Data Mining:

Concepts and Techniques

(3rd ed.)

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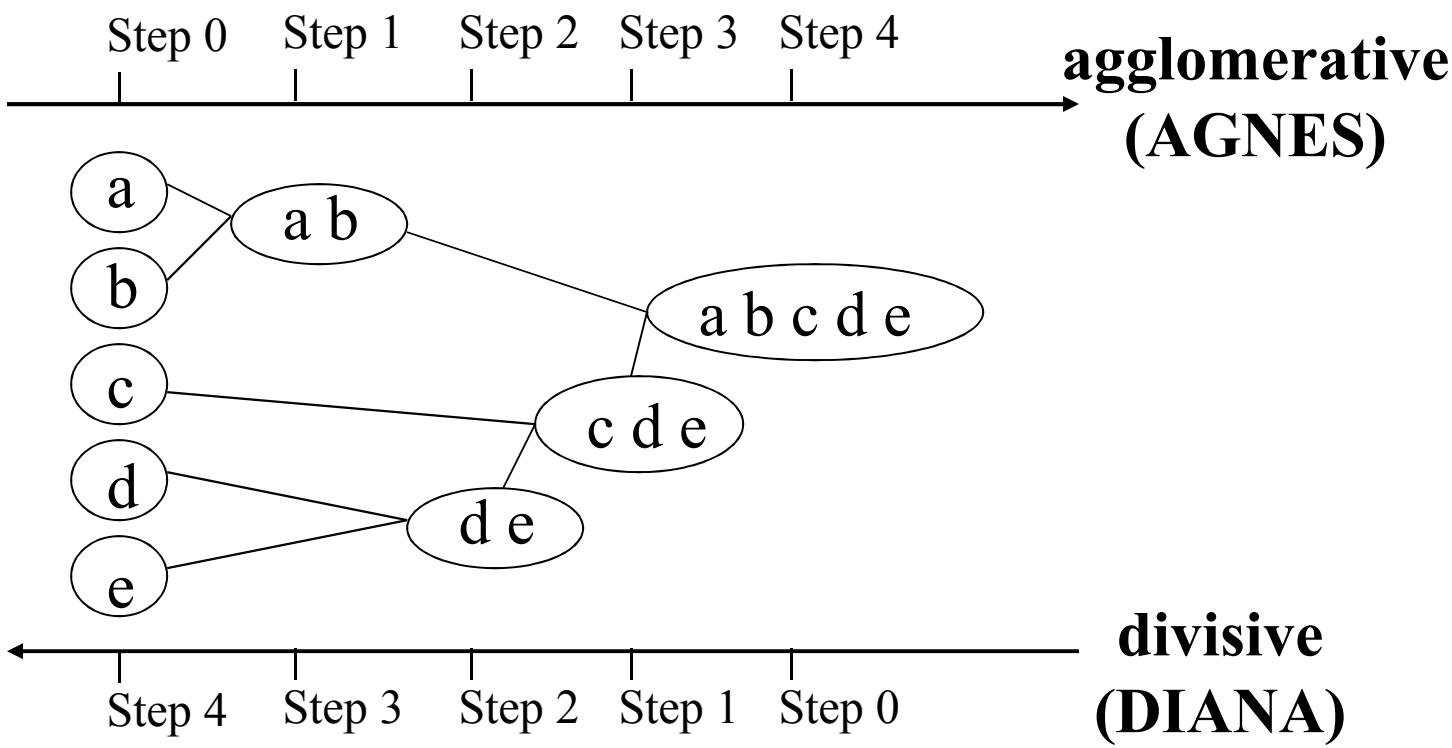
Cluster Analysis: Basic Concepts and Methods

- ✓ Cluster Analysis: Basic Concepts
- ✓ Partitioning Methods
- ✓ Density-Based Methods
- Hierarchical Methods
  - Clustering Categorical Data
- Evaluation of Clustering
- Summary

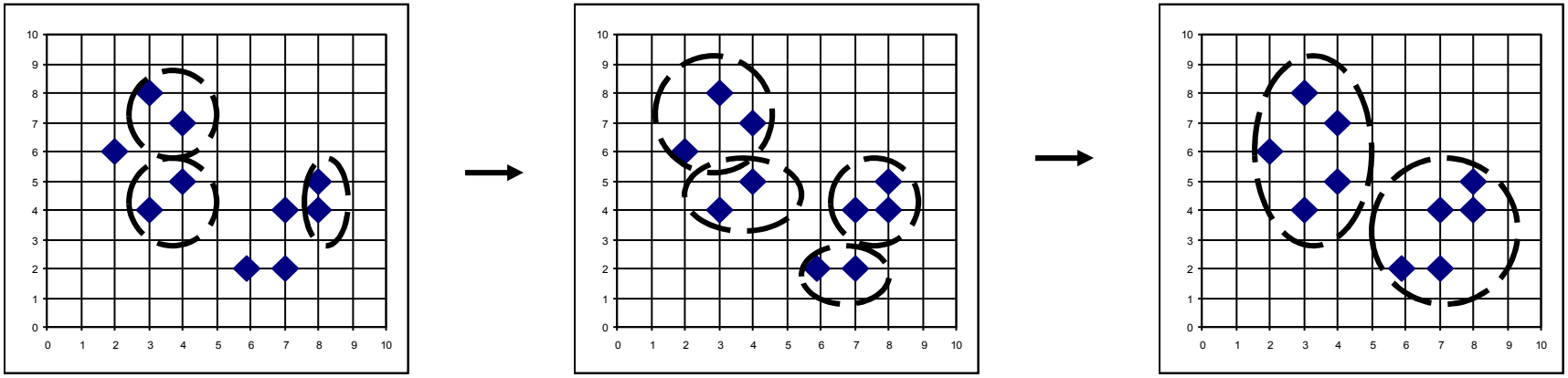
Hierarchical Clustering

- Use distance matrix as clustering criteria. This method does not require the number of clusters ***k*** as an input, but needs a termination condition



