# Clustering

CS6780 – Advanced Machine Learning
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Reading: Murphy 25.1, 25.5.1

# Supervised Learning 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
  - Signal separation: recover components of a mixed signal
  - Embeddings: find low dimensional representation of high dimensional data
  - Outlier detection: find unusual events (e.g. hackers)
  - Novelty detection: find changes in data
  - Only instances required, but no labels

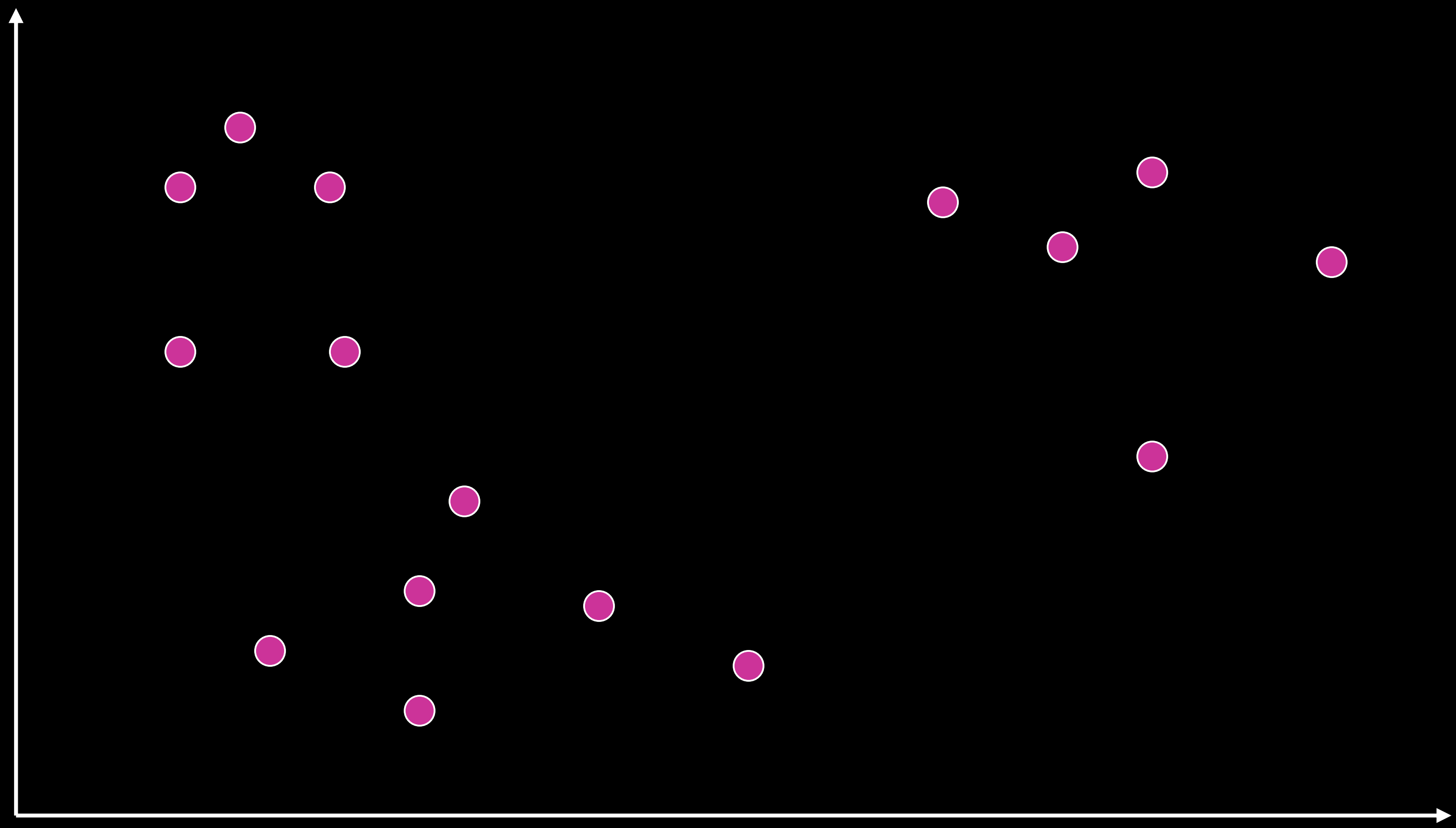
# Clustering

- 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).

