Data Mining:

Concepts and Techniques

(3rd ed.)

— Chapter 11 —

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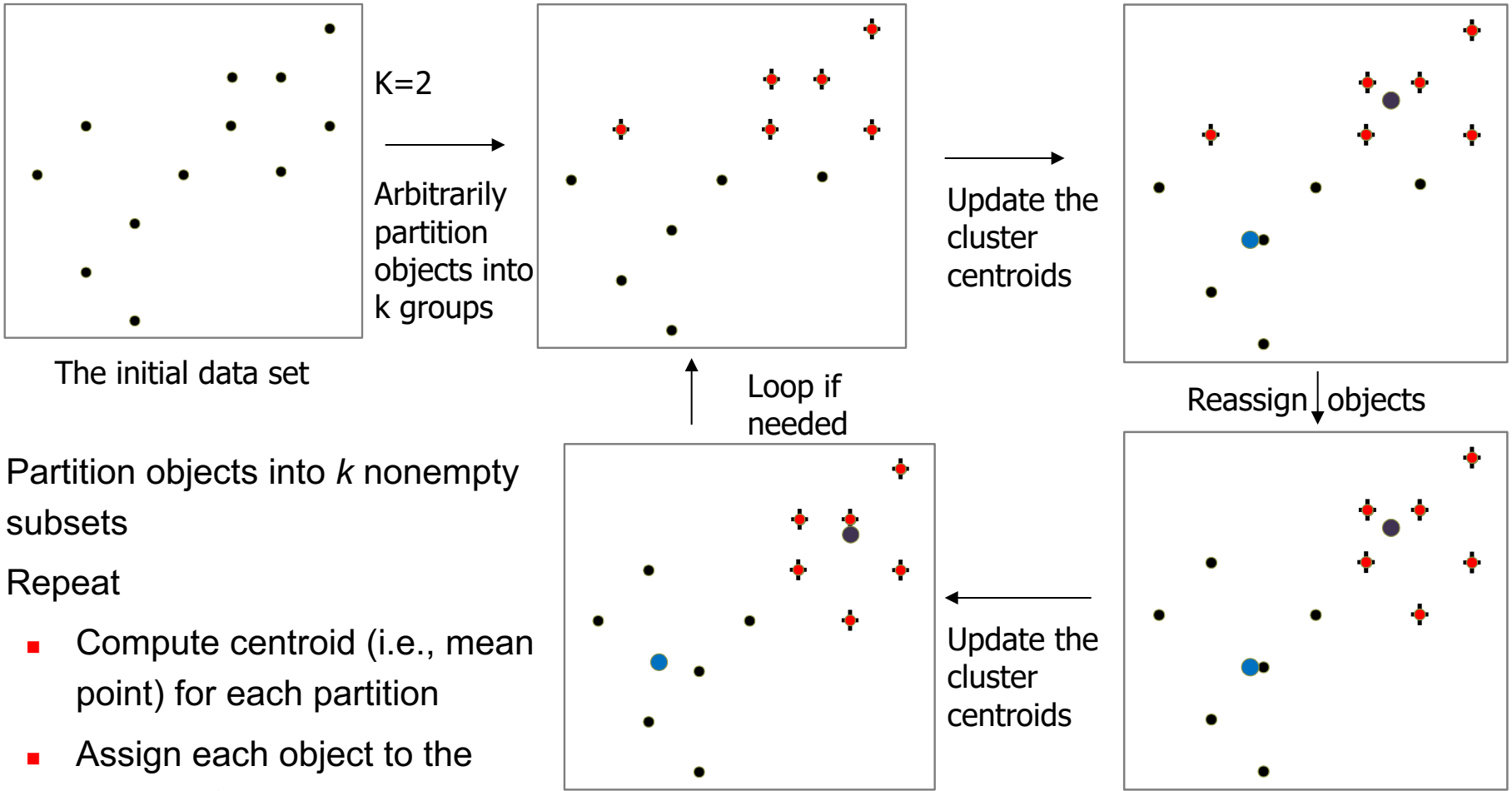
Review: Basic Cluster Analysis Methods (Chap. 10)

- Cluster Analysis: Basic Concepts
  - Group data so that object similarity is high within clusters but low across clusters
- Partitioning Methods
  - K-means and k-medoids algorithms and their refinements
- Hierarchical Methods
  - Agglomerative and divisive method, Birch, Cameleon
- Density-Based Methods
  - DBScan, Optics and DenCLu
- Grid-Based Methods
  - STING and CLIQUE (subspace clustering)
- Evaluation of Clustering
  - Assess clustering tendency, determine # of clusters, and measure clustering quality

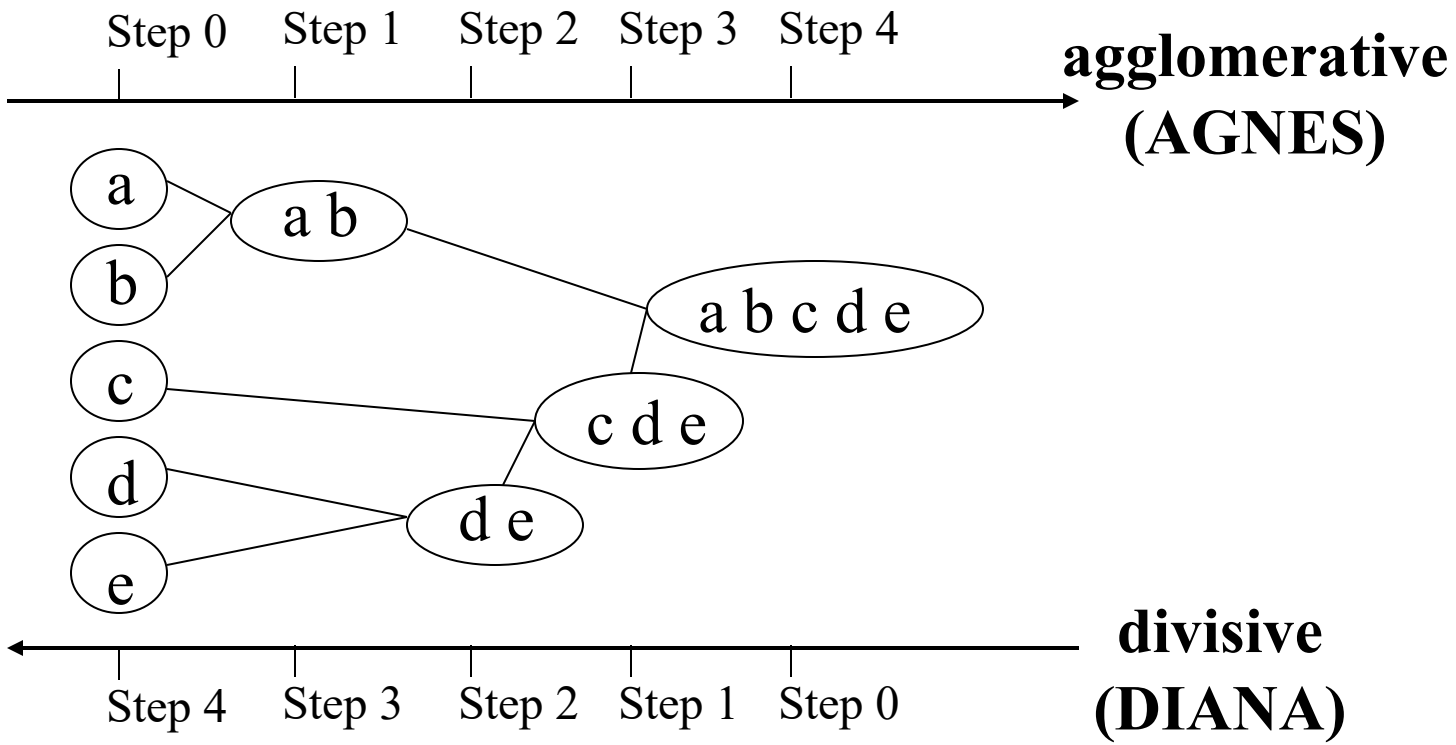
K-Means Clustering



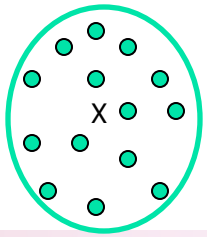
- Partition objects into *k* nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change

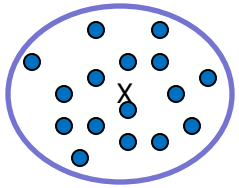
Hierarchical Clustering

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



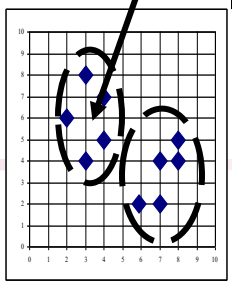
Distance between Clusters





- 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

BIRCH and the Clustering Feature (CF) Tree Structure



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

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

B = 7

L = 6

Root

CF_1	CF_2	CF_3	.....	CF_6
$child_1$	$child_2$	$child_3$		$child_6$

Non-leaf node

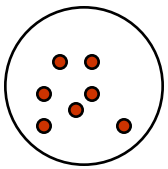
CF_1	CF_2	CF_3	.....	CF_5
$child_1$	$child_2$	$child_3$		$child_5$

Leaf node

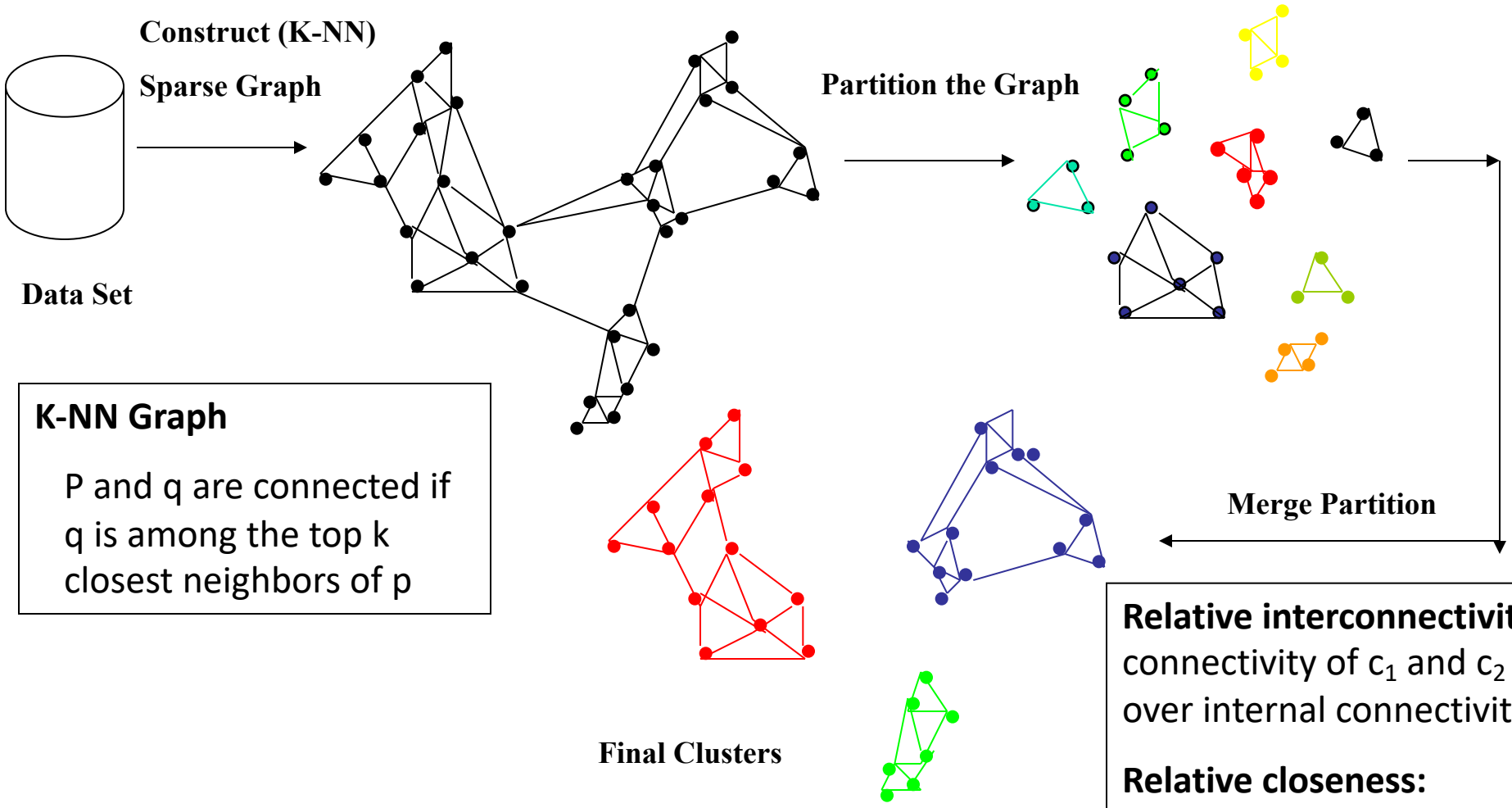
prev	CF_1	CF_2	.....	CF_6	next

Leaf node

prev	CF_1	CF_2	.....	CF_4	next



Overall Framework of CHAMELEON



K-NN Graph

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

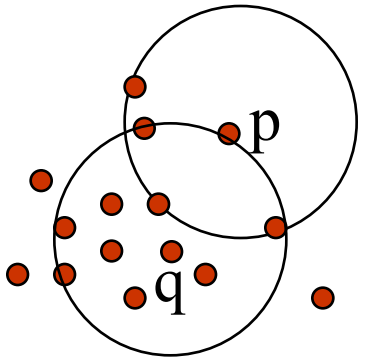
Relative interconnectivity: connectivity of c_1 and c_2 over internal connectivity

Relative closeness: closeness of c_1 and c_2 over internal closeness

Density-Based Clustering: DBSCAN

- Two parameters*:*
  - *Eps*: Maximum radius of the neighbourhood
  - *MinPts*: Minimum number of points in an Eps-neighbourhood of that point
- $N_{Eps}(p)$: {q belongs to D | dist(p,q) ≤ Eps}
- Directly density-reachable: A point *p* is directly density-reachable from a point *q* w.r.t. *Eps*, *MinPts* if
  - *p* belongs to $N_{Eps}(q)$
  - core point condition:

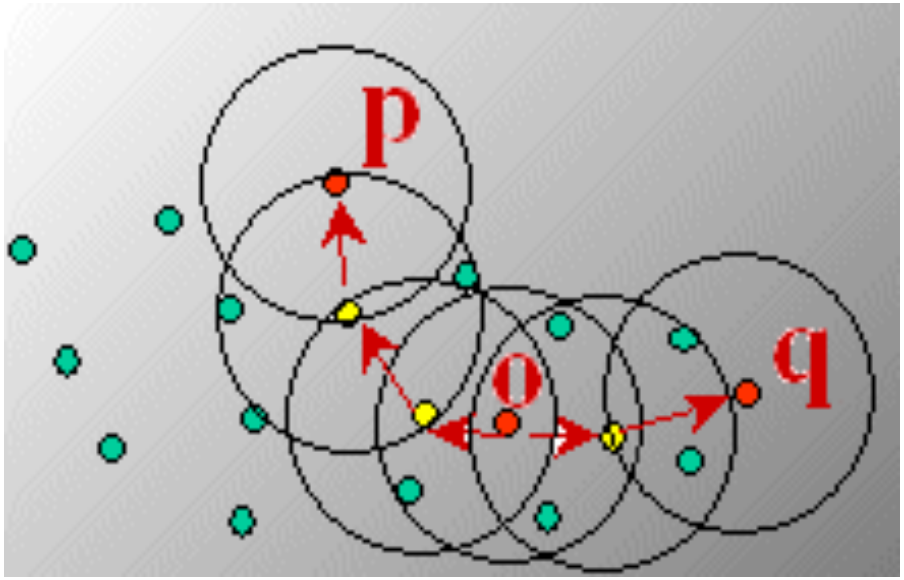
$$|N_{Eps}(q)| \geq MinPts$$

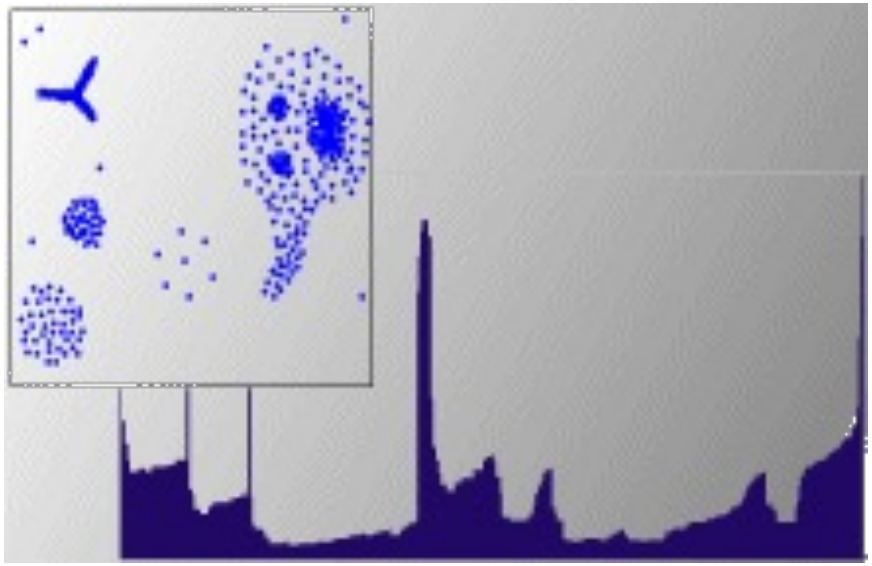


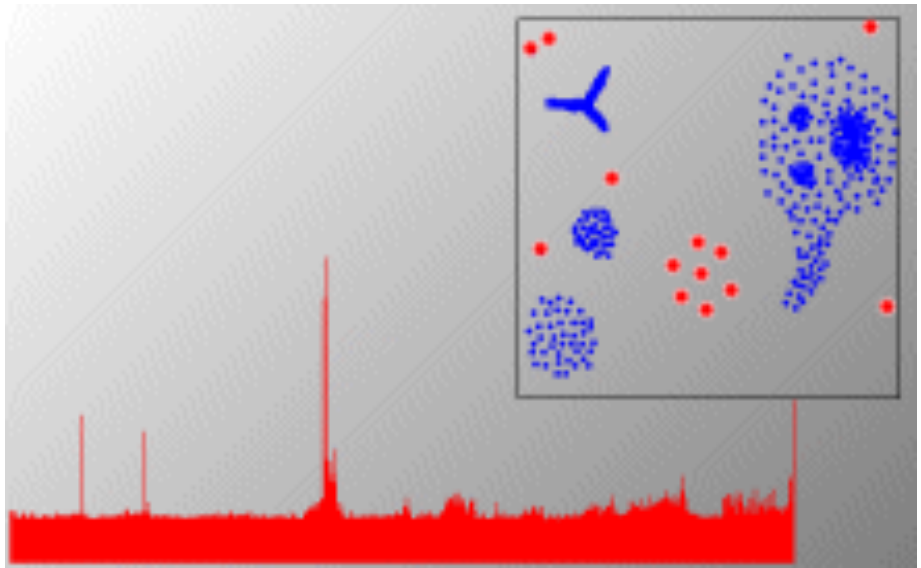
MinPts = 5

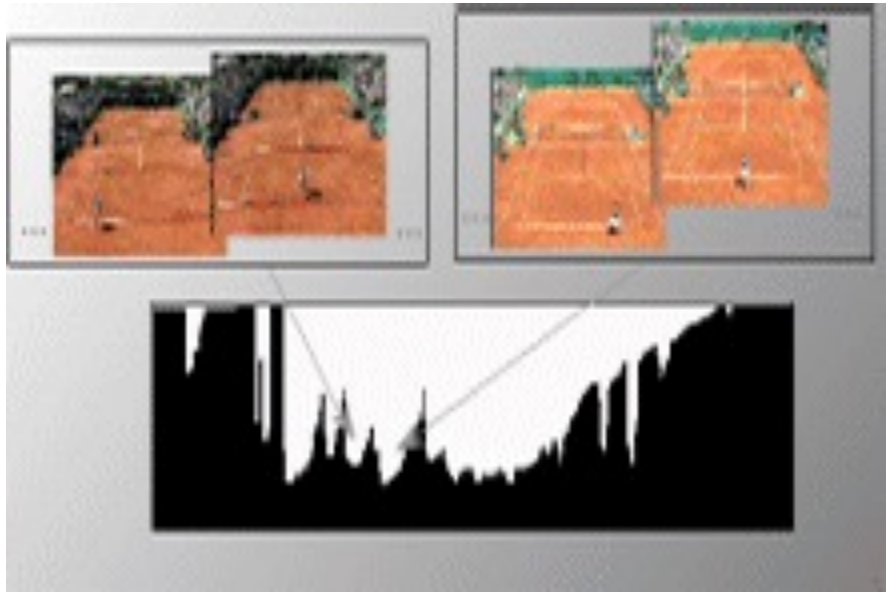
Eps = 1 cm

Density-Based Clustering: OPTICS & Its Applications

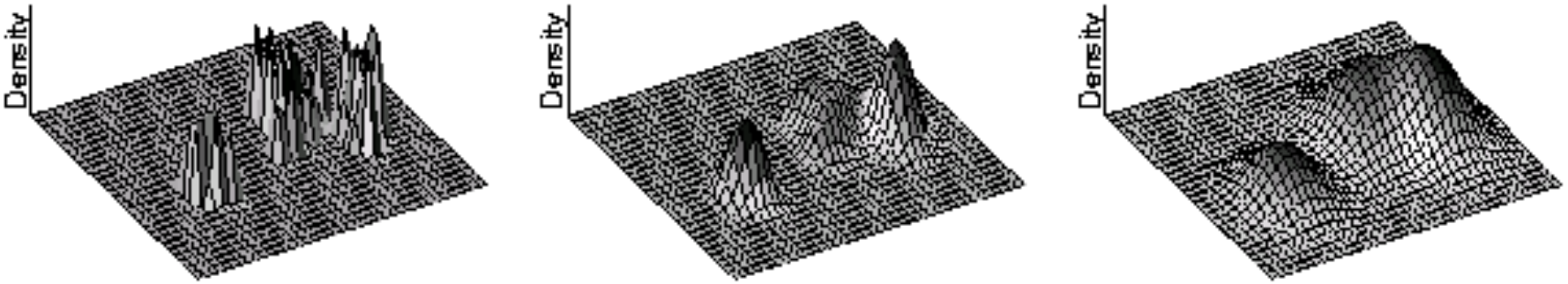






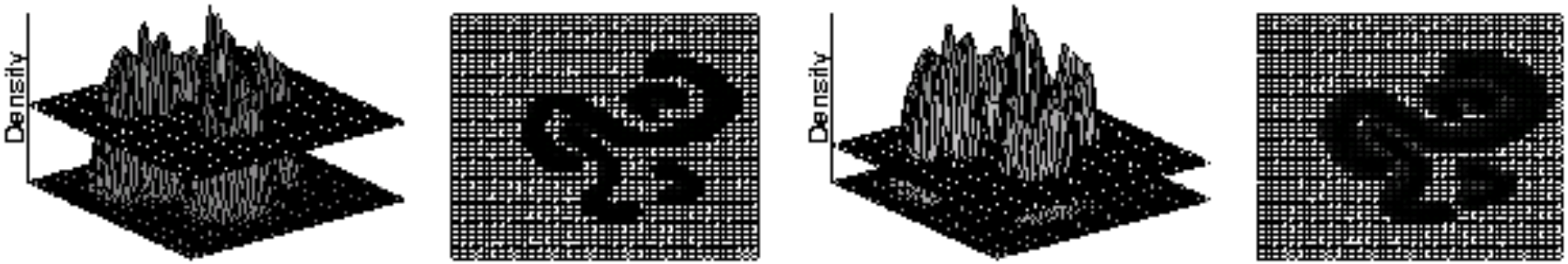


DENCLU: Center-Defined and Arbitrary



(a) $\sigma = 0.2$ (b) $\sigma = 0.6$ (d) $\sigma = 1.5$

Figure 3: Example of Center-Defined Clusters for different σ

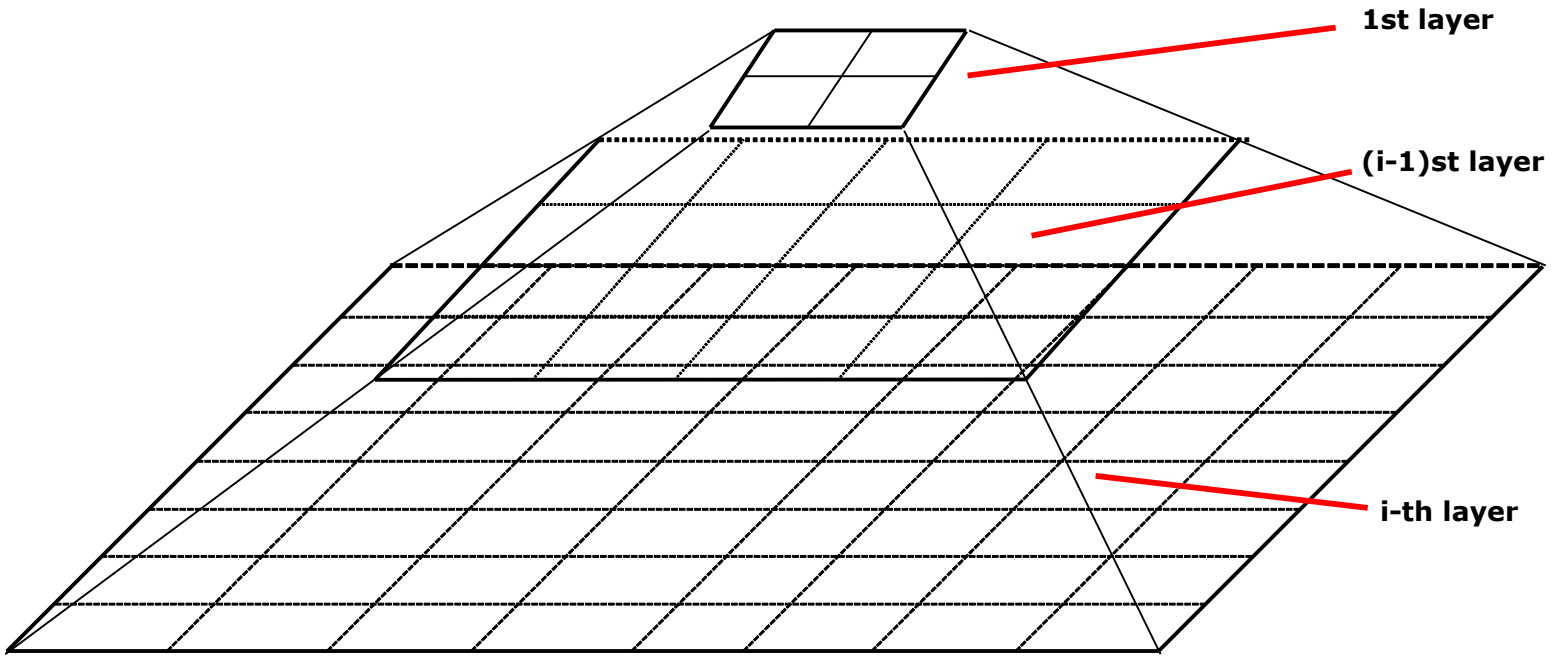


(a) $\xi = 2$ (b) $\xi = 2$ (c) $\xi = 1$ (d) $\xi = 1$

Figure 4: Example of Arbitray-Shape Clusters for different ξ

STING: A Statistical Information Grid Approach

- Wang, Yang and Muntz (VLDB'97)
- The spatial area is divided into rectangular cells
- There are several levels of cells corresponding to different levels of resolution