AGNES (Agglomerative Nesting)

- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical packages, e.g., Splus
- Use the **single-link** method and the dissimilarity matrix
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster

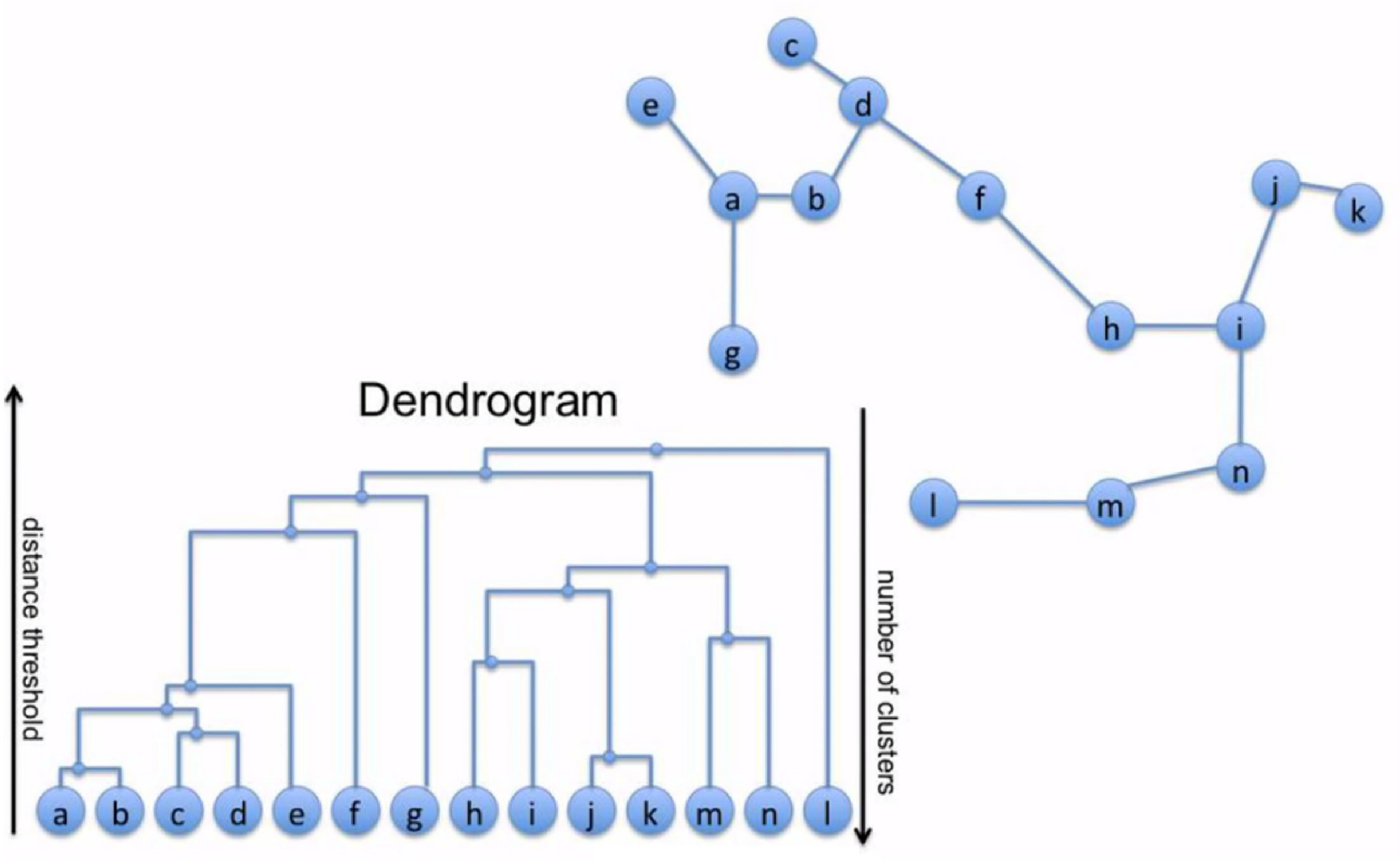


Dendrogram: Shows How Clusters are Merged

