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Artificial Intelligence

Lecture XI

Clustering

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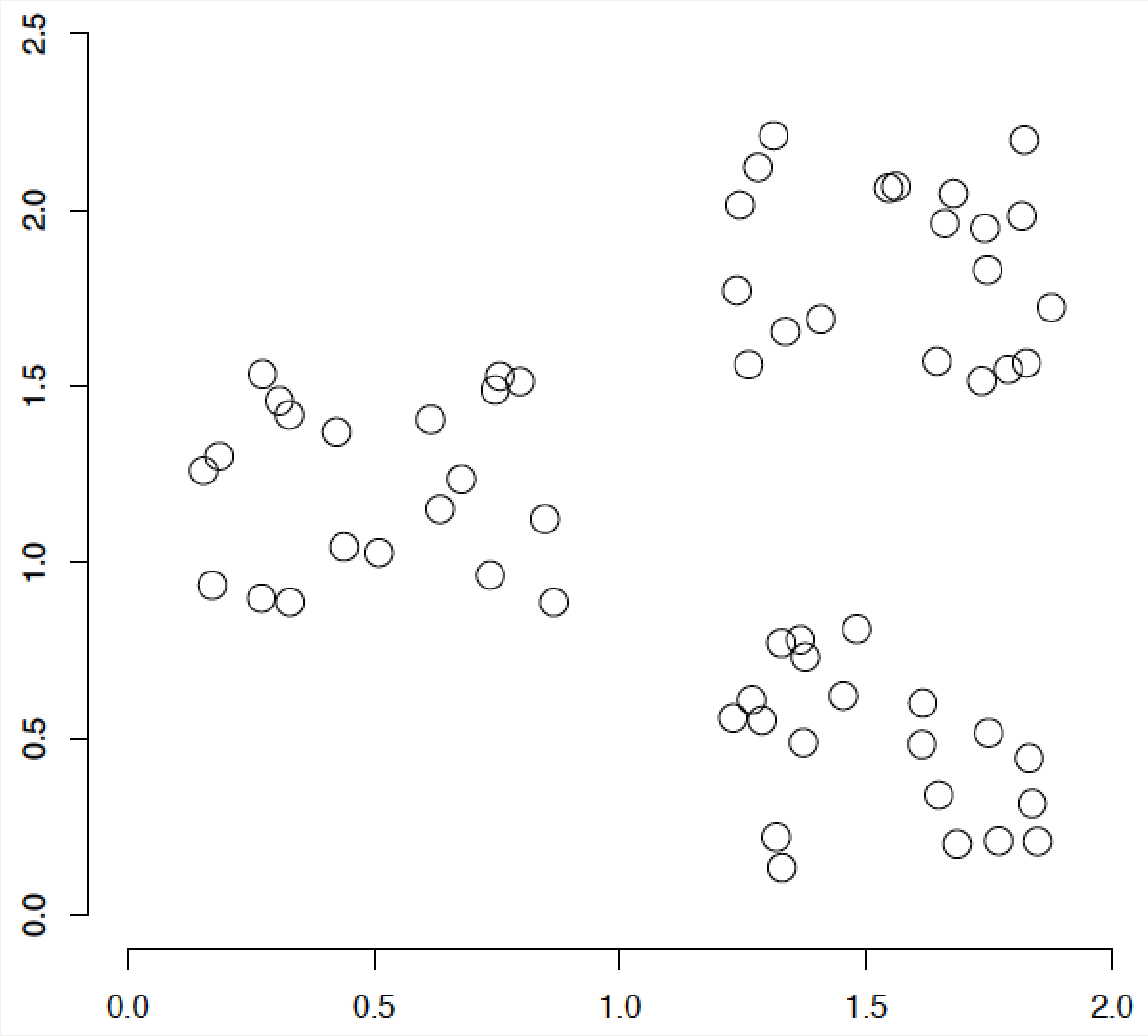
Today’s Topic: Clustering

- Introduction
- Clustering algorithms
  - Partitional
  - Hierarchical

What is clustering?