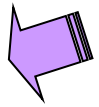
Evaluation of Clustering Quality

- 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
- Determine the Number of Clusters
  - Empirical method: # of clusters ≈√n/2
  - Elbow method: Use the turning point in the curve of sum of within cluster variance w.r.t # of clusters
  - Cross validation method
- Measuring Clustering Quality
  - Extrinsic: supervised
    - Compare a clustering against the ground truth using certain clustering quality measure
  - Intrinsic: unsupervised
    - Evaluate the goodness of a clustering by considering how well the clusters are separated, and how compact the clusters are

Outline of Advanced Clustering Analysis

- Probability Model-Based Clustering
  - Each object may take a probability to belong to a cluster
- Clustering High-Dimensional Data
  - Curse of dimensionality: Difficulty of distance measure in high-D space
- Clustering Graphs and Network Data
  - Similarity measurement and clustering methods for graph and networks
- Clustering with Constraints
  - Cluster analysis under different kinds of constraints, e.g., that raised from background knowledge or spatial distribution of the objects

Chapter 11. Cluster Analysis: Advanced Methods

- Probability Model-Based Clustering 
- Clustering High-Dimensional Data
- Clustering Graphs and Network Data
- Clustering with Constraints
- Summary

Fuzzy Set and Fuzzy Cluster

- Clustering methods discussed so far
  - Every data object is assigned to exactly one cluster
- Some applications may need for fuzzy or soft cluster assignment
  - Ex. An e-game could belong to both entertainment and software
- Methods: fuzzy clusters and probabilistic model-based clusters
- Fuzzy cluster: A fuzzy set *S:* $F_S : X \rightarrow [0, 1]$ (value between 0 and 1)
- Example: Popularity of cameras is defined as a fuzzy mapping

Camera	Sales (units)
A	50
B	1320
C	860
D	270

$$\text{Pop}(o) = \begin{cases} 1 & \text{if } 1,000 \text{ or more units of } o \text{ are sold} \\ \frac{i}{1000} & \text{if } i \ (i < 1000) \text{ units of } o \text{ are sold} \end{cases}$$

- Then, *A*(0.05), *B*(1), *C*(0.86), *D*(0.27)

Fuzzy (Soft) Clustering

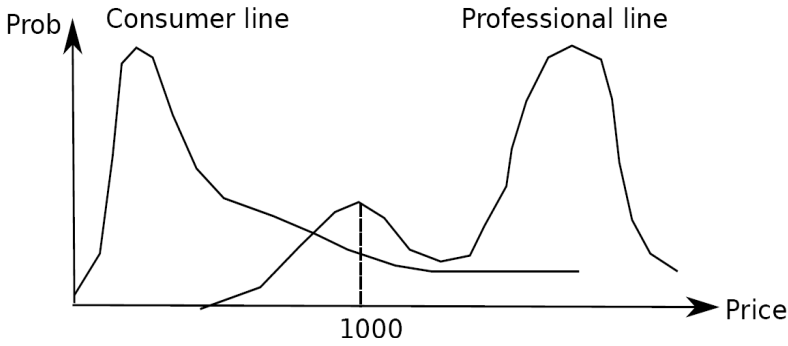
Review-id	Keywords
R_1	digital camera, lens
R_2	digital camera
R_3	lens
R_4	digital camera, lens, computer
R_5	computer, CPU
R_6	computer, computer game

$$M = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ \frac{2}{3} & \frac{1}{3} \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

- Example: Let cluster features be
  - C_1 :"digital camera" and "lens"
  - C_2: "computer"
- Fuzzy clustering
  - k fuzzy clusters C_1, …,C_k ,represented as a partition matrix M = [w_{ij}]
  - P1: for each object o_i and cluster C_j, $0 \le w_{ij} \le 1$ (fuzzy set)
  - P2: for each object o_i, $\sum_{j=1}^{k} w_{ij} = 1$, equal participation in the clustering
  - P3: for each cluster C_j , $0 < \sum_{i=1}^{n} w_{ij} < n$ ensures there is no empty cluster
- Let c_1, …, c_k as the center of the k clusters
- For an object o_i, sum of the squared error (SSE), p is a parameter:
- For a cluster C_i, SSE: $\mathrm{SSE}(C_j) = \sum_{i=1}^{n} w_{ij}^p dist(o_i, c_j)^2$ $\mathrm{SSE}(o_i) = \sum_{j=1}^{k} w_{ij}^p dist(o_i, c_j)^2$
- Measure how well a clustering fits the data: $\mathrm{SSE}(\mathcal{C}) = \sum_{i=1}^{n} \sum_{j=1}^{k} w_{ij}^p dist(o_i, c_j)^2$

Probabilistic Model-Based Clustering

- Cluster analysis is to find hidden categories.
- A hidden category (i.e., *probabilistic cluster)* is a distribution over the data space, which can be mathematically represented using a probability density function (or distribution function).
- Ex. 2 categories for digital cameras sold
  - consumer line vs. professional line
  - density functions f_1, f_2 for C_1, C_2
  - obtained by probabilistic clustering



- A **mixture model** assumes that a set of observed objects is a mixture of instances from multiple probabilistic clusters, and conceptually each observed object is generated independently
- **Out task**: infer a set of *k* probabilistic clusters that is mostly likely to generate *D* using the above data generation process

Model-Based Clustering

- A set C of k probabilistic clusters $C_1, \ldots, C_k$ with probability density functions $f_1, \ldots, f_k$, respectively, and their probabilities $\omega_1, \ldots, \omega_k$.
- Probability of an object o generated by cluster C_j is $P(o|C_j) = \omega_j f_j(o)$
- Probability of o generated by the set of cluster $\boldsymbol{C}$ is $P(o|\boldsymbol{C}) = \sum_{j=1}^{k} \omega_j f_j(o)$
- Since objects are assumed to be generated independently, for a data set D = {o_1, …, o_n}, we have,

$$P(D|\boldsymbol{C}) = \prod_{i=1}^{n} P(o_i|\boldsymbol{C}) = \prod_{i=1}^{n} \sum_{j=1}^{k} \omega_j f_j(o_i)$$

- Task: Find a set C of k probabilistic clusters s.t. $P(D|\boldsymbol{C})$ is maximized
- However, maximizing $P(D|\boldsymbol{C})$ is often intractable since the probability density function of a cluster can take an arbitrarily complicated form
- To make it computationally feasible (as a compromise), assume the probability density functions being some parameterized distributions

Univariate Gaussian Mixture Model

- O = {o_1, …, o_n} (n observed objects), Θ = {θ_1, …, θ_k} (parameters of the k distributions), and $P_j(o_i|\theta_j)$ is the probability that o_i is generated from the j-th distribution using parameter θ_j, we have

$$P(o_i|\Theta) = \sum_{j=1}^{k} \omega_j P_j(o_i|\Theta_j) \qquad P(\mathbf{O}|\Theta) = \prod_{i=1}^{n} \sum_{j=1}^{k} \omega_j P_j(o_i|\Theta_j)$$

- Univariate Gaussian mixture model
  - Assume the probability density function of each cluster follows a 1-d Gaussian distribution. Suppose that there are k clusters.
  - The probability density function of each cluster are centered at μ_j with standard deviation σ_j, θ_j, = (μ_j, σ_j), we have

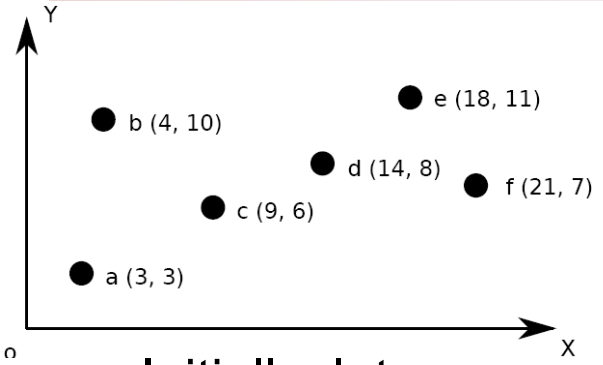
$$P(o_i|\Theta_j) = \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i-\mu_j)^2}{2\sigma^2}} \qquad P(o_i|\Theta) = \sum_{j=1}^{k} \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i-\mu_j)^2}{2\sigma^2}}$$

$$P(\mathbf{O}|\Theta) = \prod_{i=1}^{n} \sum_{j=1}^{k} \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i-\mu_j)^2}{2\sigma^2}}$$

The EM (Expectation Maximization) Algorithm

- The k-means algorithm has two steps at each iteration:
  - **Expectation Step** (E-step): Given the current cluster centers, each object is assigned to the cluster whose center is closest to the object: An object is *expected to belong to the closest cluster*
  - **Maximization Step** (M-step): Given the cluster assignment, for each cluster, the algorithm *adjusts the center* so that *the sum of distance* from the objects assigned to this cluster and the new center is minimized
- **The (EM) algorithm:** A framework to approach maximum likelihood or maximum a posteriori estimates of parameters in statistical models.
  - **E-step** assigns objects to clusters according to the current fuzzy clustering or parameters of probabilistic clusters
  - **M-step** finds the new clustering or parameters that maximize the sum of squared error (SSE) or the expected likelihood

Fuzzy Clustering Using the EM Algorithm



Iteration	E-step	M-step
1	$M^T = \begin{bmatrix} 1 & 0 & 0.48 & 0.42 & 0.41 & 0.47 \\ 0 & 1 & 0.52 & 0.58 & 0.59 & 0.53 \end{bmatrix}$	$c_1 = (8.47, 5.12),$ $c_2 = (10.42, 8.99)$
2	$M^T = \begin{bmatrix} 0.73 & 0.49 & 0.91 & 0.26 & 0.33 & 0.42 \\ 0.27 & 0.51 & 0.09 & 0.74 & 0.67 & 0.58 \end{bmatrix}$	$c_1 = (8.51, 6.11),$ $c_2 = (14.42, 8.69)$
3	$M^T = \begin{bmatrix} 0.80 & 0.76 & 0.99 & 0.02 & 0.14 & 0.23 \\ 0.20 & 0.24 & 0.01 & 0.98 & 0.86 & 0.77 \end{bmatrix}$	$c_1 = (6.40, 6.24),$ $c_2 = (16.55, 8.64)$

- Initially, let c_1 = a and c_2 = b
- 1st E-step: assign o to c_1,w. wt = $\frac{\frac{1}{dist(o,c_1)^2}}{\frac{1}{dist(o,c_1)^2}+\frac{1}{dist(o,c_2)^2}} = \frac{dist(o,c_2)^2}{dist(o,c_1)^2+dist(o,c_2)^2}$
  - $w_{c,c_1} = \frac{41}{45+41} = 0.48$
- 1st M-step: recalculate the centroids according to the partition matrix, minimizing the sum of squared error (SSE)

$$c_j = \frac{\sum_{\text{each point } o} w_{o,c_j}^2 o}{\sum_{\text{each point } o} w_{o,c_j}^2} \qquad c_1 = \left(\frac{1^2\times3+0^2\times4+0.48^2\times9+0.42^2\times14+0.41^2\times18+0.47^2\times21}{1^2+0^2+0.48^2+0.42^2+0.41^2+0.47^2}, \frac{1^2\times3+0^2\times10+0.48^2\times6+0.42^2\times8+0.41^2\times11+0.47^2\times7}{1^2+0^2+0.48^2+0.42^2+0.41^2+0.47^2}\right) = (8.47, 5.12)$$

- Iteratively calculate this until the cluster centers converge or the change is small enough

Univariate Gaussian Mixture Model

- O = {o_1, …, o_n} (n observed objects), Θ = {θ_1, …, θ_k} (parameters of the k distributions), and $P_j(o_i|\theta_j)$ is the probability that o_i is generated from the j-th distribution using parameter θ_j, we have

$$P(o_i|\Theta) = \sum_{j=1}^{k} \omega_j P_j(o_i|\Theta_j) \qquad P(\mathbf{O}|\Theta) = \prod_{i=1}^{n} \sum_{j=1}^{k} \omega_j P_j(o_i|\Theta_j)$$

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$$P(\mathbf{O}|\Theta) = \prod_{i=1}^{n} \sum_{j=1}^{k} \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i-\mu_j)^2}{2\sigma^2}}$$

Computing Mixture Models with EM

- Given n objects $O = \{o_1, \ldots, o_n\}$, we want to mine a set of parameters $\Theta = \{\theta_1, \ldots, \theta_k\}$ s.t.,$P(\mathbf{O}|\mathbf{\Theta})$ is maximized, where $\theta_j = (\mu_j, \sigma_j)$ are the mean and standard deviation of the j-th univariate Gaussian distribution
- We initially assign random values to parameters θ_j, then iteratively conduct the E- and M- steps until converge or sufficiently small change
- At the E-step, for each object o_i, calculate the probability that o_i belongs to each distribution,

$$P(\Theta_j|o_i, \mathbf{\Theta}) = \frac{P(o_i|\Theta_j)}{\sum_{l=1}^{k} P(o_i|\Theta_l)}$$

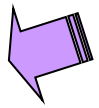
- At the M-step, adjust the parameters $\theta_j = (\mu_j, \sigma_j)$ so that the expected likelihood $P(\mathbf{O}|\mathbf{\Theta})$ is maximized

$$\mu_j = \sum_{i=1}^{n} o_i \frac{P(\Theta_j|o_i, \mathbf{\Theta})}{\sum_{l=1}^{n} P(\Theta_j|o_l, \mathbf{\Theta})} = \frac{\sum_{i=1}^{n} o_i P(\Theta_j|o_i, \mathbf{\Theta})}{\sum_{i=1}^{n} P(\Theta_j|o_i, \mathbf{\Theta})} \quad \sigma_j = \sqrt{\frac{\sum_{i=1}^{n} P(\Theta_j|o_i, \mathbf{\Theta})(o_i - u_j)^2}{\sum_{i=1}^{n} P(\Theta_j|o_i, \mathbf{\Theta})}}$$

Advantages and Disadvantages of Mixture Models

- Strength
  - Mixture models are more general than partitioning and fuzzy clustering
  - Clusters can be characterized by a small number of parameters
  - The results may satisfy the statistical assumptions of the generative models
- Weakness
  - Converge to local optimal (overcome: run multi-times w. random initialization)
  - Computationally expensive if the number of distributions is large, or the data set contains very few observed data points
  - Need large data sets
  - Hard to estimate the number of clusters

Chapter 11. Cluster Analysis: Advanced Methods

- Probability Model-Based Clustering
- Clustering High-Dimensional Data 
- Clustering Graphs and Network Data
- Clustering with Constraints
- Summary

Clustering High-Dimensional Data

- Clustering high-dimensional data (How high is high-D in clustering?)
  - Many applications: text documents, DNA micro-array data
  - Major challenges:
    - Many irrelevant dimensions may mask clusters
    - Distance measure becomes meaningless—due to equi-distance
    - Clusters may exist only in some subspaces
- Methods
  - **Subspace-clustering**: Search for clusters existing in subspaces of the given high dimensional data space
    - CLIQUE, ProClus, and bi-clustering approaches
  - **Dimensionality reduction approaches**: Construct a much lower dimensional space and search for clusters there (may construct new dimensions by combining some dimensions in the original data)
    - Dimensionality reduction methods and spectral clustering

Traditional Distance Measures May Not Be Effective on High-D Data

- Traditional distance measure could be dominated by noises in many dimensions
- Ex. Which pairs of customers are more similar?

Customer	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9	P_{10}
Ada	1	0	0	0	0	0	0	0	0	0
Bob	0	0	0	0	0	0	0	0	0	1
Cathy	1	0	0	0	1	0	0	0	0	1

- By Euclidean distance, we get,

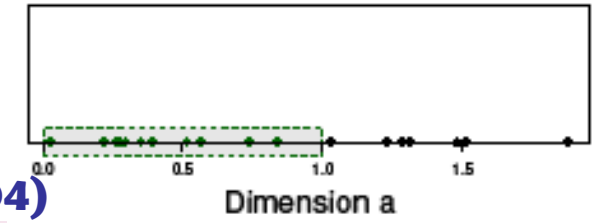
$$dist(\text{Ada}, \text{Bob}) = dist(\text{Bob}, \text{Cathy}) = dist(\text{Ada}, \text{Cathy}) = \sqrt{2}$$

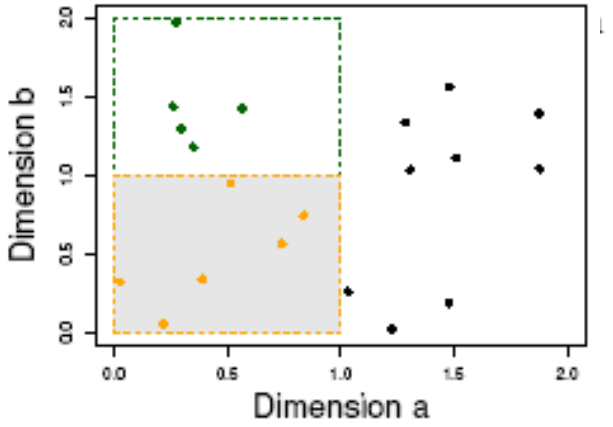
  - despite Ada and Cathy look more similar
- Clustering should not only consider dimensions but also attributes (features)
  - Feature transformation: effective if most dimensions are relevant (PCA & SVD useful when features are highly correlated/redundant)
  - Feature selection: useful to find a subspace where the data have nice clusters

The Curse of Dimensionality

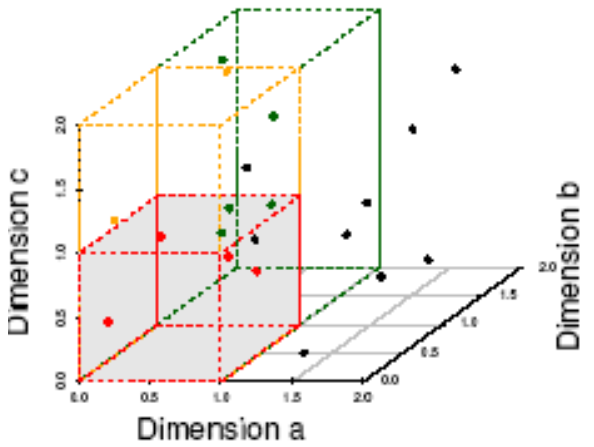
(graphs adapted from Parsons et al. KDD Explorations 2004)

- Data in only one dimension is relatively packed
- Adding a dimension "stretch" the points across that dimension, making them further apart
- Adding more dimensions will make the points further apart—high dimensional data is extremely sparse
- Distance measure becomes meaningless—due to equi-distance

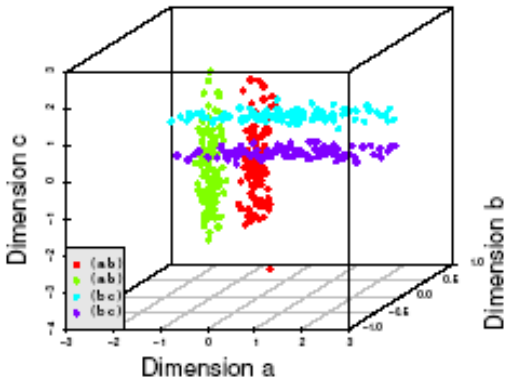




(b) 6 Objects in One Unit Bin



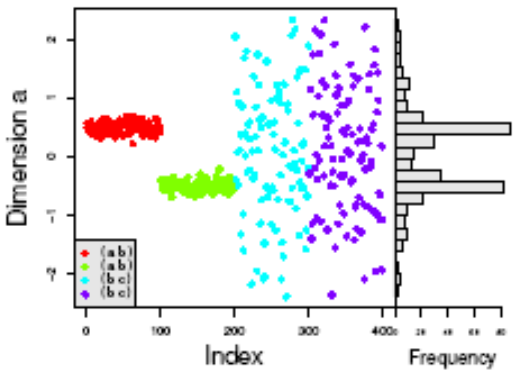
(c) 4 Objects in One Unit Bin



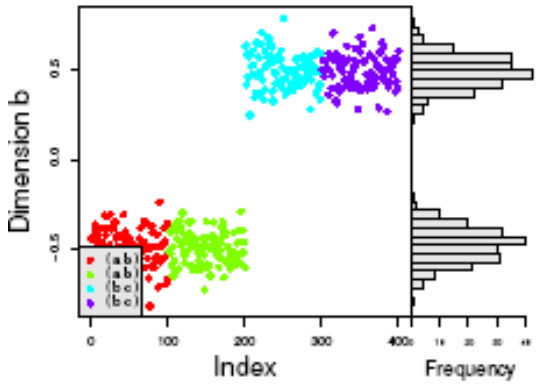
Why Subspace Clustering?

