Cluster Analysis (Part B)

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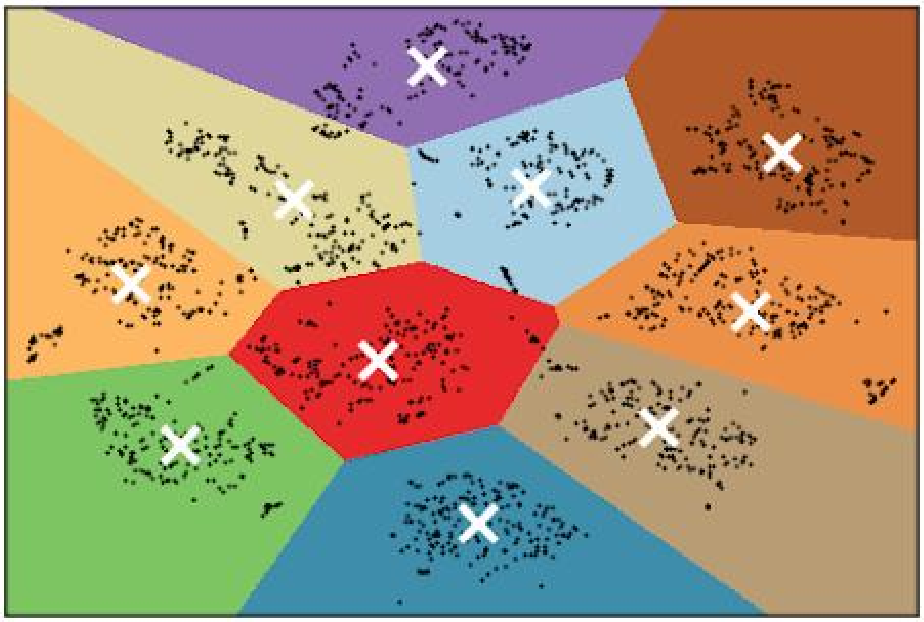
Major Clustering Approaches

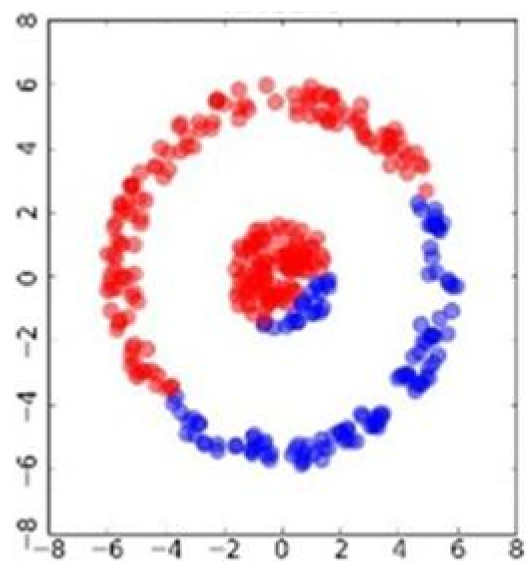
- ✓ Partitioning-based approach
  - Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors.
  - Typical methods: k-means, k-medoids, CLARA, CLARANS
- Density-based approach
  - Based on connectivity and density functions
  - Typical methods: DBSACN, OPTICS, DenClue
- Hierarchical approach
  - Create a hierarchical decomposition of the set of data (or objects) using some criterion
  - Typical methods: Agnes, Diana, BIRCH, CURE, CAMELEON
- Model-based approach
  - A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
  - Typical methods: EM, SOM

Major Clustering Approaches (cont.)

- Grid-based approach
  - Based on a multiple-level granularity structure
  - Typical methods: STING, CLIQUE, WaveCluster
- Frequent Pattern-based approach
  - Based on the analysis of frequent patterns
  - Typical methods: p-Cluster
- Support Vector approach
  - Based on the idea of mapping data points into higher dimensional feature space via a kernel function.
  - Typical methods: SVC, Kernel K-means
- Graph Theoretic approach
  - Typical methods: Spectral Clustering
- …

When K-means clustering fails





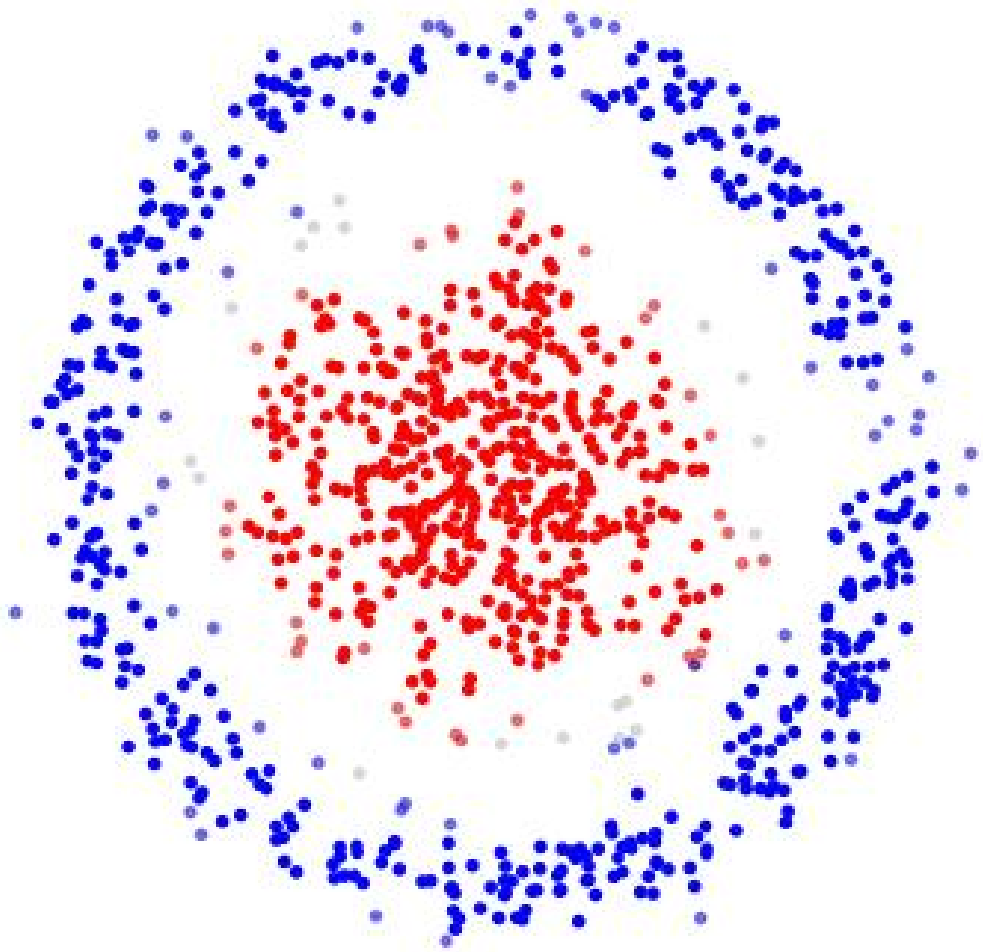
Density-based Approach

- It is based on connectivity and density functions

- Example: DBSCAN

DBSCAN

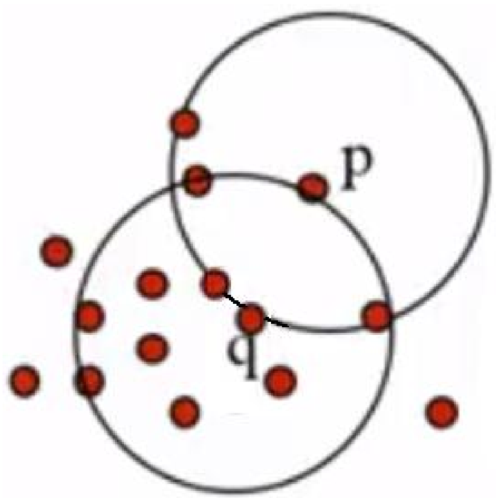
- Density-Based Spatial Clustering of Applications with Noise



Density Definition

- Cluster: maximal set of density-connected points
- Parameters:
  - ϵ: max radius of the neighborhood
  - minPts: min # of points in a ϵ-neighborhood of a point
    - The ϵ-neighborhood of a point q:

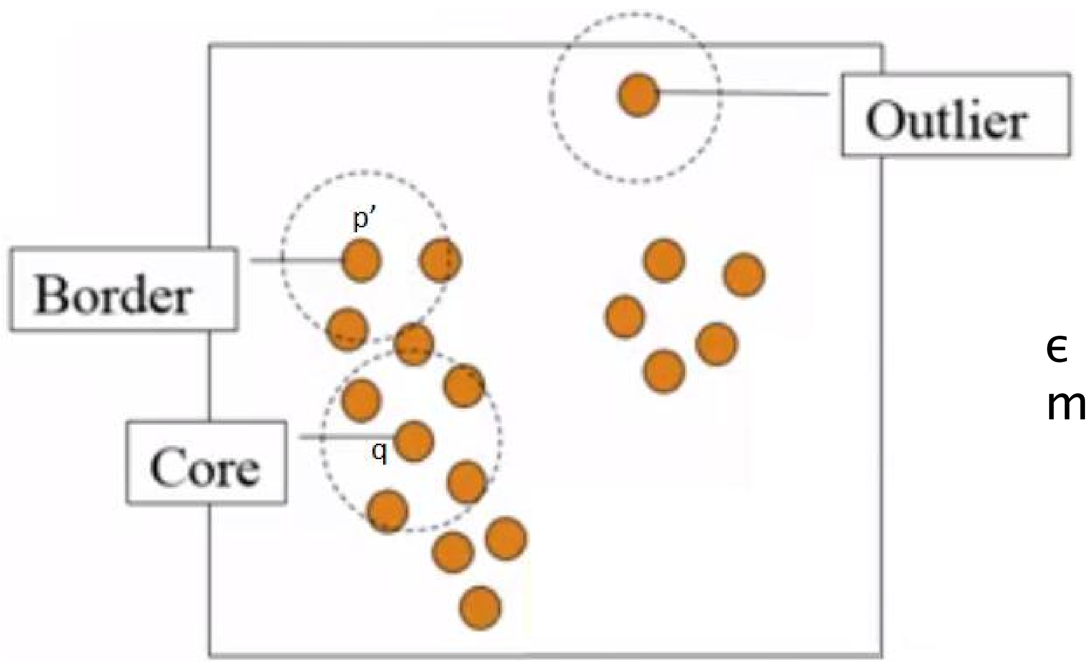
$$N_\epsilon(q) = \{p \text{ in } D \mid d(p,q) \leq \epsilon\}$$



ϵ = 1 unit
minPts = 5

Core, Border, and Outlier

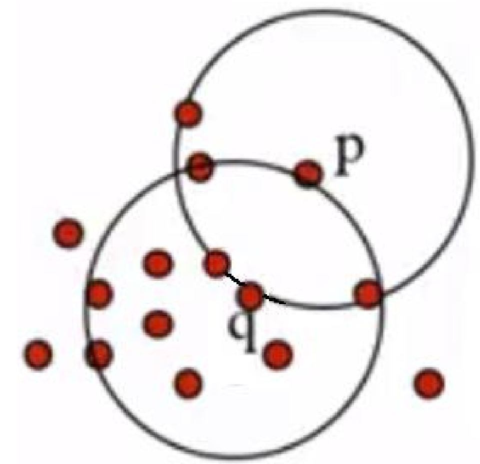
- Core point (q): dense neighborhood
- Border point (p’): in cluster, but neighborhood is not dense (reachable by the cluster)
- Outlier/noise: not in a cluster



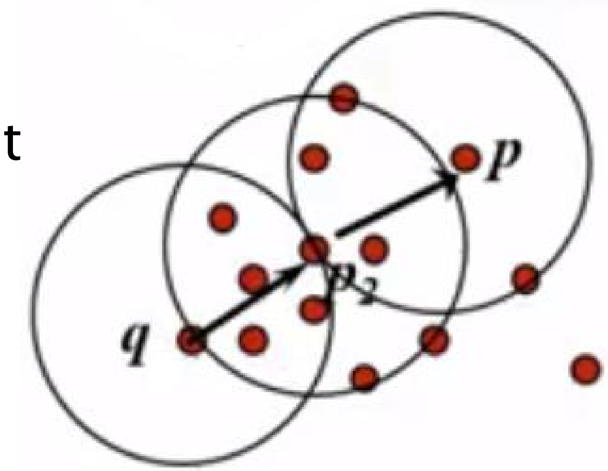
$\epsilon = 1$ unit
minPts = 5

Density Reachability

- Directly density-reachable (ϵ, minPts):
  - A point p is density directly-reachable from a point q if:
    - p in $N_\epsilon(q)$
    - Core point condition: $|N_\epsilon(q)| \geq minPts$



- Density-reachable (ϵ, minPts):
  - A point p is directly-reachable from a point q if there is a chain of points $p_1, \ldots, p_n$, $p_1=q$, $p_n=p$ such that p_{i+1} is directly density-reachable from p_i.



The DBSCAN Algorithm

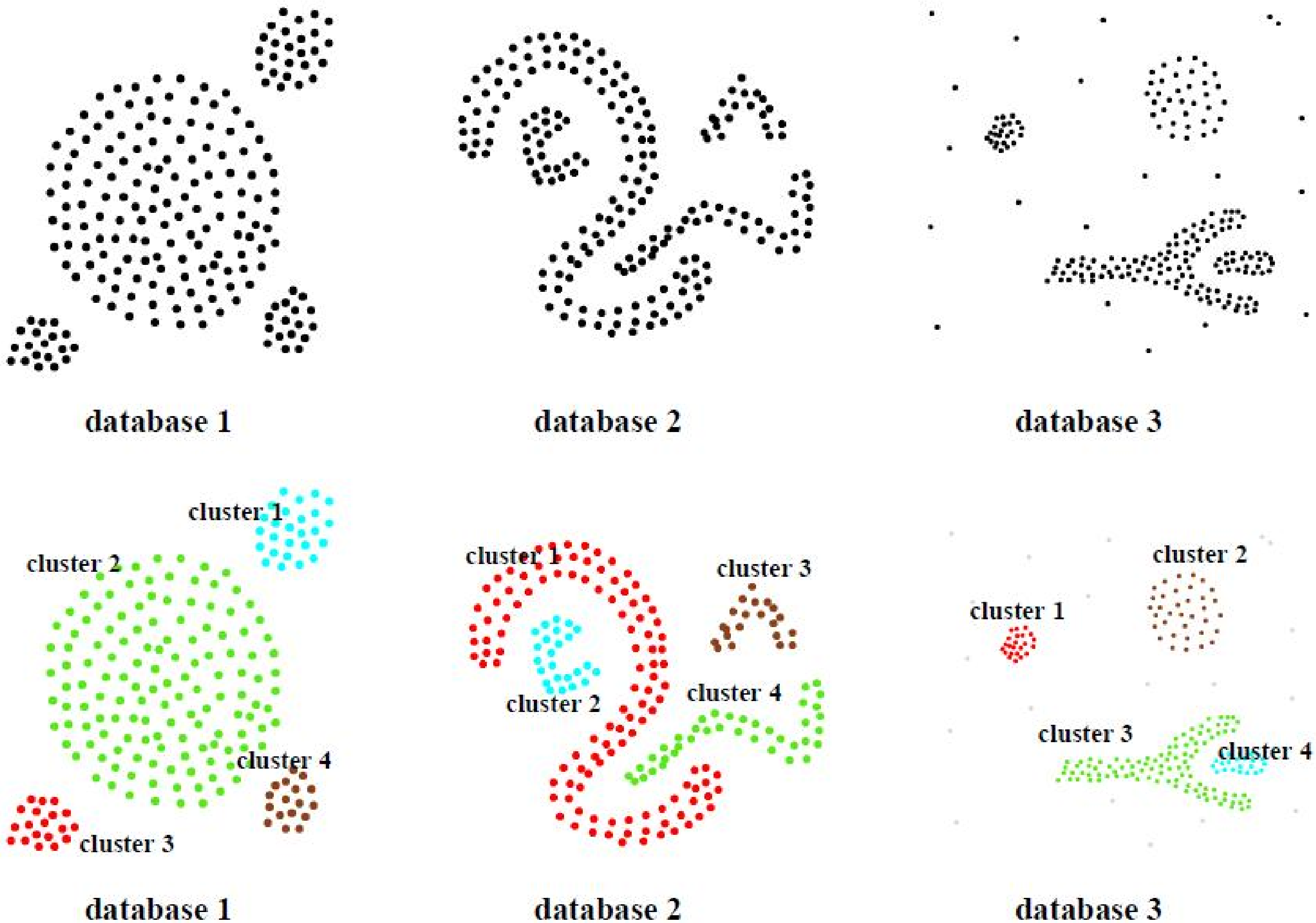
- The DBSCAN algorithm (ϵ, minPts):
  - Start with an arbitrary point p from the database
  - Retrieve all density-reachable points from p
    - If p is a core point, a cluster is formed
    - If p is a border point, no points are density reachable from p. Thus DBSCAN visits the next points of the database
  - Continue the process until all of the points have been processed.