- Clustering: the process of grouping a set of objects into classes of similar objects
  - samples within a cluster should be similar.
  - samples from different clusters should be dissimilar.
- The commonest form of *unsupervised learning*
    - Unsupervised learning = learning from raw data, as opposed to supervised data where a classification of examples is given
  - A common and important task that finds many applications in IR and other places

A data set with clear cluster structure



- How would you design an algorithm for finding the three clusters in this case?

Clustering Algorithms

- Flat algorithms
  - Usually start with a random (partial) partitioning
  - Refine it iteratively
    - *K* means clustering
    - (Model based clustering)
- Hierarchical algorithms
  - Bottom-up, agglomerative
  - (Top-down, divisive)

Hard vs. soft clustering

- Hard clustering: Each samples belongs to exactly one cluster
  - More common and easier to do
- Soft clustering: A samples can belong to more than one cluster.
  - Makes more sense for applications like creating browsable hierarchies
  - You may want to put a pair of sneakers in two clusters: (i) sports apparel and (ii) shoes
  - You can only do that with a soft clustering approach.
- We won’t do soft clustering today. See IIR 16.5, 18

Partitioning Algorithms

- Partitioning method: Construct a partition of n samples into a set of K clusters
- Given: a set of samples and the number K
- Find: a partition of K clusters that optimizes the chosen partitioning criterion
  - Globally optimal: exhaustively enumerate all partitions
  - Effective heuristic methods: K-means and K-medoids algorithms

K-Means

- Assumes samples are real-valued vectors.
- Clusters based on *centroids* (aka the *center of gravity* or 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

Select K random centers $\{s_1, s_2, \ldots s_K\}$ as seeds.
Until clustering converges or other stopping criterion:

For each s_i:

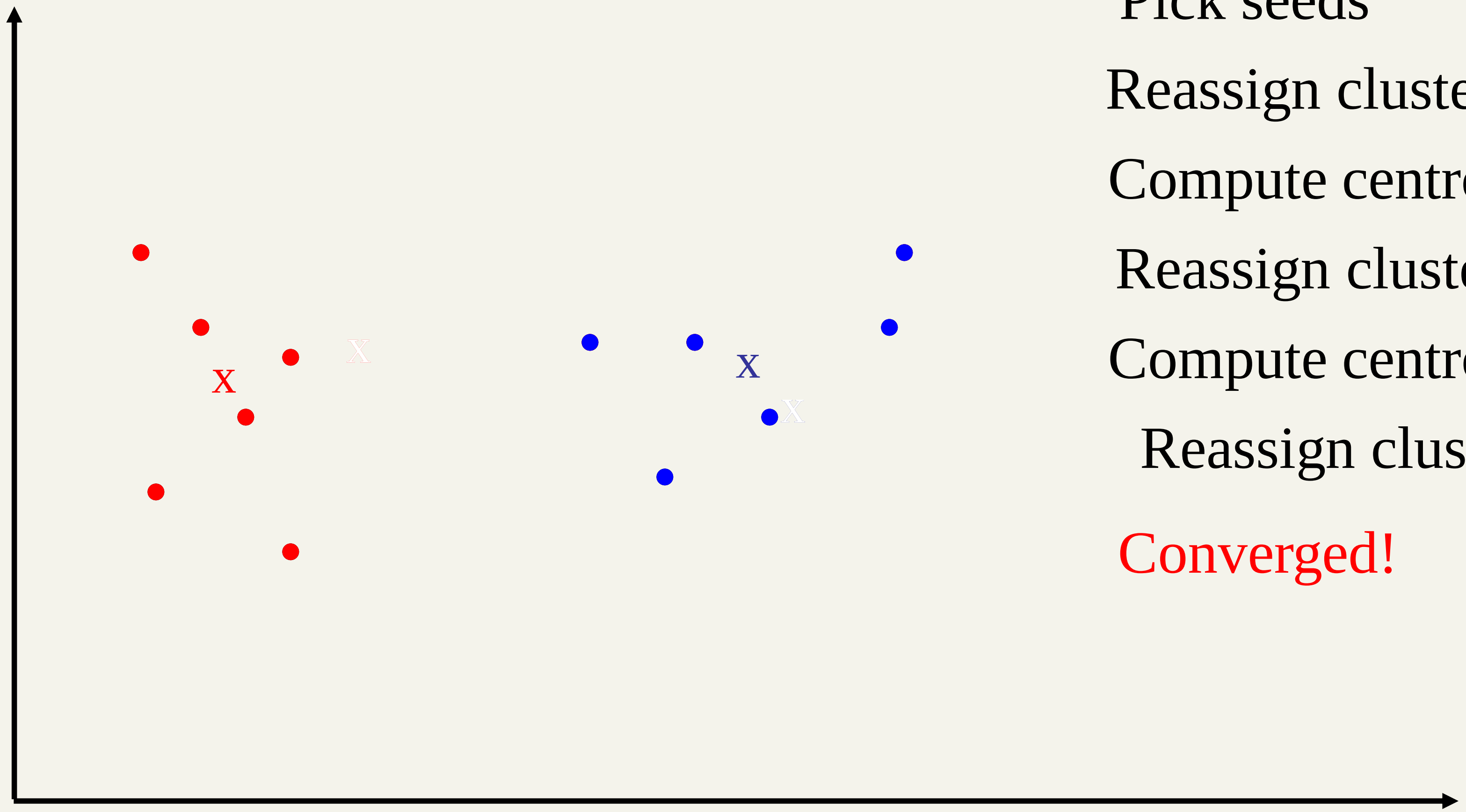
Assign d_i to the cluster c_j such that $dist(x_i, s_j)$ is minimal.