(adapted from Parsons et al. SIGKDD Explorations 2004)

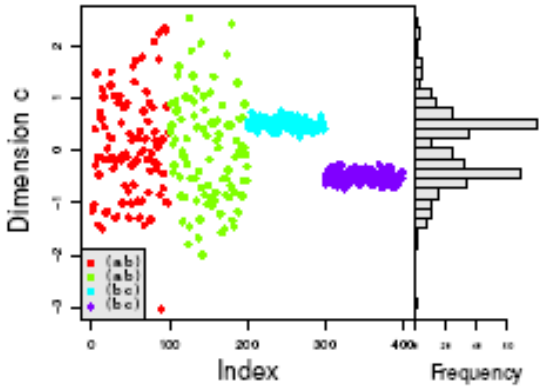
- Clusters may exist only in some subspaces
- Subspace-clustering: find clusters in all the subspaces



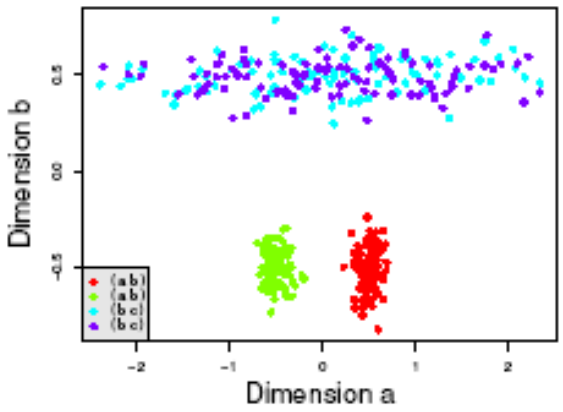
(a) Dimension a



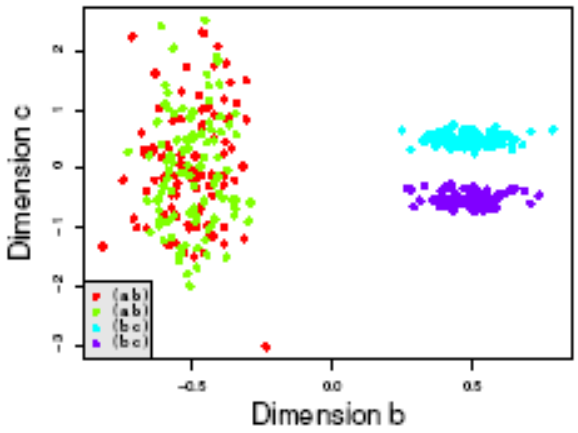
(b) Dimension b



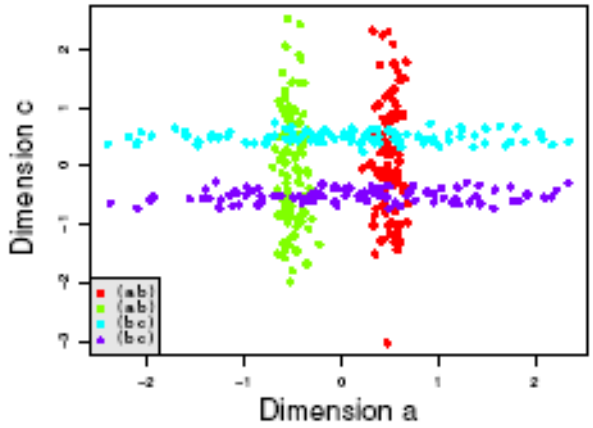
(c) Dimension c



(a) Dims a & b



(b) Dims b & c



(c) Dims a & c

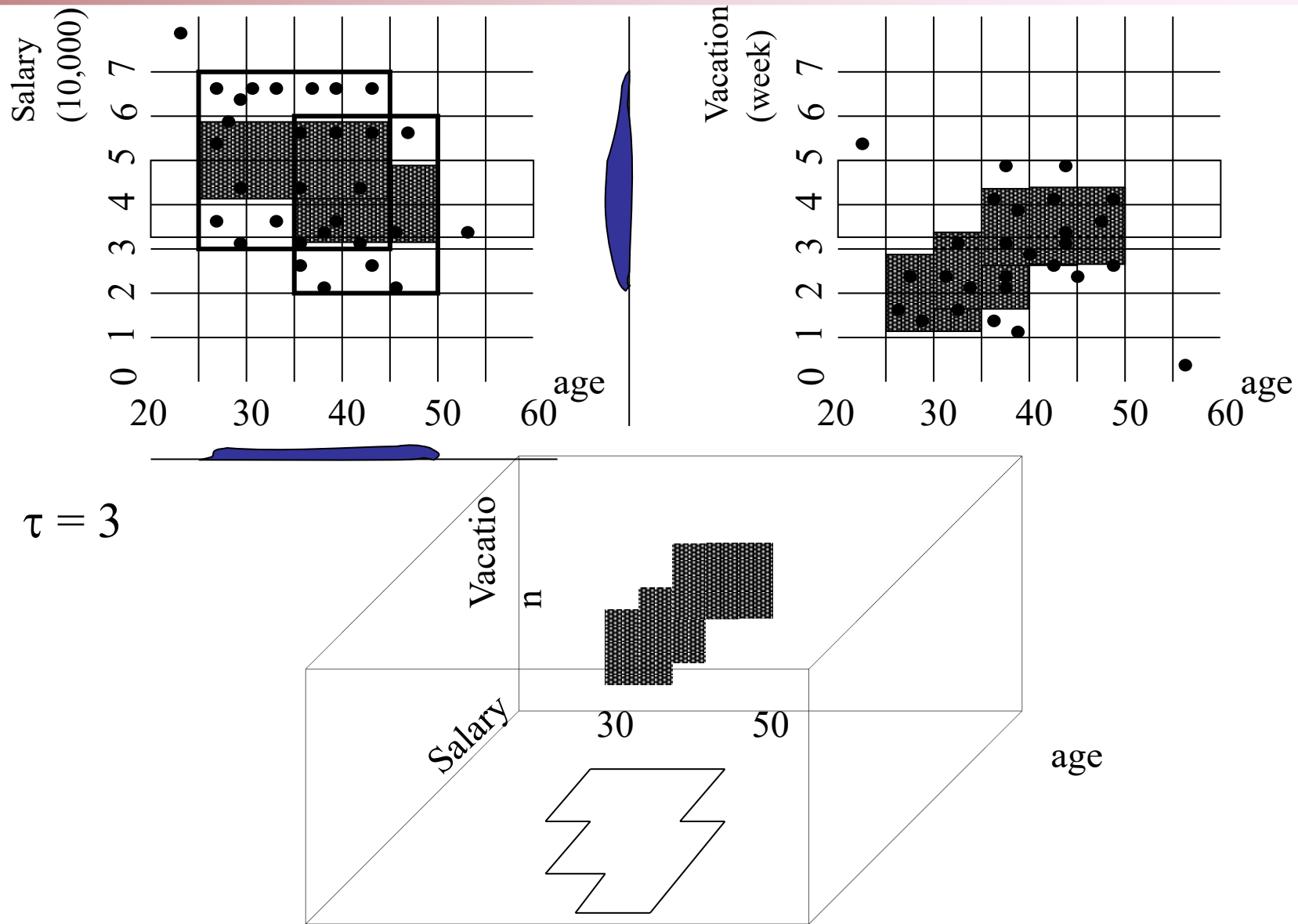
Subspace Clustering Methods

- Subspace search methods: Search various subspaces to find clusters
  - Bottom-up approaches
  - Top-down approaches
- Correlation-based clustering methods
  - E.g., PCA based approaches
- Bi-clustering methods
  - Optimization-based methods
  - Enumeration methods

Subspace Clustering Method (I): Subspace Search Methods

- Search various subspaces to find clusters
- *Bottom-up approaches*
  - Start from low-D subspaces and search higher-D subspaces only when there may be clusters in such subspaces
  - Various pruning techniques to reduce the number of higher-D subspaces to be searched
  - Ex. CLIQUE (Agrawal et al. 1998)
- *Top-down approaches*
  - Start from full space and search smaller subspaces recursively
  - Effective only if the *locality assumption* holds: restricts that the subspace of a cluster can be determined by the local neighborhood
  - Ex. PROCLUS (Aggarwal et al. 1999): a *k*-medoid-like method

CLIQUE: SubSpace Clustering with Aprori Pruning

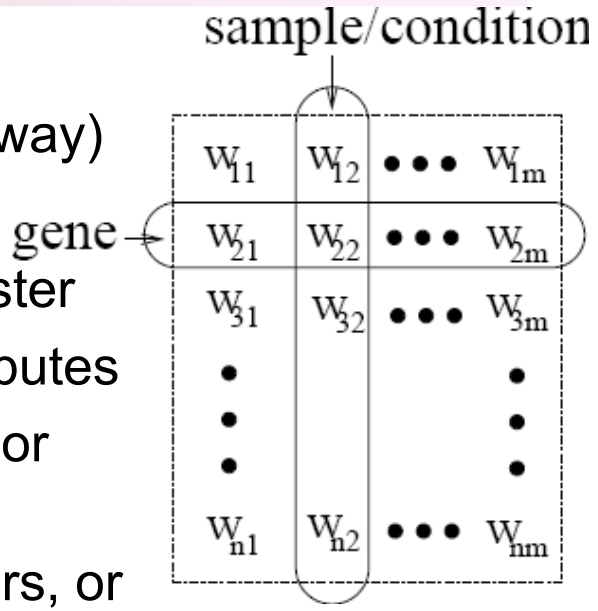


Subspace Clustering Method (II): Correlation-Based Methods

- Subspace search method: similarity based on distance or density
- Correlation-based method: based on advanced correlation models
- Ex. PCA-based approach:
  - Apply PCA (for Principal Component Analysis) to derive a set of new, uncorrelated dimensions,
  - then mine clusters in the new space or its subspaces
- Other space transformations:
  - Hough transform
  - Fractal dimensions

Subspace Clustering Method (III): Bi-Clustering Methods

- Bi-clustering: Cluster both objects and attributes simultaneously (treat objs and attrs in symmetric way)
- Four requirements:
  - Only a small set of objects participate in a cluster
  - A cluster only involves a small number of attributes
  - An object may participate in multiple clusters, or does not participate in any cluster at all
  - An attribute may be involved in multiple clusters, or is not involved in any cluster at all



- Ex 1. *Gene expression* or *microarray data:* a gene sample/condition matrix.
  - Each element in the matrix, a real number, records the expression level of a gene under a specific condition
- Ex. 2. Clustering customers and products
  - Another bi-clustering problem

	products			
customers	w_{11}	w_{12}	$\cdots$	w_{1m}
	w_{21}	w_{22}	$\cdots$	w_{2m}
	$\cdots$	$\cdots$	$\cdots$	$\cdots$
	w_{n1}	w_{n2}	$\cdots$	w_{nm}

Types of Bi-clusters

- Let A = {a_1, ..., a_n} be a set of genes, B = {b_1, …, b_n} a set of conditions
- A bi-cluster: A submatrix where genes and conditions follow some consistent patterns
- 4 types of bi-clusters (ideal cases)
  - Bi-clusters with constant values:
    - for any *i* in *I* and *j in J*, $e_{ij} = c$
  - Bi-clusters with constant values on rows:
    - $e_{ij} = c + \alpha_i$
    - Also, it can be constant values on columns
  - Bi-clusters with *coherent values* (aka. *pattern-based clusters*)
    - $e_{ij} = c + \alpha_i + \beta_j$
  - Bi-clusters with *coherent* evolutions on rows
    - e_{ij} $(e_{i1j1} - e_{i1j2})(e_{i2j1} - e_{i2j2}) \geq 0$
    - i.e., only interested in the up- or down- regulated changes across genes or conditions without constraining on the exact values

10	10	10	10	10
20	20	20	20	20
50	50	50	50	50
0	0	0	0	0

10	50	30	70	20
20	60	40	80	30
50	90	70	110	60
0	40	20	60	10

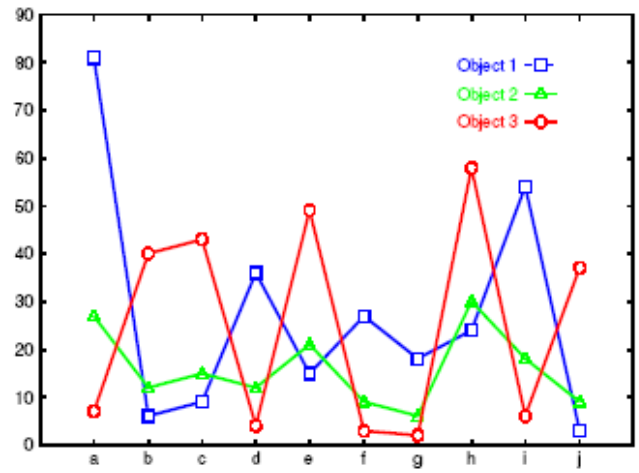
10	50	30	70	20
20	100	50	1000	30
50	100	90	120	80
0	80	20	100	10

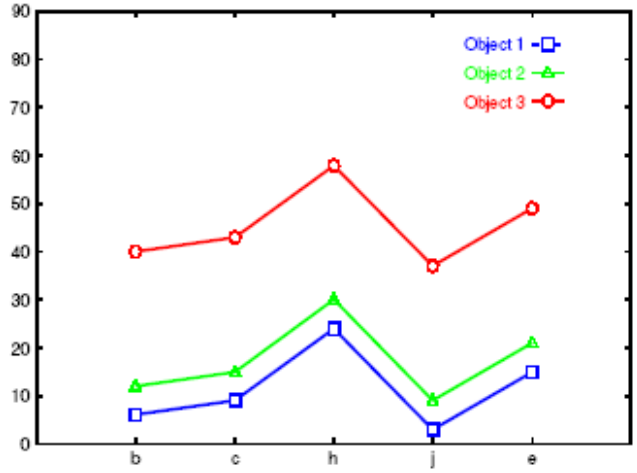
Bi-Clustering Methods

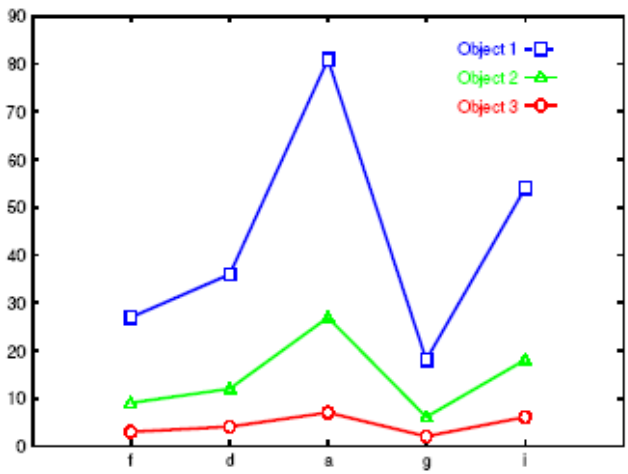
- Real-world data is noisy: Try to find approximate bi-clusters
- Methods: Optimization-based methods vs. enumeration methods
- Optimization-based methods
  - Try to find a submatrix at a time that achieves the best significance as a bi-cluster
  - Due to the cost in computation, greedy search is employed to find local optimal bi-clusters
  - Ex. δ-Cluster Algorithm (Cheng and Church, ISMB'2000)
- Enumeration methods
  - Use a tolerance threshold to specify the degree of noise allowed in the bi-clusters to be mined
  - Then try to enumerate all submatrices as bi-clusters that satisfy the requirements
  - Ex. δ-pCluster Algorithm (H. Wang et al.' SIGMOD'2002, MaPle: Pei et al., ICDM'2003)

Bi-Clustering for Micro-Array Data Analysis

- Left figure: Micro-array “raw” data shows 3 genes and their values in a multi-D space: Difficult to find their patterns
- Right two: Some subsets of dimensions form nice shift and scaling patterns
- No globally defined similarity/distance measure
- Clusters may not be exclusive
  - An object can appear in multiple clusters







Bi-Clustering (I): δ-Bi-Cluster

- For a submatrix *I x J,* the mean of the *i*-th row: $e_{iJ} = \frac{1}{|J|} \sum_{j \in J} e_{ij}$
  - The mean of the *j*-th column: $e_{Ij} = \frac{1}{|I|} \sum_{i \in I} e_{ij}$
  - The mean of all elements in the submatrix is

$$e_{IJ} = \frac{1}{|I||J|} \sum_{i \in I, j \in J} e_{ij} = \frac{1}{|I|} \sum_{i \in I} e_{iJ} = \frac{1}{|J|} \sum_{j \in J} e_{Ij}$$

  - The quality of the submatrix as a bi-cluster can be measured by the *mean squared residue* value

$$H(I \times J) = \frac{1}{|I||J|} \sum_{i \in I, j \in J} (e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2$$

- A submatrix *I x J* is **δ-bi-cluster** if $H(I \times J) \leq \delta$ where $\delta \geq 0$ is a threshold. When $\delta = 0$, *I x J* is a perfect bi-cluster with coherent values. By setting $\delta > 0$, a user can specify the tolerance of average noise per element against a perfect bi-cluster
  - residue(e_{ij}) = $e_{ij} - e_{iJ} - e_{Ij} + e_{IJ}$

Bi-Clustering (I): The δ-Cluster Algorithm

- **Maximal δ-bi-cluster** is a **δ**-bi-cluster *I x J* such that there does not exist another **δ**-bi-cluster *I′ x J′ which* contains *I x J*
- Computing is costly: Use heuristic greedy search to obtain local optimal clusters
- Two phase computation: deletion phase and additional phase
- Deletion phase: Start from the whole matrix, iteratively remove rows and columns while the mean squared residue of the matrix is over **δ**
  - At each iteration, for each row/*column*, compute the *mean squared residue:*

$$d(i) = \frac{1}{|J|}\sum_{j \in J}(e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2 \qquad d(j) = \frac{1}{|I|}\sum_{i \in I}(e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2$$

  - Remove the row or column of the largest mean squared residue
- Addition phase:
  - Expand iteratively the **δ**-bi-cluster *I x J* obtained in the deletion phase as long as the **δ**-bi-cluster requirement is maintained
  - Consider all the rows/columns not involved in the current bi-cluster *I x J* by calculating their mean squared residues
  - A row/column of the smallest mean squared residue is added into the current **δ**-bi-cluster
- It finds only one **δ**-bi-cluster, thus needs to run multiple times: replacing the elements in the output bi-cluster by random numbers

Bi-Clustering (II): δ-pCluster

- Enumerating all bi-clusters (δ-pClusters) [H. Wang, et al., Clustering by pattern similarity in large data sets. SIGMOD'02]
- Since a submatrix *I x J* is a bi-cluster with (perfect) coherent values iff $e_{i1j1} - e_{i2j1} = e_{i1j2} - e_{i2j2}$. For any 2 *x* 2 submatrix of *I x J*, define *p-score*

$$p\text{-score}\begin{pmatrix} e_{i_1j_1} & e_{i_1j_2} \\ e_{i_2j_1} & e_{i_2j_2} \end{pmatrix} = |(e_{i_1j_1} - e_{i_2j_1}) - (e_{i_1j_2} - e_{i_2j_2})|$$

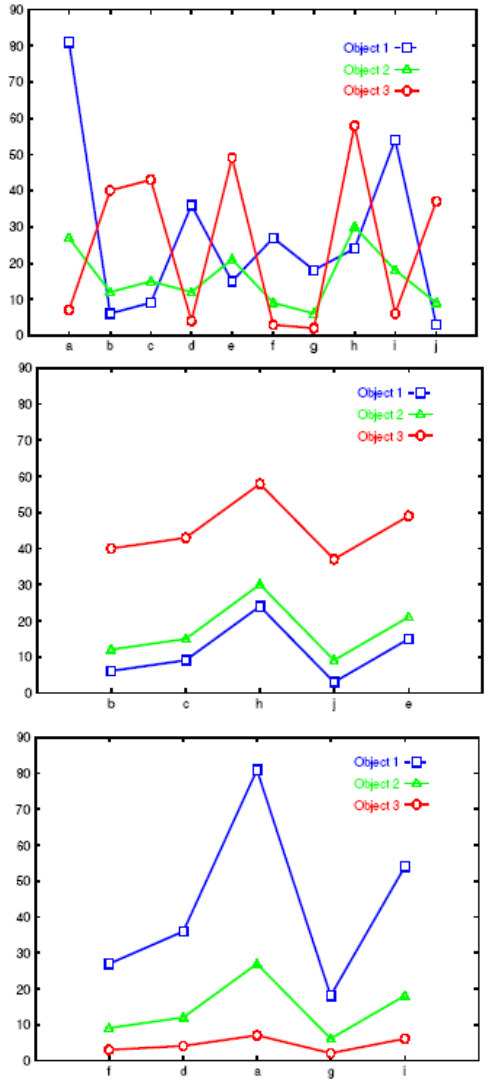
- A submatrix *I x J* is a **δ-pCluster** (pattern-based cluster) if the *p*-score of every 2 *x* 2 submatrix of *I x J* is at most δ, where δ ≥ 0 is a threshold specifying a user's tolerance of noise against a perfect bi-cluster
- The *p*-score controls the noise on every element in a bi-cluster, while the mean squared residue captures the average noise
- **Monotonicity**: If *I* x *J* is a δ-pClusters, every *x* x *y* (*x,y* ≥ 2) submatrix of *I* x *J* is also a δ-pClusters.
- A δ-pCluster is **maximal** if no more row or column can be added into the cluster and retain δ-pCluster: We only need to compute all maximal δ-pClusters.

MaPle: Efficient Enumeration of δ-pClusters

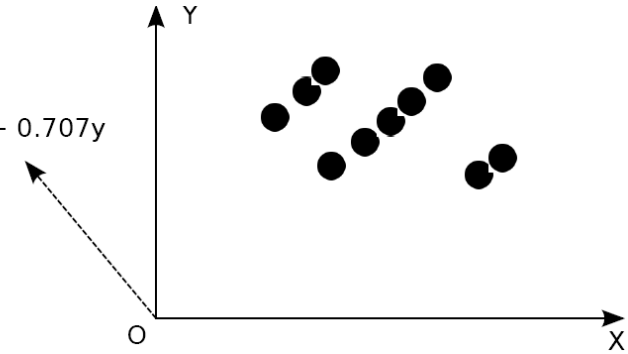
- Pei et al., MaPle: Efficient enumerating all maximal δ-pClusters. ICDM'03
- Framework: Same as pattern-growth in frequent pattern mining (based on the downward closure property)
- For each condition combination J, find the maximal subsets of genes I such that I x J is a δ-pClusters
  - If I x J is not a submatrix of another δ-pClusters
  - then I x J is a maximal δ-pCluster.
- Algorithm is very similar to mining frequent closed itemsets
- Additional advantages of δ-pClusters:
  - Due to averaging of δ-cluster, it may contain outliers but still within δ-threshold
  - Computing bi-clusters for scaling patterns, take logarithmic on

$$\frac{d_{xa} / d_{ya}}{d_{xb} / d_{yb}} < \delta$$

will lead to the p-score form



Dimensionality-Reduction Methods

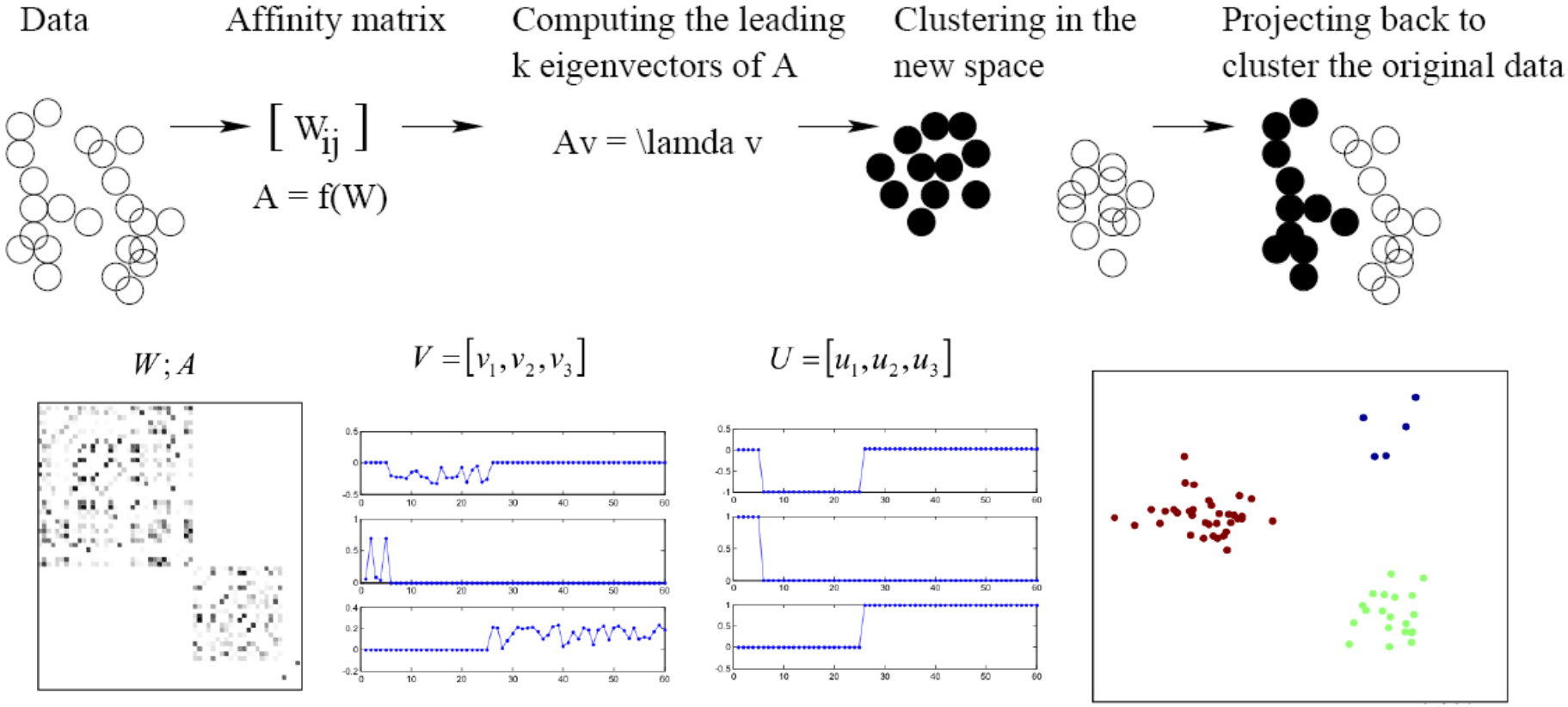


- Dimensionality reduction: In some situations, it is more effective to construct a new space instead of using some subspaces of the original data
- Ex. To cluster the points in the right figure, any subspace of the original one, X and Y, cannot help, since all the three clusters will be projected into the overlapping areas in X and Y axes.
  - Construct a new dimension as the dashed one, the three clusters become apparent when the points projected into the new dimension
- Dimensionality reduction methods
  - Feature selection and extraction: But may not focus on clustering structure finding
  - Spectral clustering: Combining feature extraction and clustering (i.e., use the *spectrum* of the similarity matrix of the data to perform dimensionality reduction for clustering in fewer dimensions)
    - Normalized Cuts (Shi and Malik, CVPR'97 or PAMI'2000)
    - The Ng-Jordan-Weiss algorithm (NIPS'01)

Spectral Clustering: The Ng-Jordan-Weiss (NJW) Algorithm

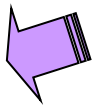
- Given a set of objects o_1, …, o_n, and the distance between each pair of objects, dist(o_i, o_j), find the desired number k of clusters
- Calculate an affinity matrix W, where σ is a scaling parameter that controls how fast the affinity W_{ij} decreases as dist(o_i, o_j) increases. In NJW, set $W_{ij} = 0$ $D_{ii} = \sum_{j=1}^{n} W_{ij}$
- Derive a matrix A = *f*(W). NJW defines a matrix D to be a diagonal matrix s.t. D_{ii} is the sum of the i-th row of W, i.e., $W_{ij} = e^{-\frac{dist(o_i, o_j)}{\sigma^2}}$
  Then, A is set to $A = D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$
- A spectral clustering method finds the k leading eigenvectors of A
  - A vector v is an eigenvector of matrix A if Av = λv, where λ is the corresponding eigen-value
- Using the k leading eigenvectors, project the original data into the new space defined by the k leading eigenvectors, and run a clustering algorithm, such as *k*-means, to find k clusters
- Assign the original data points to clusters according to how the transformed points are assigned in the clusters obtained

