CS5824: Advanced Machine Learning

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COMPUTER SCIENCE
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Cluster Analysis: An Introduction

Cluster Analysis: An Introduction

- What Is Cluster Analysis?
- Applications of Cluster Analysis
- Cluster Analysis: Requirements and Challenges
- Cluster Analysis: A Multi-Dimensional Categorization
- An Overview of Typical Clustering Methodologies
- An Overview of Clustering Different Types of Data
- An Overview of User Insights and Clustering

What Is Cluster Analysis?

- **What is a cluster?**
  - A cluster is a collection of data objects which are
    - Similar (or related) to one another within the same group (i.e., cluster)
    - Dissimilar (or unrelated) to the objects in other groups (i.e., clusters)
- **Cluster analysis** (or **clustering, data segmentation**, ...)
  - Given a set of data points, partition them into a set of groups (i.e., clusters) which are as similar as possible
- Cluster analysis is unsupervised learning (i.e., no predefined classes)
  - This contrasts with classification (i.e., supervised learning)
- Typical ways to use/apply cluster analysis
  - As a stand-alone tool to get insight into data distribution, or
  - As a preprocessing (or intermediate) step for other algorithms (e.g., Outlier detection)

What Is Good Clustering?

- A good clustering method will produce high quality clusters which should have
  - **High intra-class similarity**: Cohesive within clusters
  - **Low inter-class similarity**: Distinctive between clusters
- **Quality function**
  - There is usually a separate "quality" function that measures the "goodness" of a cluster
  - It is hard to define "similar enough" or "good enough"
    - The answer is typically highly subjective
- There exist many similarity measures and/or functions for different applications
- Similarity measure is critical for cluster analysis

Cluster Analysis: Applications

- A key intermediate step for other data mining tasks
  - Generating a compact summary of data for classification, pattern discovery, hypothesis generation and testing, etc.
  - Outlier detection: Outliers—those “far away” from any cluster
- Data summarization, compression, and reduction
  - Ex. Image processing: Vector quantization
- Collaborative filtering, recommendation systems, or customer segmentation
  - Find like-minded users or similar products
- Dynamic trend detection
  - Clustering stream data and detecting trends and patterns
- Multimedia data analysis, biological data analysis and social network analysis
  - Ex. Clustering images or video/audio clips, gene/protein sequences, etc.

Considerations for Cluster Analysis

- **Partitioning criteria**
  - Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable, e.g., grouping topical terms)
- **Separation of clusters**
  - Exclusive (e.g., one customer belongs to only one region) vs. nonexclusive (e.g., one document may belong to more than one class)
- **Similarity measure**
  - Distance-based (e.g., Euclidean, road network, vector) vs. connectivity-based (e.g., density or contiguity)
- **Clustering space**
  - Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)

Requirements and Challenges

- **Quality**
  - Ability to deal with different types of attributes: Numerical, categorical, text, multimedia, networks, and mixture of multiple types
  - Discovery of clusters with arbitrary shape
  - Ability to deal with noisy data
- **Scalability**
  - Clustering all the data instead of only on samples
  - High dimensionality
  - Incremental or stream clustering and insensitivity to input order
- **Constraint-based clustering**
  - User-given preferences or constraints; domain knowledge; user queries
- **Interpretability and usability**
  - The final generated clusters should be semantically meaningful and useful

Partitioning Methods

Partitioning Algorithms: Basic Concepts

- Partitioning method: Discovering the groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions
- K-partitioning method: Partitioning a dataset ***D*** of ***n*** objects into a set of ***K*** clusters so that an objective function is optimized (e.g., the sum of squared distances is minimized, where c_k is the centroid or medoid of cluster C_k)
  - A typical objective function: **Sum of Squared Errors (SSE)**

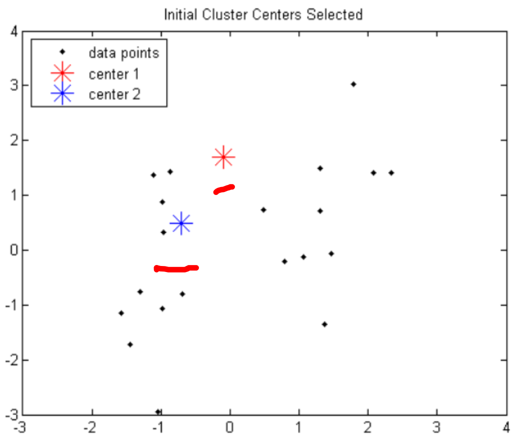
$$SSE(C) = \sum_{k=1}^{K} \sum_{x_{i \in c_k}} \|x_i - c_k\|^2$$

- Problem definition: Given K, find a partition of K clusters that optimizes the chosen partitioning criterion
  - Global optimal: Needs to exhaustively enumerate all partitions
  - Heuristic methods (i.e., greedy algorithms): K-Means, K-Medians, K-Medoids, etc.

The K-Means Clustering Method

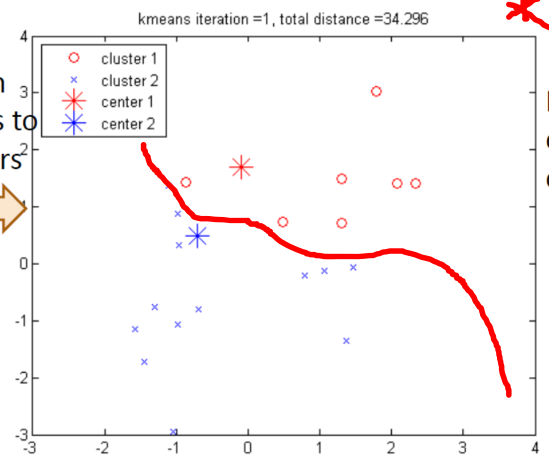
- *K-Means* (MacQueen'67, Lloyd'57/'82)
  - Each cluster is represented by the center of the cluster
- Given K, the number of clusters, the *K-Means* clustering algorithm is outlined as follows
  - Select K points as initial centroids
  - **Repeat**
    - Form K clusters by assigning each point to its closest centroid
    - Re-compute the centroids (i.e., mean point) of each cluster
  - **Until** convergence criterion is satisfied
- Different kinds of measures can be used
  - Manhattan distance (L_1 norm), Euclidean distance (L_2 norm), Cosine similarity

Example: K-Means Clustering

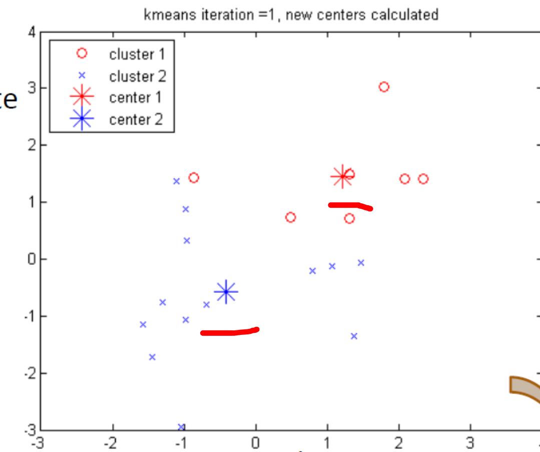


The original data points & randomly select K = 2 centroids

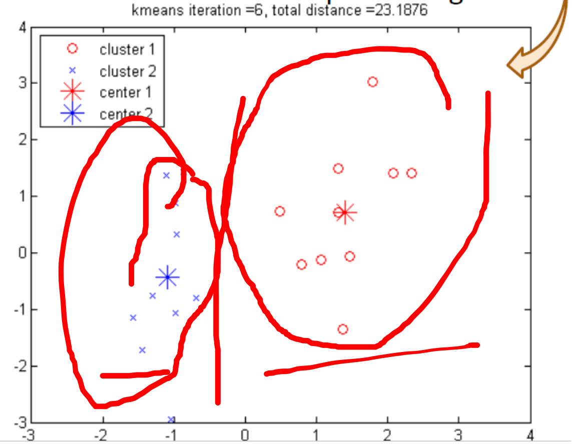
Assign points to clusters



Recompute cluster centers



Redo point assignment



Execution of the K-Means Clustering Algorithm

Select K points as initial centroids

Repeat

- Form K clusters by assigning each point to its closest centroid
- Re-compute the centroids (i.e., *mean point*) of each cluster