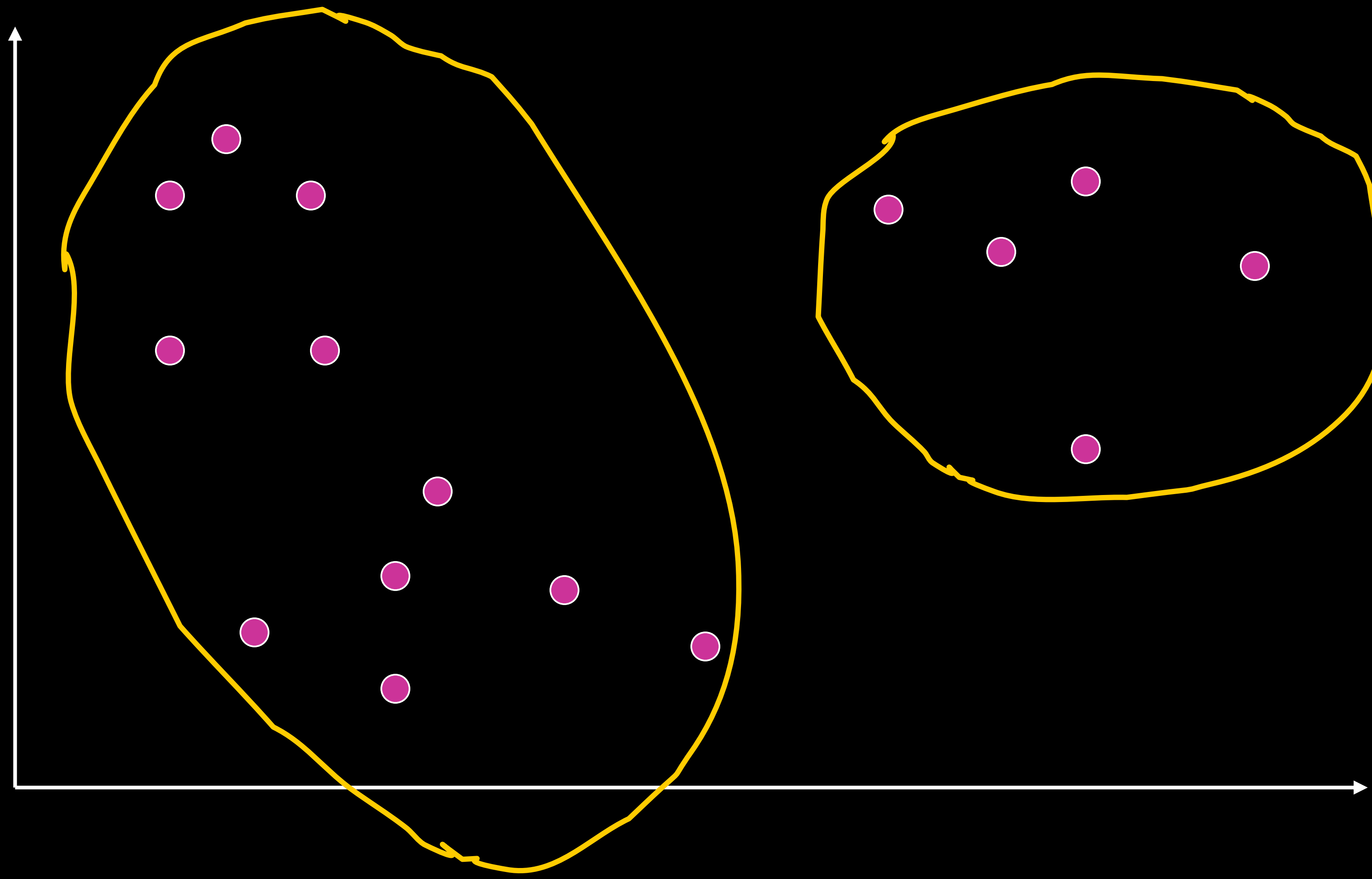
# Applications of Clustering

- Exploratory data analysis
- Cluster retrieved documents in search engine
- Detecting near duplicates
  - Entity resolution
    - E.g. “Thorsten Joachims” == “Thorsten B Joachims”
  - Cheating detection
- Automated (or semi-automated) creation of taxonomies
  - E.g. phylogenetic tree
- Compression