Spectral Clustering: Illustration and Comments



- Spectral clustering: Effective in tasks like image processing
- Scalability challenge: Computing eigenvectors on a large matrix is costly
- Can be combined with other clustering methods, such as bi-clustering

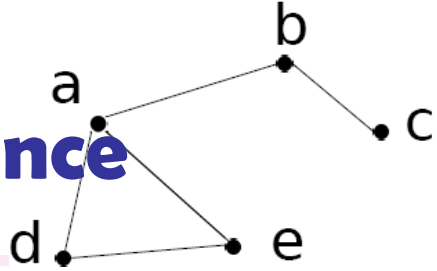
Chapter 11. Cluster Analysis: Advanced Methods

- Probability Model-Based Clustering
- Clustering High-Dimensional Data
- Clustering Graphs and Network Data 
- Clustering with Constraints
- Summary

Clustering Graphs and Network Data

- Applications
  - Bi-partite graphs, e.g., customers and products, authors and conferences
  - Web search engines, e.g., click through graphs and Web graphs
  - Social networks, friendship/coauthor graphs
- Similarity measures
  - Geodesic distances
  - Distance based on random walk (SimRank)
- Graph clustering methods
  - Minimum cuts: FastModularity (Clauset, Newman & Moore, 2004)
  - Density-based clustering: SCAN (Xu et al., KDD'2007)

Similarity Measure (I): Geodesic Distance



- Geodesic distance (A, B): length (i.e., # of edges) of the shortest path between A and B (if not connected, defined as infinite)
- **Eccentricity** of v, eccen(v): The largest geodesic distance between v and any other vertex $u \in V - \{v\}$.
  - E.g., eccen(a) = eccen(b) = 2; eccen(c) = eccen(d) = eccen(e) = 3
- **Radius** of graph G: The minimum eccentricity of all vertices, i.e., the distance between the "most central point" and the "farthest border"
  - $r = \min_{v \in V} eccen(v)$
  - E.g., radius (g) = 2
- **Diameter** of graph G: The maximum eccentricity of all vertices, i.e., the largest distance between any pair of vertices in G
  - $d = \max_{v \in V} eccen(v)$
  - E.g., diameter (g) = 3
- A **peripheral vertex** is a vertex that achieves the diameter.
  - E.g., Vertices c, d, and e are peripheral vertices

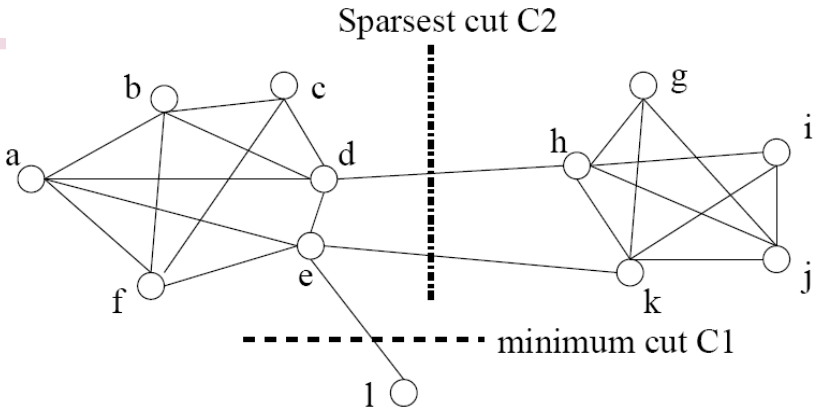
SimRank: Similarity Based on Random Walk and Structural Context

- SimRank: structural-context similarity, i.e., based on the similarity of its neighbors
- In a directed graph G = (V,E),
  - *individual in-neighborhood* of v: I(v) = {u | (u, v) ∈ E}
  - *individual out-neighborhood* of v: O(v) = {w | (v, w) ∈ E}
- Similarity in SimRank: $s(u,v) = \frac{C}{|I(u)||I(v)|} \sum_{x \in I(u)} \sum_{y \in I(v)} s(x,y)$
  - Initialization: $s_0(u,v) = \begin{cases} 0 & \text{if } u \neq v \\ 1 & \text{if } u = v \end{cases}$
  - Then we can compute s_{i+1} from s_i based on the definition
- Similarity based on random walk: in a strongly connected component
  - Expected distance: $d(u,v) = \sum_{t:u \rightsquigarrow v} P[t]l(t)$
  - Expected meeting distance: $m(u,v) = \sum_{t:(u,v) \rightsquigarrow (x,x)} P[t]l(t)$
  - Expected meeting probability: $p(u,v) = \sum_{t:(u,v) \rightsquigarrow (x,x)} P[t]C^{l(t)}$

$$P[t] = \begin{cases} \prod_{i=1}^{k-1} \frac{1}{|O(w_i)|} & \text{if } l(t) > 0 \\ 0 & \text{if } l(t) = 0. \end{cases}$$

P[t] is the probability of the tour

Graph Clustering: Sparsest Cut



- G = (V,E). The *cut set* of a cut is the set of edges {(u, v) ∈ E | u ∈ S, v ∈ T } and S and T are in two partitions
- *Size* of the cut: # of edges in the cut set
- Min-cut (e.g., C_1) is not a good partition
- A better measure: **Sparsity**: $$\Phi = \frac{\text{the size of the cut}}{\min\{|S|, |T|\}}$$
- A cut is ***sparsest*** if its sparsity is not greater than that of any other cut
- Ex. Cut C2 = ({a, b, c, d, e, f, l}, {g, h, i, j, k}) is the sparsest cut
- For k clusters, the **modularity** of a clustering assesses the quality of the clustering: $$Q = \sum_{i=1}^{k} \left(\frac{l_i}{|E|} - \left(\frac{d_i}{2|E|}\right)^2\right)$$

  l_i: # edges between vertices in the i-th cluster
  d_i: the sum of the degrees of the vertices in the i-th cluster
- The *modularity* of a clustering of a graph is the difference between the fraction of all edges that fall into individual clusters and the fraction that would do so if the graph vertices were randomly connected
- The optimal clustering of graphs maximizes the modularity

Graph Clustering: Challenges of Finding Good Cuts

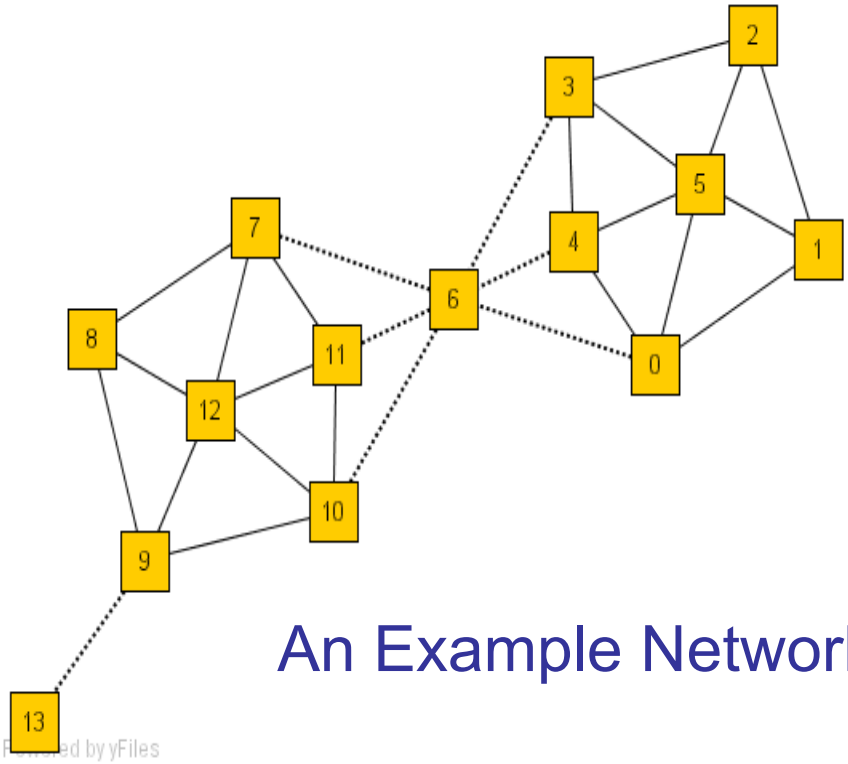
- High computational cost
  - Many graph cut problems are computationally expensive
  - The sparsest cut problem is NP-hard
  - Need to tradeoff between efficiency/scalability and quality
- Sophisticated graphs
  - May involve weights and/or cycles.
- High dimensionality
  - A graph can have many vertices. In a similarity matrix, a vertex is represented as a vector (a row in the matrix) whose dimensionality is the number of vertices in the graph
- Sparsity
  - A large graph is often sparse, meaning each vertex on average connects to only a small number of other vertices
  - A similarity matrix from a large sparse graph can also be sparse

Two Approaches for Graph Clustering

- Two approaches for clustering graph data
  - Use *generic clustering methods* for high-dimensional data
  - *Designed specifically for clustering graphs*
- Using clustering methods for high-dimensional data
  - Extract a similarity matrix from a graph using a similarity measure
  - A generic clustering method can then be applied on the similarity matrix to discover clusters
  - Ex. Spectral clustering: approximate optimal graph cut solutions
- Methods specific to graphs
  - Search the graph to find well-connected components as clusters
  - Ex. SCAN (Structural Clustering Algorithm for Networks)
    - X. Xu, N. Yuruk, Z. Feng, and T. A. J. Schweiger, “SCAN: A Structural Clustering Algorithm for Networks”, KDD'07

SCAN: Density-Based Clustering of Networks

- How many clusters?
- What size should they be?
- What is the best partitioning?
- Should some points be segregated?

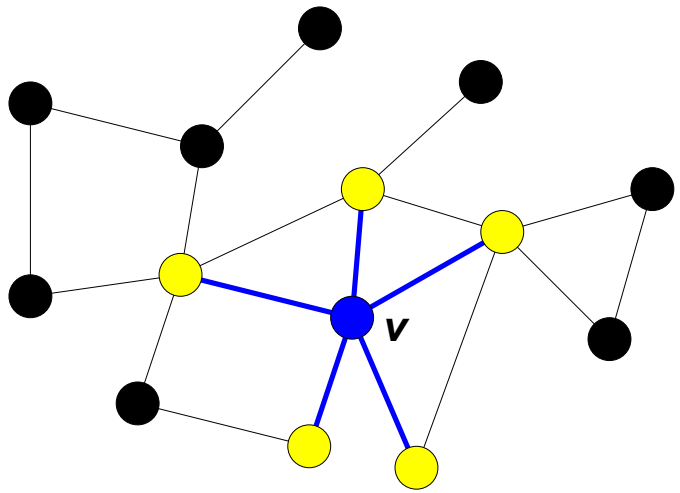


An Example Network

- Application: Given simply information of who associates with whom, could one identify clusters of individuals with common interests or special relationships (families, cliques, terrorist cells)?

A Social Network Model

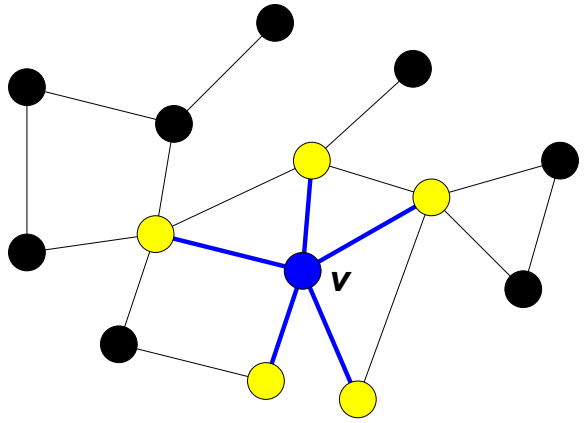
- Cliques, hubs and outliers
  - Individuals in a tight social group, or clique, know many of the same people, regardless of the size of the group
  - Individuals who are hubs know many people in different groups but belong to no single group. Politicians, for example bridge multiple groups
  - Individuals who are outliers reside at the margins of society. Hermits, for example, know few people and belong to no group
- The Neighborhood of a Vertex
  - Define $\Gamma(v)$ as the immediate neighborhood of a vertex (i.e. the set of people that an individual knows)



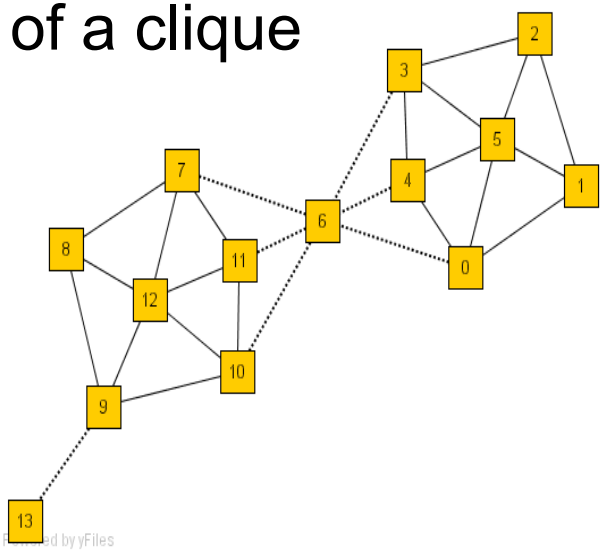
Structure Similarity

- The desired features tend to be captured by a measure we call Structural Similarity

$$\sigma(v,w) = \frac{|\Gamma(v) \bigcap \Gamma(w)|}{\sqrt{|\Gamma(v)||\Gamma(w)|}}$$



- Structural similarity is large for members of a clique and small for hubs and outliers



Structural Connectivity [1]

- ε-Neighborhood: $N_\varepsilon(v) = \{w \in \Gamma(v) \mid \sigma(v,w) \geq \varepsilon\}$
- Core: $CORE_{\varepsilon,\mu}(v) \Leftrightarrow \mid N_\varepsilon(v) \mid \geq \mu$
- Direct structure reachable:

$$DirRECH_{\varepsilon,\mu}(v,w) \Leftrightarrow CORE_{\varepsilon,\mu}(v) \wedge w \in N_\varepsilon(v)$$

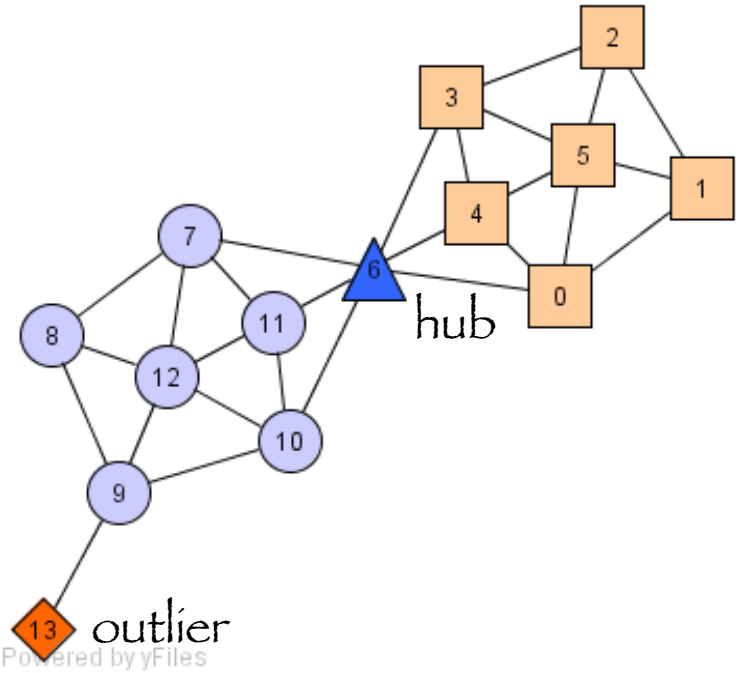
- Structure reachable: transitive closure of direct structure reachability
- Structure connected:

$$CONNECT_{\varepsilon,\mu}(v,w) \Leftrightarrow \exists u \in V : RECH_{\varepsilon,\mu}(u,v) \wedge RECH_{\varepsilon,\mu}(u,w)$$

[1] M. Ester, H. P. Kriegel, J. Sander, & X. Xu (KDD'96) “A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases

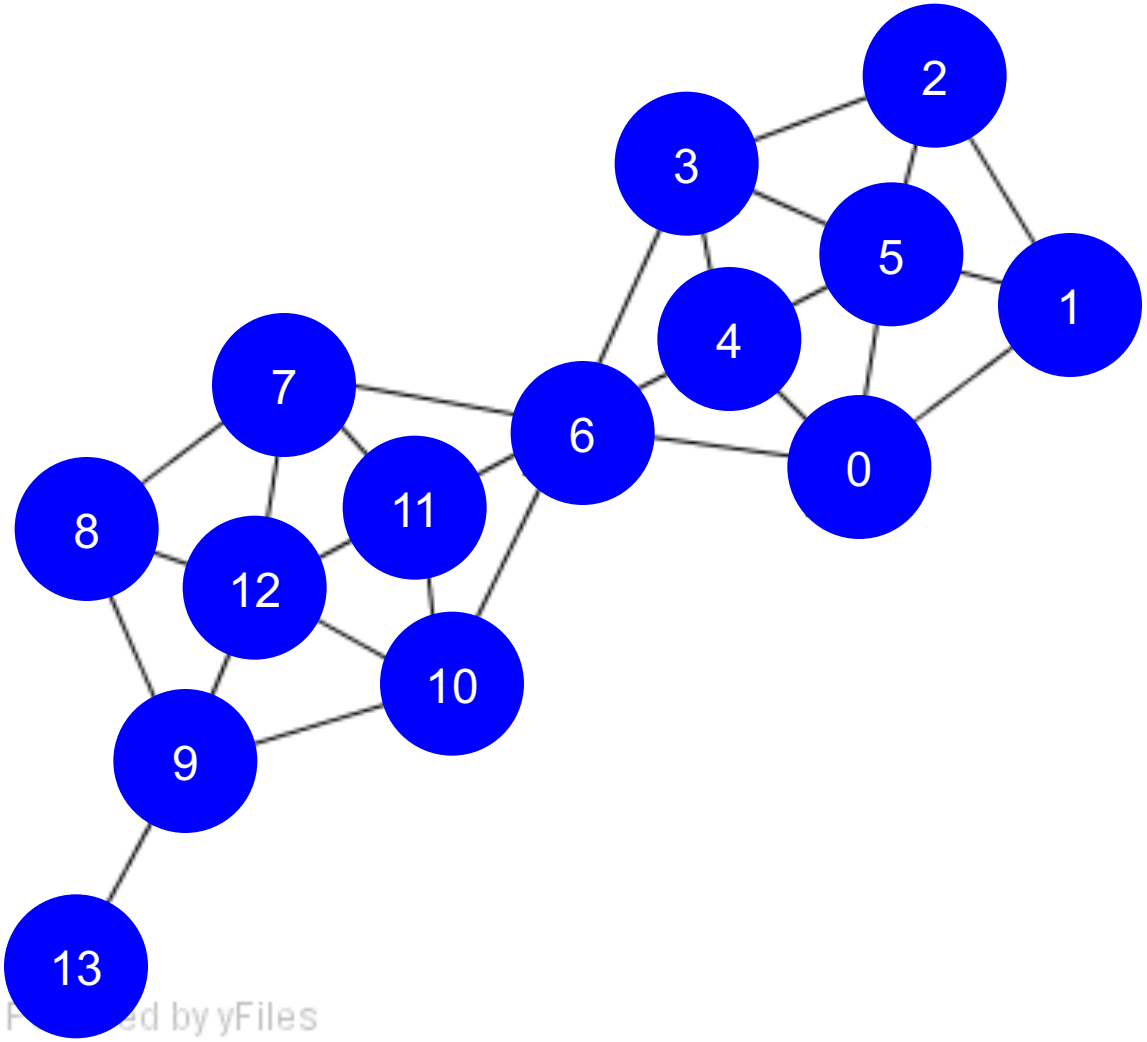
Structure-Connected Clusters

- Structure-connected cluster C
  - Connectivity: $\forall v, w \in C : CONNECT_{\varepsilon,\mu}(v, w)$
  - Maximality: $\forall v, w \in V : v \in C \wedge REACH_{\varepsilon,\mu}(v, w) \Rightarrow w \in C$
- Hubs:
  - Not belong to any cluster
  - Bridge to many clusters
- Outliers:
  - Not belong to any cluster
  - Connect to less clusters



Algorithm

$\mu = 2$
$\varepsilon = 0.7$



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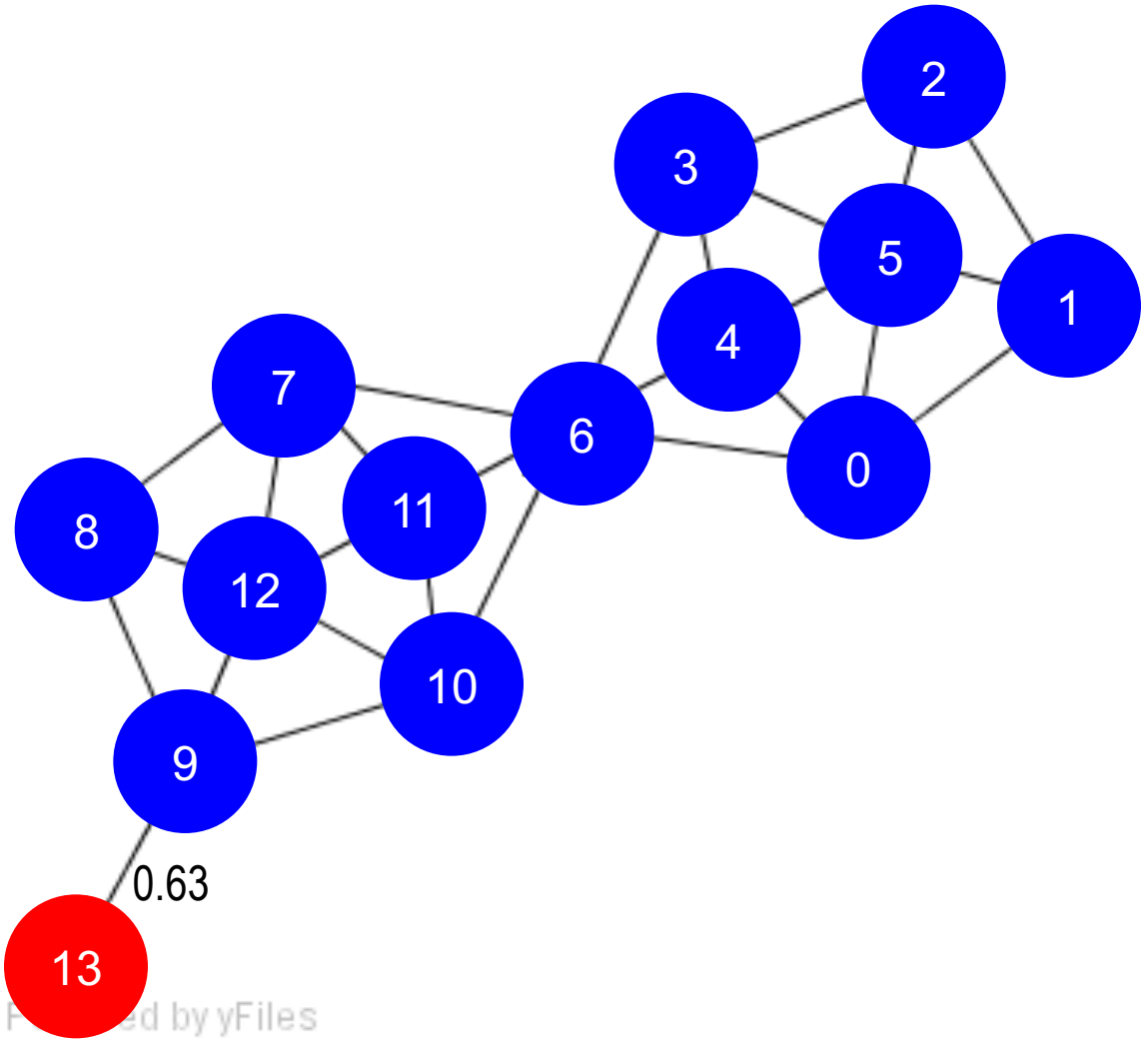

