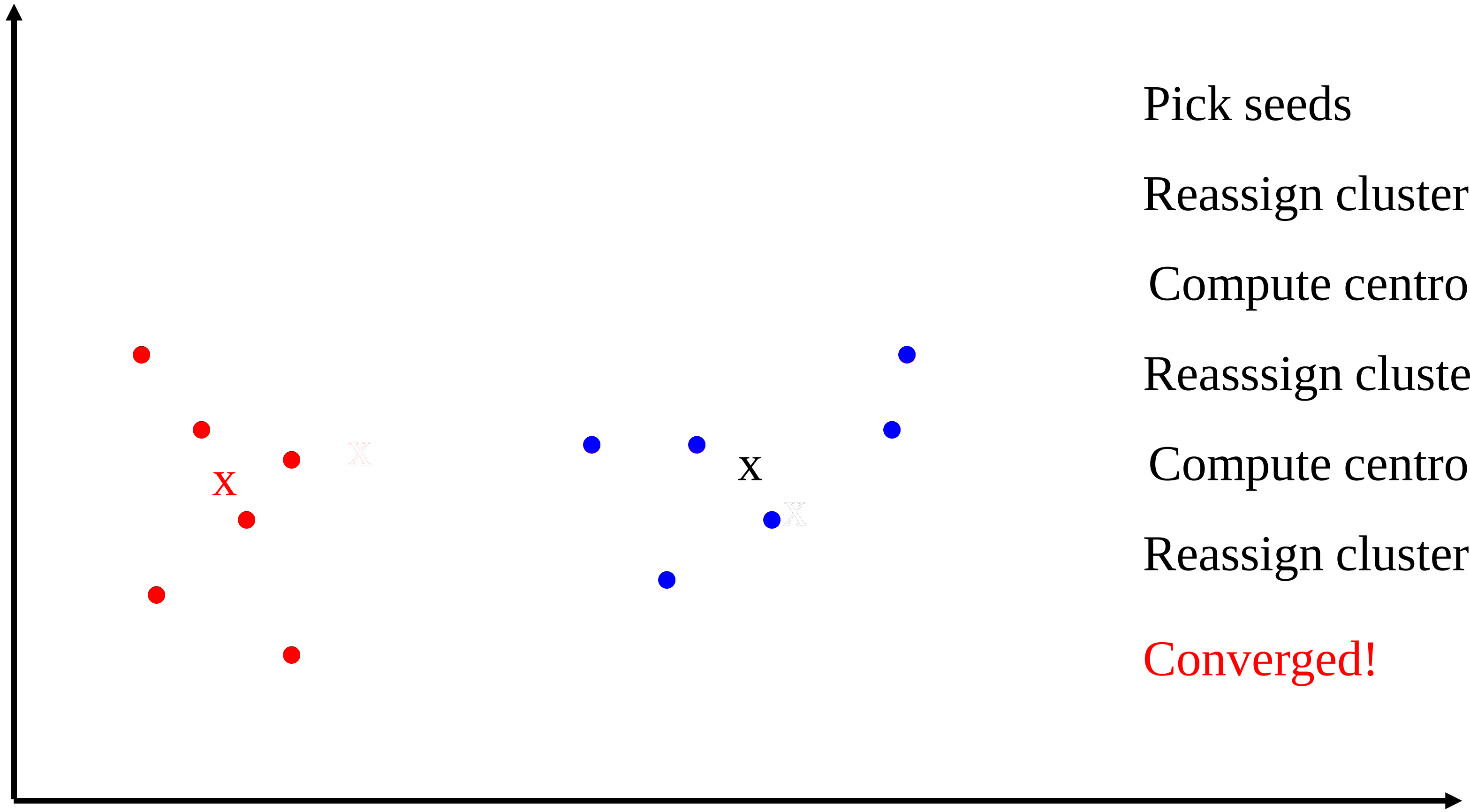
$$\vec{\mu}(\mathrm{c}) = \frac{1}{|c|}\sum_{\vec{x} \in c} \vec{x}$$

- **Reassignment of instances to clusters is based on distance to the current cluster centroids.**

K-Means Algorithm

- Input: k = number of clusters, distance measure d
- Select k random instances $\{s_1, s_2, \ldots s_k\}$ as seeds.
- Until clustering converges or other stopping criterion:
  - For each instance x_i:
    - Assign x_i to the cluster c_j such that $d(x_i, s_j)$ is min.
  - For each cluster c_j *//update the centroid of each cluster*
    - $s_j = \mu(c_j)$

K-means Example
(k=2)



Pick seeds

Reassign clusters

Compute centroids

Reasssign clusters

Compute centroids

Reassign clusters

Converged!

Time Complexity

- **Assume computing distance between two instances is O(*m*) where *m* is the dimensionality of the vectors.**
- **Reassigning clusters for *n* points: O(*kn*) distance computations, or O(*knm*).**
- **Computing centroids: Each instance gets added once to some centroid: O(*nm*).**
- **Assume these two steps are each done once for *i* iterations: O(*iknm*).**
- **Linear in all relevant factors, assuming a fixed number of iterations, more efficient than HAC.**

Buckshot Algorithm

Problem

- Results can vary based on random seed selection, especially for high-dimensional data.
- Some seeds can result in poor convergence rate, or convergence to sub-optimal clusterings.

Idea: Combine HAC and K-means clustering.

- First randomly take a sample of instances of size $\sqrt{n}$
- Run group-average HAC on this sample
- Use the results of HAC as initial seeds for K-means.
- Overall algorithm is efficient and avoids problems of bad seed selection.