# Clustering Example



# Clustering Example



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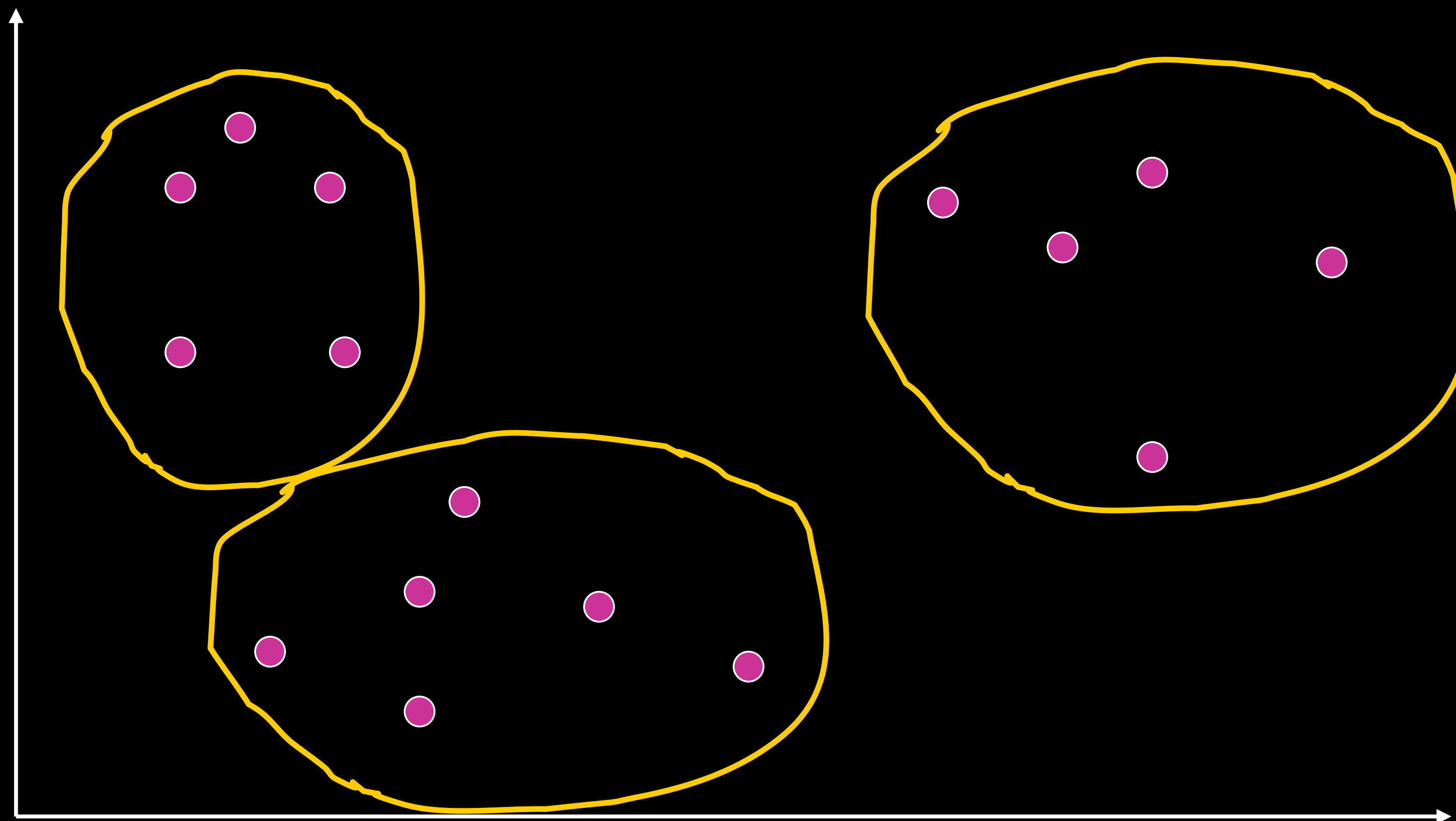

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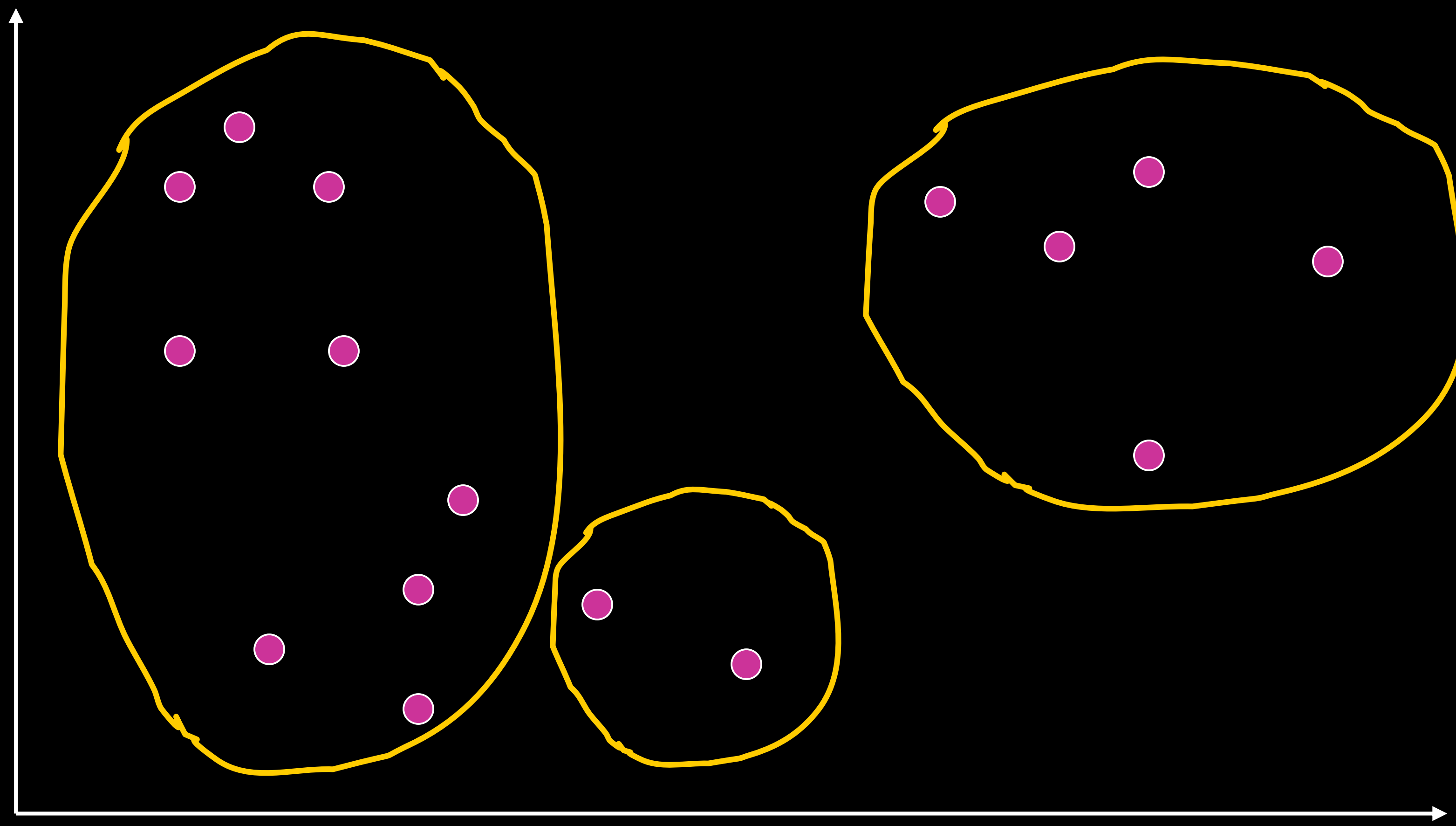