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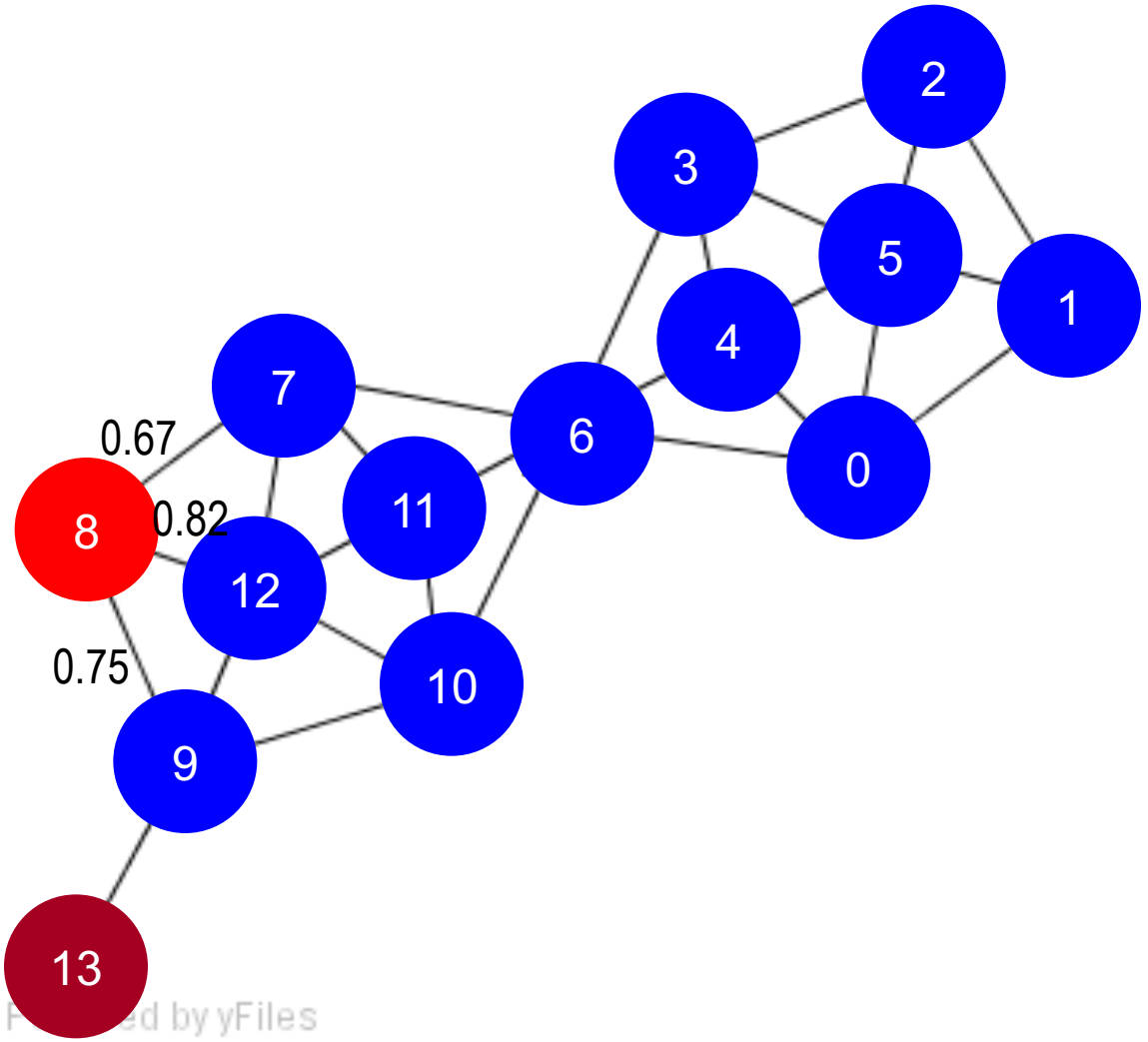

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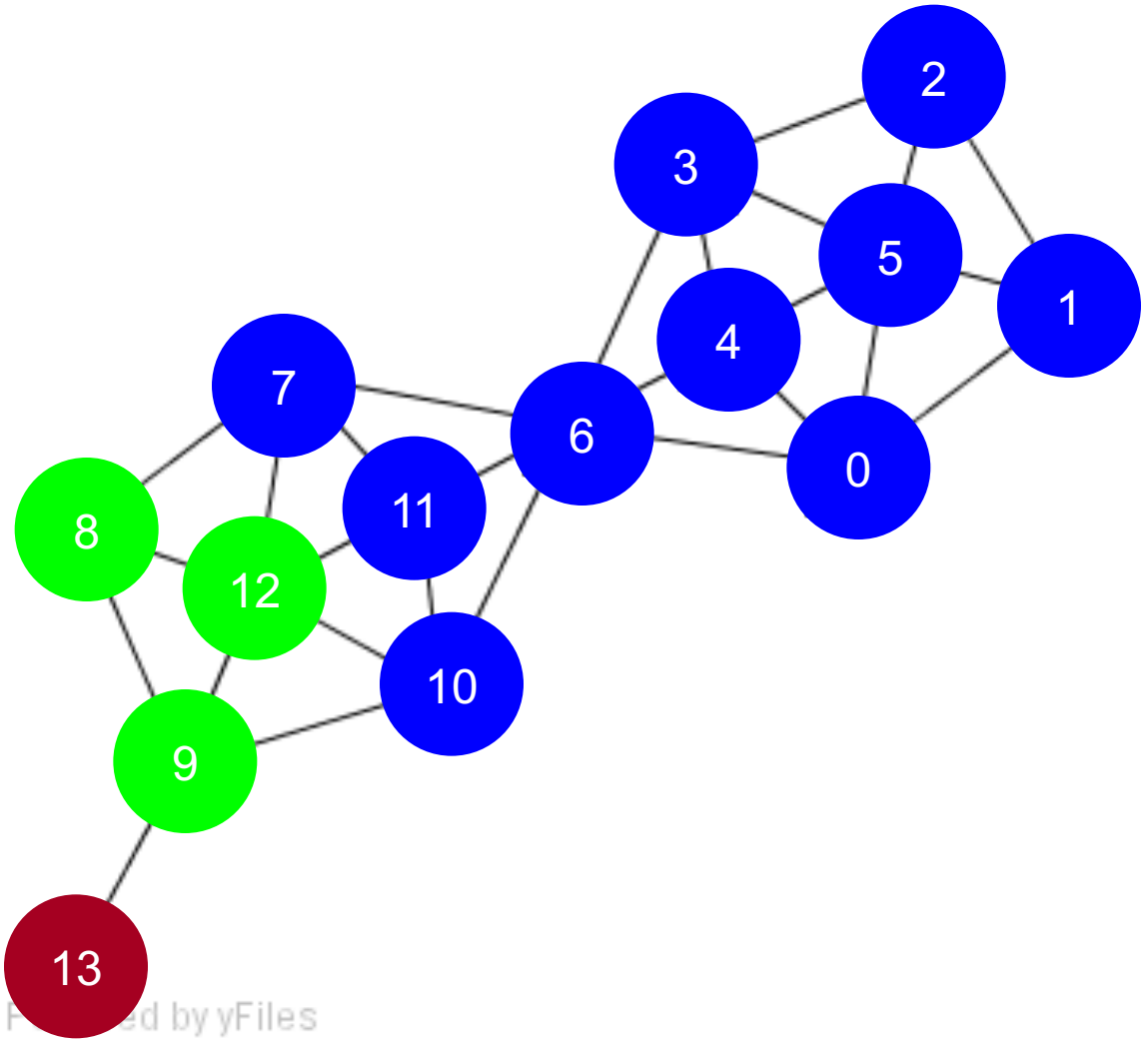

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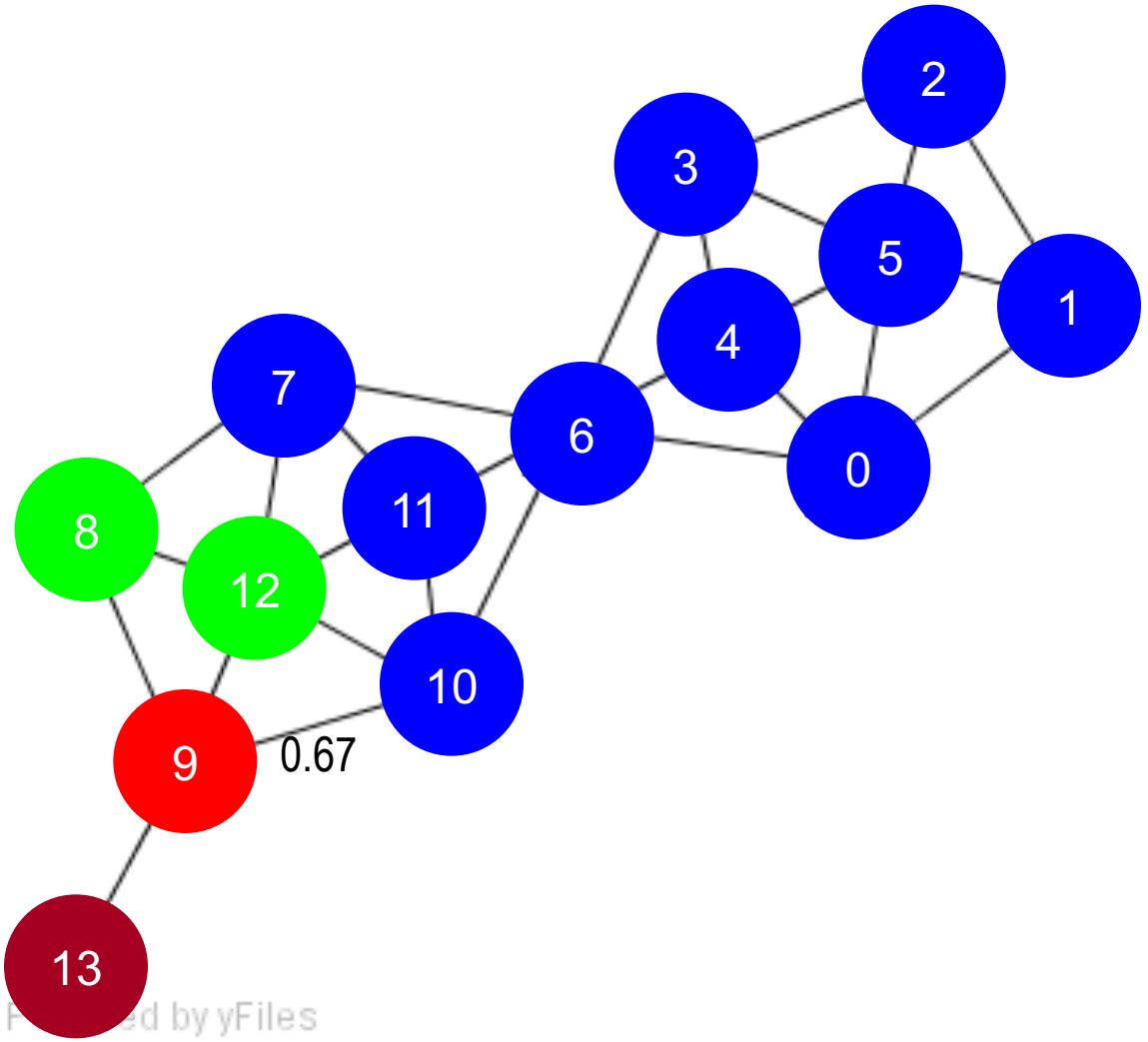

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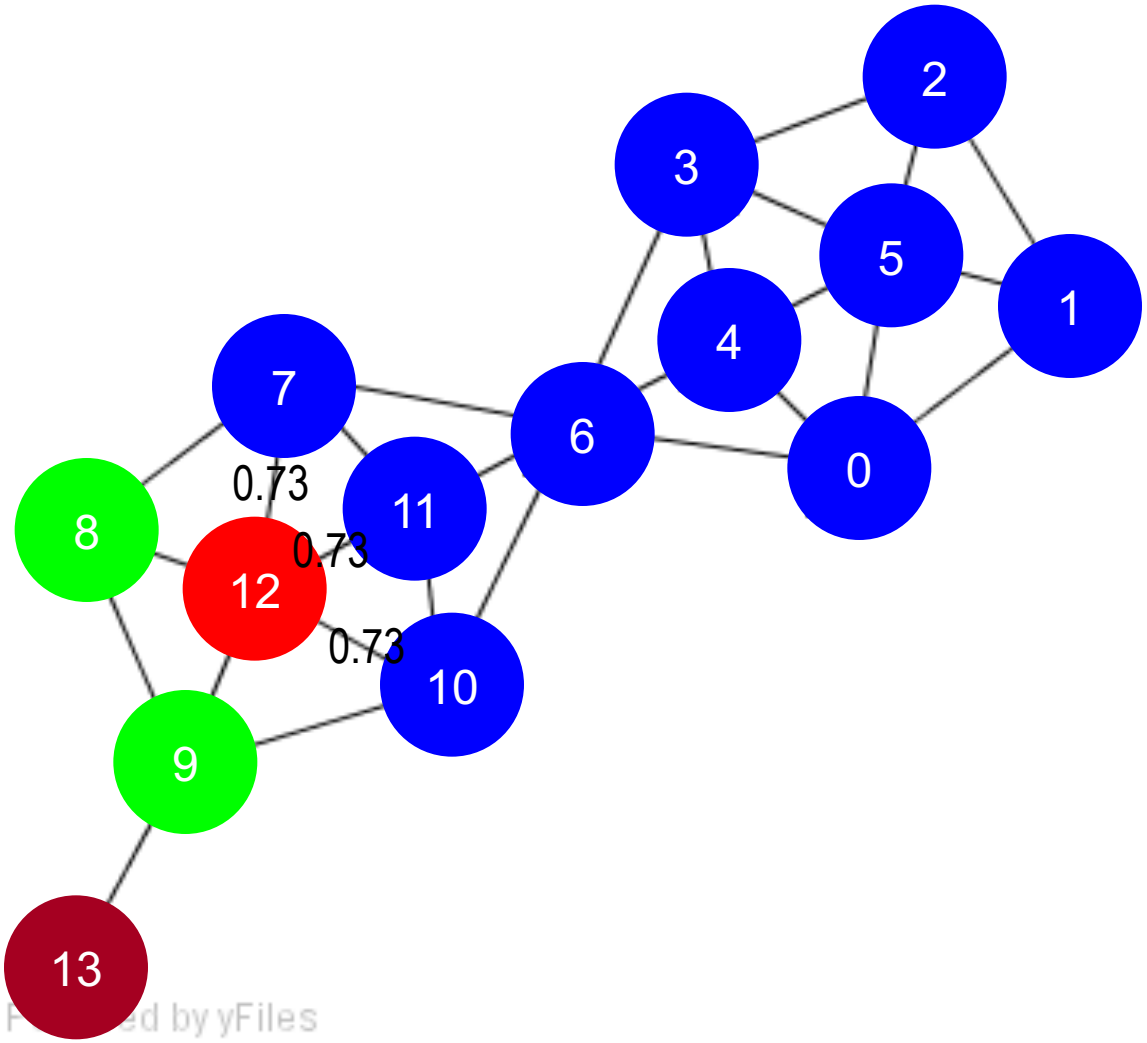

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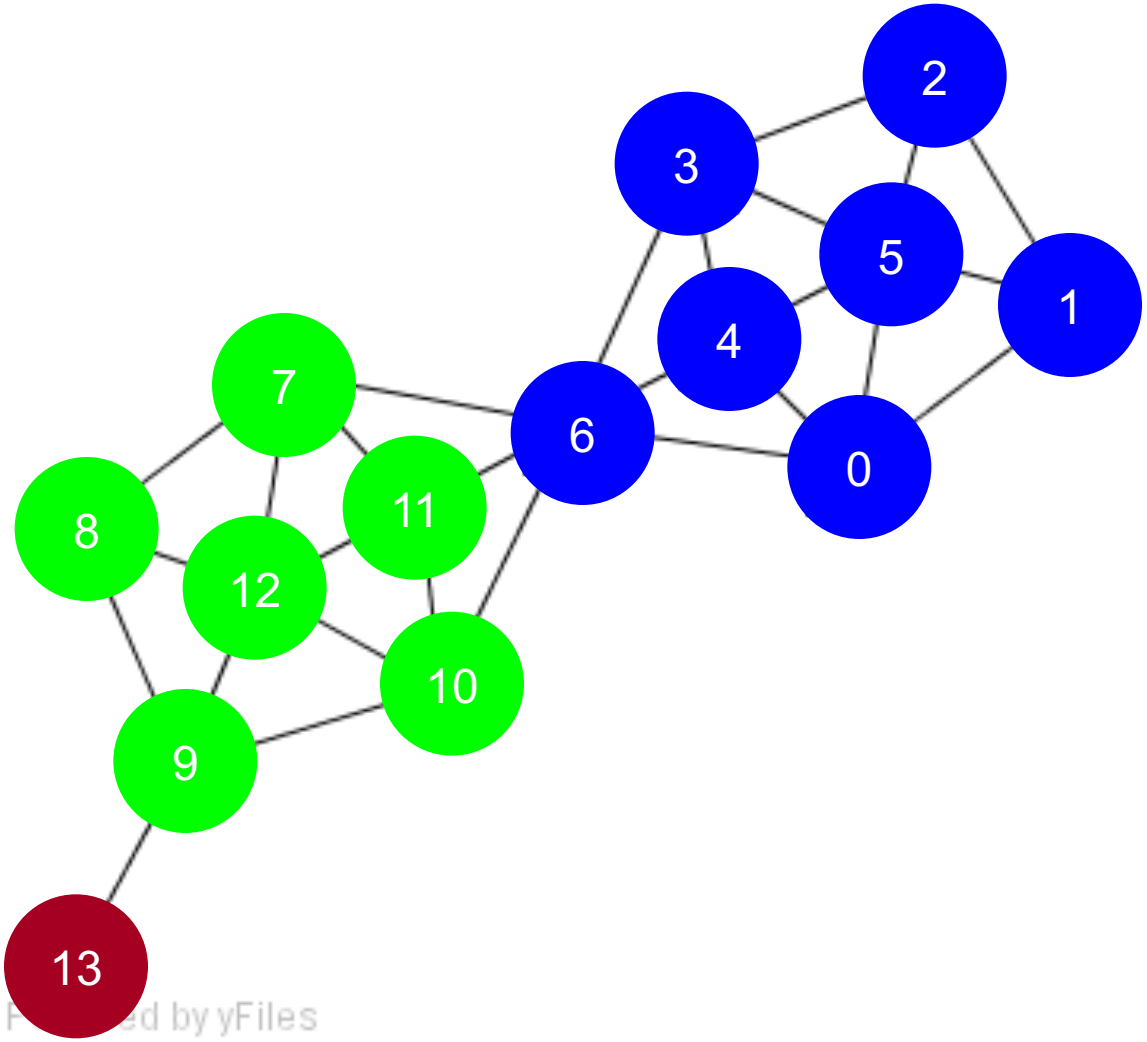

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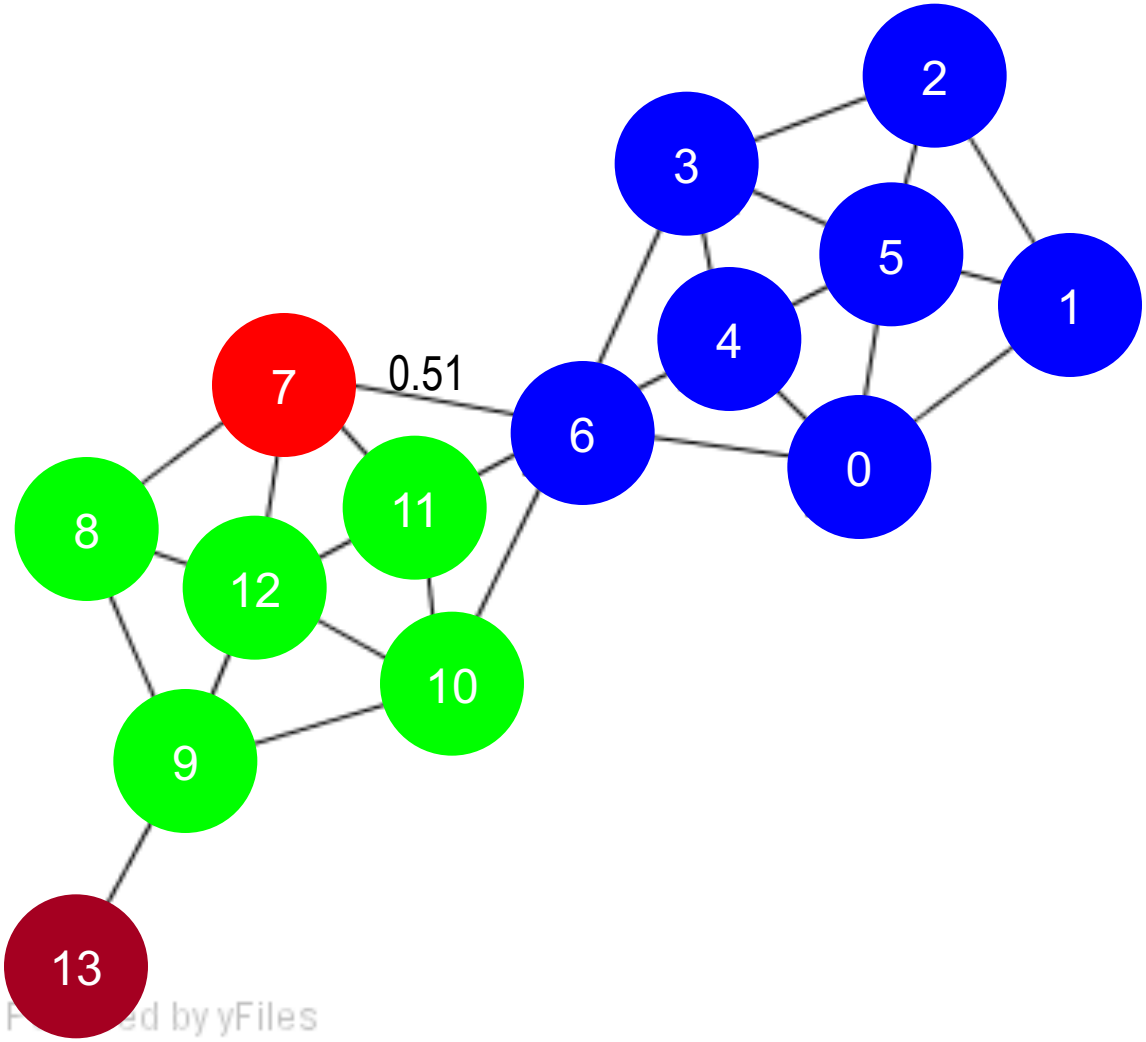

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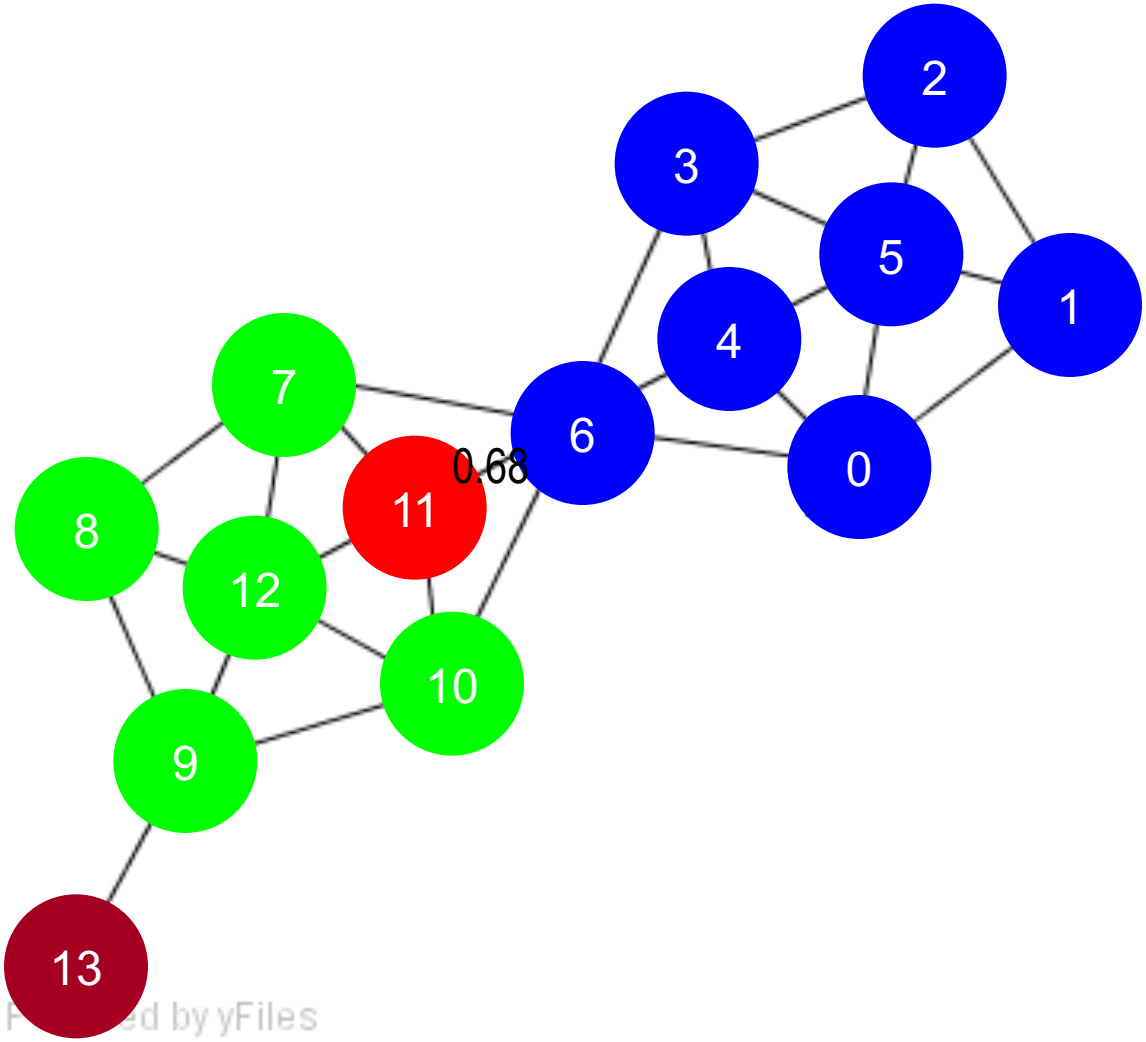