Example – Original Points

database 1 database 2 database 3

M. Ester et al., A density-based algorithm for discovering clusters in large spatial databases with noise, 1996

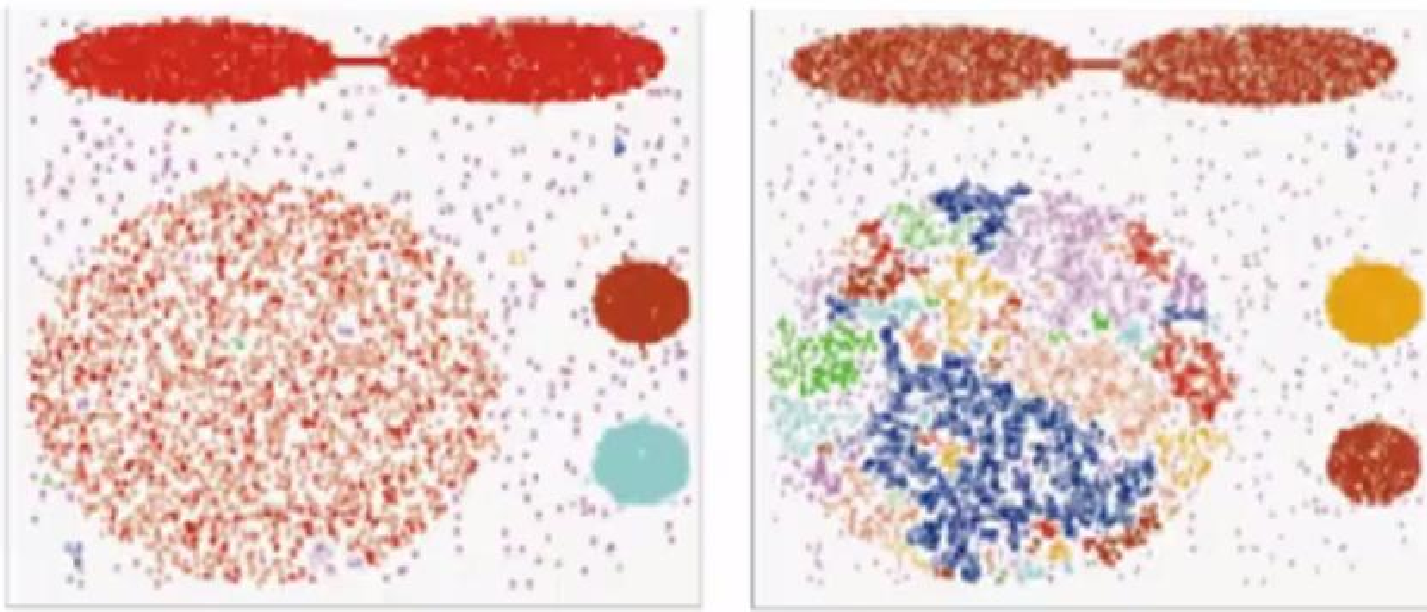
Discovered Clusters



M. Ester et al., A density-based algorithm for discovering clusters in large spatial databases with noise, 1996

Sensitivity to Parameters

- minPts = 4
  - (a) $\epsilon = 0.5$
  - (b) $\epsilon = 0.4$

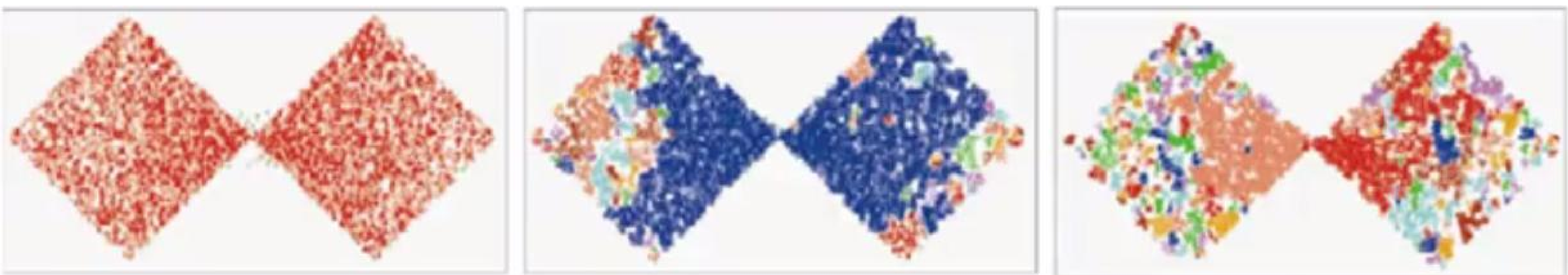


(a) (b)

J. Sander et al., The Algorithm GDBSCAN and Its Applications, 1998

Sensitivity to Parameters

- minPts = 4
  - (a) $\epsilon = 5.0$
  - (b) $\epsilon = 3.5$
  - (c) $\epsilon = 3.0$



(a) (b) (c)

J. Sander et al., The Algorithm GDBSCAN and Its Applications, 1998

Further Reading

- The OPTICS Clustering Algorithm
  - M. Ankerst, MM. Breunig, H-P. Kriegel, J. Sander, OPTICS: Ordering Points To Identify the Clustering Structure, ACM SIGMOD international conference on Management of data, pp. 49-60, 1999.

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- M. Ester, H-P. Kriegel , J. Sander, X. Xu. "A density-based algorithm for discovering clusters in large spatial databases with noise", 1996.

  [Highest impact paper award, 2014]

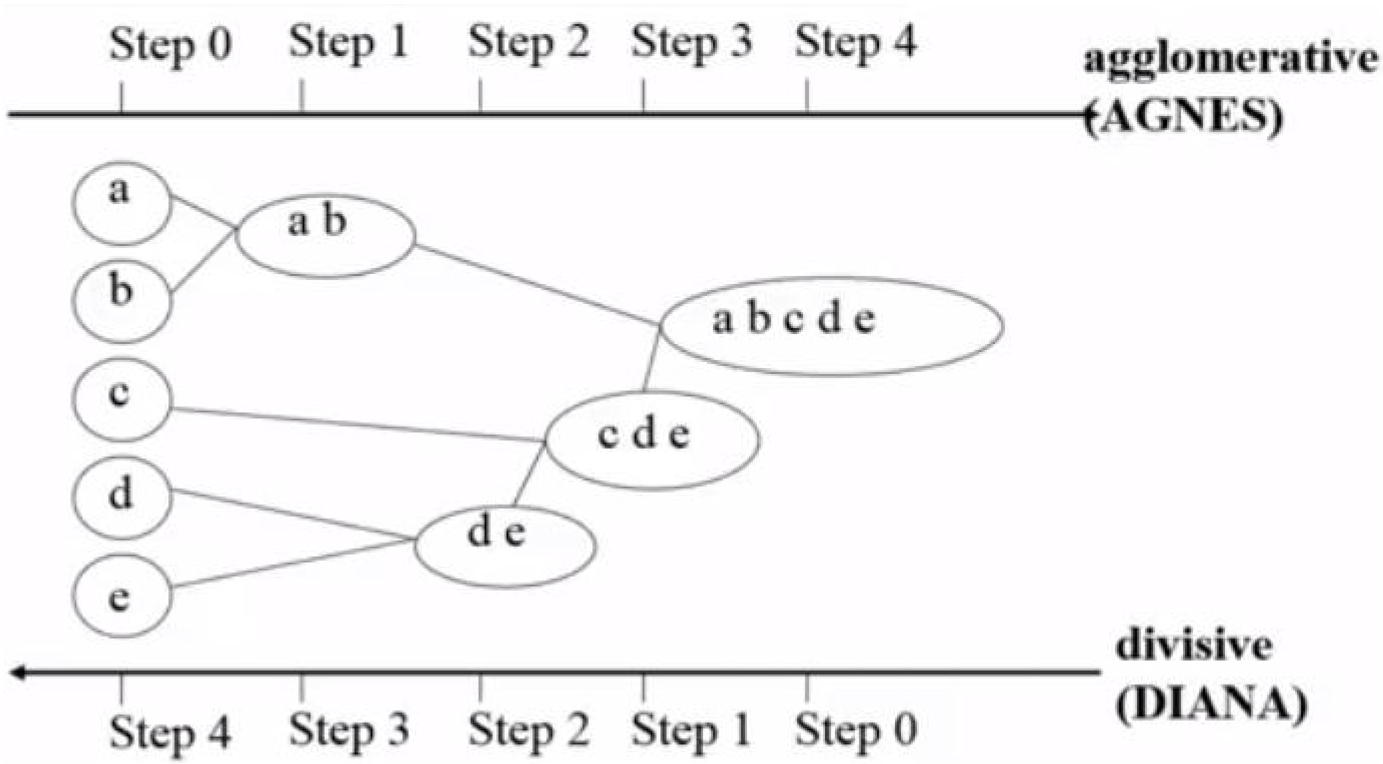
- J. Sander, M. Ester, H-P. Kriegel, X. Xu. Density-Based Clustering in Spatial Databases: The Algorithm GDBSCAN and Its Applications, 1998.