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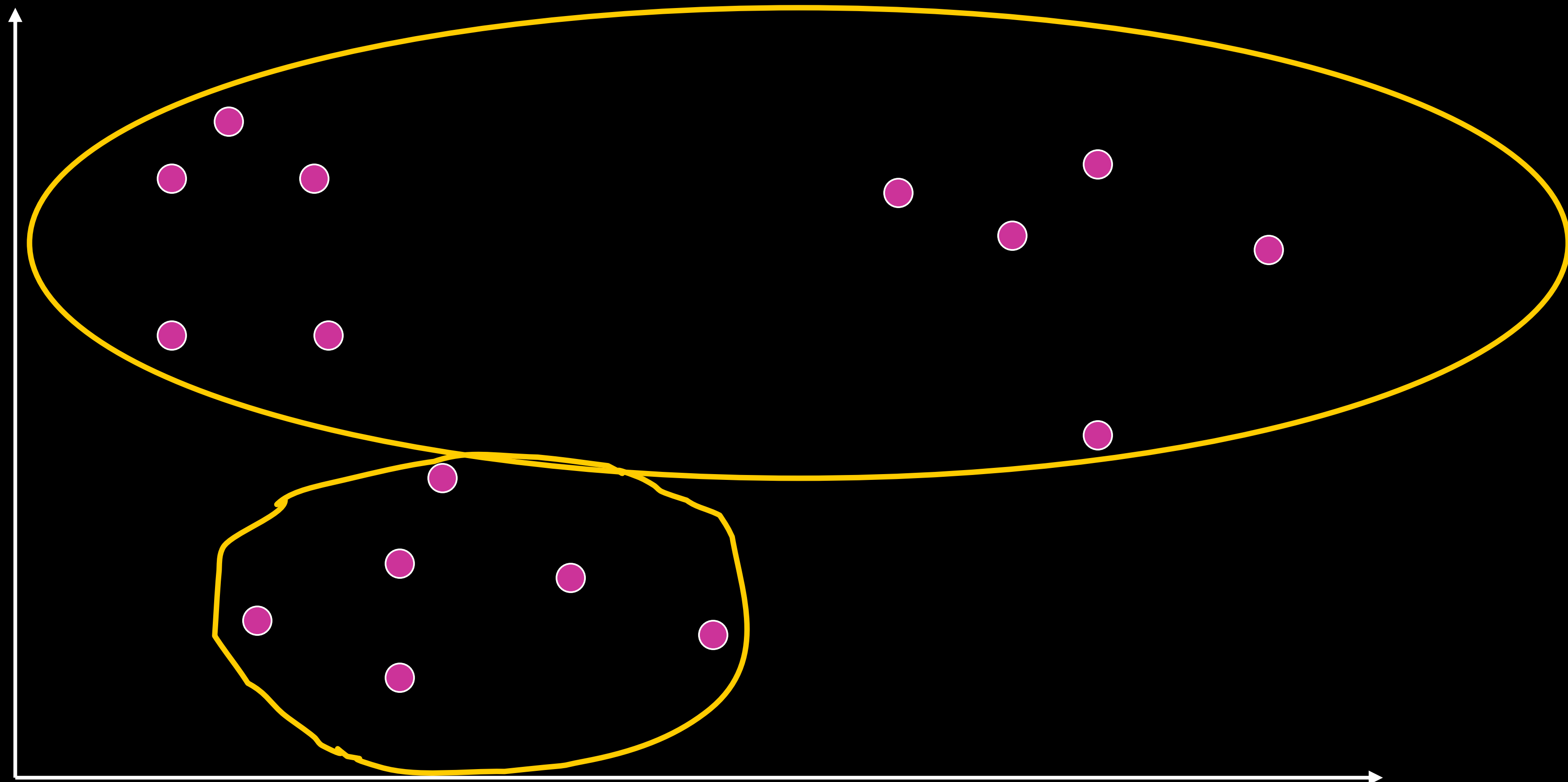