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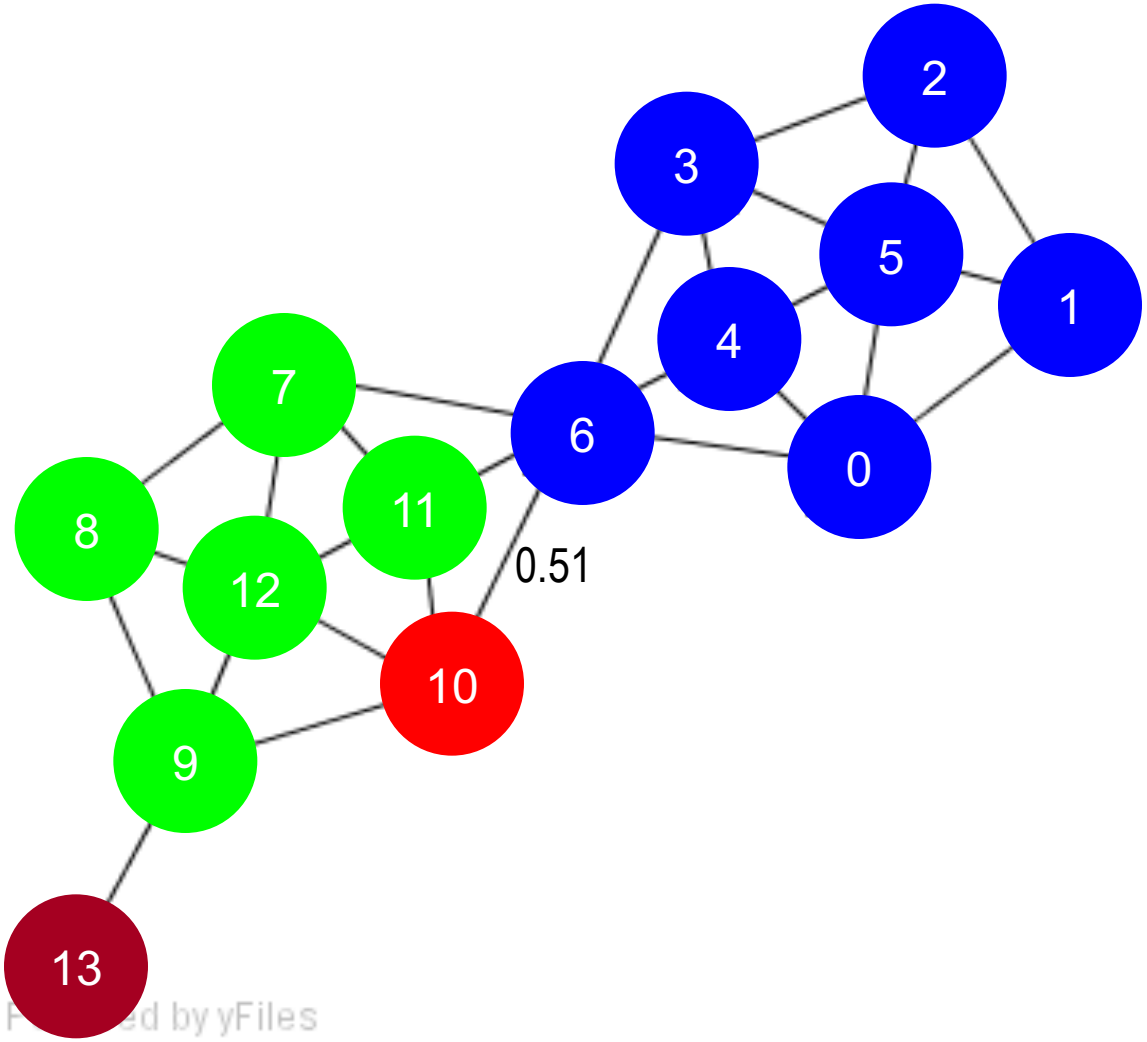

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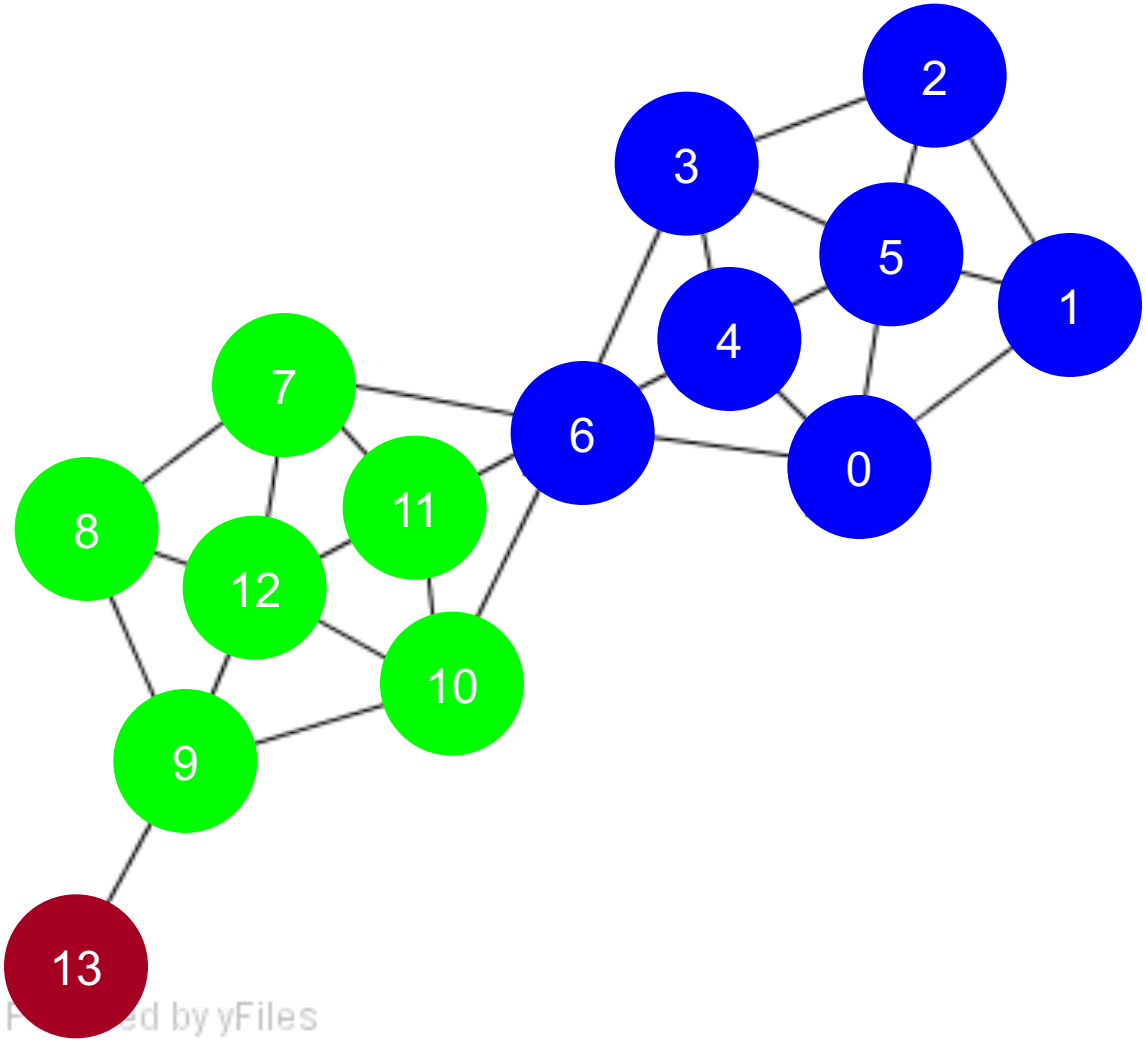

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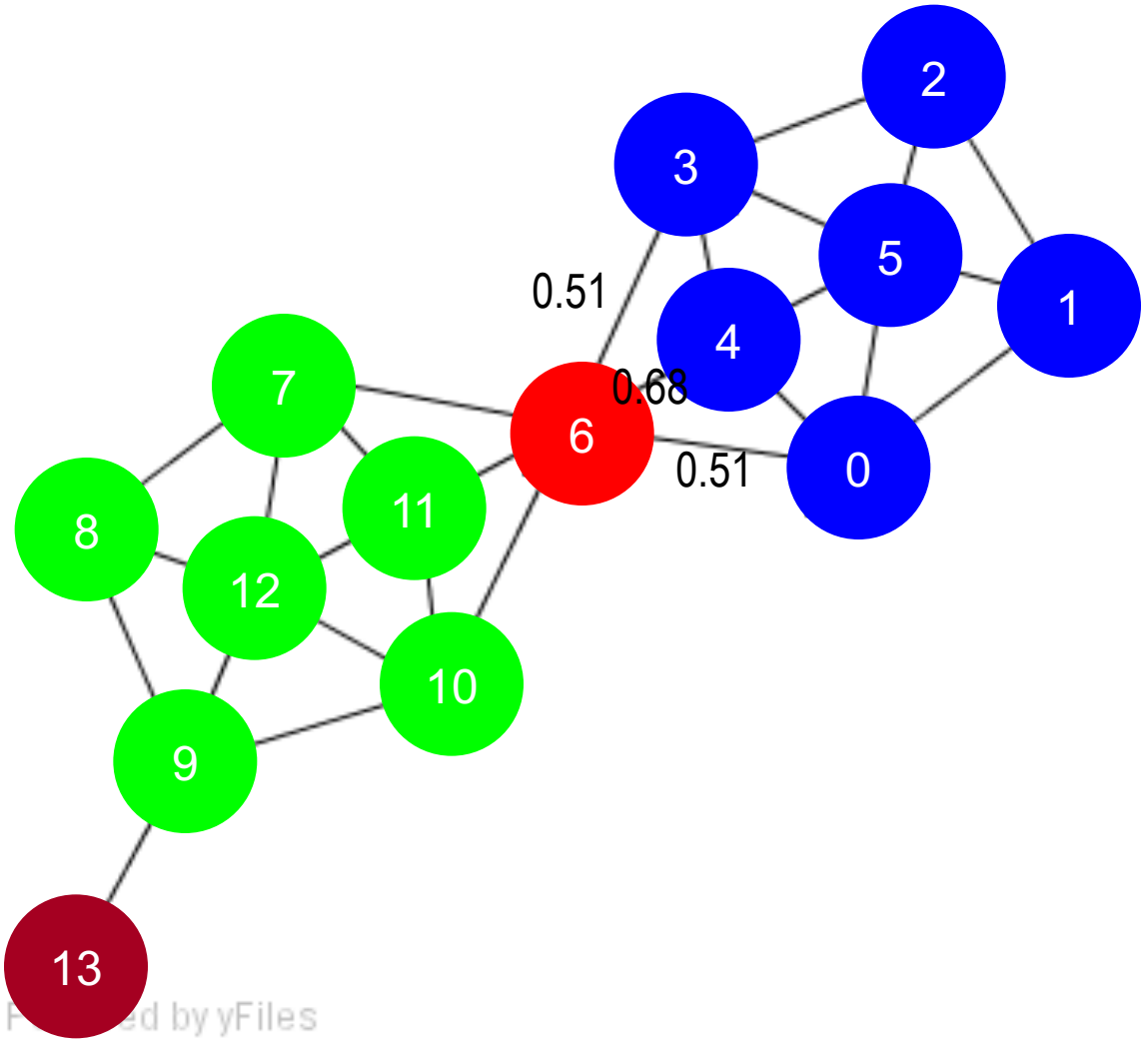

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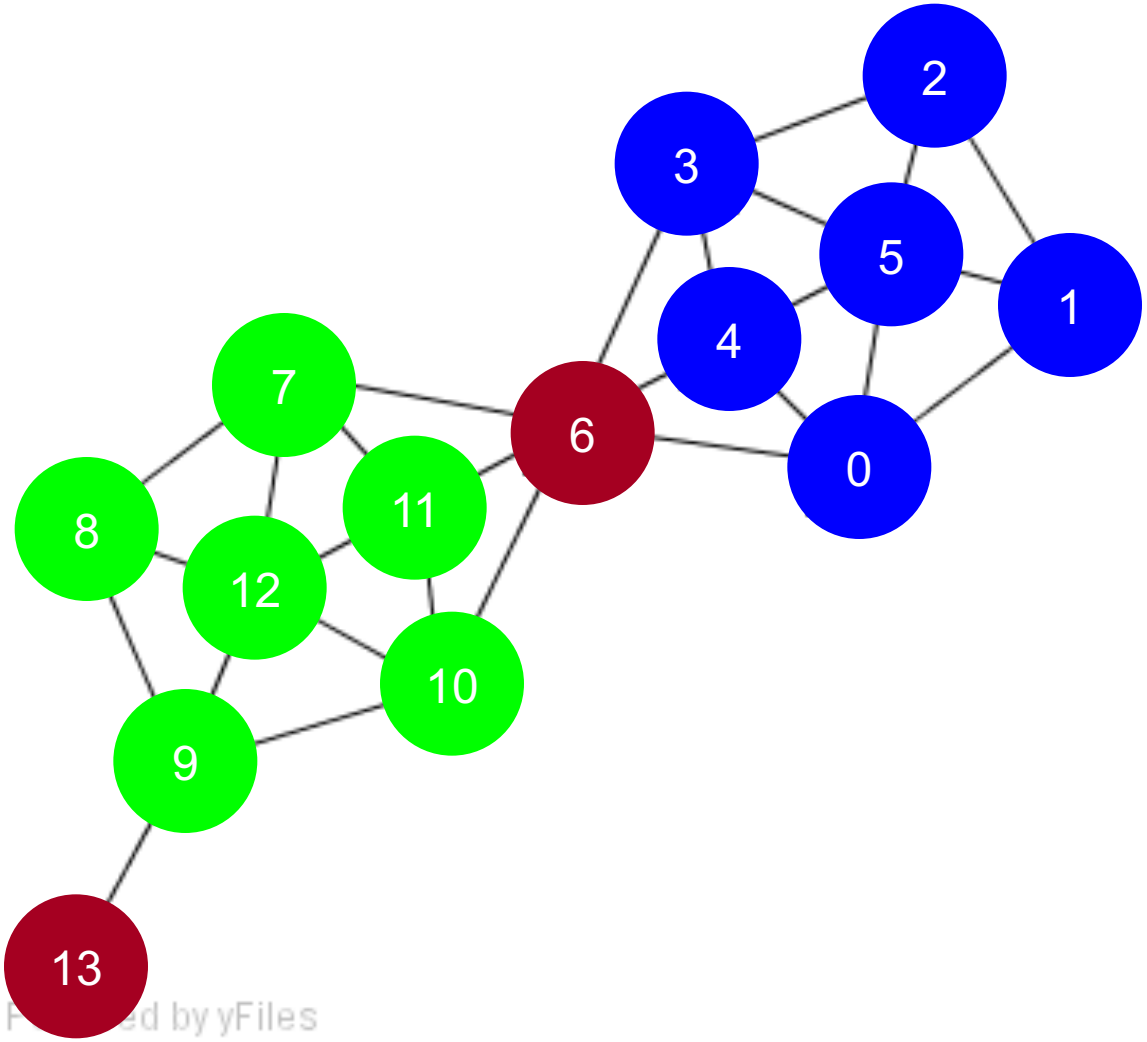
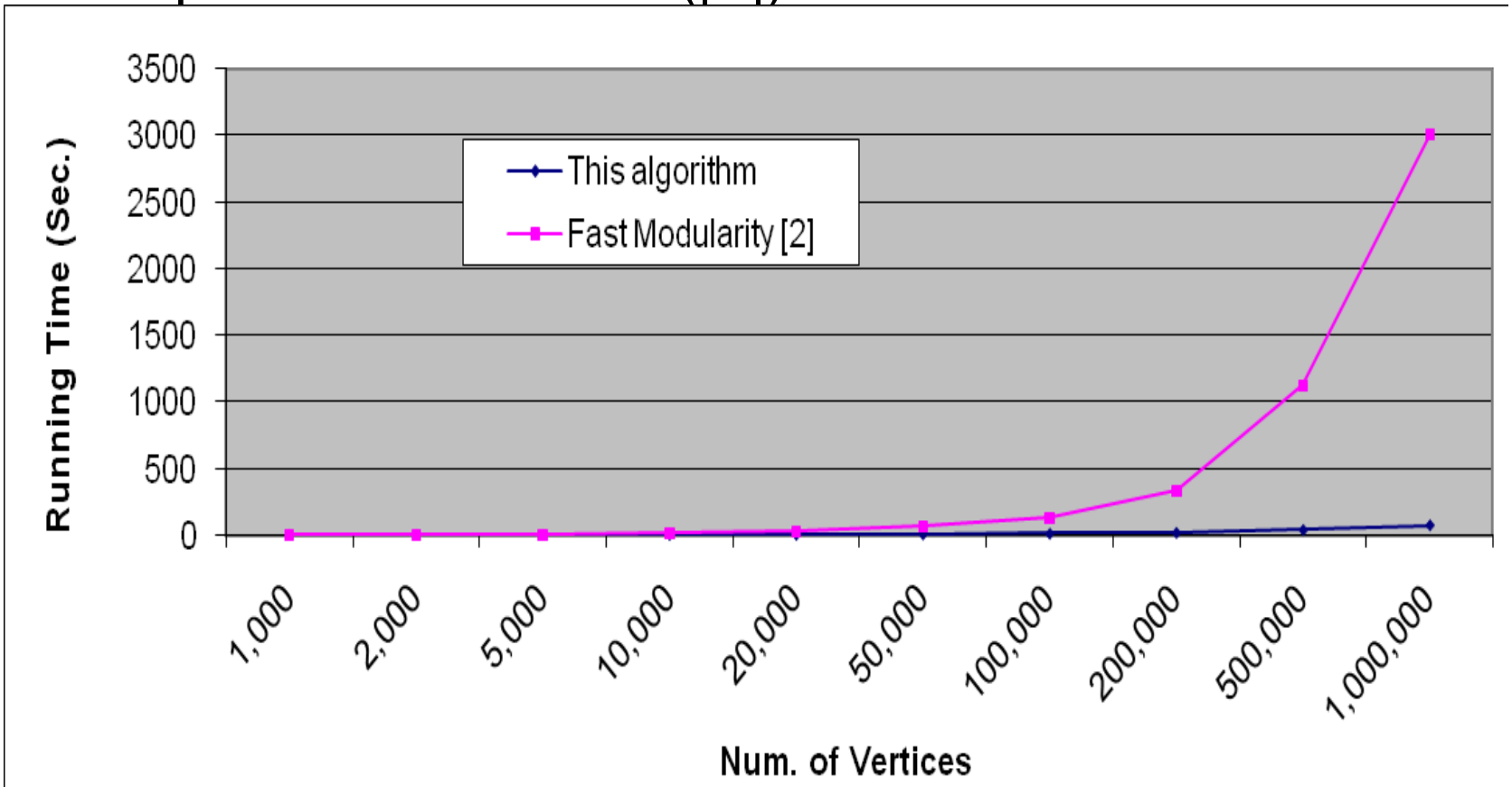


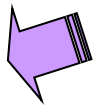
Running Time

- Running time = $O(|E|)$
- For sparse networks = $O(|V|)$



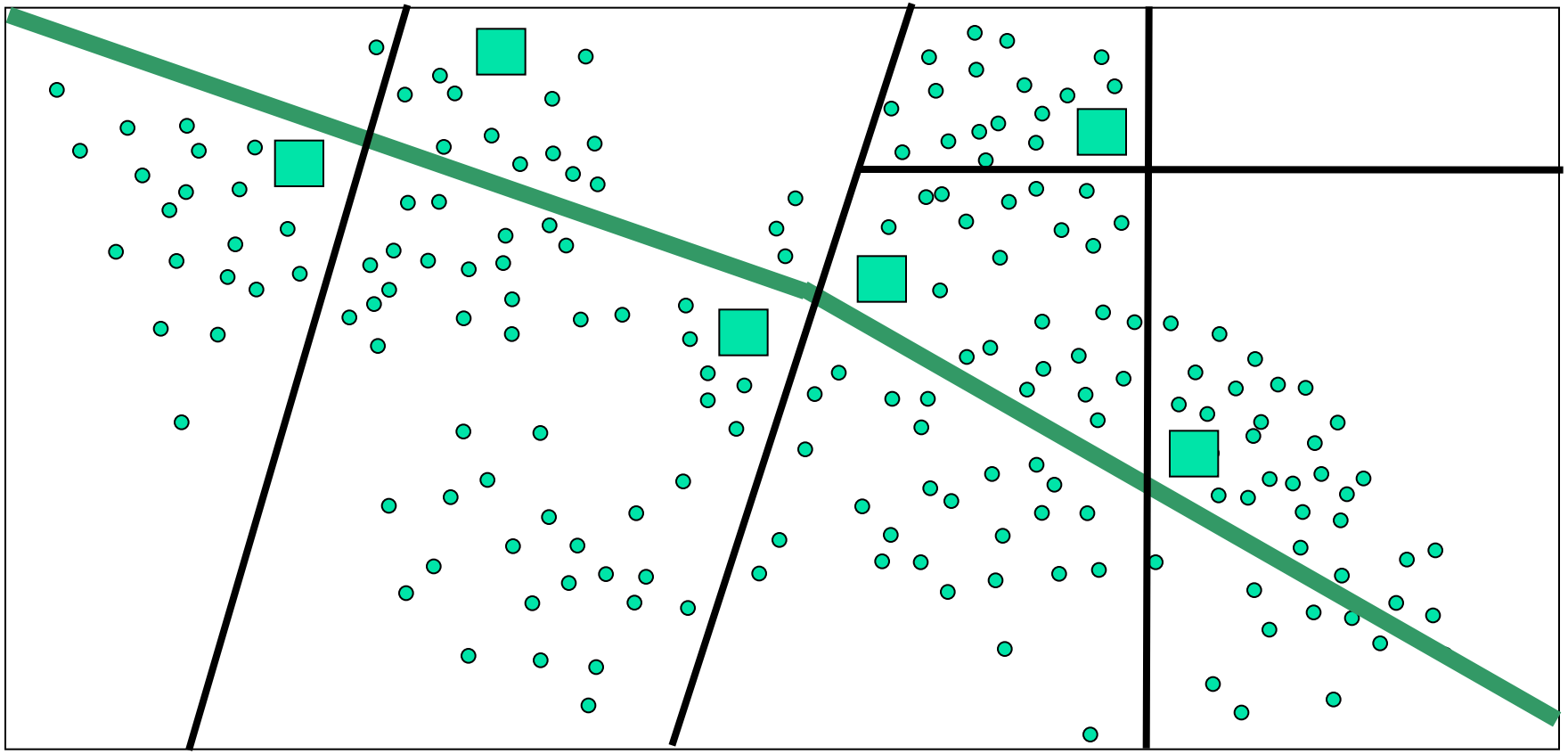
[2] A. Clauset, M. E. J. Newman, & C. Moore, *Phys. Rev. E* **70**, 066111 (2004).

Chapter 11. Cluster Analysis: Advanced Methods

- Probability Model-Based Clustering
- Clustering High-Dimensional Data
- Clustering Graphs and Network Data
- Clustering with Constraints 
- Summary

Why Constraint-Based Cluster Analysis?