Hierarchical Approach

- Create a hierarchical decomposition of the set of data (or objects) using some criterion

- Two categories:
  - Agglomerative (bottom-up)
  - Divisive (top-down)

Dendrogram



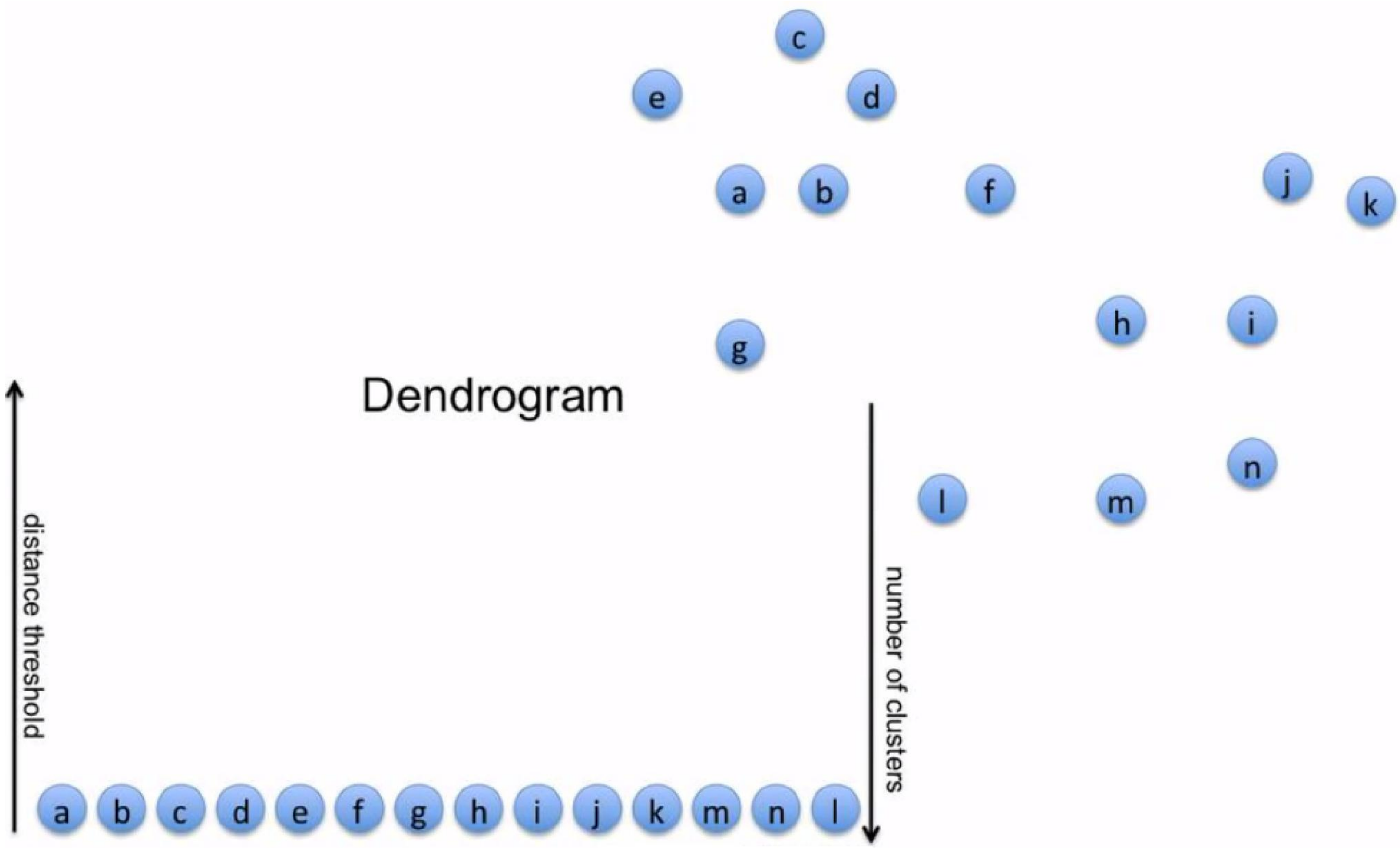
AGNES (Agglomerative Nesting)
DIANA (Divisive Analysis)

Agglomerative Clustering

- The algorithm:
  - Start with a collection C on n singleton clusters
    - Each cluster contains one data point: $c_i = \{\boldsymbol{x_i}\}$
  - Repeat
    - Find a pair of clusters that are closest: min $D(c_i, c_j)$
    - Merge the clusters c_i and c_j into a new cluster c_{i+j}
    - Remove c_i and c_j from the collection C, then add c_{i+j}
  - Until only one cluster left

Example

- Cluster distance measure: single link



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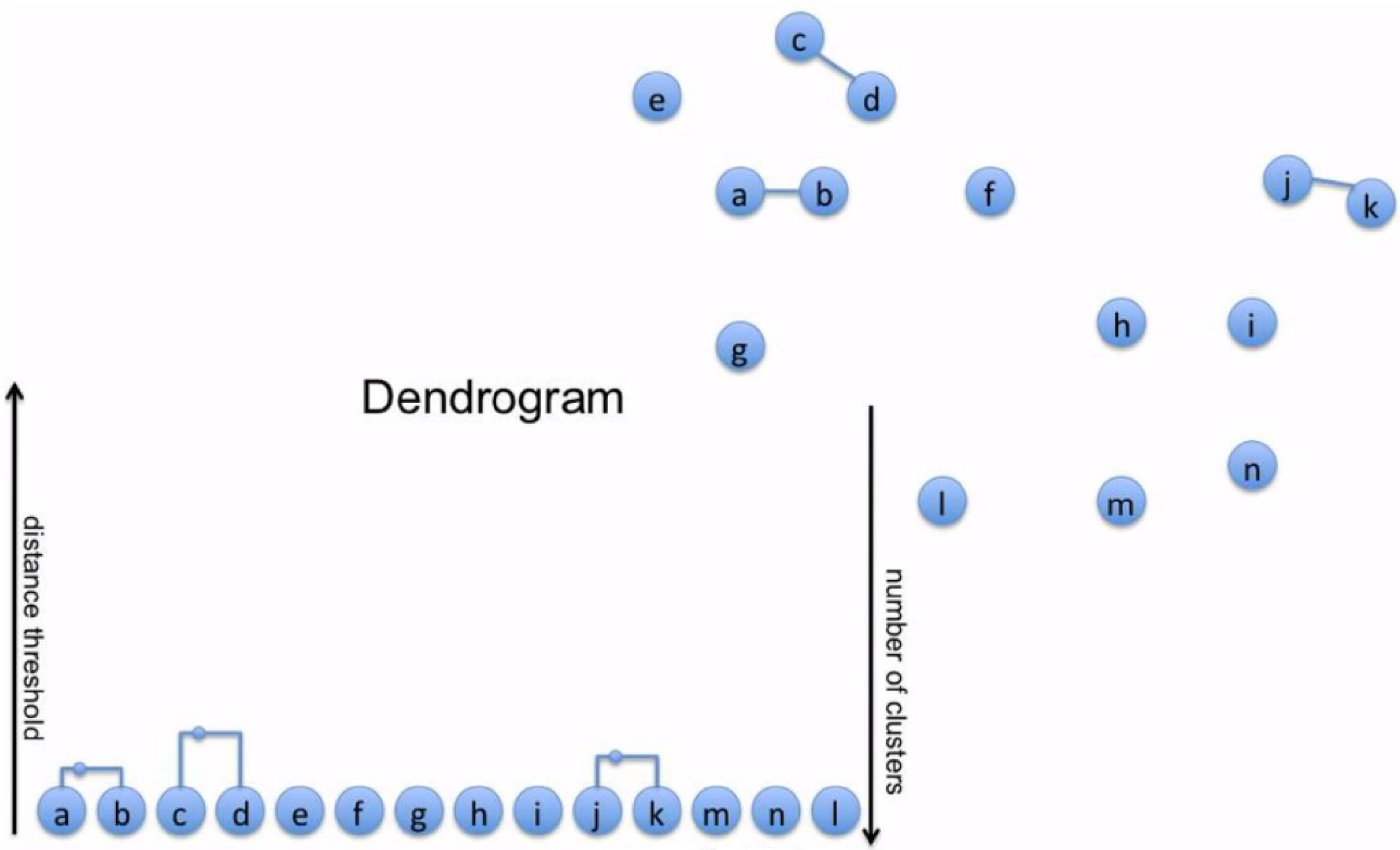
Example (cont.)