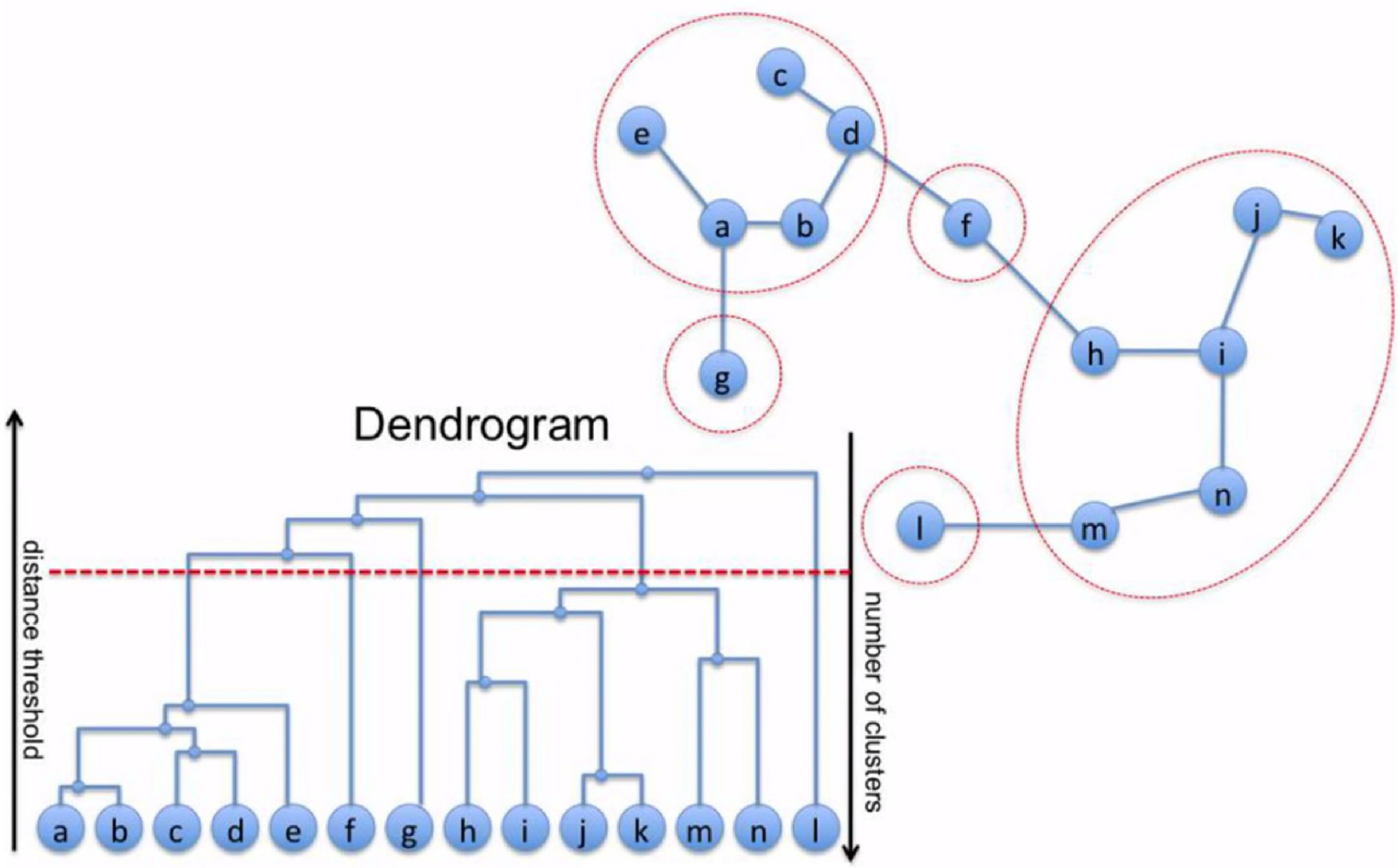
Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram

A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster

Dendrogram: Shows How Clusters are Merged

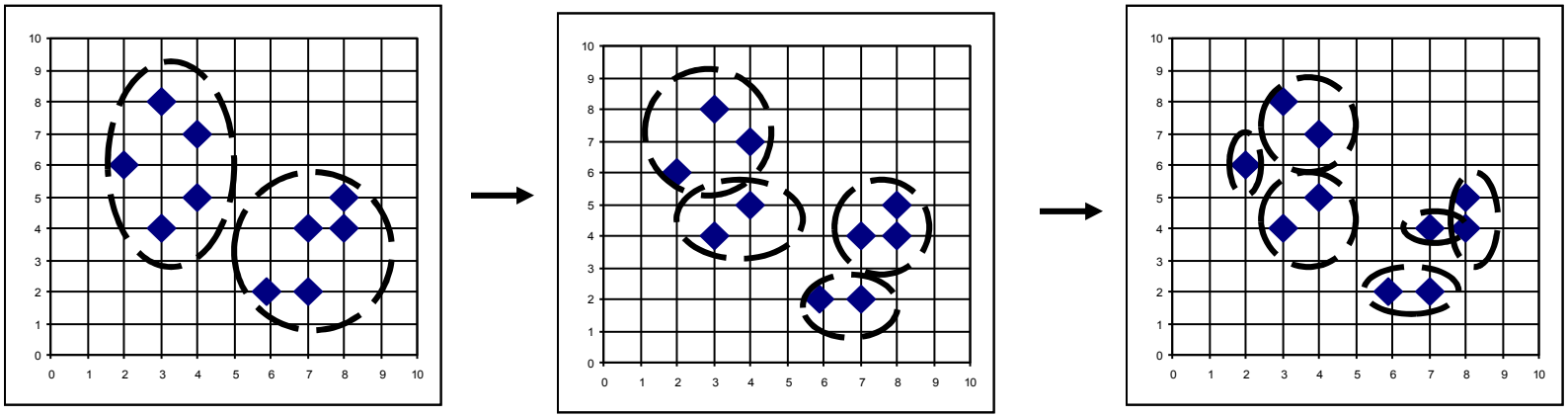


Dendrogram: Shows How Clusters are Merged

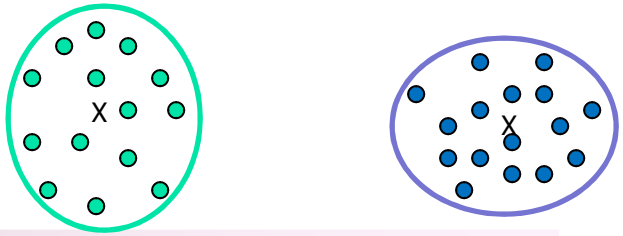


DIANA (Divisive Analysis)

- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical analysis packages, e.g., Splus
- Inverse order of AGNES
- Eventually each node forms a cluster on its own



Distance between Clusters



- Single link: smallest distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = min(t_{ip}, t_{jq})$
- Complete link: largest distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = max(t_{ip}, t_{jq})$
- Average: avg distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = avg(t_{ip}, t_{jq})$
- Centroid: distance between the centroids of two clusters, i.e., $dist(K_i, K_j) = dist(C_i, C_j)$
- Medoid: distance between the medoids of two clusters, i.e., $dist(K_i, K_j) = dist(M_i, M_j)$
  - Medoid: a chosen, centrally located object in the cluster

Centroid, Radius and Diameter of a Cluster (for numerical data sets)

- Centroid: the "middle" of a cluster

$$C_m = \frac{\sum_{i=1}^{N}(t_{ip})}{N}$$

- Radius: square root of average distance from any point of the cluster to its centroid

$$R_m = \sqrt{\frac{\sum_{i=1}^{N}(t_{ip} - c_m)^2}{N}}$$

- Diameter: square root of average mean squared distance between all pairs of points in the cluster

$$D_m = \sqrt{\frac{\sum_{i=1}^{N}\sum_{i=1}^{N}(t_{ip} - t_{iq})^2}{N(N-1)}}$$

Extensions to Hierarchical Clustering

- Major weakness of agglomerative clustering methods
  - Can never undo what was done previously
  - Do not scale well: time complexity of at least $O(n^2)$, where n is the number of total objects
- Integration of hierarchical & distance-based clustering
  - BIRCH (1996): uses CF-tree and incrementally adjusts the quality of sub-clusters – (CF: Clustering Feature)
  - CHAMELEON (1999): hierarchical clustering using dynamic modeling

BIRCH (Balanced Iterative Reducing and Clustering Using Hierarchies)

- Zhang, Ramakrishnan & Livny, SIGMOD'96
- Incrementally construct a CF (Clustering Feature) tree, a hierarchical data structure for multiphase clustering
  - Phase 1: scan DB to build an initial in-memory CF tree (a multi-level compression of the data that tries to preserve the inherent clustering structure of the data)
  - Phase 2: use an arbitrary clustering algorithm to cluster the leaf nodes of the CF-tree
- *Scales linearly*: finds a good clustering with a single scan and improves the quality with a few additional scans
- *Weakness:* handles only numeric data, and sensitive to the order of the data record

Clustering Feature Vector in BIRCH

Clustering Feature (CF): ***CF = (N, LS, SS)***

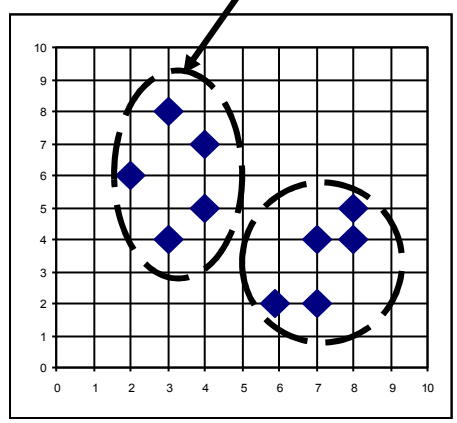
N: **Number of data points**

LS: linear sum of N points: $\sum_{i=1}^{N} X_i$

SS: square sum of N points

$$SS = \sum_{i=1}^{N} X_i^2$$

CF = (5, (16,30),(54,190))