Until convergence criterion is satisfied

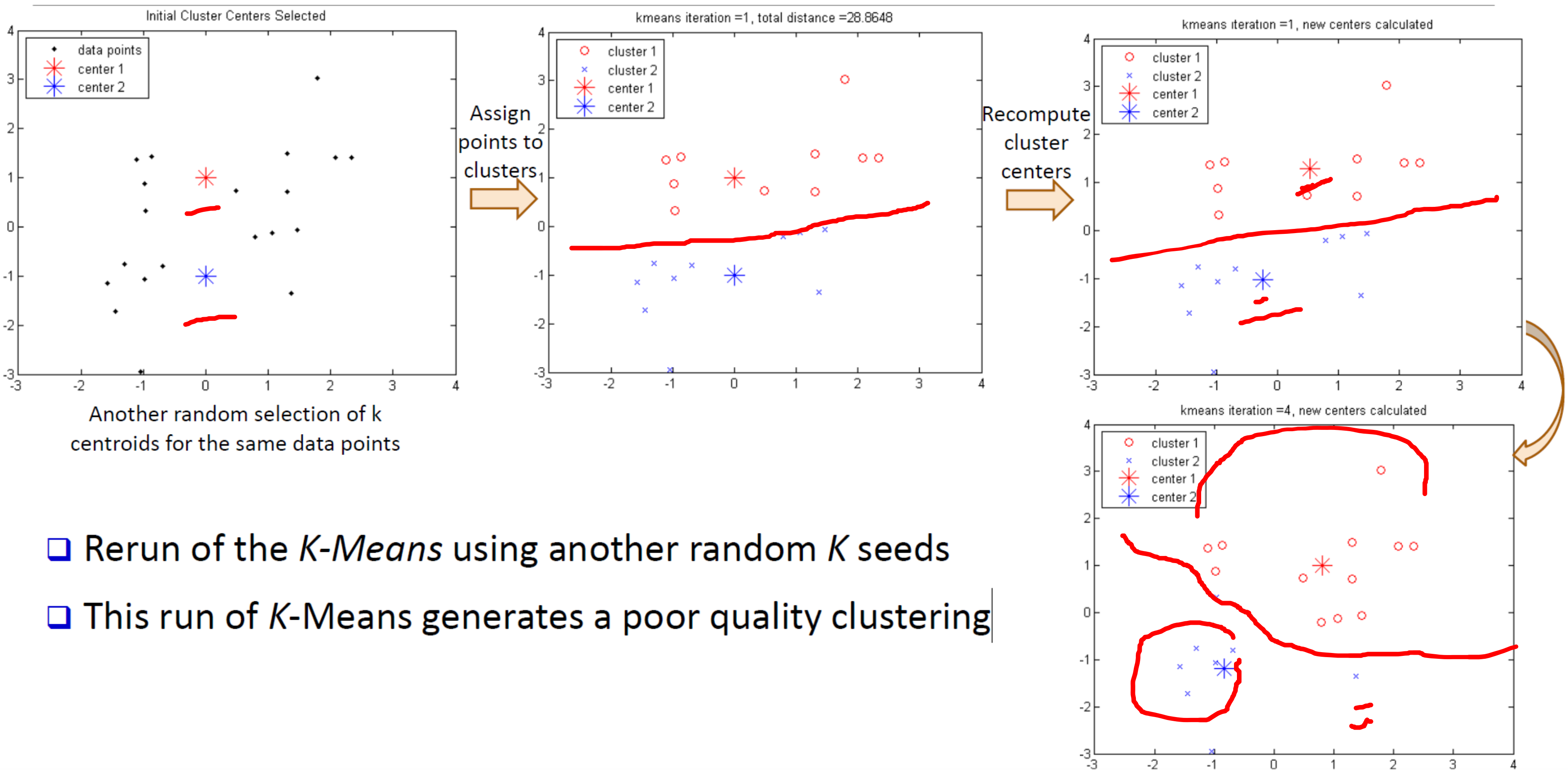
Discussion on the K-Means Method

- Efficiency: O(tKn) where n: # of objects, K: # of clusters, and t: # of iterations
  - Normally, K, t << n; thus, an efficient method
- K-means clustering often terminates at a local optimal
  - Initialization can be important to find high-quality clusters
- Need to specify K, the number of clusters, in advance
  - There are ways to automatically determine the "best" K
  - In practice, one often runs a range of values and selects the "best" K value
- Sensitive to noisy data and outliers
  - Variations: Using K-medians, K-medoids, etc.
- K-means is applicable only to objects in a continuous n-dimensional space
  - Using the K-modes for categorical data
- Not suitable to discover clusters with non-convex shapes
  - Using density-based clustering, etc.

Variations of K-Means

- There are many variants of the K-Means method, varying in different aspects
- Choosing better initial centroid estimates
  - K-means++, Intelligent K-Means, Genetic K-Means
- Choosing different representative prototypes for the clusters
  - K-Medoids, K-Medians, K-Modes
- Applying feature transformation techniques
  - Weighted K-Means, Kernel K-Means

Poor Initialization in K-Means May Lead to Poor Clustering

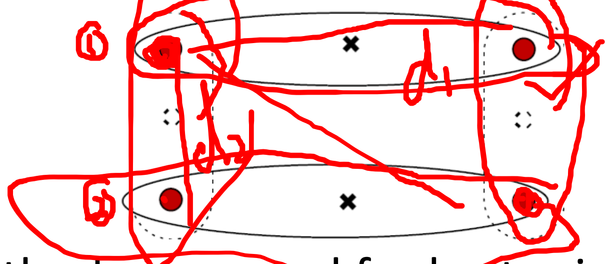


Another random selection of k centroids for the same data points

- Rerun of the *K-Means* using another random *K* seeds
- This run of *K*-Means generates a poor quality clustering

Initialization of K-Means: Problem and Solution

- Different initializations may generate rather different clustering results (some could be far from optimal)
- Original proposal (MacQueen'67): Select K seeds randomly
  - Need to run the algorithm multiple times using different seeds



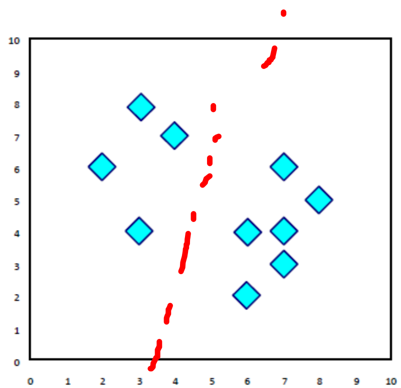
$d_1 \rightarrow d_2$

- There are many methods proposed for better initialization of K seeds
  - K-Means++ (Arthur & Vassilvitskii'07):
    - The first centroid is selected at random
    - The next centroid selected is the one that is farthest from the currently selected (selection is based on a weighted probability score)
    - The selection continues until K centroids are obtained