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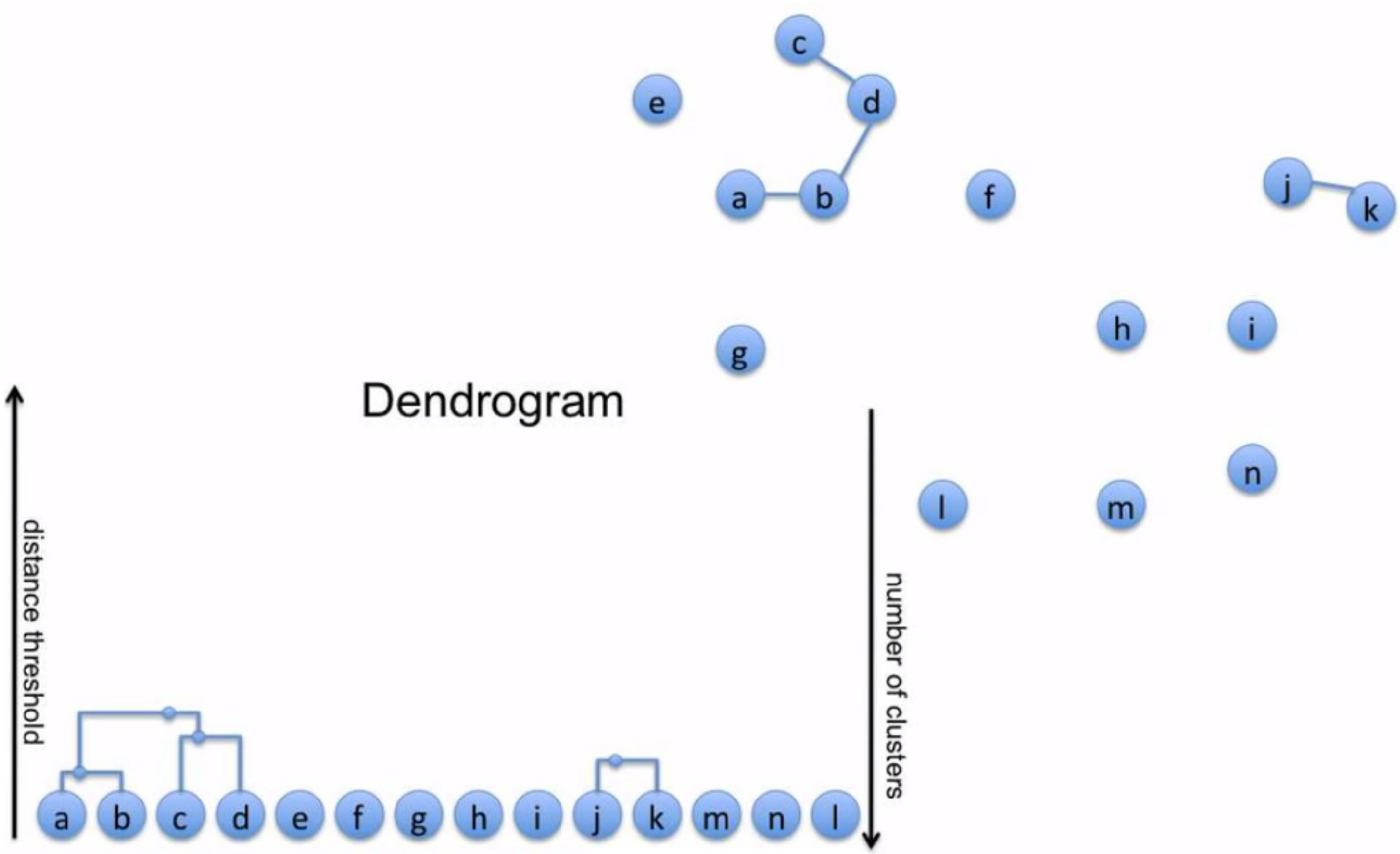
Example (cont.)



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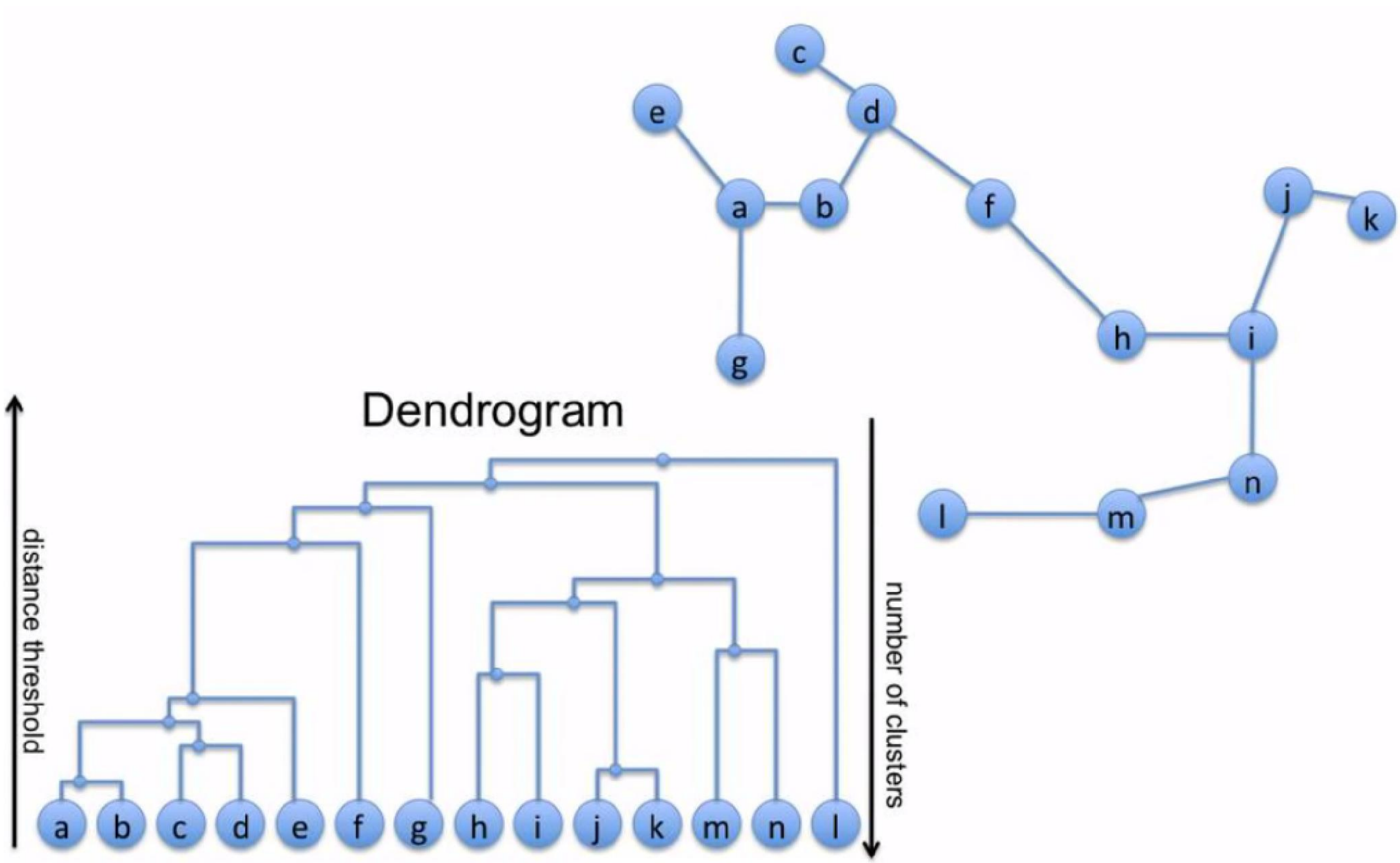
Example (cont.)