# Similarity (Distance) Measures

- Euclidian distance ($L_2$ norm):

$$L_2(\vec{x}, \vec{x}') = \sqrt{\sum_{i=1}^{N} \left(x_i - x_i'\right)^2}$$

- $L_1$ norm:

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

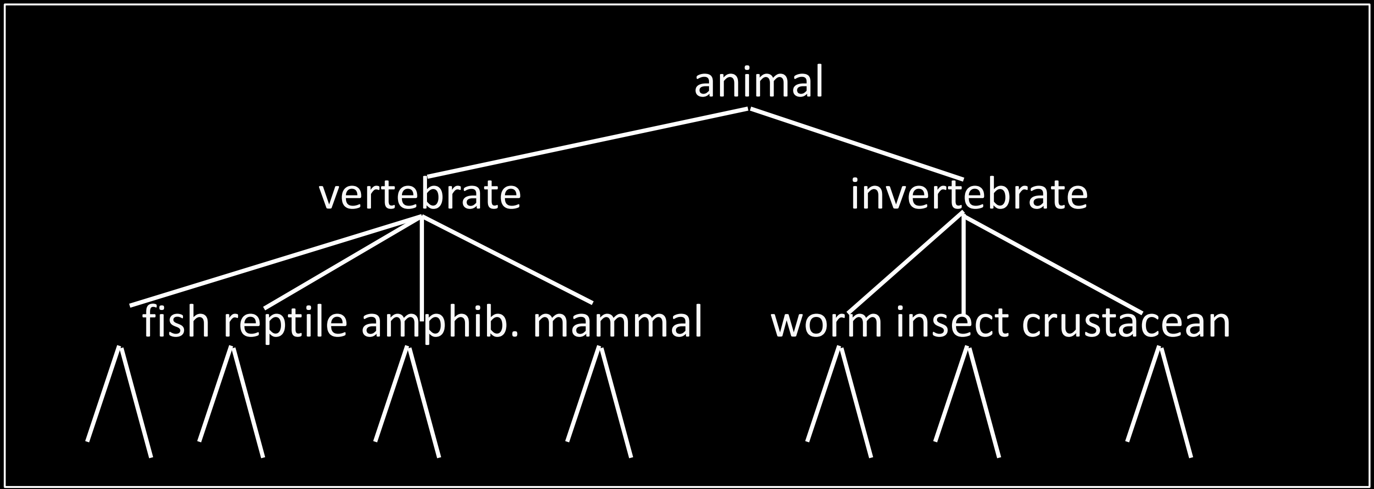
- Cosine similarity:

$$\cos(\vec{x}, \vec{x}') = \frac{\vec{x} * \vec{x}'}{\|\vec{x}\| \, \|\vec{x}'\|}$$

- Kernels

# Hierarchical Clustering

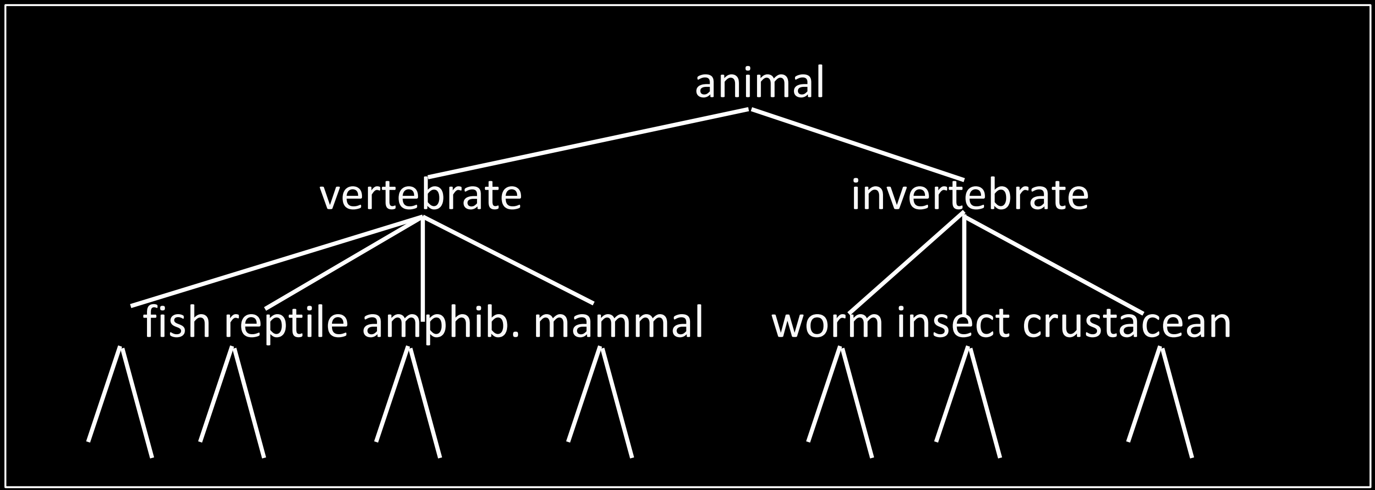
- Build a tree-based hierarchical taxonomy from a set of unlabeled examples.