Handling Outliers: From K-Means to K-Medoids

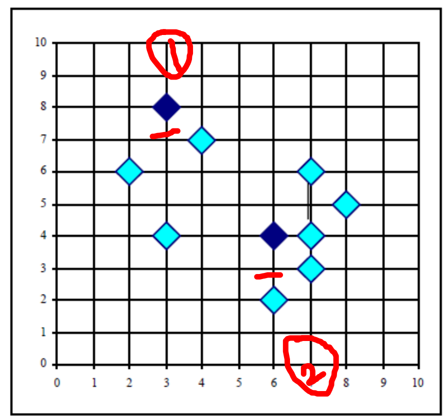
- The K-Means algorithm is sensitive to outliers!—since an object with an extremely large value may substantially distort the distribution of the data
- K-Medoids: Instead of taking the mean value of the object in a cluster as a reference point, medoids can be used, which is the most centrally located object in a cluster
- The K-Medoids clustering algorithm:
  - Select K points as the initial representative objects (i.e., as initial K medoids)
  - **Repeat**
    - Assigning each point to the cluster with the closest medoid
    - Randomly select a non-representative object oi
    - Compute the total cost S of swapping the medoid m with oi
    - If S < 0, then swap m with oi to form the new set of medoids
  - **Until** convergence criterion is satisfied

PAM: A Typical K-Medoids Algorithm

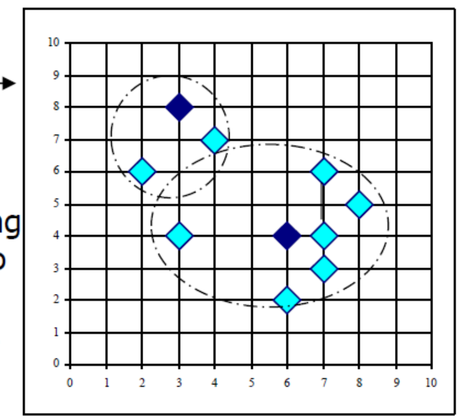


$K = 2$

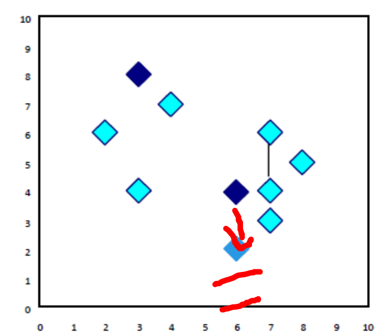
Arbitrary choose K objects as initial medoids



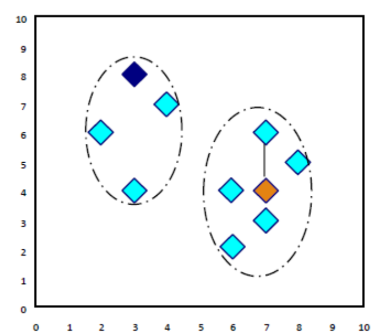
Assign each remaining object to nearest medoids



Randomly select a non-medoid object, O_{random}



Compute total cost of swapping



Swapping O and O_{ramdom}

If quality is improved

Select initial K medoids randomly

Repeat

Object re-assignment

Swap medoid m with o_i if it improves the clustering quality

Until convergence criterion is satisfied

Discussion on K-Medoids Clustering

- K-Medoids Clustering: Find representative objects (medoids) in clusters
- PAM (Partitioning Around Medoids: Kaufmann & Rousseeuw 1987)
  - Starts from an initial set of medoids, and
  - Iteratively replaces one of the medoids by one of the non-medoids if it improves the total sum of the squared errors (SSE) of the resulting clustering
  - PAM works effectively for small data sets but does not scale well for large data sets (due to the computational complexity)
  - Computational complexity: PAM: O(K(n − K)2) (quite expensive!)
- Efficiency improvements on PAM
  - CLARA (Kaufmann & Rousseeuw, 1990):
  - PAM on samples; O(Ks2 + K(n − K)), s is the sample size
  - CLARANS (Ng & Han, 1994): Randomized re-sampling, ensuring efficiency + quality

K-Medians: Handling Outliers by Computing Medians

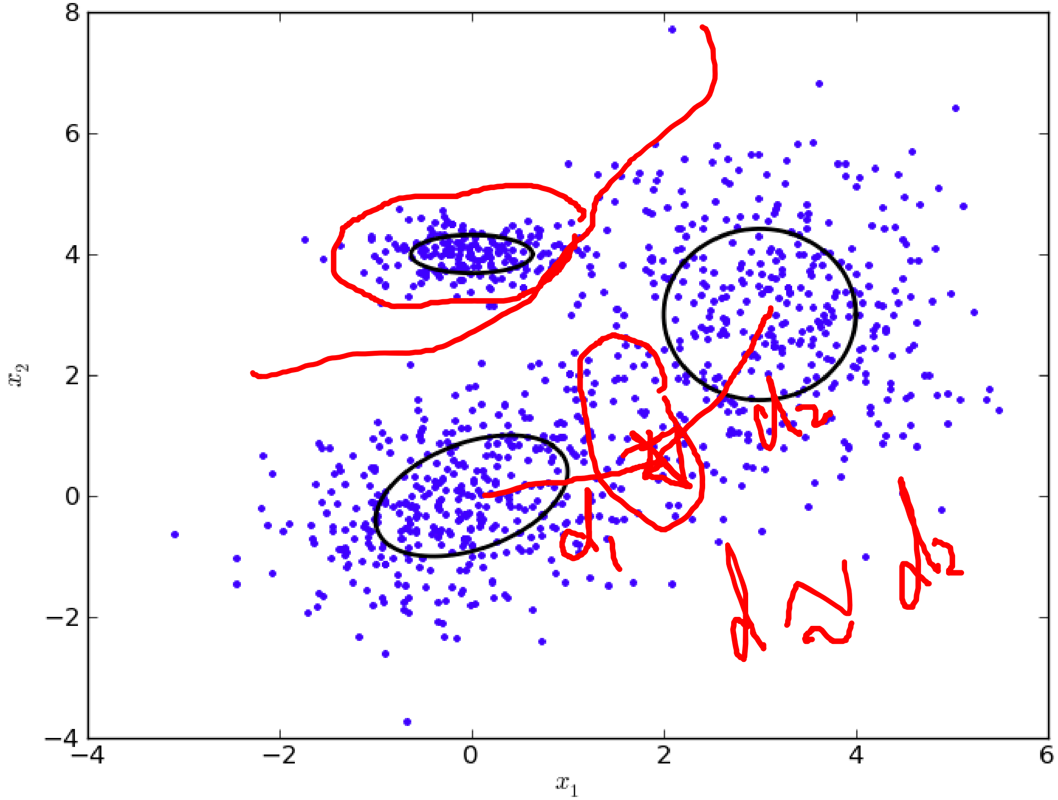
- Medians are less sensitive to outliers than means
  - Think of the median salary vs. mean salary of a large firm when adding a few top executives!
- K-Medians: Instead of taking the mean value of the objects in a cluster as a reference point, medians are used (L1-norm as the distance measure)
- The criterion function for the K-Medians algorithm: $S = \sum_{k=1}^{K} \sum_{x_i \in C_k} | x_{ij} - med_{kj} |$
- The K-Medians clustering algorithm:
  - Select K points as the initial representative objects (i.e., as initial K medians)
  - **Repeat**
    - Assign every point to its nearest median
    - Re-compute the median using the median of each individual feature
  - **Until** convergence criterion is satisfied