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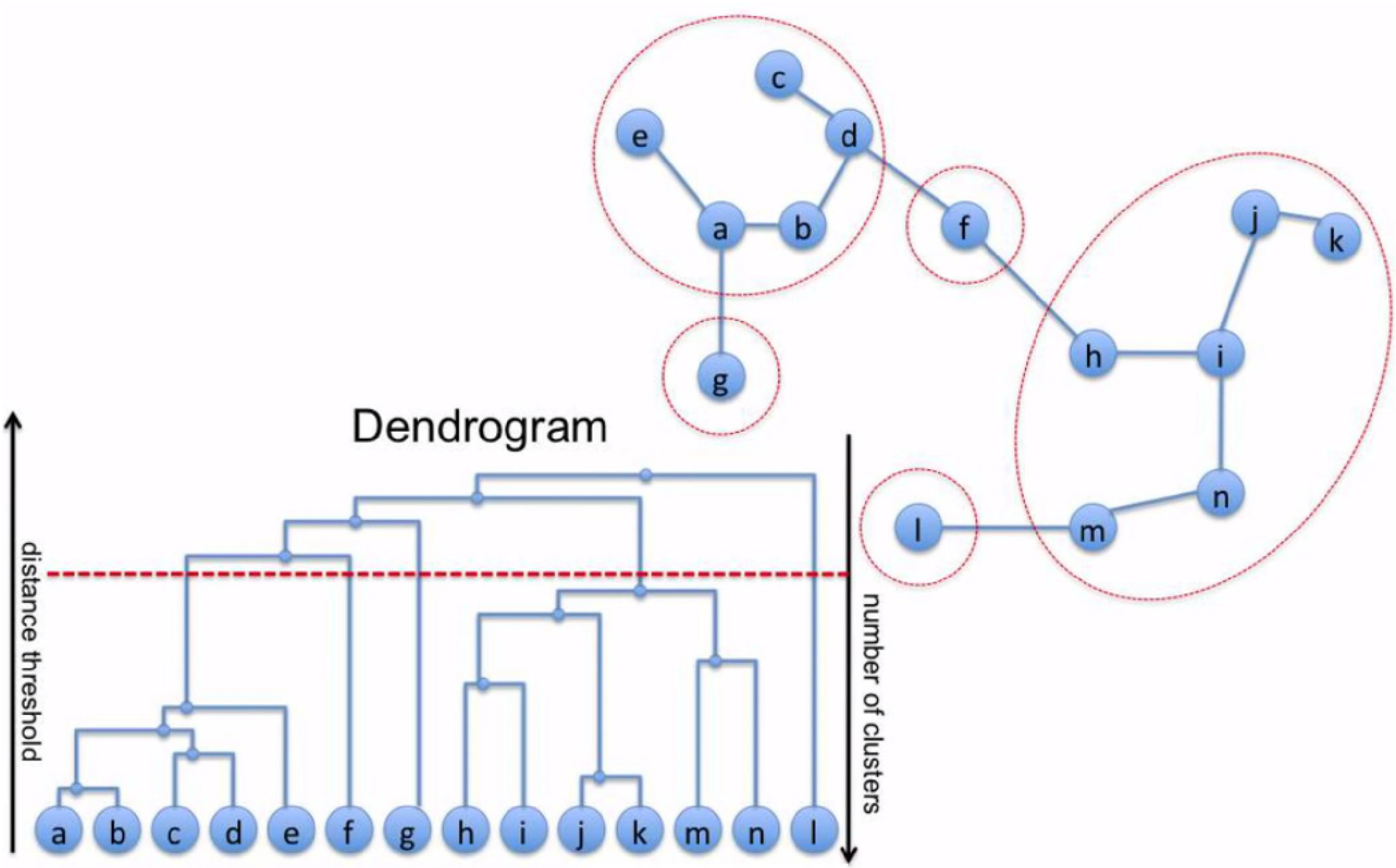
Example (cont.)



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Cluster Distance Measure

- Single link: $D(C_1, C_2) = \min(\boldsymbol{x_1}, \boldsymbol{x_2})$
  - Distance between the closest elements in clusters
- Complete link: $D(C_1, C_2) = \mathrm{m}ax(\boldsymbol{x_1}, \boldsymbol{x_2})$
  - Distance between the farthest elements in clusters
- Average link: average all pairwise distances
  - Less affected by outliers
- Centroids: distance between centroids (mean) of clusters
- Ward's method: sum of deviations from the centroid
  - The smaller, the better for merging.

Further Reading

- The Birch Clustering Algorithm
  - T. Zhang, R. Ramakrishnan, M. Livny, BIRCH: an efficient data clustering method for very large databases, Proceedings of the ACM SIGMOD international conference on Management of data, SIGMOD, pp 103-114, 1996.

- The CHAMELEON Clustering Algorithm
  - G. Karypis, E-H. Han, V. Kumar, CHAMELEON: A Hierarchical Clustering Algorithm Using Dynamic Modeling, IEEE Computer 32(8): 68-75, 1999.

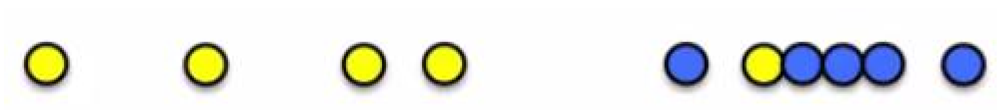
Model-based Approach

- A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other

- Example: EM Clustering
  - EM: Expectation-Maximization

Mixture Models in 1-D

- Case 1
  - Assume the data points come from two Gaussians with unknown parameters
  - We know each point comes from which Gaussian



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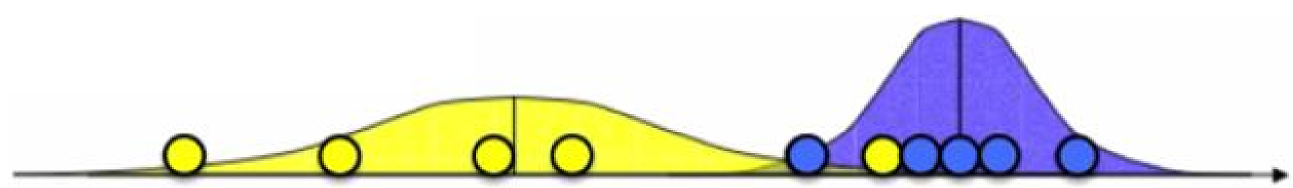
Mixture Models in 1-D

- Case 1
  - Assume the data points come from two Gaussians with unknown parameters
  - We know each point comes from which Gaussian

$$\mu_b = \frac{x_1 + x_2 + \ldots + x_{n_b}}{n_b}$$

$$\sigma_b^2 = \frac{(x_1 - \mu_b)^2 + \ldots + (x_n - \mu_b)^2}{n_b}$$



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Mixture Models of 1-D

- Case 2
  - We <u>don't know the sources</u>
  - We know the parameters of the Gaussians

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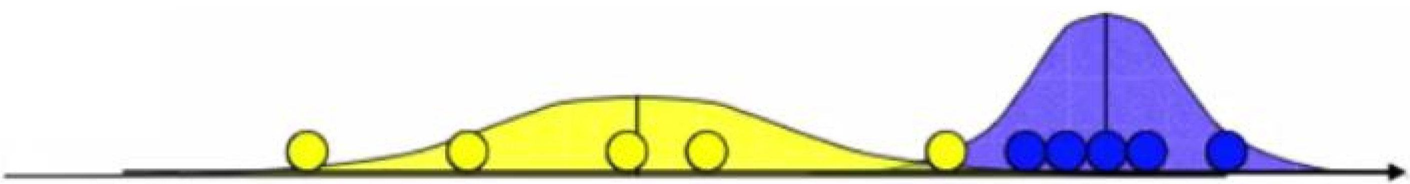
Mixture Models of 1-D