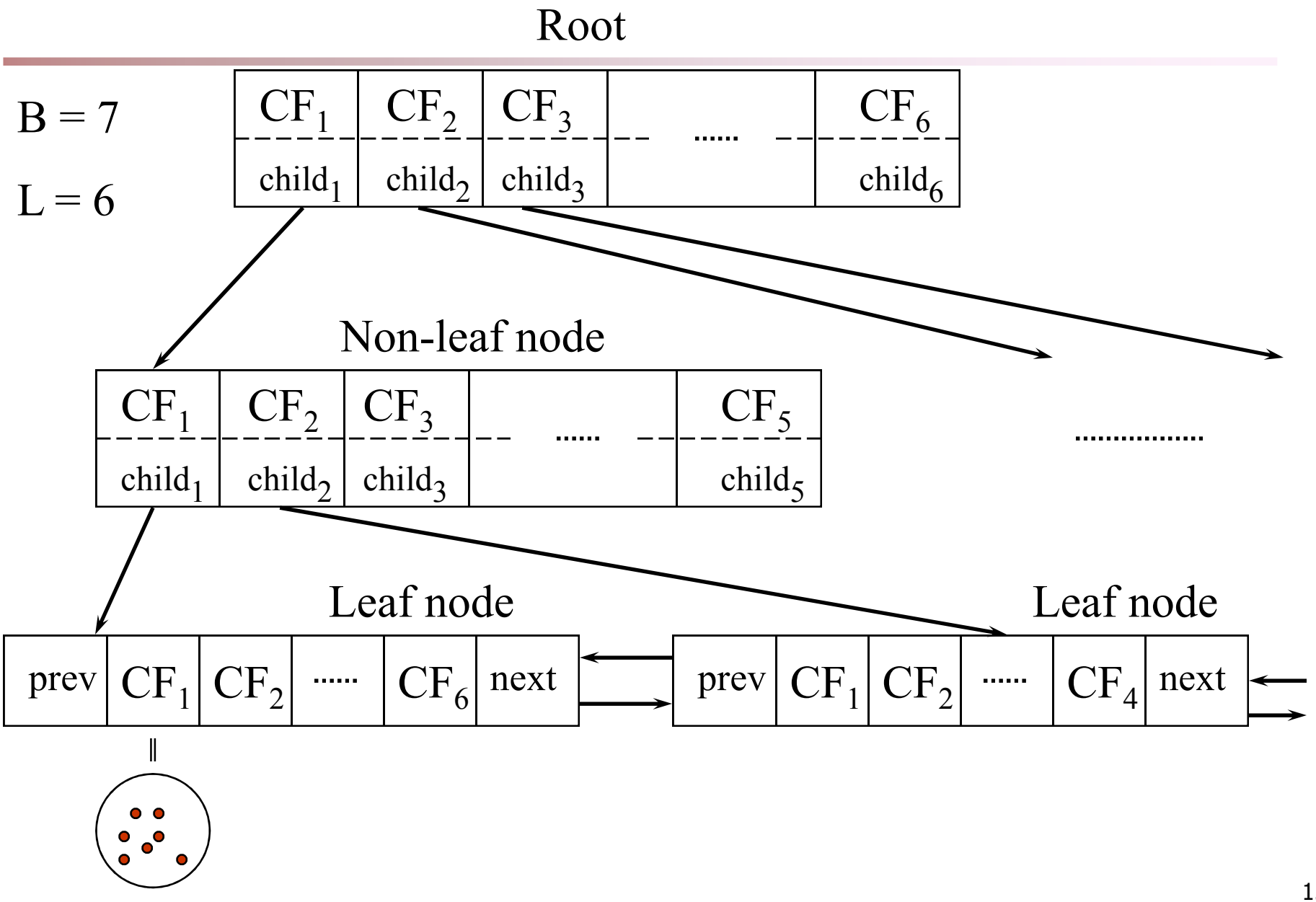


(3,4)
(2,6)
(4,5)
(4,7)
(3,8)

CF-Tree in BIRCH

- Clustering feature:
  - Summary of the statistics for a given subcluster: the 0-th, 1st, and 2nd moments of the subcluster from the statistical point of view
  - Registers crucial measurements for computing cluster and utilizes storage efficiently
- A CF tree is a height-balanced tree that stores the clustering features for a hierarchical clustering
  - A nonleaf node in a tree has descendants or “children”
  - The nonleaf nodes store sums of the CFs of their children
- A CF tree has two parameters
  - Branching factor: max # of children
  - Threshold: max diameter of sub-clusters stored at the leaf nodes