K-Modes: Clustering Categorical Data

- K-Means cannot handle non-numerical (categorical) data
  - Mapping categorical value to 1/0 cannot generate quality clusters
- K-Modes: An extension to K-Means by replacing means of clusters with modes
  - Mode: The value that appears most often in a set of data values
- Dissimilarity measure between object X and the center of a cluster Z
  - $\Phi(x_j, z_j) = 1 - \frac{n_j^r}{n_l}$ when $x_j = z_j$; 1 when $x_j \neq z_j$
  - where z_j is the categorical value of attribute j in Z_l, n_l is the number of objects in cluster l, and n_j^r is the number of objects whose attribute value is r
- This dissimilarity measure (distance function) is **frequency-based**
- Algorithm is still based on iterative object cluster assignment and centroid update

Gaussian Mixture Models and E-M algorithm

Hard Clustering Can Be Difficult



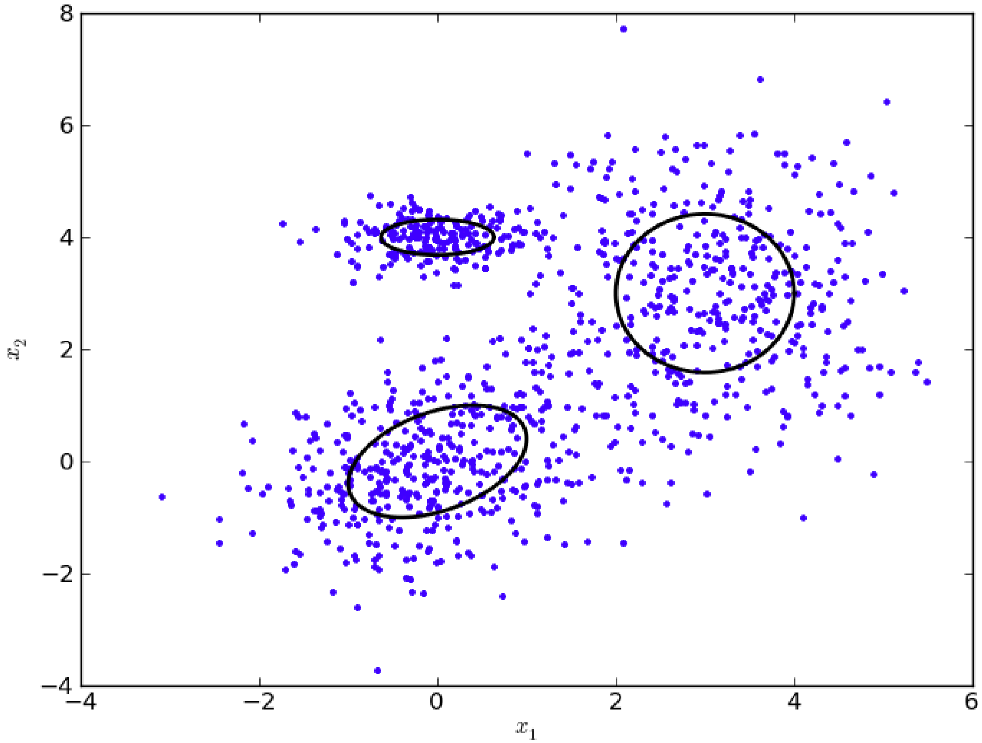
Soft Clustering

k: # cluster

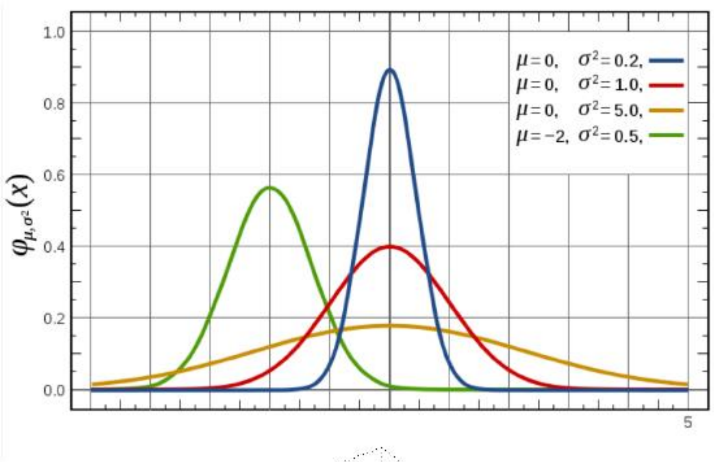
- Every object *i* is assigned to one cluster *j* with a probability
  - $P(z_i = j) \in [0,1]$ and $\sum_j P(z_i = j) = 1$
  - Where z_i is a hidden variable of which cluster x_i belongs to.

i

$Pr(z_i = j)$



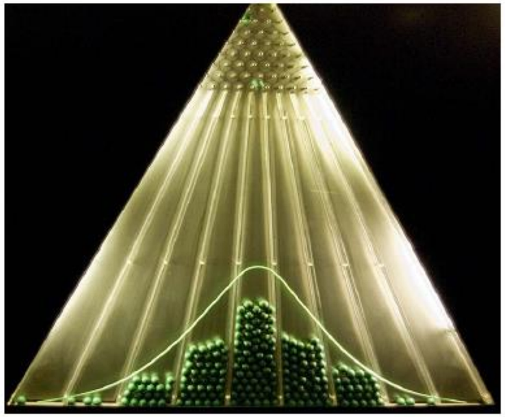
Gaussian Distribution

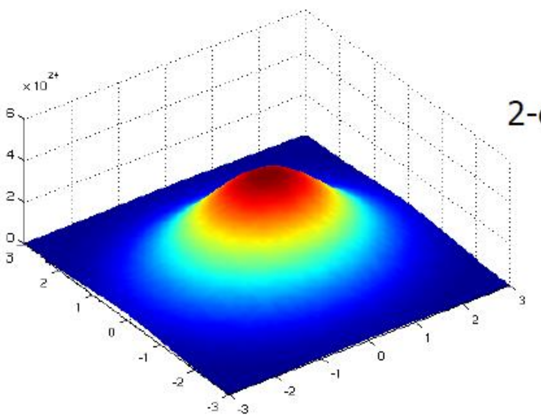


1-d Gaussian

$$\mathcal{N}(\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Bean machine: drop ball with pins



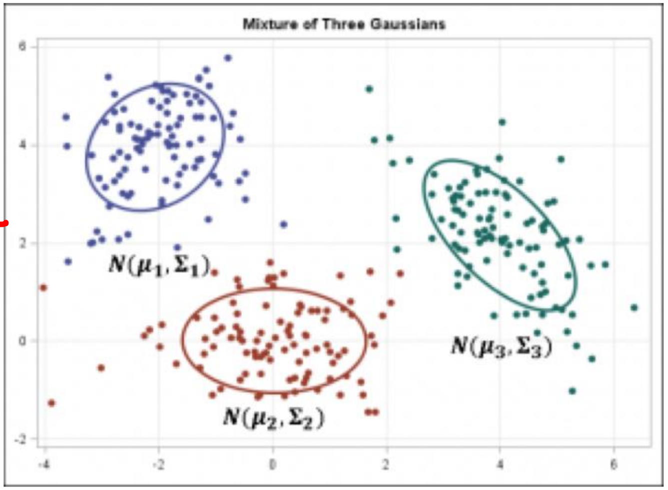


2-d Gaussian

$$f_{\mathbf{x}}(x_1,\ldots,x_k) = \frac{\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)}{\sqrt{(2\pi)^k|\boldsymbol{\Sigma}|}}$$

From wikipedia and http://home.dei.polimi.it

Gaussian Mixture Model



- Assumptions
  - Each data point comes from one of K classes.
  - The cluster prior distribution w_j is unknown.
  - Each class c_j follows a Gaussian distribution:

$$P\left(x \middle| c_j, \theta_j\right) = \frac{1}{\sqrt{2\pi\sigma_j^2}} e^{-\frac{(x-\mu_j)^2}{2\sigma_j^2}}$$