- Case 2
  - We don't know the sources
  - We know the parameters of the Gaussians

$$P(b \mid x_i) = \frac{P(x_i \mid b)P(b)}{P(x_i \mid b)P(b) + P(x_i \mid a)P(a)}$$

$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left\{-\frac{(x_i - \mu_i)^2}{2\sigma_b^2}\right\}$$



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Expectation-Maximization

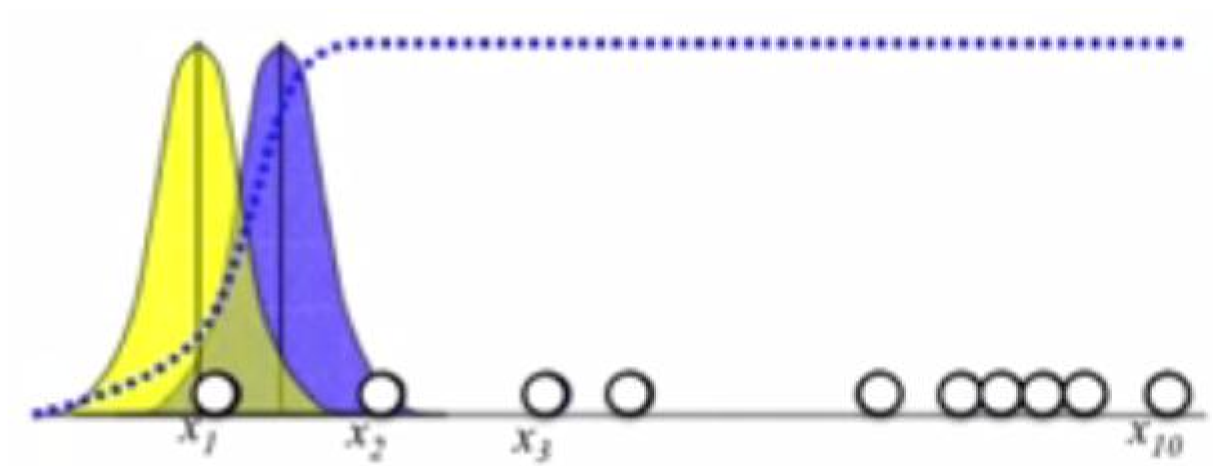
- Chicken and egg problem!
  - We need parameters to guess source of points
  - We need to know source to estimate parameters
- EM algorithm
  - Start with two randomly placed Gaussians
  - REPEAT
    - Use the Gaussians to determine which point comes from which Gaussian (Case 2)
    - Adjust parameters to fit points assigned to them (Case 1)
  - UNTIL Convergence

Expectation-Maximization (cont.)

- Chicken and egg problem!
  - We need parameters to guess source of points
  - We need to know source to estimate parameters
- EM algorithm
  - Start with two randomly placed Gaussians
  - REPEAT
    - Use the Gaussians to determine which point comes from which Gaussian (E-step)
    - Adjust parameters to fit points assigned to them (M-step)
  - UNTIL Convergence

EM Visualization

- Initialization



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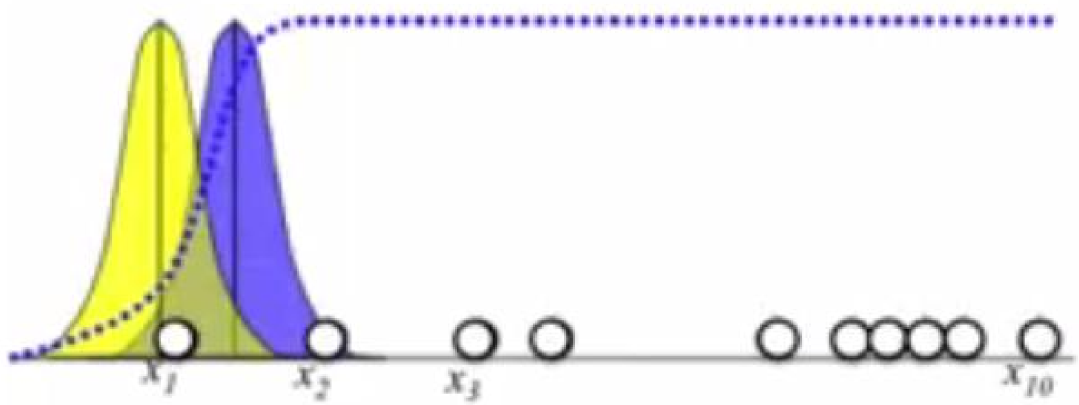
EM Visualization (cont.)

- Initialization

$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left\{-\frac{(x_i - \mu_b)^2}{2\sigma_b^2}\right\}$$

$$b_i = P(b \mid x_i) = \frac{P(x_i \mid b)P(b)}{P(x_i \mid b)P(b) + P(x_i \mid a)P(a)}$$

$$a_i = P(a \mid x_i) = 1 - b_i$$



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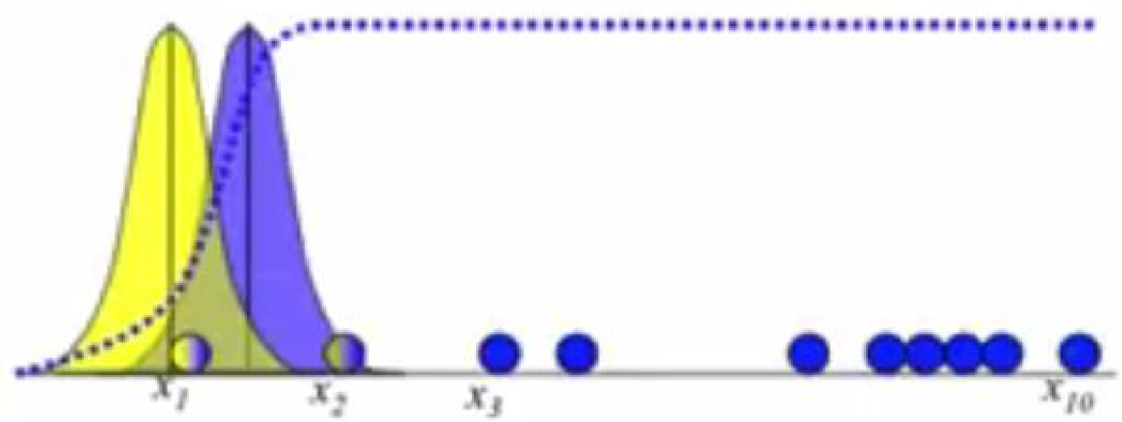
EM Visualization (E-Step)

$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left\{ -\frac{(x_i - \mu_b)^2}{2\sigma_b^2} \right\}$$

$$b_i = P(b \mid x_i) = \frac{P(x_i \mid b)P(b)}{P(x_i \mid b)P(b) + P(x_i \mid a)P(a)}$$

$$a_i = P(a \mid x_i) = 1 - b_i$$



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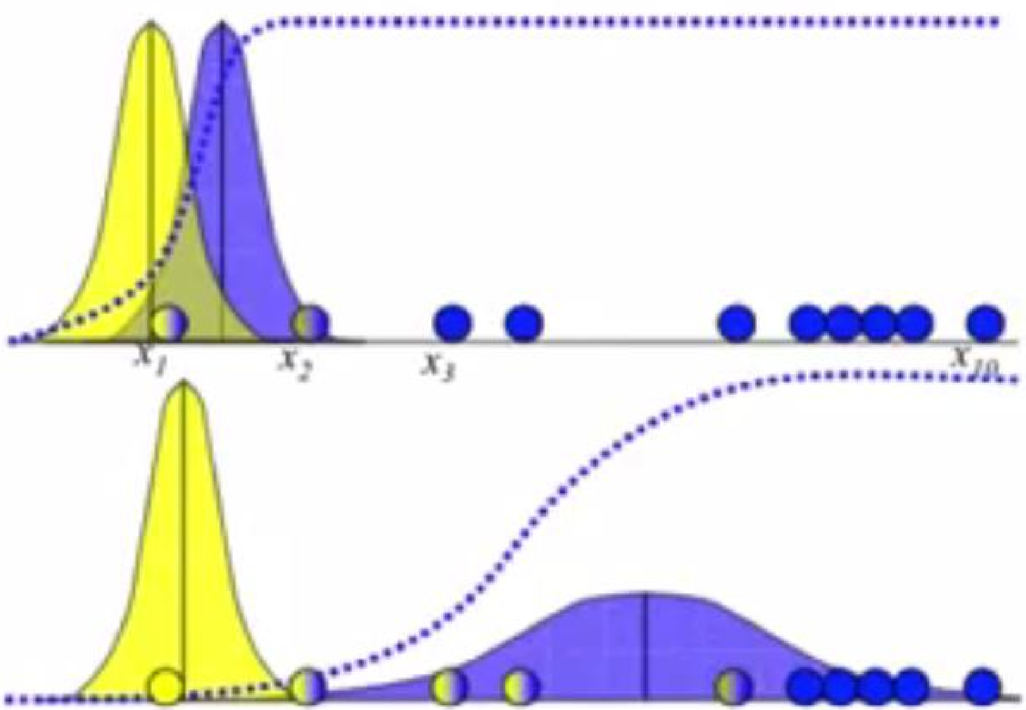
EM Visualization (M-Step)