The CF Tree Structure



The Birch Algorithm

- Cluster Diameter

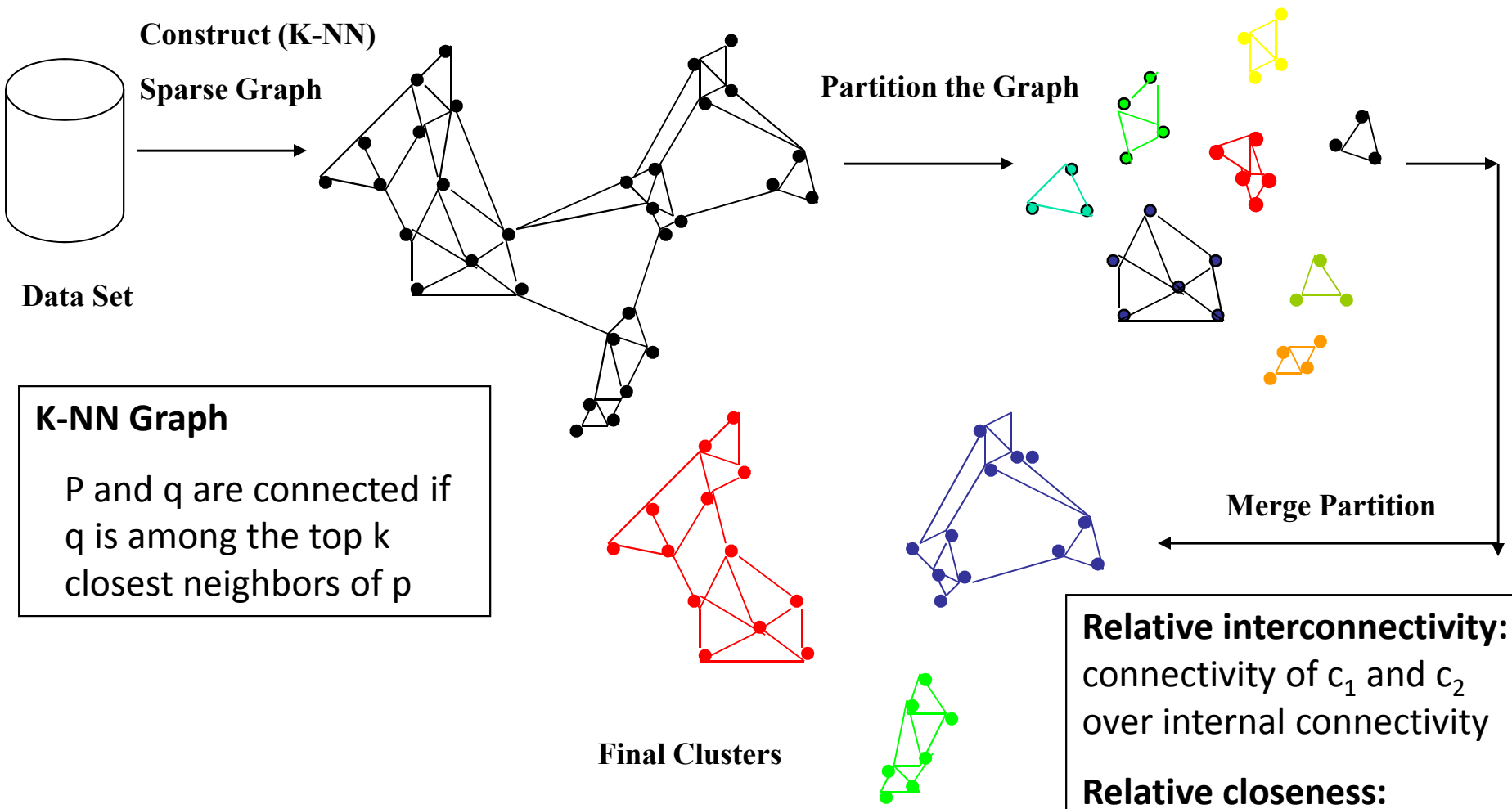
$$\sqrt{\frac{1}{n(n-1)}\sum(x_i - x_j)^2}$$

- For each point in the input
  - Find closest leaf entry
  - Add point to leaf entry and update CF
  - If entry diameter > max_diameter, then split leaf, and possibly parents
- Algorithm is O(n)
- Concerns
  - Sensitive to insertion order of data points
  - Since we fix the size of leaf nodes, so clusters may not be so natural
  - Clusters tend to be spherical given the radius and diameter measures

CHAMELEON: Hierarchical Clustering Using Dynamic Modeling (1999)

- CHAMELEON: G. Karypis, E. H. Han, and V. Kumar, 1999
- Measures the similarity based on a dynamic model
  - Two clusters are merged only if the *interconnectivity* and *closeness (proximity)* between two clusters are high *relative to* the internal interconnectivity of the clusters and closeness of items within the clusters
- Graph-based, and a two-phase algorithm
  1. Use a graph-partitioning algorithm: cluster objects into a large number of relatively small sub-clusters
  2. Use an agglomerative hierarchical clustering algorithm: find the genuine clusters by repeatedly combining these sub-clusters

Overall Framework of CHAMELEON



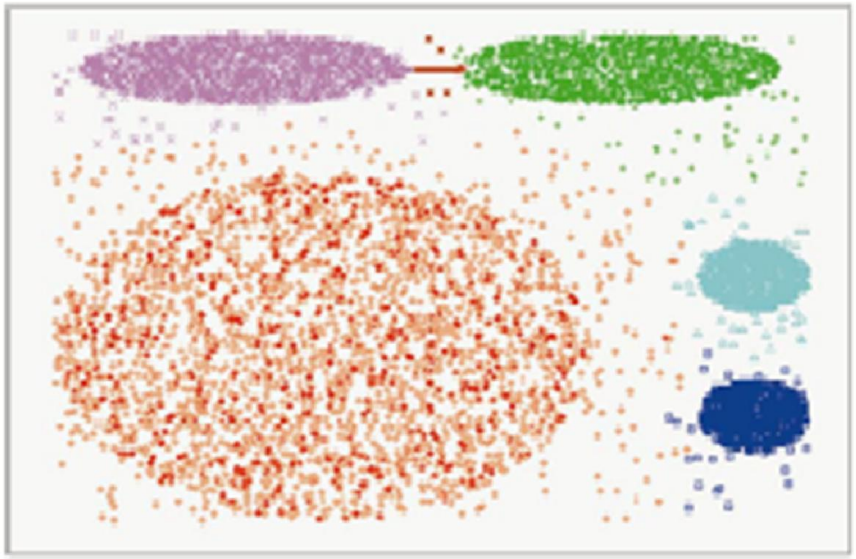
K-NN Graph

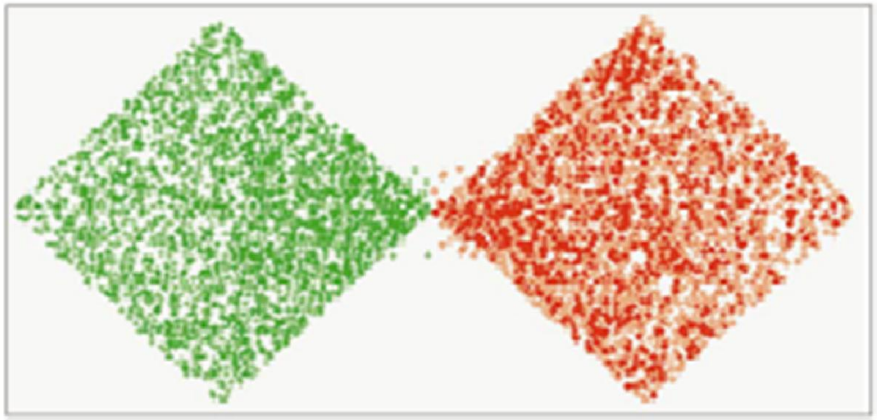
P and q are connected if q is among the top k closest neighbors of p