(Update the seeds to the centroid of each cluster)

For each cluster c_j

$s_j = \mu(c_j)$

K Means Example (K=2)



Pick seeds

Reassign clusters

Compute centroids

Reassign clusters

Compute centroids

Reassign clusters

Converged!

K Means Examples

- Find the suitable clusters to classify the following data sets:

1- { 1, 2, 1.5, 1.2, 2.5, 3.8}
2- {1 , 2, 5, 7, 10, 15, 19}

- Find the R value that make the following data set separable into three clusters, then find the clusters:

1- {10, 20, 7, 2, R, 15,100}

Termination conditions

- Several possibilities, e.g.,
  - A fixed number of iterations.
  - samples partition unchanged.
  - Centroid positions don't change.

Does this mean that the samples in a cluster are unchanged?

Convergence

- Why should the *K*-means algorithm ever reach a *fixed point*?
  - A state in which clusters don't change.
- *K*-means is a special case of a general procedure known as the *Expectation Maximization (EM) algorithm*.
  - EM is known to converge.
  - Number of iterations could be large.
    - But in practice usually isn't

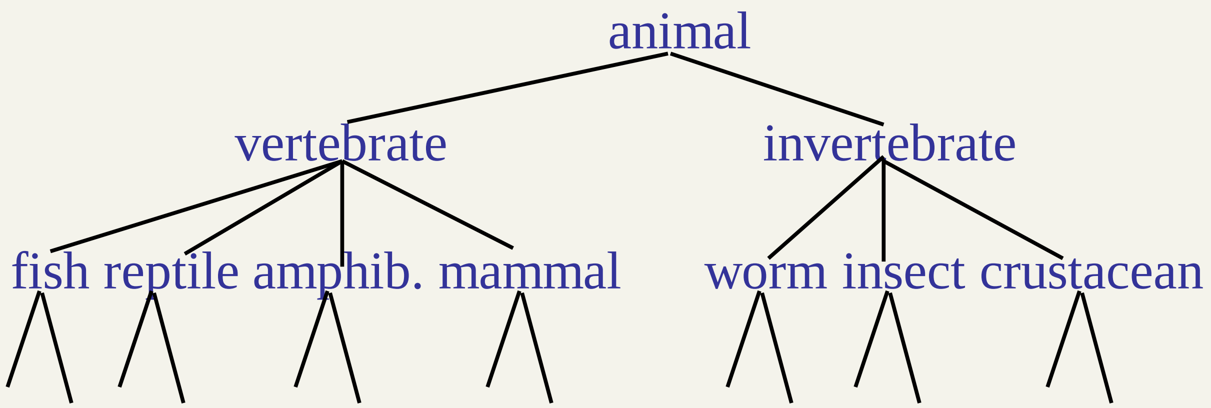
Lower case

Convergence of *K*-Means

- Define goodness measure of cluster *k* as sum of squared distances from cluster centroid:
  - $G_k = \Sigma_i (s_i - c_k)^2$ (sum over all s_i in cluster *k*)
- $G = \Sigma_k G_k$
- Reassignment monotonically decreases G since each vector is assigned to the closest centroid.