$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left\{-\frac{(x_i - \mu_b)^2}{2\sigma_b^2}\right\}$$

$$b_i = P(b \mid x_i) = \frac{P(x_i \mid b)P(b)}{P(x_i \mid b)P(b) + P(x_i \mid a)P(a)}$$

$$a_i = P(a \mid x_i) = 1 - b_i$$

$$\mu_b = \frac{b_1 x_1 + b_2 x_2 + \ldots + b_n x_n}{b_1 + b_2 + \ldots + b_n}$$

$$\sigma_b^2 = \frac{b_1(x_1 - \mu_b)^2 + \ldots + b_n(x_n - \mu_b)^2}{b_1 + b_2 + \ldots + b_n}$$

$$\mu_a = \frac{a_1 x_1 + a_2 x_2 + \ldots + a_n x_n}{a_1 + a_2 + \ldots + a_n}$$

$$\sigma_a^2 = \frac{a_1(x_1 - \mu_a)^2 + \ldots + a_n(x_n - \mu_a)^2}{a_1 + a_2 + \ldots + a_n}$$

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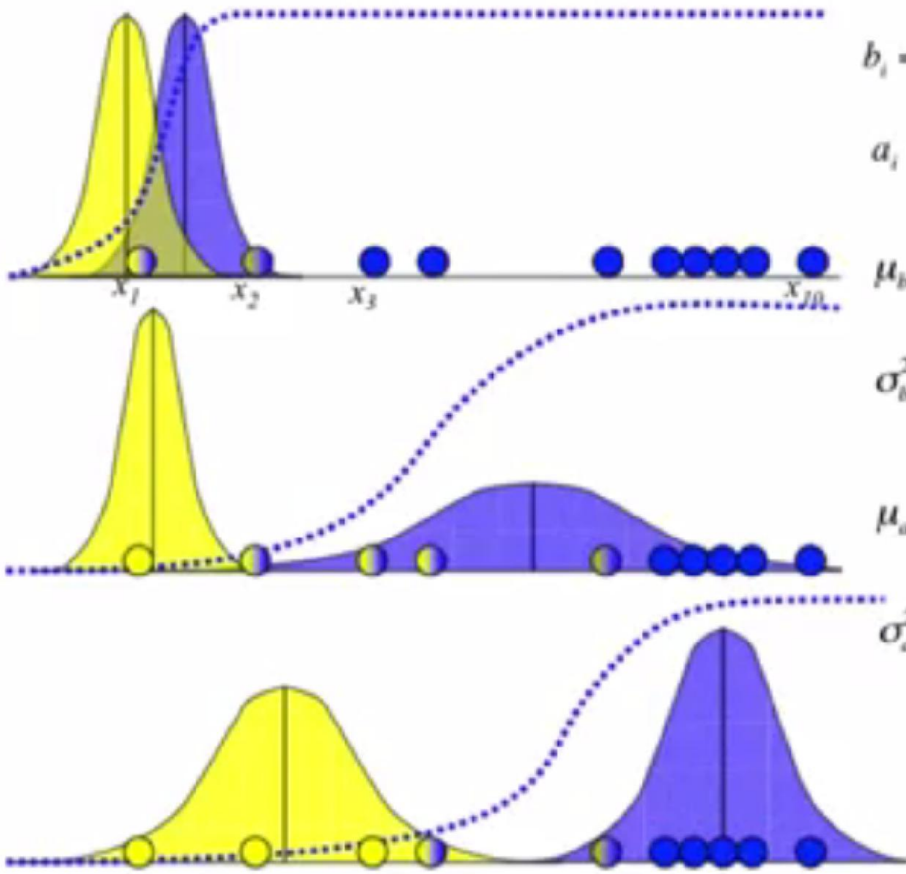
EM Visualization (E-Step)



$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left\{-\frac{(x_i - \mu_b)^2}{2\sigma_b^2}\right\}$$

$$b_i = P(b \mid x_i) = \frac{P(x_i \mid b)P(b)}{P(x_i \mid b)P(b) + P(x_i \mid a)P(a)}$$

$$a_i = P(a \mid x_i) = 1 - b_i$$

$$\mu_b = \frac{b_1 x_1 + b_2 x_2 + \ldots + b_n x_n}{b_1 + b_2 + \ldots + b_n}$$

$$\sigma_b^2 = \frac{b_1(x_1 - \mu_b)^2 + \ldots + b_n(x_n - \mu_b)^2}{b_1 + b_2 + \ldots + b_n}$$

$$\mu_a = \frac{a_1 x_1 + a_2 x_2 + \ldots + a_n x_n}{a_1 + a_2 + \ldots + a_n}$$

$$\sigma_a^2 = \frac{a_1(x_1 - \mu_a)^2 + \ldots + a_n(x_n - \mu_a)^2}{a_1 + a_2 + \ldots + a_n}$$

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EM Clustering

- Soft computing clustering
  - Clusters overlap
- K-means clustering is a special case of (hard) EM.
- Sensitive to the initialization
- How to pick K?

Further Reading

- The SOM and Spectral Clustering Algorithms
- Grid-based Clustering
- Subspace Clustering
- Collaborative Clustering
- …

Measuring Clustering Quality

- Two methods: extrinsic vs. intrinsic

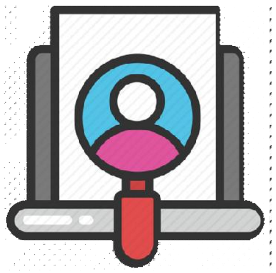
- Extrinsic: supervised, i.e., the ground truth is available
  - Compare clustering results against the ground truth labels

- Intrinsic: unsupervised, i.e., the ground truth is unavailable
  - Evaluate the goodness of a clustering by considering how well the clusters are separated
    - e.g. Entropy (purity)

Measuring Clustering Quality (cont.)

- Clustering quality measure: $Q(C, C_g)$, for a clustering C given the ground truth C_g.
- Q is good if it satisfies the following 4 essential criteria
  - Cluster homogeneity: the purer, the better
  - Cluster completeness: should assign objects belong to the same category in the ground truth to the same cluster
  - Rag bag: putting a heterogeneous object into a pure cluster should be penalized more than putting it into a rag bag (i.e., miscellaneous or the "other" category)
  - Small cluster preservation: splitting a small category into pieces is more harmful than splitting a large category into pieces

Measuring Clustering Quality (cont.)

- Clustering quality:
  - User inspection → 
  - Sum of squared error → $SSE = \sum_{j=1}^{k} \sum_{x \in C_j} \left\| \boldsymbol{x} - \boldsymbol{\mu}_j \right\|^2$
  - Entropy → $E_{total}(\Omega) = \sum_{w \in \Omega} \frac{m_w}{m} \times E(w)$
  - Silhouette Index → …
  - …

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Measuring Clustering Quality (cont.)

- Total clustering entropy

$$E_{total}(\Omega) = \sum_{w \in \Omega} \frac{m_w}{m} \times E(w),$$

where $\Omega = \{w_1, w_2, \dots, w_k\}$,
m_w is the number of points in cluster w,
m is the total number of points

- Entropy of a single cluster w

$$E(w) = -\sum_{c \in C} \frac{|w_c|}{m_w} \times \log_2 \frac{|w_c|}{m_w},$$

where c is a class in the set C of all classes,
$|w_c|$ is the number of points classified as c in cluster w

References

- Jiawei Han, Micheline Kamber and Jian Pei, Data Mining: Concepts and Techniques, 3rd edition, 2006.
- M. Ankerst, MM. Breunig, H-P. Kriegel, J. Sander, OPTICS: Ordering Points To Identify the Clustering Structure, ACM SIGMOD international conference on Management of data, pp. 49-60, 1999.
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