- 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.
- Basic algorithm:

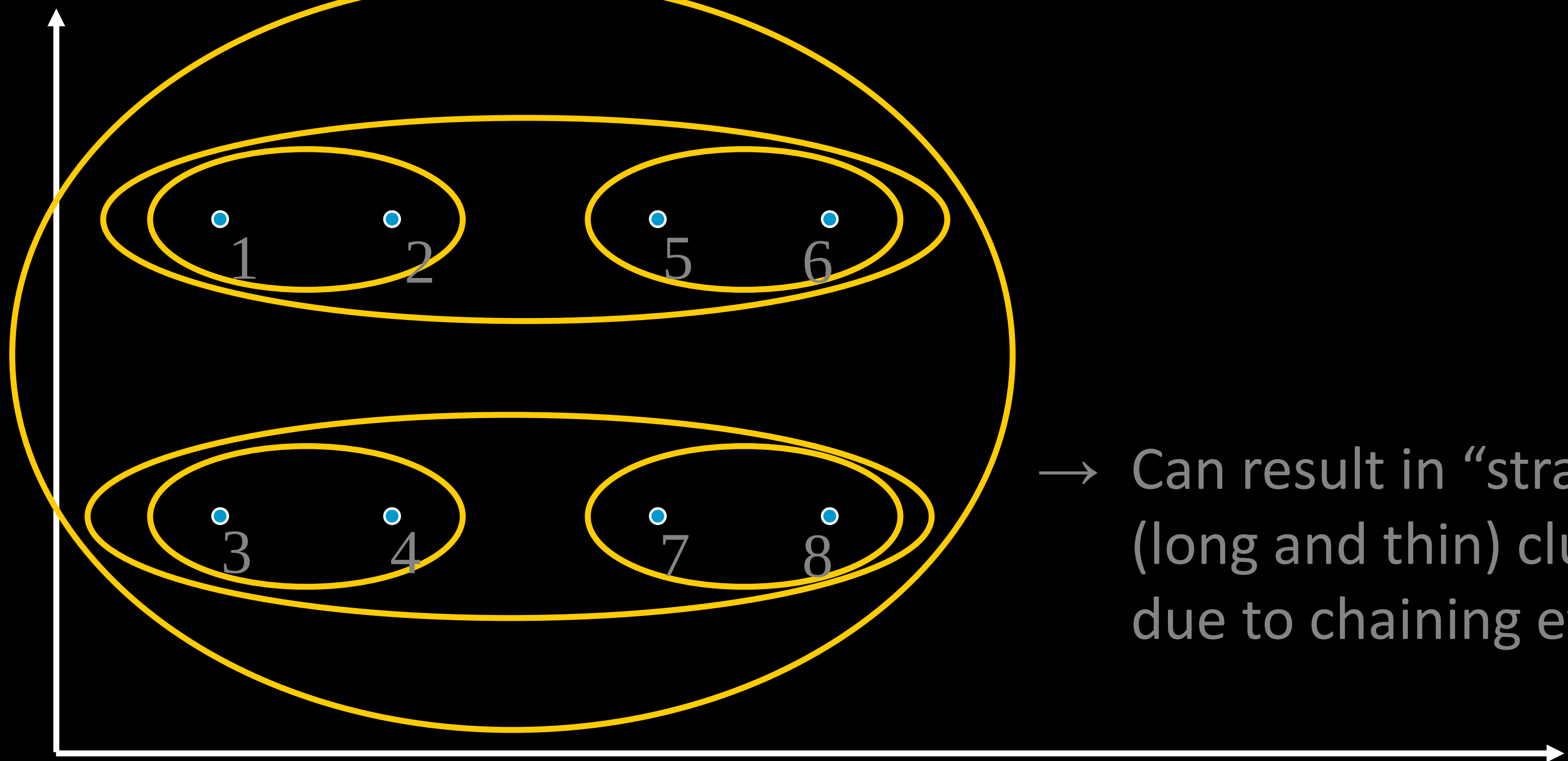
  - Start with all instances in their own cluster.
  - Until there is only one cluster:
    - Among the current clusters, determine the two clusters, $c_i$ and $c_j$, that are most similar.
    - Replace $c_i$ and $c_j$ with a single cluster $c_i \cup c_j$

- The history of merging forms a binary tree or hierarchy.