Hierarchical Clustering

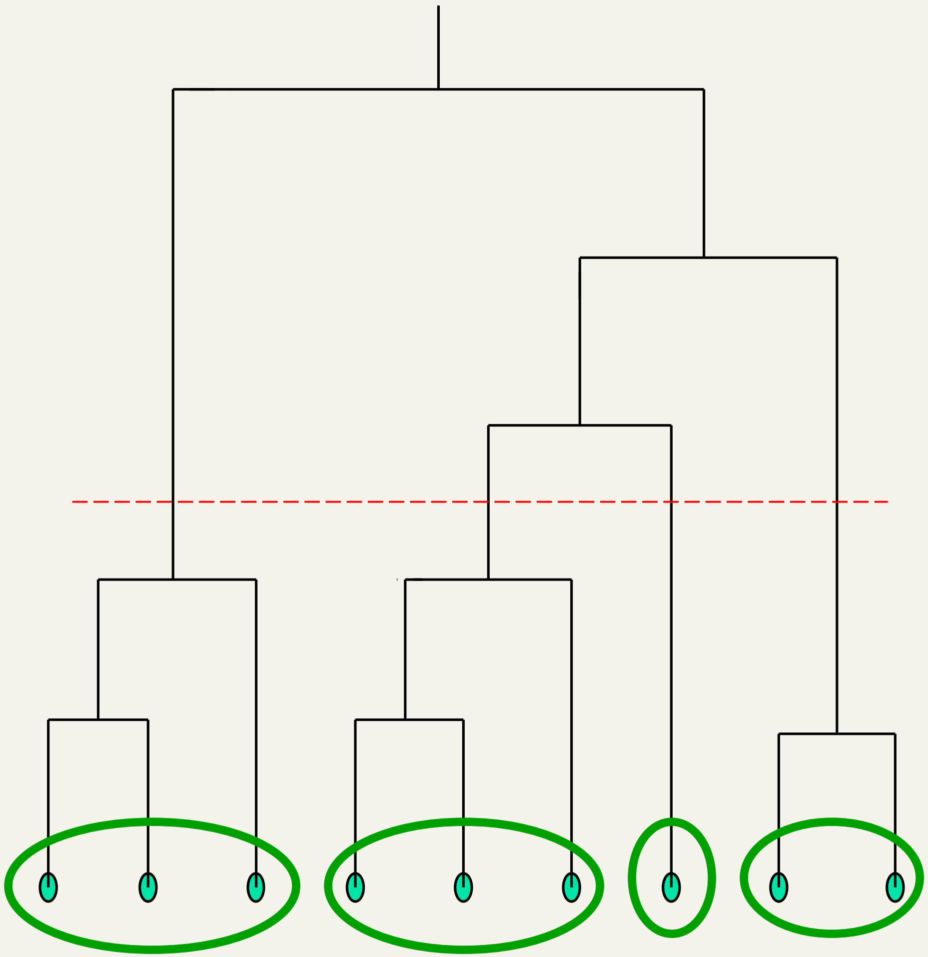
- Build a tree-based hierarchical taxonomy (*dendrogram*) from a set of samples.



- One approach: recursive application of a partitional clustering algorithm.

Dendogram: Hierarchical Clustering

- Clustering obtained by cutting the dendrogram at a desired level: each connected component forms a cluster.



Hierarchical Agglomerative Clustering (HAC)

- Starts with each doc 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.