- Need user feedback: Users know their applications the best
- Less parameters but more user-desired constraints, e.g., an ATM allocation problem: obstacle & desired clusters



Categorization of Constraints

- Constraints on instances: specifies how a pair or a set of instances should be grouped in the cluster analysis
  - Must-link vs. cannot link constraints
    - must-link(x, y): x and y should be grouped into one cluster
  - Constraints can be defined using variables, e.g.,
    - cannot-link(x, y) if dist(x, y) > d
- Constraints on clusters: specifies a requirement on the clusters
  - E.g., specify the min # of objects in a cluster, the max diameter of a cluster, the shape of a cluster (e.g., a convex), # of clusters (e.g., k)
- Constraints on similarity measurements: specifies a requirement that the similarity calculation must respect
  - E.g., driving on roads, obstacles (e.g., rivers, lakes)
- Issues: Hard vs. soft constraints; conflicting or redundant constraints

Constraint-Based Clustering Methods (I): Handling Hard Constraints

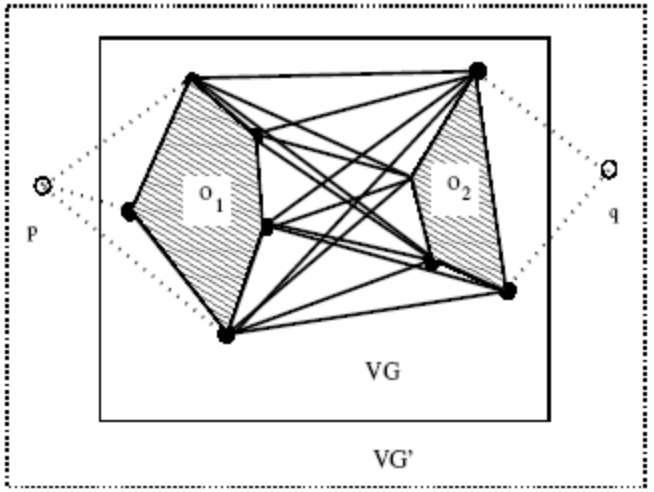
- Handling hard constraints: Strictly respect the constraints in cluster assignments
- Example: The COP-k-means algorithm
  - Generate super-instances for must-link constraints
    - Compute the transitive closure of the must-link constraints
    - To represent such a subset, replace all those objects in the subset by the mean.
    - The super-instance also carries a weight, which is the number of objects it represents
  - Conduct modified k-means clustering to respect cannot-link constraints
    - Modify the center-assignment process in k-means to a *nearest feasible center assignment*
    - An object is assigned to the nearest center so that the assignment respects all cannot-link constraints

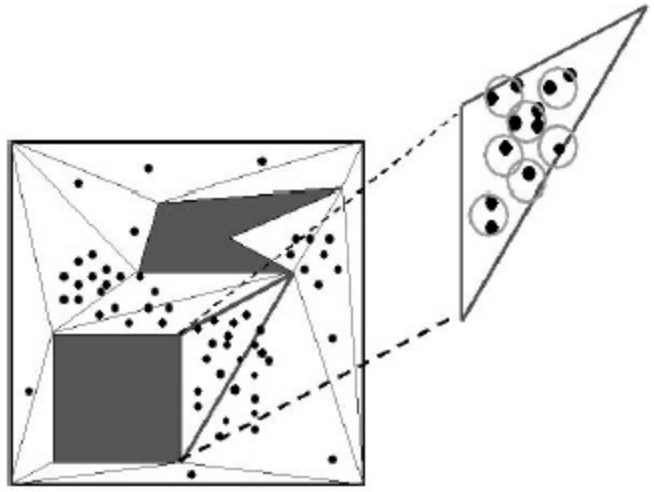
Constraint-Based Clustering Methods (II): Handling Soft Constraints

- Treated as an optimization problem: When a clustering violates a soft constraint, a penalty is imposed on the clustering
- Overall objective: Optimizing the clustering quality, and minimizing the constraint violation penalty
- Ex. CVQE (Constrained Vector Quantization Error) algorithm: Conduct k-means clustering while enforcing constraint violation penalties
- Objective function: Sum of distance used in k-means, adjusted by the constraint violation penalties
  - Penalty of a *must-link* violation
    - If objects x and y must-be-linked but they are assigned to two different centers, c_1 and c_2, dist(c_1, c_2) is added to the objective function as the penalty
  - Penalty of a cannot-link violation
    - If objects x and y cannot-be-linked but they are assigned to a common center c, dist(c, c′), between c and c′ is added to the objective function as the penalty, where c′ is the closest cluster to c that can accommodate x or y

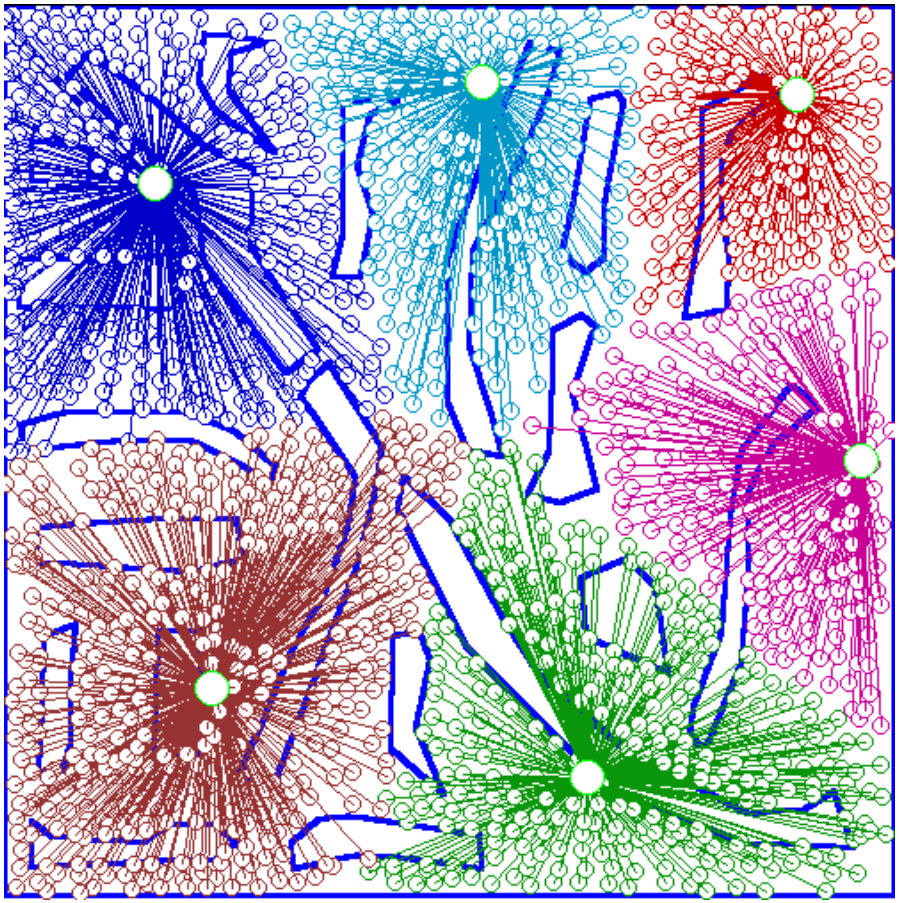
Speeding Up Constrained Clustering

- It is costly to compute some constrained clustering
- Ex. Clustering with obstacle objects: Tung, Hou, and Han. Spatial clustering in the presence of obstacles, ICDE'01
- K-medoids is more preferable since k-means may locate the ATM center in the middle of a lake
- Visibility graph and shortest path
- Triangulation and micro-clustering
- Two kinds of join indices (shortest-paths) worth pre-computation
  - VV index: indices for any pair of obstacle vertices
  - MV index: indices for any pair of micro-cluster and obstacle indices

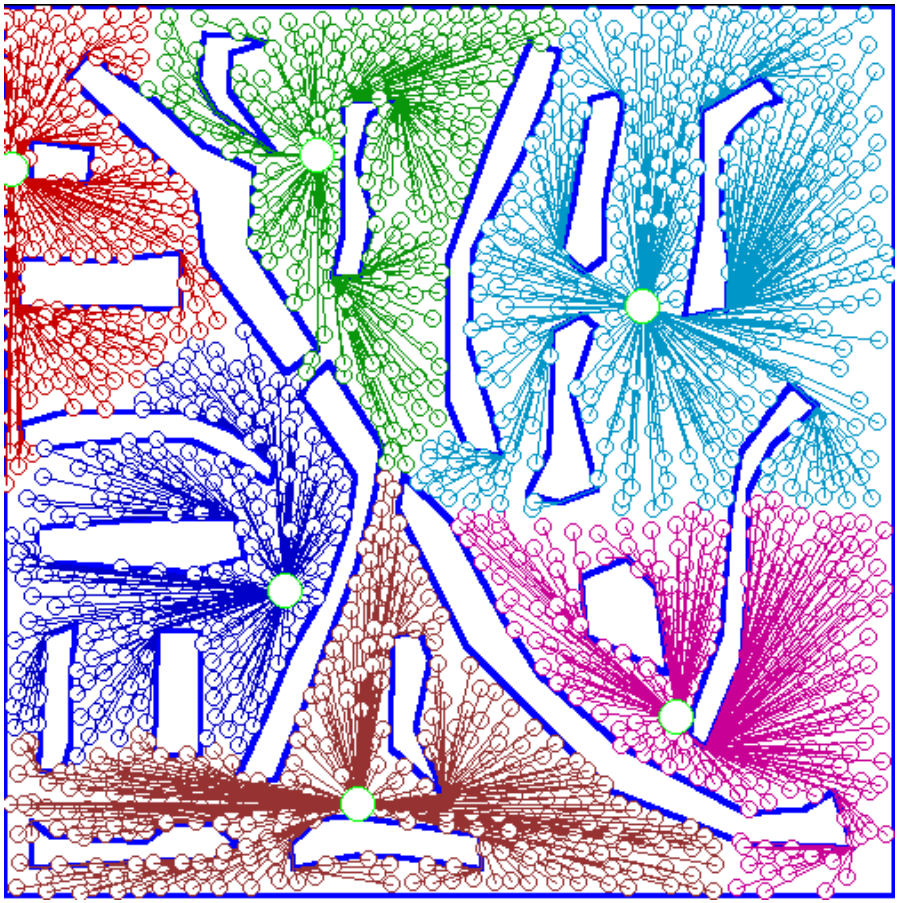




An Example: Clustering With Obstacle Objects

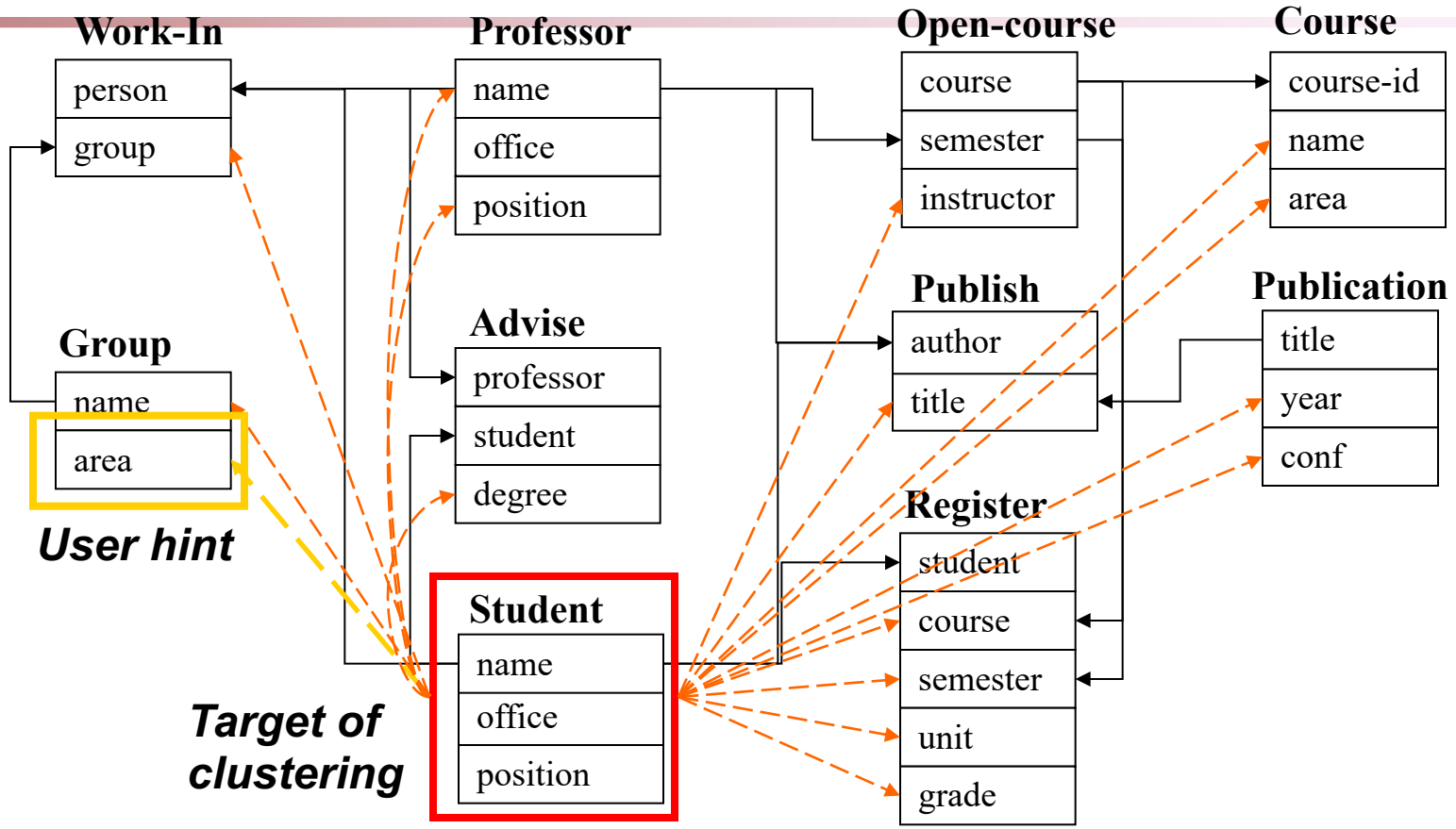


Not Taking obstacles into account



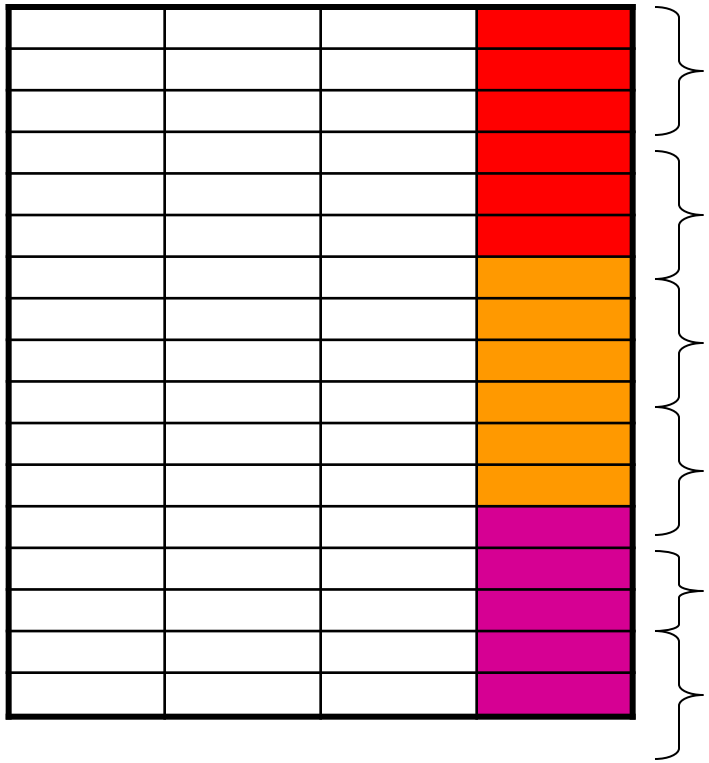
Taking obstacles into account

User-Guided Clustering: A Special Kind of Constraints



- X. Yin, J. Han, P. S. Yu, "Cross-Relational Clustering with User's Guidance", KDD'05
- User usually has a goal of clustering, e.g., clustering students by research area
- User specifies his clustering goal to CrossClus

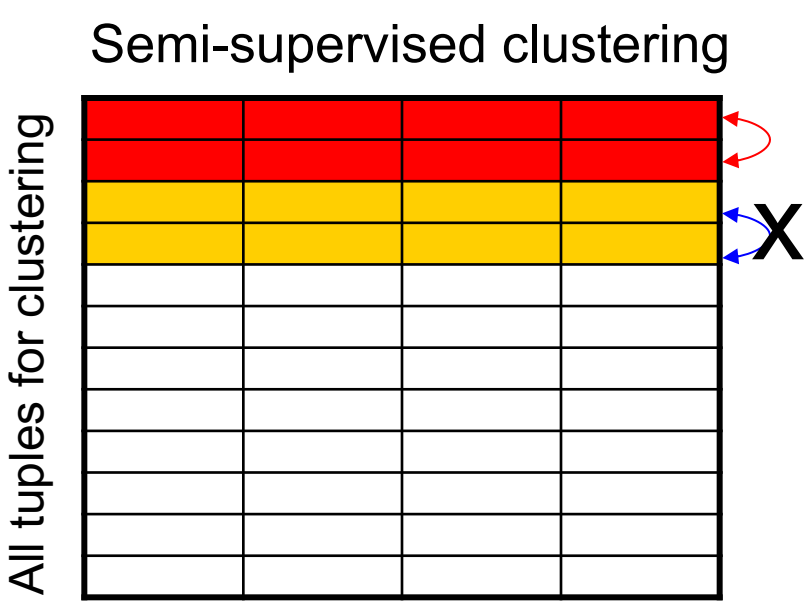
Comparing with Classification

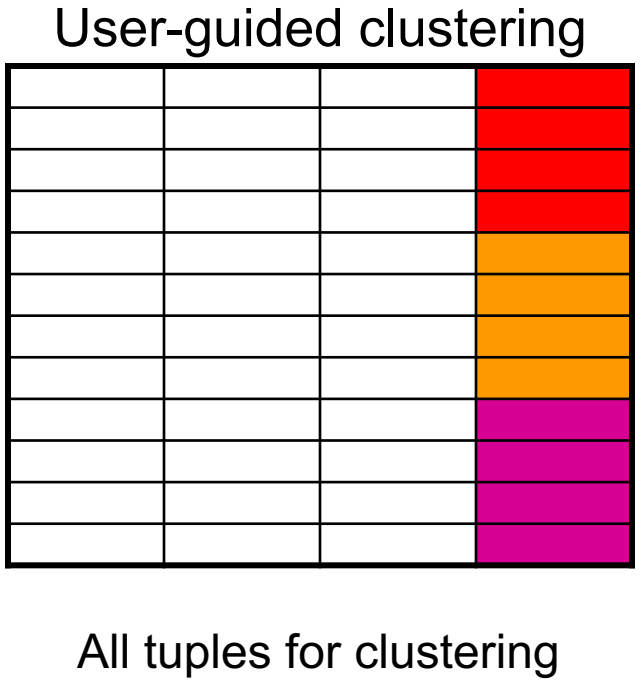


- User-specified *feature* (in the form of *attribute*) is used as a hint, not class labels
  - The attribute may contain too many or too few distinct values, e.g., a user may want to cluster students into 20 clusters instead of 3
  - Additional features need to be included in cluster analysis

Comparing with Semi-Supervised Clustering

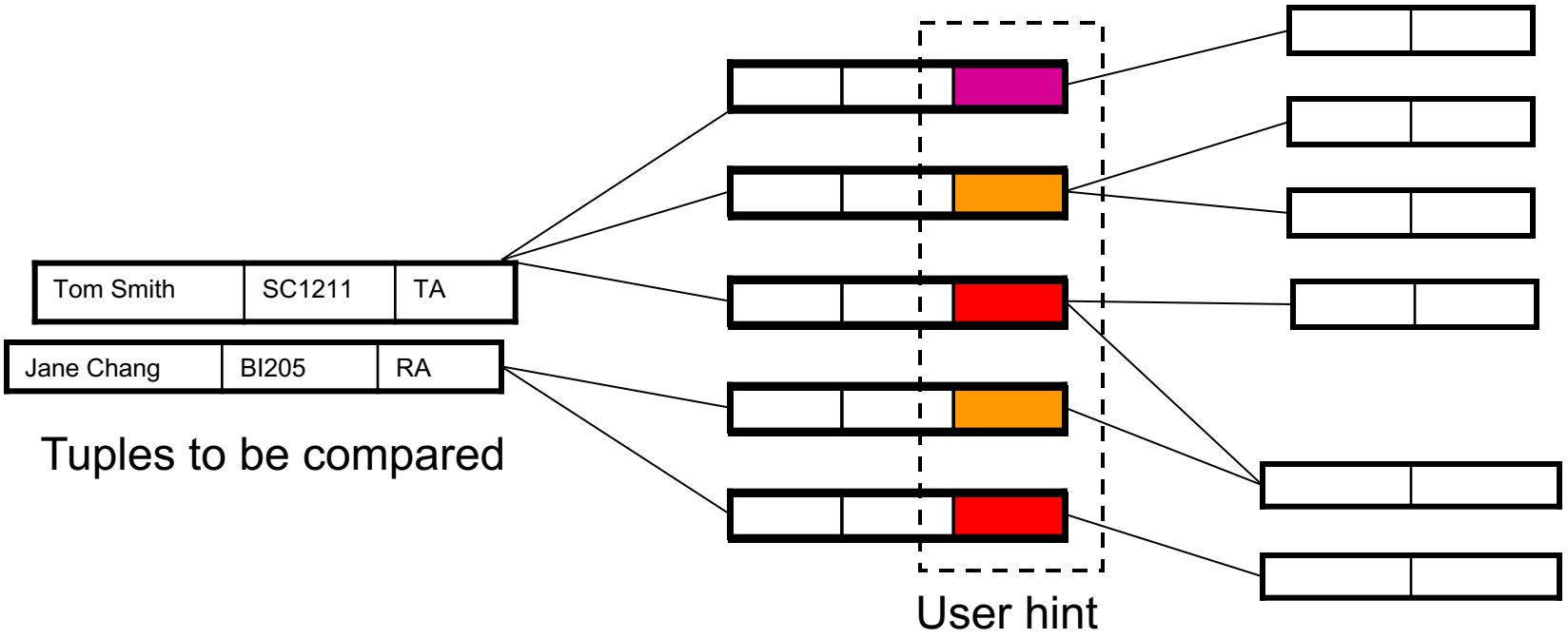
- Semi-supervised clustering: User provides a training set consisting of “similar” (“must-link) and “dissimilar” (“cannot link”) pairs of objects
- User-guided clustering: User specifies an attribute as a hint, and more relevant features are found for clustering





Why Not Semi-Supervised Clustering?

- Much information (in multiple relations) is needed to judge whether two tuples are similar
- A user may not be able to provide a good training set
- It is much easier for a user to specify an attribute as a hint, such as a student's *research area*



CrossClus: An Overview

- Measure *similarity between features* by how they group objects into clusters
- Use a heuristic method to search for pertinent features
  - *Start from user-specified feature and gradually expand search range*
- Use *tuple ID propagation* to create feature values
  - Features can be easily created during the expansion of search range, by propagating IDs
- Explore three clustering algorithms: *k*-means, *k*-medoids, and hierarchical clustering

Multi-Relational Features

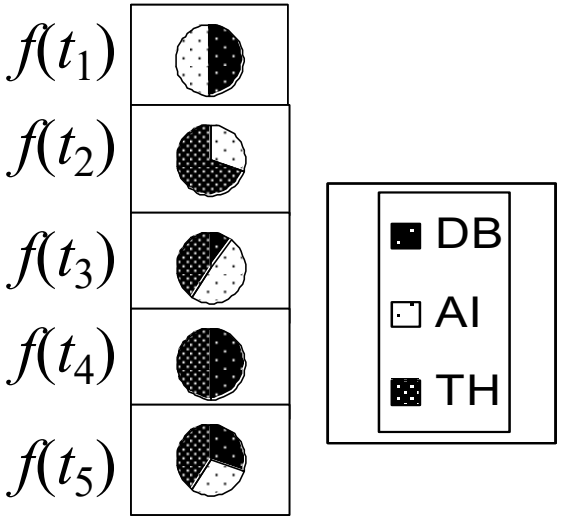
- A multi-relational feature is defined by:
  - A join path, e.g., *Student* → *Register* → *OpenCourse* → *Course*
  - An attribute, e.g., *Course.area*
  - (For numerical feature) an aggregation operator, e.g., sum or average
- Categorical feature *f* = [*Student* → *Register* → *OpenCourse* → *Course*, *Course.area*, null]

areas of courses of each student

Tuple	Areas of courses		
	DB	***AI***	***TH***
t_1	5	5	0
t_2	0	3	7
t_3	1	5	4
t_4	5	0	5
t_5	3	3	4

Values of feature f

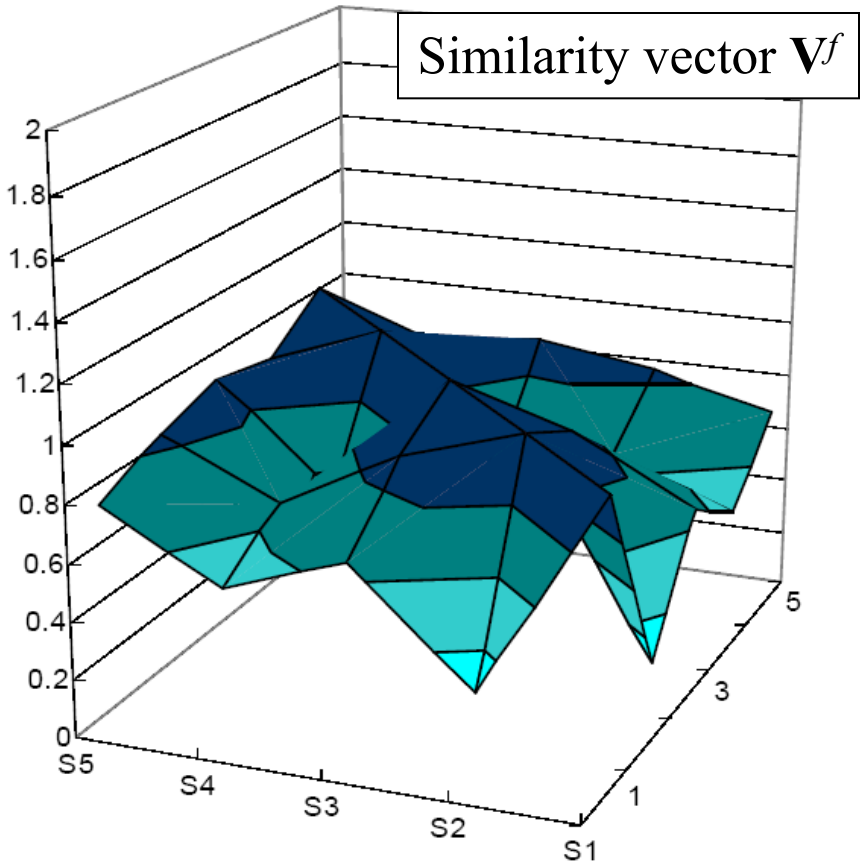
Tuple	Feature *f*		
	DB	***AI***	***TH***
t_1	0.5	0.5	0
t_2	0	0.3	0.7
t_3	0.1	0.5	0.4
t_4	0.5	0	0.5
t_5	0.3	0.3	0.4



Representing Features

- Similarity between tuples t_1 and t_2 w.r.t. categorical feature f
  - Cosine similarity between vectors $f(t_1)$ and $f(t_2)$

$$\mathrm{sim}_f(t_1, t_2) = \frac{\sum_{k=1}^{L} f(t_1).p_k \cdot f(t_2).p_k}{\sqrt{\sum_{k=1}^{L} f(t_1).p_k^{\,2}} \cdot \sqrt{\sum_{k=1}^{L} f(t_2).p_k^{\,2}}}$$