  - The parameters for each class μ_j, σ_j are unknown (need to be learned).
  - The probability of x_i is the sum over all classes,

$$P(x_i|\theta) = \sum_{j=1}^{K} P\left(x_i \middle| c_j, \theta_j\right) P(c_j)$$

w_j

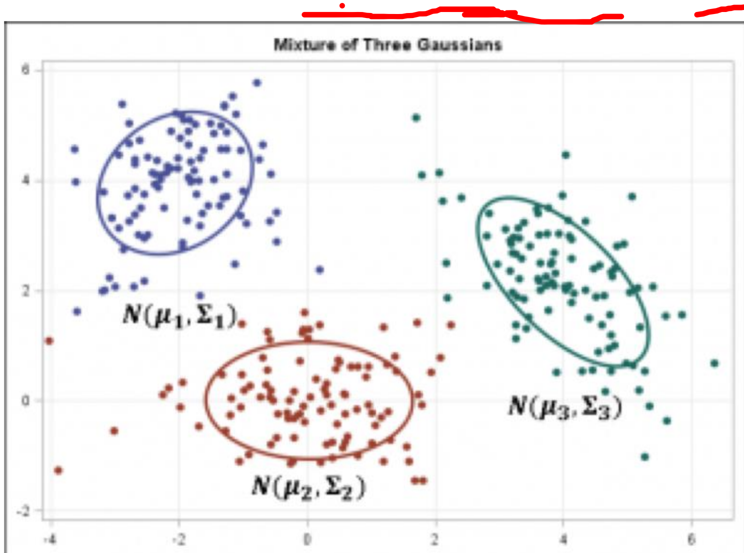
Soft Clustering with Gaussian Mixture Model

- Every object i is assigned to one cluster j with a probability
  - $P(z_i = j) \in [0,1]$ and $\sum_j P(z_i = j) = 1$
  - Where z_i is a hidden variable of which cluster x_i belongs to.

Assume the parameters of the GMM have been learned

- The probability of x_i belonging to cluster c_j :

$$P(z_i = c_j | x_i) \propto P(x_i, z_i = c_j) = w_j P(x_i | z_i = c_j)$$



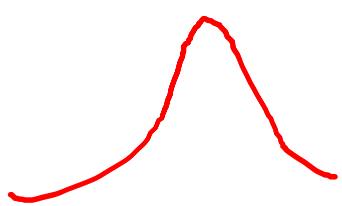
Cluster prior probabilities

Probability density function of each cluster

P(Cj)

The E-M(Expectation Maximization) Algorithm

- A framework to approach maximum likelihood or maximum a posteriori estimates of parameters in statistical models.
- Expectation Step: Assignment
  - Assigns objects to clusters according to the current soft clustering or parameters of probabilistic clusters
  - $w_{ij}^{t+1} = P\left(z_i = j \middle| x_i, \theta_j^t\right) \propto w_j P\left(x_i \middle| z_i = j, \theta_j^t\right)$ ⇐ Joint probability of x_i and its cluster c_j
- Maximization Step:
  - finds the new parameters of each cluster that maximize the expected likelihood
  - $\theta_{t+1} = argmax_{\theta} \Sigma_i \Sigma_j w_{ij}^{t+1} log L(x_i, z_j | \theta)$



Example: Applying E-M algorithm to 1-D GMM

- Iteratively do the following two steps
  - **E-Step**: Evaluate the soft clustering probability according to $\mu_j^t, \sigma_j^t, w_j^t$
    - $w_{ij}^{t+1} = \frac{w_j^t P\left(x_i \middle| \mu_j^t, \sigma_j^t\right)}{\Sigma_k w_k^t P\left(x_i \middle| \mu_k^t, \sigma_k^t\right)}$
  - **M-Step**: Find the new parameters μ_j^t, σ_j^t that maximize log likelihood. In Gaussian distribution, this is equivalent to do parameter estimation when each data point has a weight.
    - $\mu_j^{t+1} = \frac{\Sigma_i w_{ij}^{t+1} x_i}{\Sigma_i w_{ij}^{t+1}}, \left(\sigma_j^2\right)^{t+1} = \frac{\Sigma_i w_{ij}^{t+1} (x_i - \mu_j^{t+1})^2}{\Sigma_i w_{ij}^{t+1}}$ ⇦ Weighted average means and variance
    - $w_j^{t+1} = \frac{\Sigma_i w_{ij}^{t+1}}{n}$

Gaussian Mixture Model

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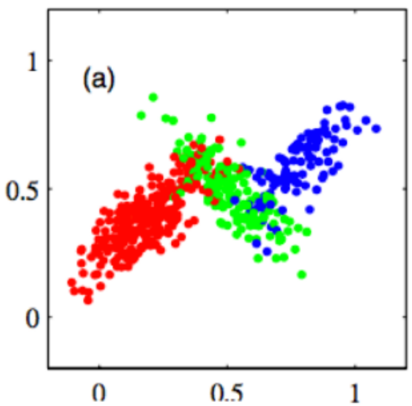
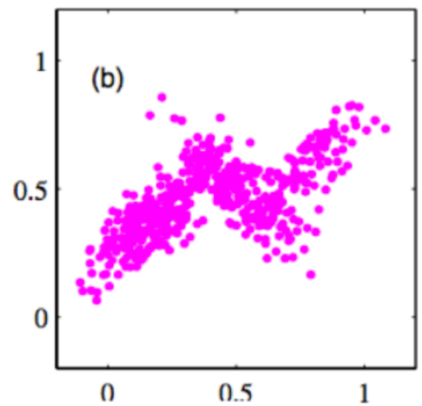
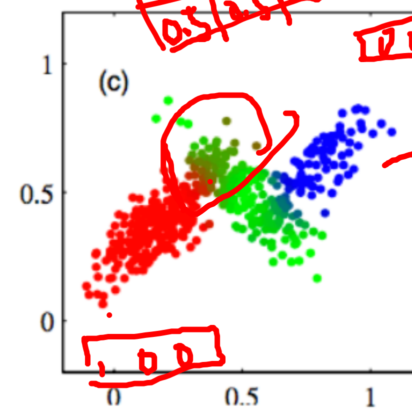
- Example of applying Gaussian Mixture Model



The data points belong to three classes. Each class follows a Gaussian distribution.