Closest pair of clusters

- Many variants to defining closest pair of clusters
- **Single-link**
- **Complete-link**
- **Centroid**
- **Average-link**

Single Link Agglomerative Clustering

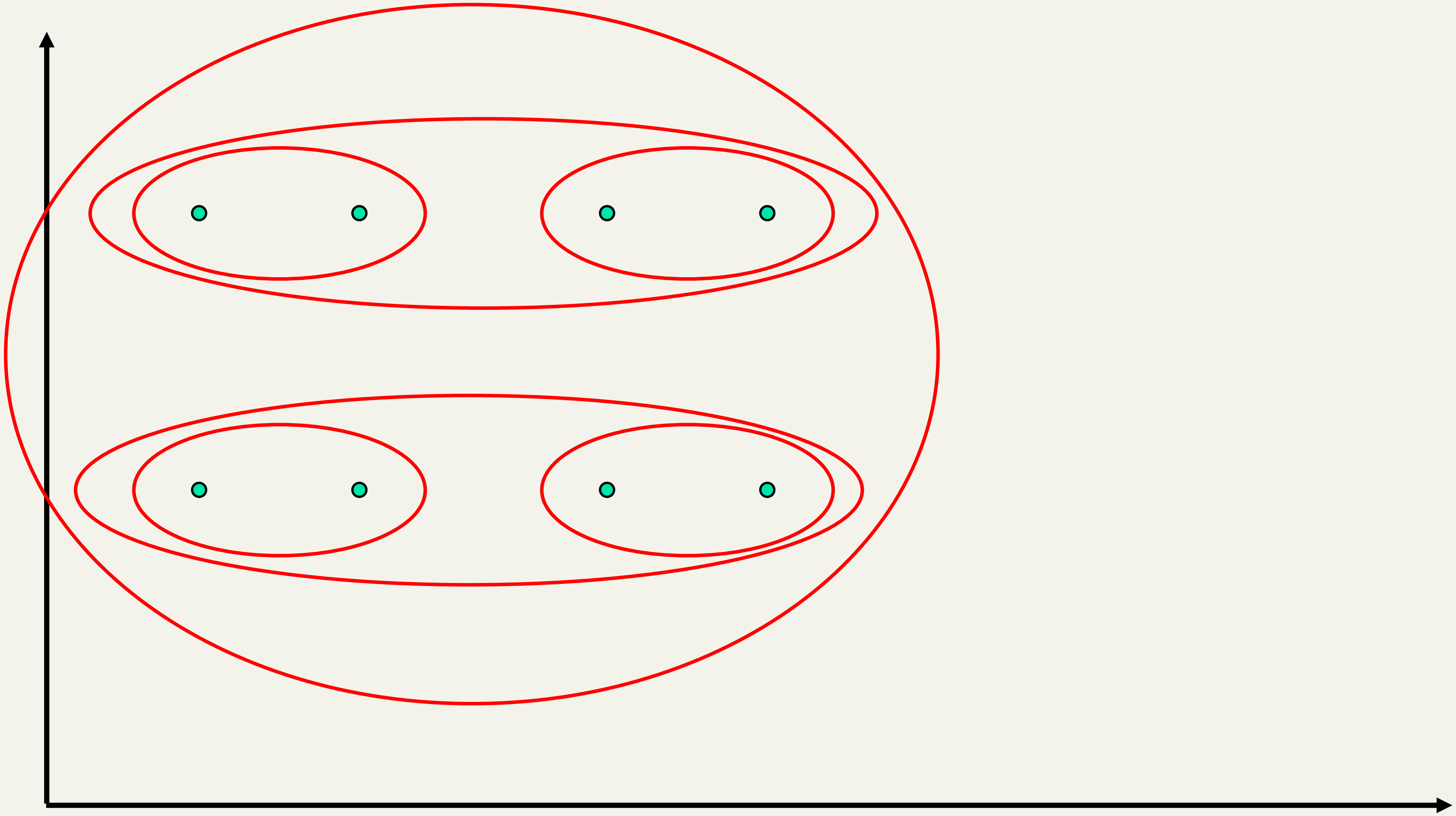
- Use maximum similarity of pairs:

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

- Can result in "straggly" (long and thin) clusters due to chaining effect.
- After merging c_i and c_j, the similarity of the resulting cluster to another cluster, c_k, is:

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

Single Link Example



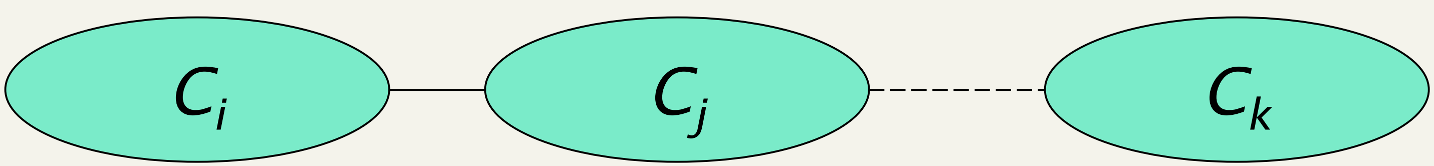
Complete Link Agglomerative Clustering

- Use minimum similarity of pairs:

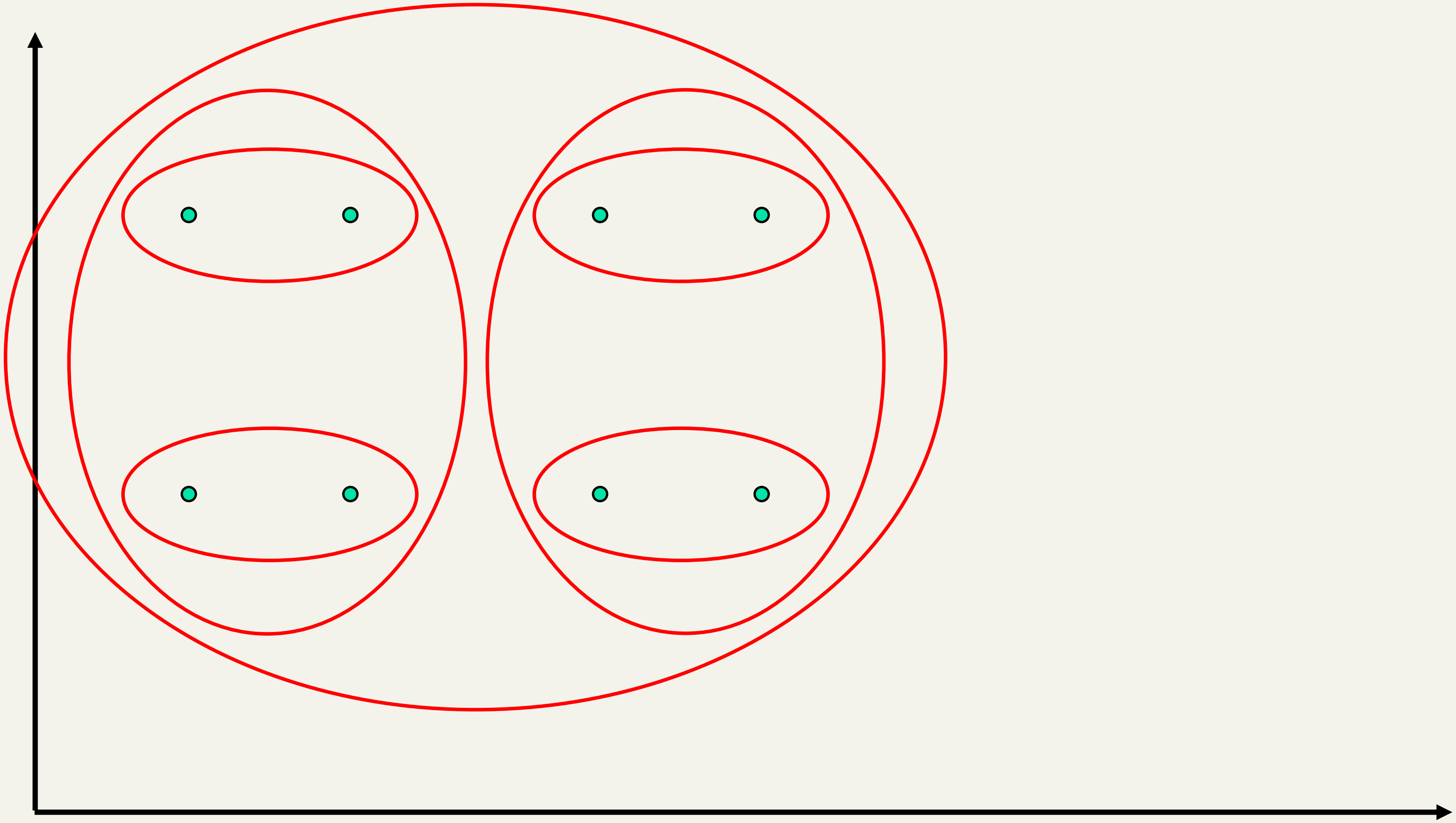
$$sim(c_i, c_j) = \min_{x \in c_i, y \in c_j} sim(x, y)$$