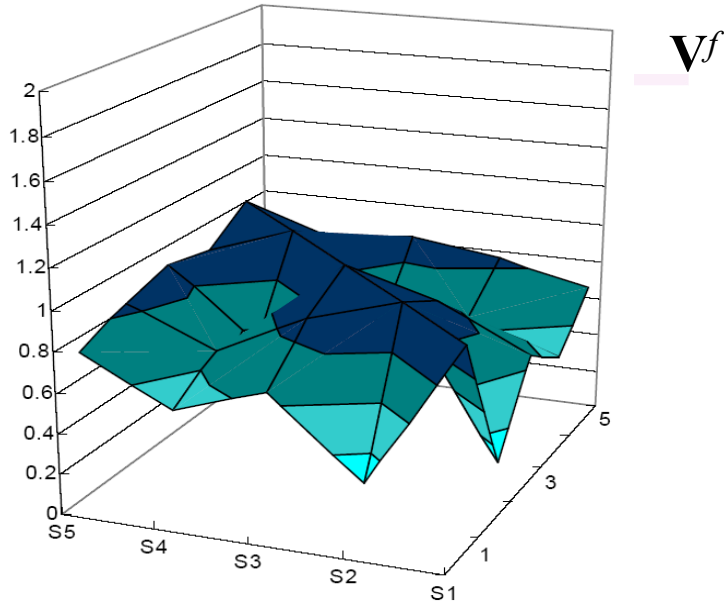


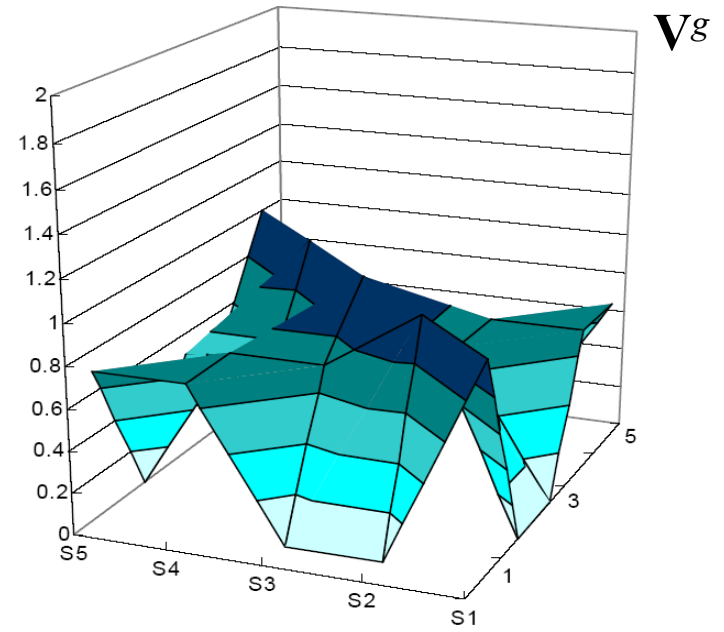
- Most important information of a feature f is how f groups tuples into clusters
- f is represented by similarities between every pair of tuples indicated by f
- The horizontal axes are the tuple indices, and the vertical axis is the similarity
- This can be considered as a vector of N x N dimensions

Similarity Between Features

Values of Feature f and g

	Feature f (course)				Feature g (group)		
	DB	AI	TH		Info sys	Cog sci	Theory
t_1	0.5	0.5	0		1	0	0
t_2	0	0.3	0.7		0	0	1
t_3	0.1	0.5	0.4		0	0.5	0.5
t_4	0.5	0	0.5		0.5	0	0.5
t_5	0.3	0.3	0.4		0.5	0.5	0

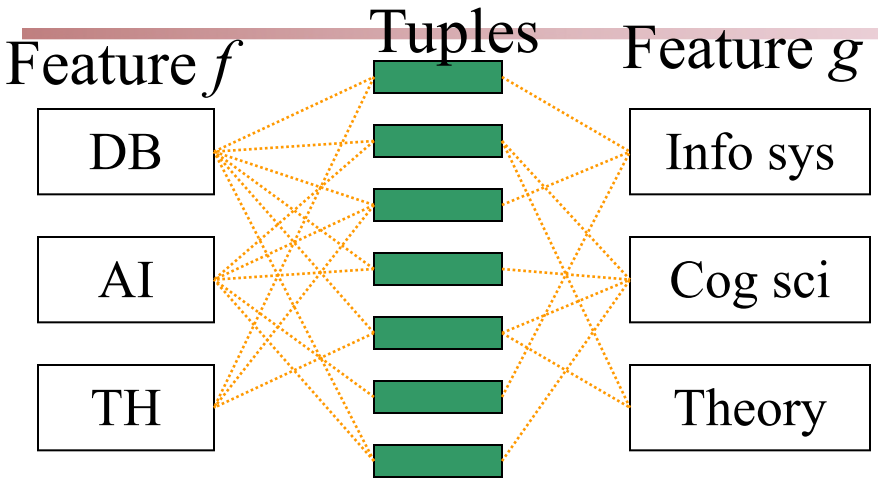




Similarity between two features – cosine similarity of two vectors

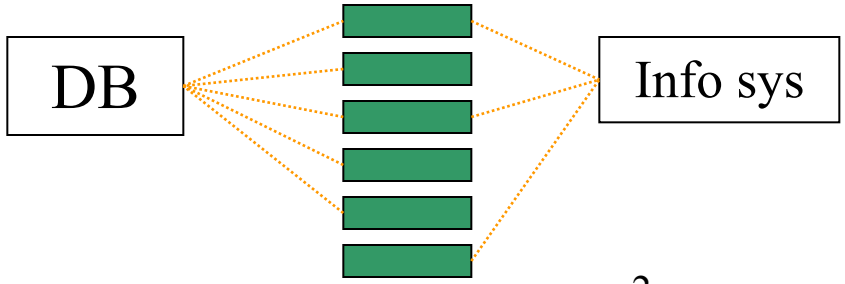
$$sim(f,g) = \frac{V^f \cdot V^g}{|V^f||V^g|}$$

Computing Feature Similarity



Similarity between feature values w.r.t. the tuples

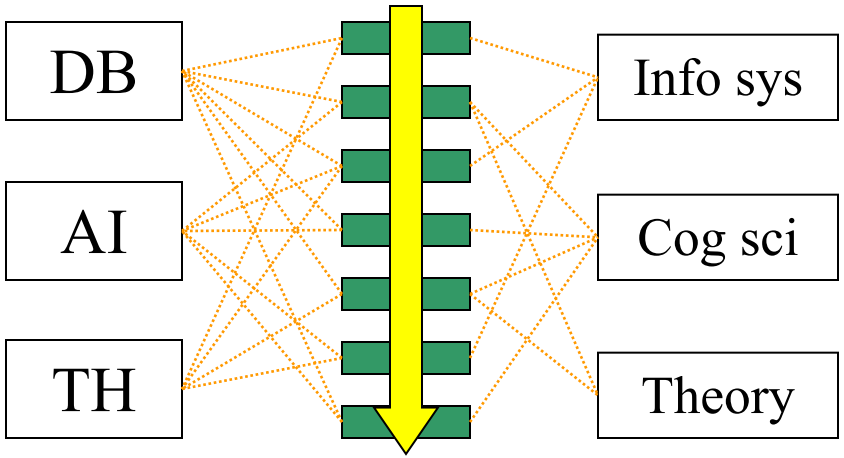
$$sim(f_k, g_q) = \sum_{i=1 \text{ to } N} f(t_i).p_k \cdot g(t_i).p_q$$



$$V^f \cdot V^g = \sum_{i=1}^{N} \sum_{j=1}^{N} sim_f(t_i, t_j) \cdot sim_g(t_i, t_j) = \sum_{k=1}^{l} \sum_{q=1}^{m} sim(f_k, g_q)^2$$

Tuple similarities, hard to compute

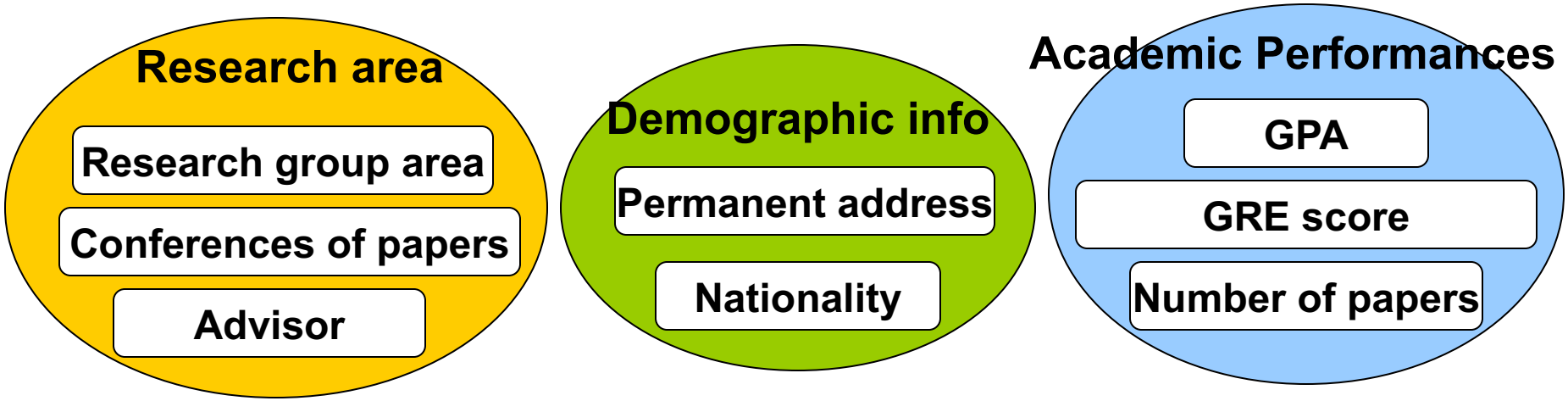
Feature value similarities, easy to compute



Compute similarity between each pair of feature values by one scan on data

Searching for Pertinent Features

- Different features convey different aspects of information

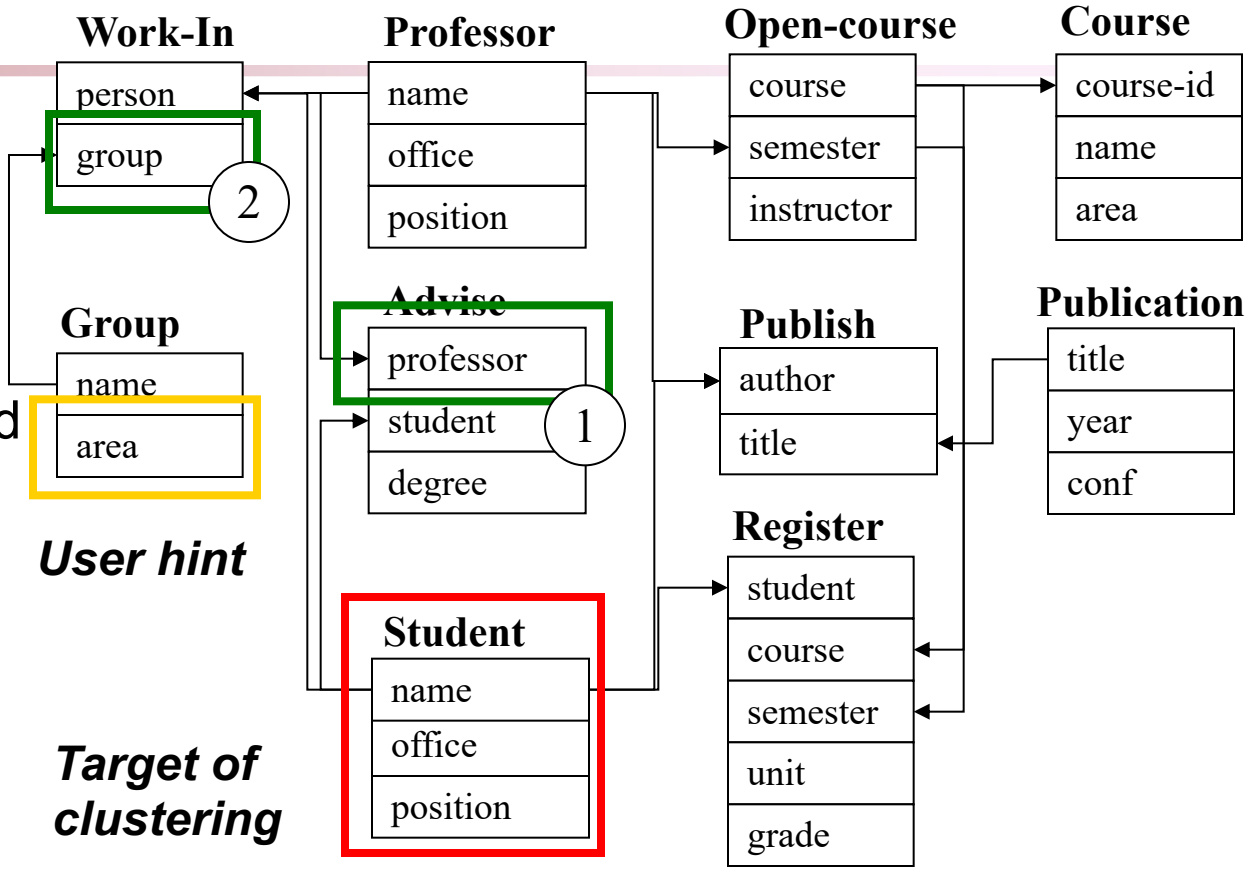


- Features conveying same aspect of information usually cluster tuples in more similar ways
  - Research group areas vs. conferences of publications
- Given user specified feature
  - Find pertinent features by computing feature similarity

Heuristic Search for Pertinent Features

Overall procedure

1. Start from the user-specified feature
2. Search in neighborhood of existing pertinent features
3. Expand search range gradually



- Tuple ID propagation is used to create multi-relational features
  - IDs of target tuples can be propagated along any join path, from which we can find tuples joinable with each target tuple

Clustering with Multi-Relational Features

- Given a set of L pertinent features $f_1, \ldots, f_L$, similarity between two tuples

$$\text{sim}(t_1, t_2) = \sum_{i=1}^{L} \text{sim}_{f_i}(t_1, t_2) \cdot f_i.weight$$

  - Weight of a feature is determined in feature search by its similarity with other pertinent features
- Clustering methods
  - CLARANS [Ng & Han 94], a scalable clustering algorithm for non-Euclidean space
  - K-means
  - Agglomerative hierarchical clustering

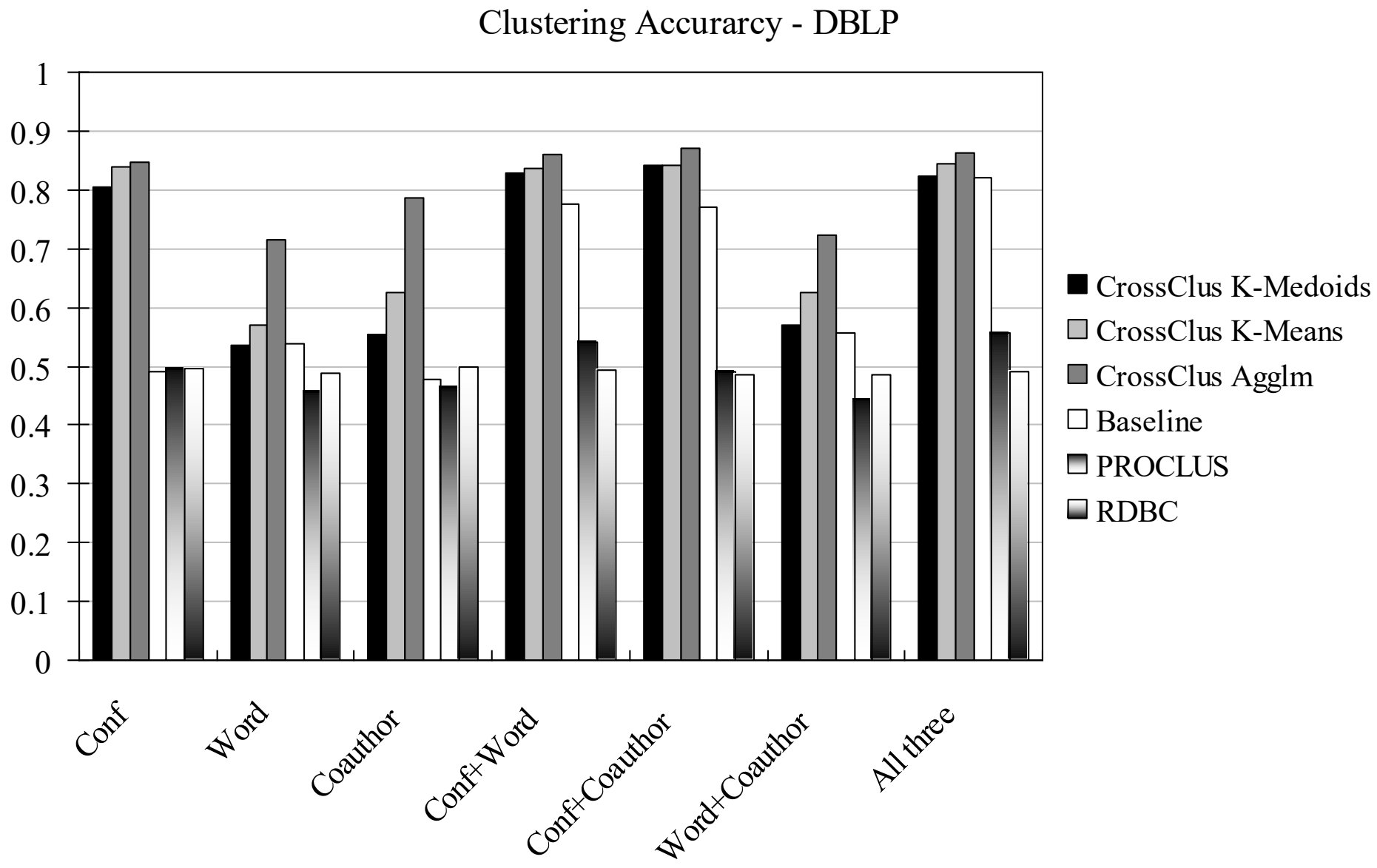
Experiments: Compare CrossClus with

- Baseline: Only use the user specified feature
- PROCLUS [Aggarwal, et al. 99]: a state-of-the-art subspace clustering algorithm
  - Use a subset of features for each cluster
  - We convert relational database to a table by propositionalization
  - User-specified feature is forced to be used in every cluster
- RDBC [Kirsten and Wrobel'00]
  - A representative ILP clustering algorithm
  - Use neighbor information of objects for clustering
  - User-specified feature is forced to be used

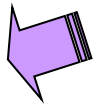
Measure of Clustering Accuracy

- Accuracy
  - Measured by manually labeled data
    - We manually assign tuples into clusters according to their properties (e.g., professors in different research areas)
  - Accuracy of clustering: Percentage of pairs of tuples in the same cluster that share common label
    - This measure favors many small clusters
    - We let each approach generate the same number of clusters

DBLP Dataset



Chapter 11. Cluster Analysis: Advanced Methods

- Probability Model-Based Clustering
- Clustering High-Dimensional Data
- Clustering Graphs and Network Data
- Clustering with Constraints
- Summary 

Summary

- Probability Model-Based Clustering
  - Fuzzy clustering
  - Probability-model-based clustering
  - The EM algorithm
- Clustering High-Dimensional Data
  - Subspace clustering: bi-clustering methods
  - Dimensionality reduction: Spectral clustering
- Clustering Graphs and Network Data
  - Graph clustering: min-cut vs. sparsest cut
  - High-dimensional clustering methods
  - Graph-specific clustering methods, e.g., SCAN
- Clustering with Constraints
  - Constraints on instance objects, e.g., Must link vs. Cannot Link
  - Constraint-based clustering algorithms

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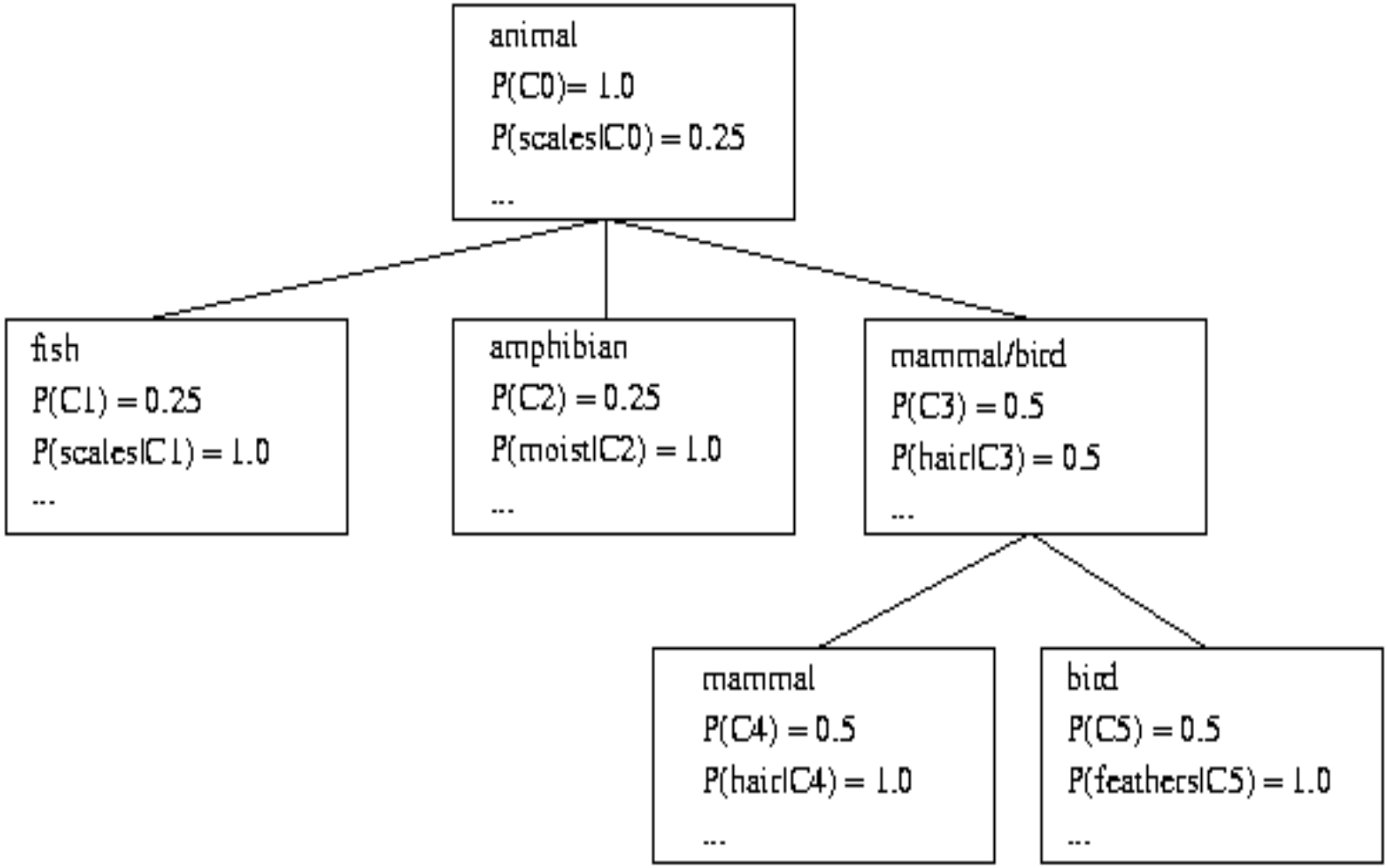
Slides Not to Be Used in Class

Conceptual Clustering

- Conceptual clustering
  - A form of clustering in machine learning
  - Produces a classification scheme for a set of unlabeled objects
  - Finds characteristic description for each concept (class)
- COBWEB (Fisher'87)
  - A popular a simple method of incremental conceptual learning
  - Creates a hierarchical clustering in the form of a classification tree
  - Each node refers to a concept and contains a probabilistic description of that concept

COBWEB Clustering Method

A classification tree



More on Conceptual Clustering

- Limitations of COBWEB
  - The assumption that the attributes are independent of each other is often too strong because correlation may exist
  - Not suitable for clustering large database data – skewed tree and expensive probability distributions
- CLASSIT
  - an extension of COBWEB for incremental clustering of continuous data
  - suffers similar problems as COBWEB
- AutoClass (Cheeseman and Stutz, 1996)
  - Uses Bayesian statistical analysis to estimate the number of clusters
  - Popular in industry

Neural Network Approaches

- Neural network approaches
  - Represent each cluster as an exemplar, acting as a "prototype" of the cluster
  - New objects are distributed to the cluster whose exemplar is the most similar according to some distance measure
- Typical methods
  - SOM (Soft-Organizing feature Map)
  - Competitive learning
    - Involves a hierarchical architecture of several units (neurons)
    - Neurons compete in a "winner-takes-all" fashion for the object currently being presented

Self-Organizing Feature Map (SOM)

- SOMs, also called topological ordered maps, or Kohonen Self-Organizing Feature Map (KSOMs)
- It maps all the points in a high-dimensional source space into a 2 to 3-d target space, s.t., the distance and proximity relationship (i.e., topology) are preserved as much as possible
- Similar to k-means: cluster centers tend to lie in a low-dimensional manifold in the feature space
- Clustering is performed by having several units competing for the current object
  - The unit whose weight vector is closest to the current object wins
  - The winner and its neighbors learn by having their weights adjusted
- SOMs are believed to resemble processing that can occur in the brain
- Useful for visualizing high-dimensional data in 2- or 3-D space

Web Document Clustering Using SOM

- The result of SOM clustering of 12088 Web articles
- The picture on the right: drilling down on the keyword "mining"
- Based on websom.hut.fi Web page