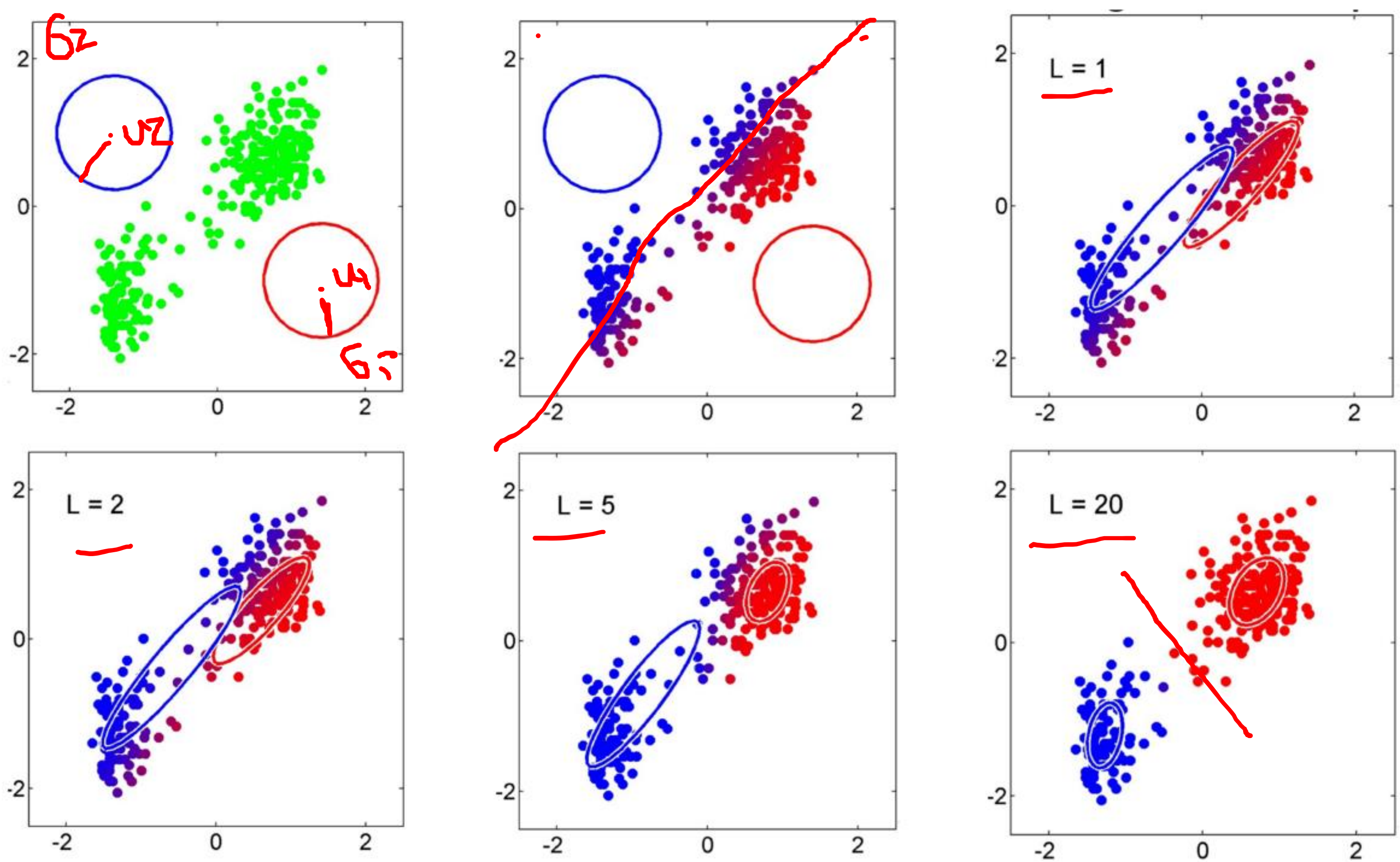
We hide the class information.



Cluster information inferred by GMM.

- We can use E-M algorithm to learn the parameters.

Example: Applying E-M algorithm to GMM



Gaussian Mixture Model – Strength and Weakness

- Advantages
  - Mixture models are more general than partitioning: different densities and sizes of clusters
  - Clusters can be characterized by a small number of parameters
  - The results satisfy the statistical assumptions of generative models
- Disadvantages
  - Converge to local optimal ⇦ Overcome it by running multi-times w. random initialization
  - Computationally more expensive
  - Hard to estimate the number of clusters
  - Can only deal with spherical clusters

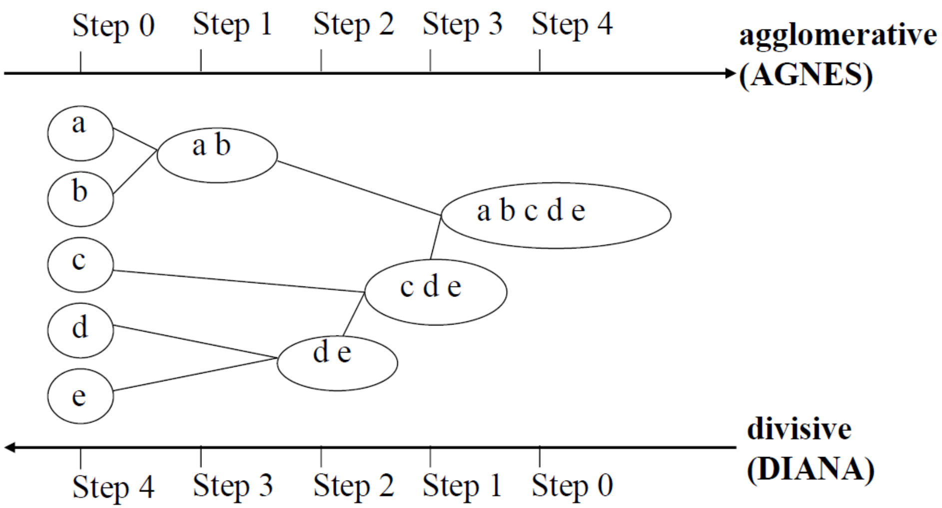
Hierarchical Methods

Hierarchical Clustering Methods

- Basic Concepts of Hierarchical Algorithms
- Agglomerative Clustering Algorithms
- Divisive Clustering Algorithms
- Extensions to Hierarchical Clustering

Hierarchical Clustering: Basic Concepts

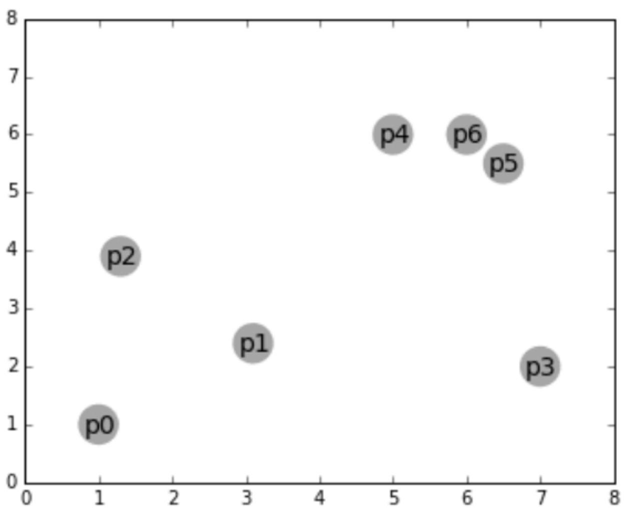
- Hierarchical clustering
  - Generate a clustering hierarchy (drawn as a dendrogram)
  - Not required to specify K, the number of clusters
  - More deterministic
  - No iterative refinement

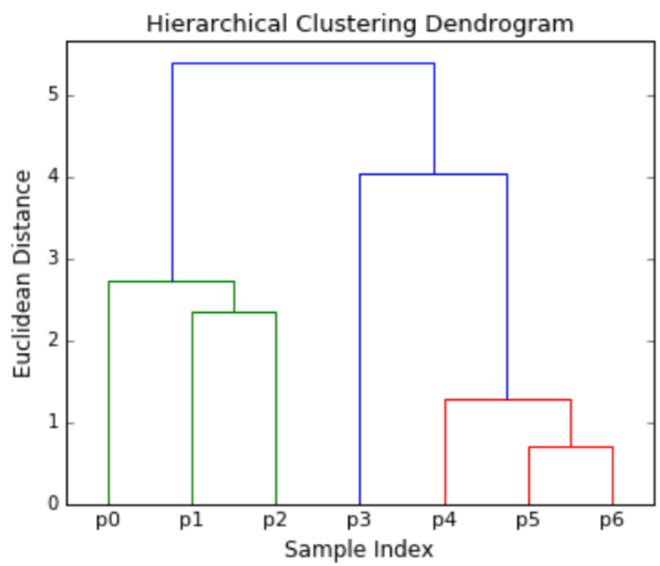


- Two categories of algorithms:
  - **Agglomerative**: Start with singleton clusters, continuously merge two clusters at a time to build a bottom-up hierarchy of clusters
  - **Divisive**: Start with a huge macro-cluster, split it continuously into two groups, generating a top-down hierarchy of clusters