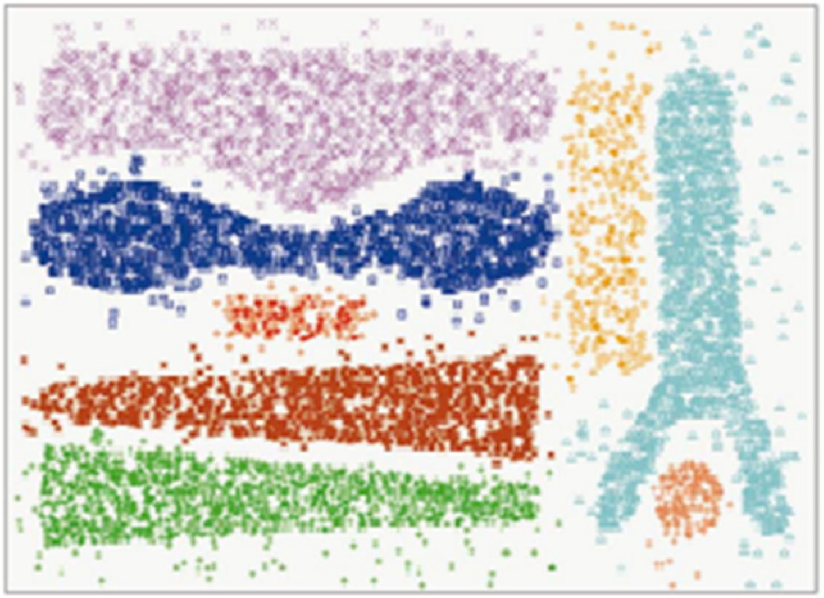
Relative interconnectivity: connectivity of c_1 and c_2 over internal connectivity

Relative closeness: closeness of c_1 and c_2 over internal closeness

CHAMELEON (Clustering Complex Objects)







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ROCK: Clustering Categorical Data

- ROCK: RObust Clustering using linKs
  - S. Guha, R. Rastogi & K. Shim, ICDE'99
- Major ideas
  - Use links to measure similarity/proximity
  - Not distance-based
- Algorithm: sampling-based clustering
  - Draw random sample
  - Cluster with links
  - Label data in disk
- Experiments
  - mushroom data, congressional voting

Similarity Measure in ROCK

- Traditional measures for categorical data may not work well, e.g., Jaccard coefficient
- Example: Two groups (clusters) of transactions
  - C_1 .<a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
  - C_2 .<a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}
- Jaccard co-efficient may lead to wrong clustering result
  - C_1: 0.2 ({a, b, c}, {b, d, e}} to 0.5 ({a, b, c}, {a, b, d})
  - C_1 & C_2: could be as high as 0.5 ({a, b, c}, {a, b, f})

- Jaccard co-efficient-based similarity function: $Sim(T_1, T_2) = \frac{|T_1 \cap T_2|}{|T_1 \cup T_2|}$
  - Ex. Let T_1 = {a, b, c}, T_2= {c, d, e}

$$Sim(T_1, T_2) = \frac{|\{c\}|}{|\{a, b, c, d, e\}|} = \frac{1}{5} = 0.2$$

Link Measure in ROCK

- Clusters
  - C_1. <a, b, c, d, e>: {a, b, c}, {a, b, d}, {a, b, e}, {a, c, d}, {a, c, e}, {a, d, e}, {b, c, d}, {b, c, e}, {b, d, e}, {c, d, e}
  - C_2. <a, b, f, g>: {a, b, f}, {a, b, g}, {a, f, g}, {b, f, g}
- Neighbors
  - Two transactions are neighbors if **sim**(T_1,T_2) > threshold
  - Let T_1 = {a, b, c}, T_2= {c, d, e}, T_3 = {a, b, f} and threshold = 0.5
    - T_1 connected to: {a,b,d}, {a,b,e}, {a,c,d}, {a,c,e}, {b,c,d}, {b,c,e}, {a,b,f}, {a,b,g}
    - T_2 connected to: {a,c,d}, {a,c,e}, {a,d,e}, {b,c,e}, {b,d,e}, {b,c,d}
    - T_3 connected to: {a,b,c}, {a,b,d}, {a,b,e}, {a,b,g}, {a,f,g}, {b,f,g}
- **Link Similarity**
  - Link similarity between two transactions is the # of common neighbors
  - link(T_1, T_2) = *4, since they have 4 common neighbors*
    - {a, c, d}, {a, c, e}, {b, c, d}, {b, c, e}
  - link(T_1, T_3) = *3, since they have 3 common neighbors*
    - {a, b, d}, {a, b, e}, {a, b, g}