# 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.

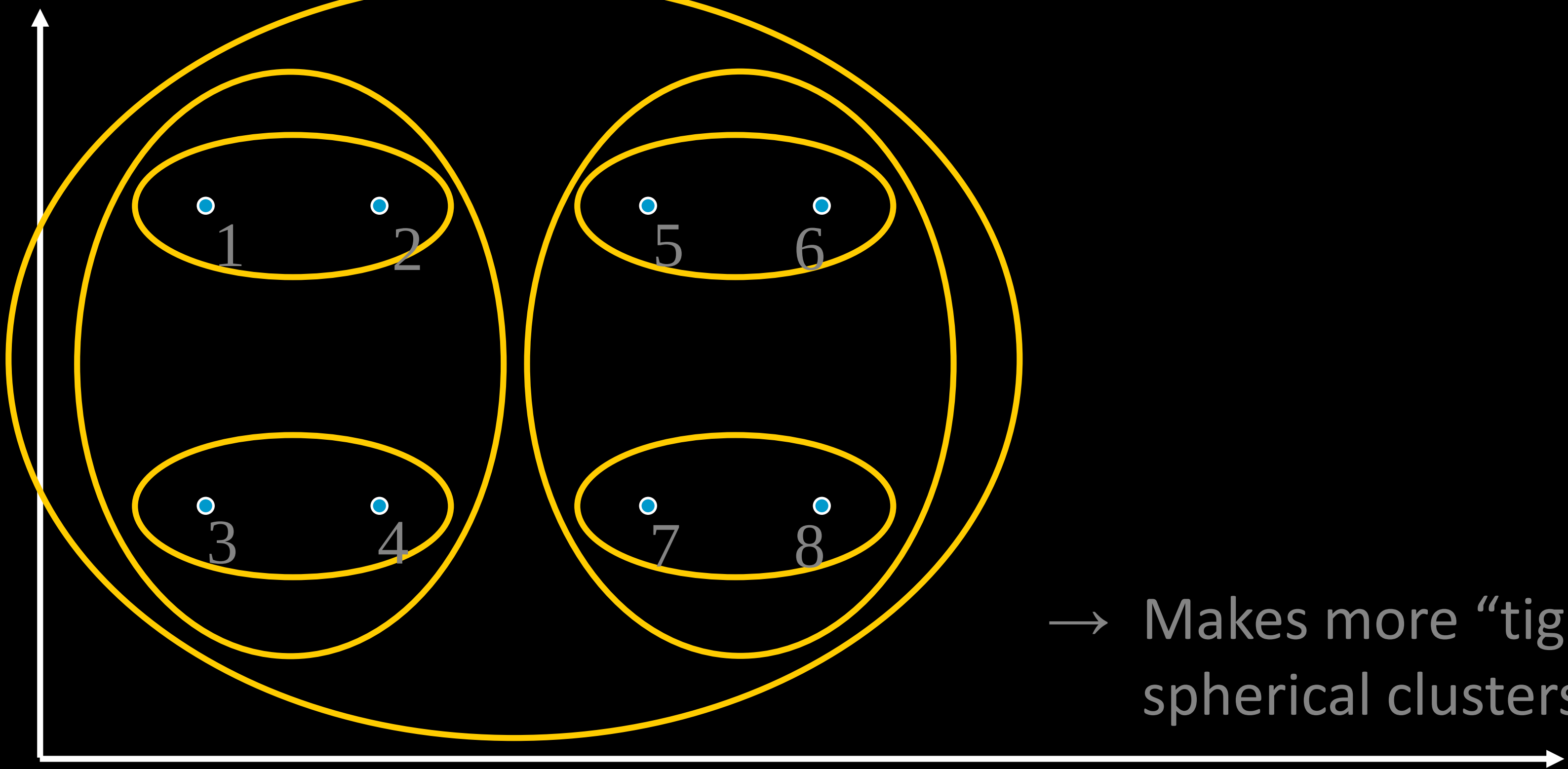
# Single-Link HAC




→ Can result in “straggly” (long and thin) clusters due to chaining effect.

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

# Complete-Link HAC




→ Makes more "tight," spherical clusters.

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

# 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 $O(n)$ merging iterations,
  - must find smallest distance pair of clusters → Maintain heap $O(n^2 \log n)$
  - it must compute the distance between the most recently created cluster and each other existing cluster. Can this be done in constant time?

→ $O(n^2 \log n)$ overall.

# 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

| | x1 | x2 | x3 | x4 | x5 |
|---|---|---|---|---|---|
| x1 | 1 | 0.8 | 0.2 | 0.7 | 0.3 |
| x2 | 0.8 | 1 | 0.1 | 0.5 | 0.2 |
| x3 | 0.2 | 0.1 | 1 | 0.9 | 0.5 |
| x4 | 0.7 | 0.5 | 0.9 | 1 | 0.4 |
| x5 | 0.3 | 0.2 | 0.5 | 0.4 | 1 |

Merge x3,x4
replace with max

| | x1 | x2 | c1 | x5 |
|---|---|---|---|---|
| x1 | 1 | 0.8 | 0.7 | 0.3 |
| x2 | 0.8 | 1 | 0.5 | 0.2 |
| c1 | 0.7 | 0.5 | 1 | 0.5 |
| x5 | 0.3 | 0.2 | 0.5 | 1 |

Merge x1,x2
replace with max

| | c2 | c1 | x5 |
|---|---|---|---|
| c2 | 1 | 0.7 | 0.3 |
| c1 | 0.7 | 1 | 0.5 |
| x5 | 0.3 | 0.5 | 1 |