Dendrogram: Shows How Clusters are Merged

- **Dendrogram**: Decompose a set of data objects into a tree of clusters by multi-level nested partitioning
- A **clustering** of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster



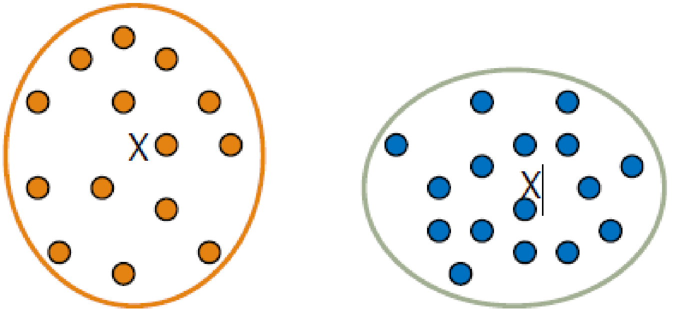


Hierarchical clustering generates a dendrogram (a hierarchy of clusters)

Agglomerative Clustering Algorithm

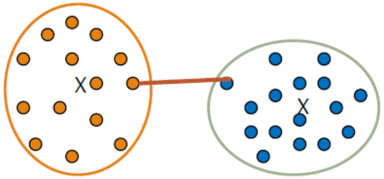
- AGNES (AGglomerative NESting) (Kaufmann and Rousseeuw, 1990)
  - Continuously merge nodes that have the least dissimilarity
  - Eventually all nodes belong to the same cluster

- Agglomerative clustering varies on different similarity measures among clusters
  - Single link (nearest neighbor)
  - Complete link (diameter)
  - Average link (group average)
  - Centroid link (centroid similarity)

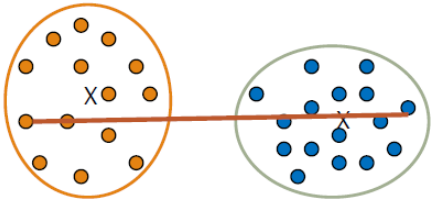


Single Link vs. Complete Link in Hierarchical Clustering

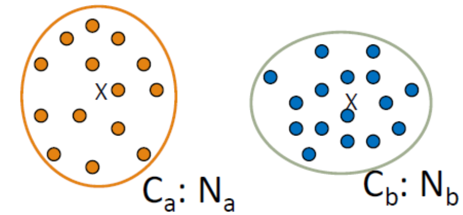
- **Single link (nearest neighbor)**
  - **Def.** The similarity between two clusters is the similarity between
    their most similar (nearest neighbor) members
  - Local similarity-based: Emphasizing more on close regions, ignoring the overall structure of the cluster
  - Capable of clustering non-elliptical shaped group of objects
  - Sensitive to noise and outliers



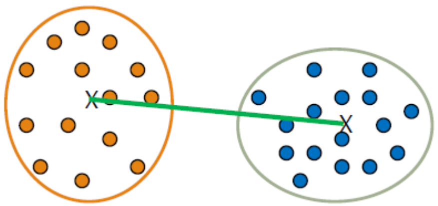
- **Complete link (diameter)**
  - **Def.** The similarity between two clusters is the similarity between their most dissimilar members
  - Merge two clusters to form one with the smallest diameter
  - Nonlocal in behavior, obtaining compact shaped clusters
  - Sensitive to outliers



Agglomerative Clustering: Average vs. Centroid Links



- Agglomerative clustering with **average link**
  - **Average link**: The average distance between an element in one cluster and an element in the other (i.e., all pairs in two clusters)
  - Expensive to compute

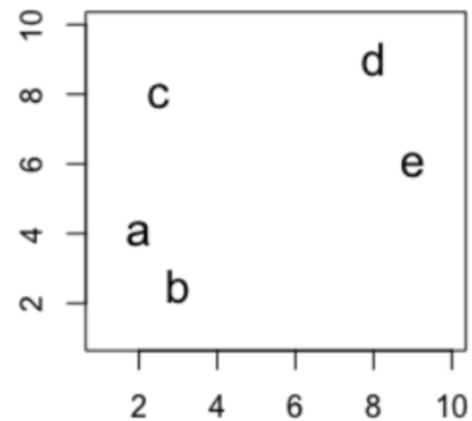


- Agglomerative clustering with **centroid link**
  - **Centroid link**: The distance between the centroids of two clusters
- **Group Averaged Agglomerative Clustering (GAAC)**
  - Let two clusters C_a and C_b be merged into C_{aUb}. The new centroid is: $c_{a \cup b} = \dfrac{N_a c_a + N_b c_b}{N_a + N_b}$
    - N_a is the cardinality of cluster C_a, and c_a is the centroid of C_a
  - The similarity measure for GAAC is the average of their distances
- Agglomerative clustering with **Ward's criterion**
  - Ward's criterion: The increase in the value of the SSE criterion for the clustering obtained by merging them into $C_a\ U\ C_b$:

$$W(C_{a \cup b}, c_{a \cup b}) - W(C, c) = \frac{N_a N_b}{N_a + N_b} d(c_a, c_b)$$

Agglomerative Clustering: Example of Single Link

- 2-D Data points
  - a(2,4)
  - b(3,2)
  - c(2,8)
  - d(8,9)
  - e(9,6)

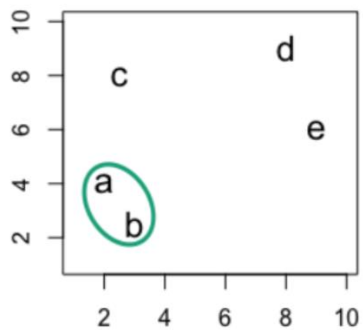


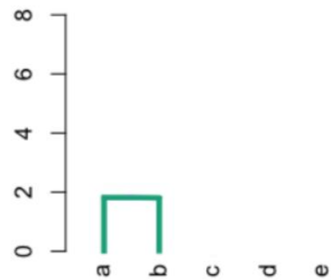
Distance Matrix

	a	b	c	d	e
a	0				
b	2.2	0			
c	4	6.1	0		
d	7.8	8.6	6.1	0	
e	7.3	7.2	7.3	3.2	0

Agglomerative Clustering: Example of Single Link

- 2-D Data points





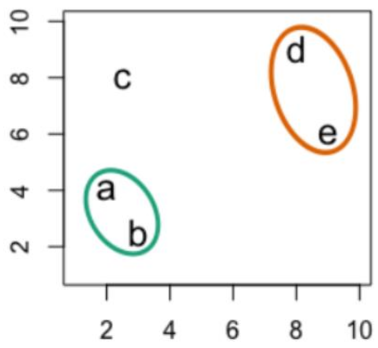
Distance Matrix

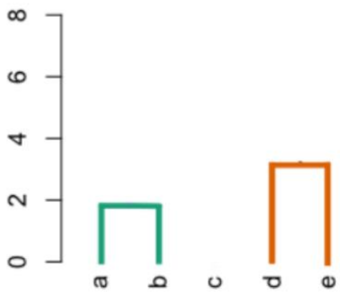
	a,b	c	d	e
a,b	0			
c	4	0		
d	7.8	6.1	0	
e	7.2	7.3	3.2	0

- Update distance
  - Distance((a,b), c) = min(Distance(a,c), Distance(b,c)) = min(4, 6.1)=4
  - Distance((a,b), d) = min(Distance(a,d), Distance(b,d)) = min(7.8, 8.6)=7.8
  - Distance((a,b), e) = min(Distance(a,e), Distance(b,e)) = min(7.3, 7.2)=7.2