Mushroom Data Set

- http://archive.ics.uci.edu/ml/datasets/Mushroom

- Number of Instances: 8124
- Number of Attributes: 22 (all nominally valued) including cap shape, cap color, odor, etc.
- Missing Attribute Values: 2480 of them (denoted by "?")
- Class Distribution:
  - edible: 4208 (51.8%)
  - poisonous: 3916 (48.2%)
  - total: 8124 instances

Clustering result for mushroom data

Traditional Hierarchical Algorithm					
Cluster No	No of Edible	No of Poisonous	Cluster No	No of Edible	No of Poisonous
1	666	478	11	120	144
2	283	318	12	128	140
3	201	188	13	144	163
4	164	227	14	198	163
5	194	125	15	131	211
6	207	150	16	201	156
7	233	238	17	151	140
8	181	139	18	190	122
9	135	78	19	175	150
10	172	217	20	168	206
ROCK					
Cluster No	No of Edible	No of Poisonous	Cluster No	No of Edible	No of Poisonous
1	96	0	12	48	0
2	0	256	13	0	288
3	704	0	14	192	0
4	96	0	15	32	72
5	768	0	16	0	1728
6	0	192	17	288	0
7	1728	0	18	0	8
8	0	32	19	192	0
9	0	1296	20	16	0
10	0	8	21	0	36
11	48	0			

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Assessing Clustering Tendency

- Assess if non-random structure exists in the data by measuring the probability that the data is generated by a uniform data distribution
- Test spatial randomness by statistic test: Hopkins Static
  - Given a dataset D regarded as a sample of a random variable o, determine how far away o is from being uniformly distributed in the data space
  - Sample *n* points, $p_1, \ldots, p_n$, uniformly from D. For each p_i, find its nearest neighbor in D: $x_i = min\{dist(p_i, v)\}$ where v in D
  - Sample *n* points, $q_1, \ldots, q_n$, uniformly from D. For each q_i, find its nearest neighbor in D – $\{q_i\}$: $y_i = min\{dist(q_i, v)\}$ where v in D and $v \neq q_i$
  - Calculate the Hopkins Statistic: $H = \frac{\sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i + \sum_{i=1}^{n} y_i}$
  - If D is uniformly distributed, $\sum x_i$ and $\sum y_i$ will be close to each other and H is close to 0.5. If D is highly skewed, H is close to 0

Determine the Number of Clusters

- Empirical method
  - # of clusters ≈$\sqrt{n/2}$ for a dataset of n points
- Elbow method
  - Use the turning point in the curve of sum of within cluster variance w.r.t the # of clusters
- Cross validation method
  - Divide a given data set into *m* parts
  - Use *m* – 1 parts to obtain a clustering model
  - Use the remaining part to test the quality of the clustering
    - E.g., For each point in the test set, find the closest centroid, and use the sum of squared distance between all points in the test set and the closest centroids to measure how well the model fits the test set
  - For any k > 0, repeat it *m* times, compare the overall quality measure w.r.t. different *k's*, and find # of clusters that fits the data the best

Measuring Clustering Quality

- Two methods: extrinsic vs. intrinsic
- Extrinsic: supervised, i.e., the ground truth is available
  - Compare a clustering against the ground truth using certain clustering quality measure
  - Ex. BCubed precision and recall metrics
- Intrinsic: unsupervised, i.e., the ground truth is unavailable
  - Evaluate the goodness of a clustering by considering how well the clusters are separated, and how compact the clusters are
  - Ex. Silhouette coefficient

Measuring Clustering Quality: Extrinsic Methods

- 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 “other” category)
  - Small cluster preservation: splitting a small category into pieces is more harmful than splitting a large category into pieces

Measuring Clustering Quality

- Clustering quality
  - User inspection
  - Sum of squared error
  - Entropy
  - Silhouette Index
  - Calinski-Harabasz Index
  - …

$$\mathrm{SSE} = \sum_{j=1}^{k} \sum_{x \in C_j} distance(x, m_j)^2$$

$$entropy(D_i) = -\sum_{i=1}^{k} P_i(c_i) \log_2 P_i(c_i),$$

$$entropy_{total}(D) = \sum_{i=1}^{k} \frac{|D_i|}{|D|} \times entropy(D_i)$$

$$SI_k = \frac{1}{n} \sum_{i=1}^{n} \frac{(b_i - a_i)}{max(a_i, b_i)}$$

$$CH(k) = \frac{[trace\ B\ /\ K-1]}{[trace\ W\ /\ N-K]} \text{ for } K \in \mathbb{N}$$

$$trace\ B = \sum_{k=1}^{K} |C_k| \| \overline{C}_k - \overline{x} \|^2$$

$$trace\ W = \sum_{k=1}^{K} \sum_{i=1}^{N} w_{k,i} \| x_i - \overline{C}_k \|^2$$

Summary

- Cluster analysis groups objects based on their similarity and has wide applications
- Clustering algorithms can be categorized into partitioning methods, hierarchical methods, density-based methods, grid-based methods, and model-based methods
- K-means and K-medoids algorithms are popular partitioning-based clustering algorithms
- DBSCAN, OPTICS, and DENCLU are interesting density-based algorithms
- Birch and Chameleon are interesting hierarchical clustering algorithms, and there are also probabilistic hierarchical clustering algorithms
- ROCK algorithm is used to cluster categorical data.
- Quality of clustering results can be evaluated in various ways

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