Merge c1,c2
replace with max

| | c3 | x5 |
|---|---|---|
| c3 | 1 | 0.5 |
| x5 | 0.5 | 1 |

# 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:

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

# Non-Hierarchical Clustering

- K-means clustering (“hard”)
- Mixtures of Gaussians and training via Expectation maximization Algorithm (“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

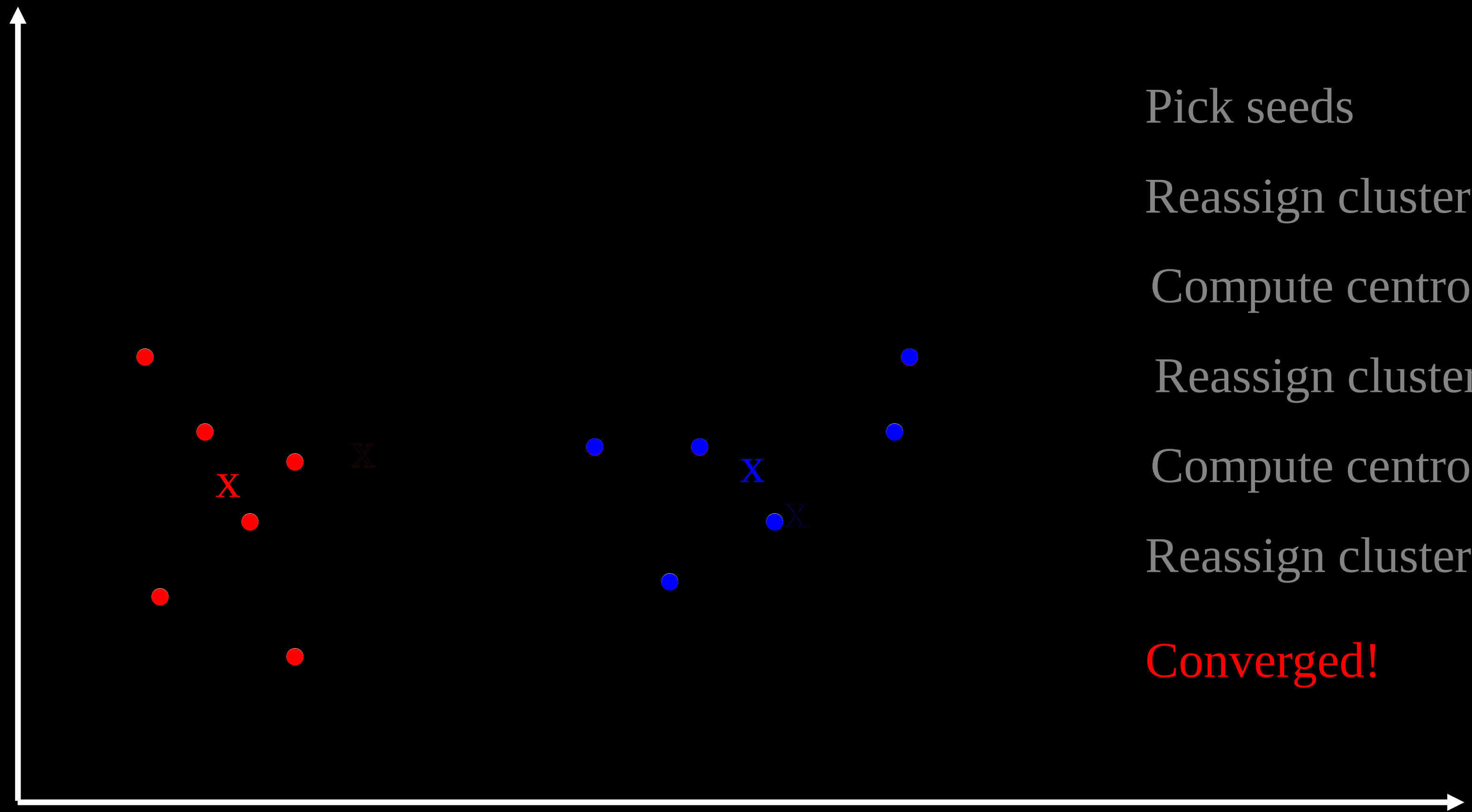
# K-Means Algorithm

- Input: $k$ = number of clusters, Euclidian distance $d$
- 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*
    - $s_j = \mu(c_j)$

Note: Clusters represented via ***centroids***

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

# K-means Example
## (k=2)




Pick seeds

Reassign clusters

Compute centroids

Reassign clusters

Compute centroids

Reassign clusters

Converged!

# Time Complexity

- Assume computing distance between two instances is O($N$) where $N$ is the dimensionality of the vectors.
- Reassigning clusters for $n$ points: O($kn$) distance computations, or O($knN$).
- Computing centroids: Each instance gets added once to some centroid: O($nN$).
- Assume these two steps are each done once for $i$ iterations: O($iknN$).
- Linear in all relevant factors, assuming a fixed number of iterations.

# 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 $n^{1/2}$
- 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.

# Non-Hierarchical Clustering

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