- Makes "tighter," spherical clusters that are typically preferable.
- After merging c_i and c_j, the similarity of the resulting cluster to another cluster, c_k, is:

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



Complete Link Example



Group Average Agglomerative Clustering

- Similarity of two clusters = average similarity of all pairs within merged cluster.

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

- Compromise between single and complete link.
- Two options:
  - Averaged across all ordered pairs in the merged cluster
  - Averaged over all pairs *between* the two original clusters
- No clear difference in efficacy

Computing Group Average Similarity

- 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 Is A Good Clustering?

- Internal criterion: A good clustering will produce high quality clusters in which:
  - the intra-class (that is, intra-cluster) similarity is high
  - the inter-class similarity is low
  - The measured quality of a clustering depends on both the samples representation and the similarity measure used

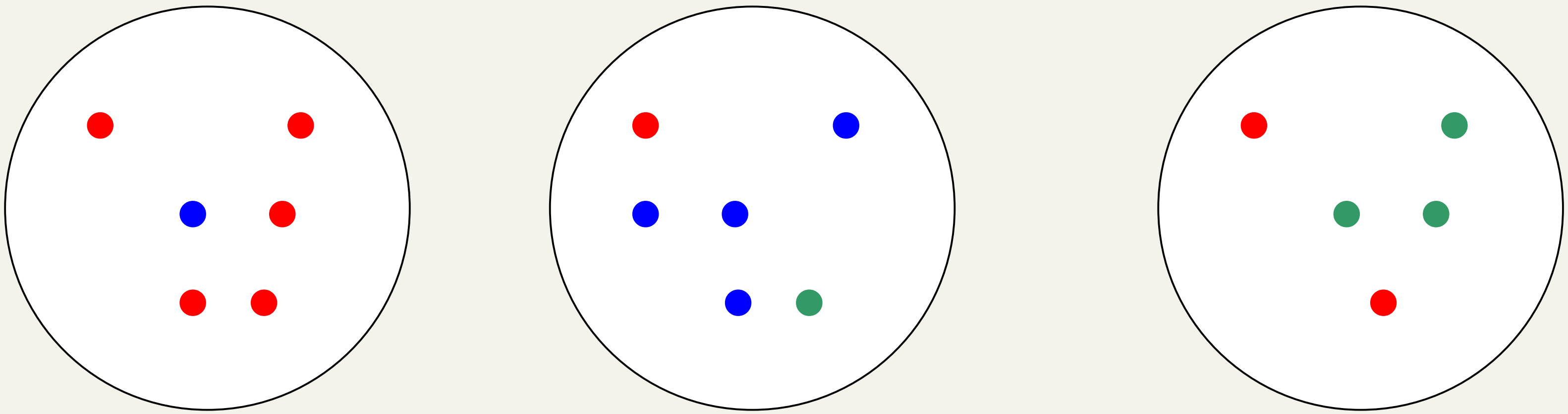
External Evaluation of Cluster Quality

- Simple measure: purity, the ratio between the dominant class in the cluster π_i and the size of cluster ω_i

$$Purity(\omega_i) = \frac{1}{n_i} \max_j (n_{ij}) \quad j \in C$$

- Biased because having *n* clusters maximizes purity
- Others are entropy of classes in clusters (or mutual information between classes and clusters)

Purity example



Cluster I　　　　Cluster II　　　　Cluster III

Cluster I: Purity = 1/6 (max(5, 1, 0)) = 5/6

Cluster II: Purity = 1/6 (max(1, 4, 1)) = 4/6

Cluster III: Purity = 1/5 (max(2, 0, 3)) = 3/5