Agglomerative Clustering: Example of Single Link

- 2-D Data points





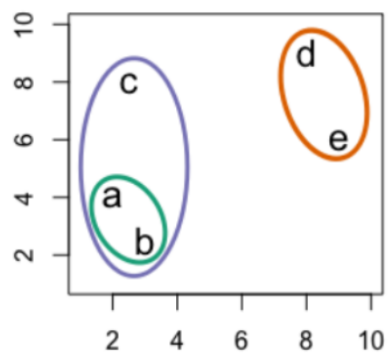
Distance Matrix

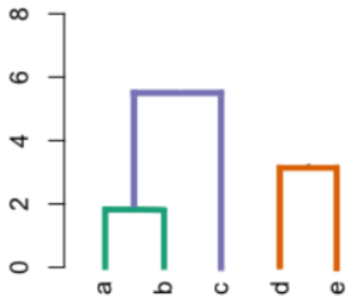
	a,b	c	d,e
a,b	0		
c	4	0	
d,e	7.2	6.1	0

- Update distance
  - Distance((d,e), (a,b)) = min(Distance(d,(a,b)), Distance(e,(a,b)) = 7.2
  - Distance((d,e), c) = min(Distance(d,c), Distance(e,c)) = 6.1

Agglomerative Clustering: Example of Single Link

- 2-D Data points





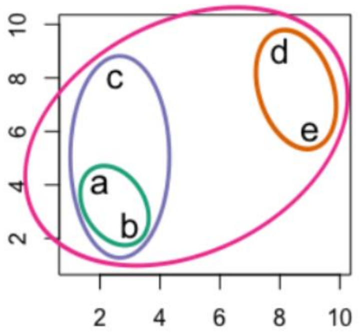
Distance Matrix

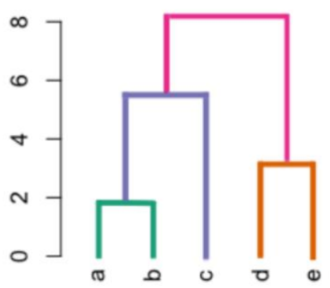
	a,b,c	d,e
a,b,c	0	
d,e	6.1	0

- Update distance
  - Distance((d,e), (c,(a,b)))= min(Distance((d,e),(a,b)), Distance((d,e),c) = 6.1

Agglomerative Clustering: Example of Single Link

- 2-D Data points

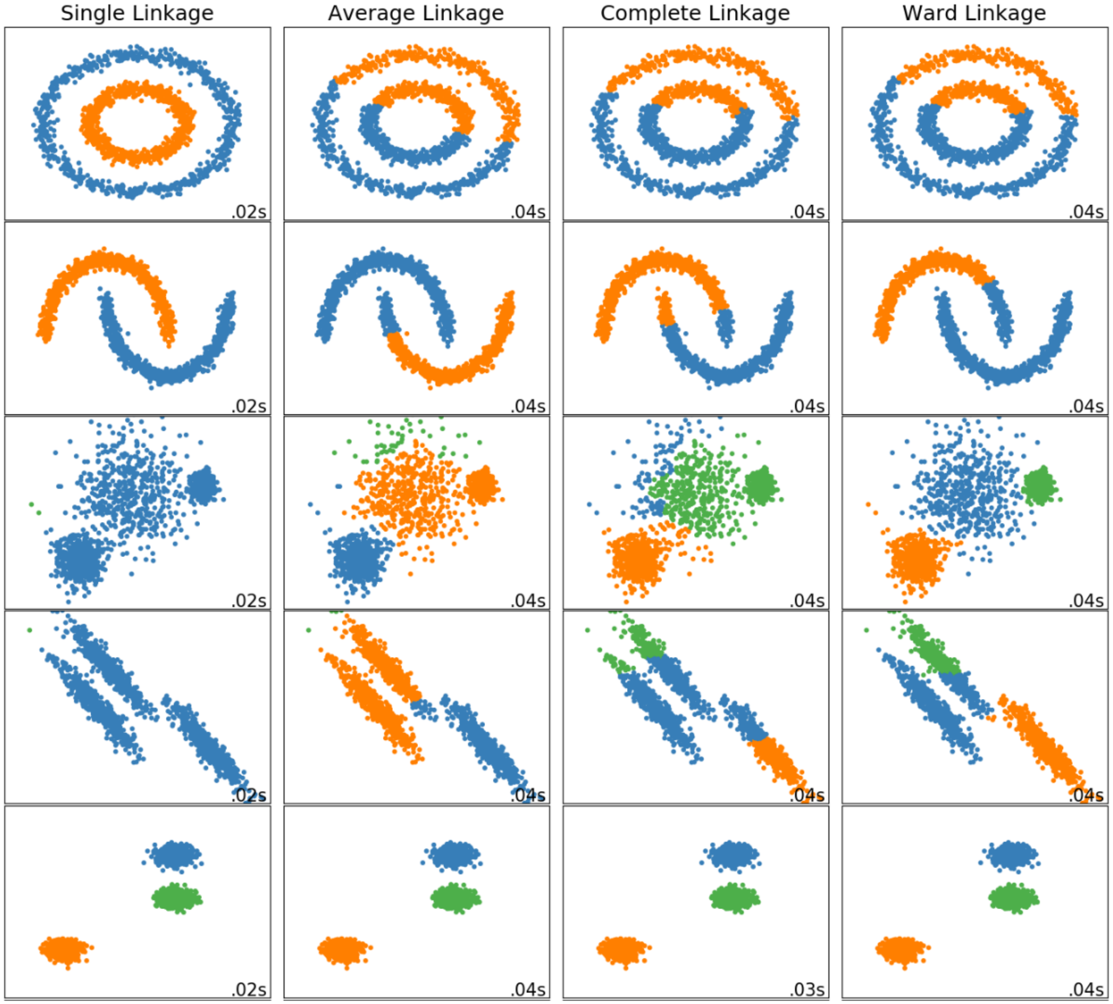




Distance Matrix

	a,b,c,d,e
a,b,c,d,e	0

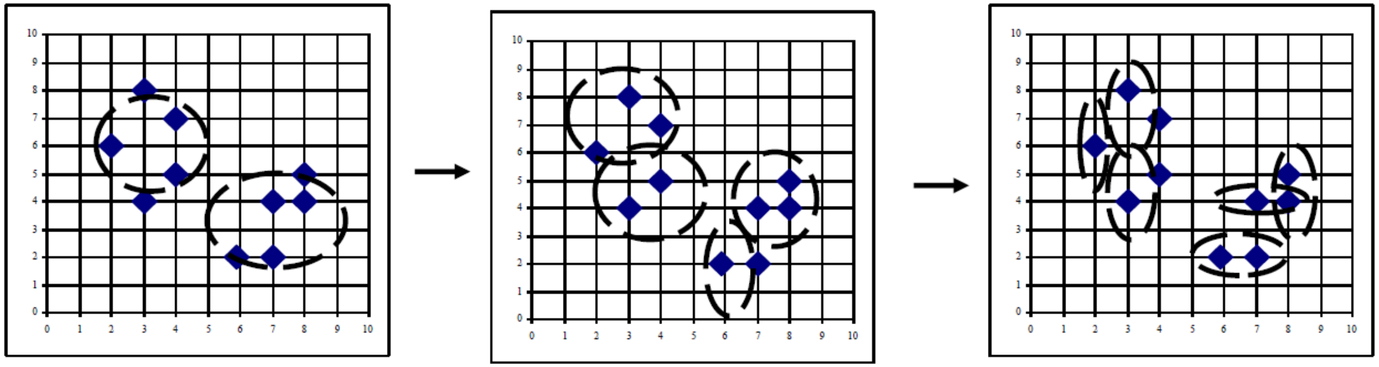
Comparison of Different Linkage Methods



- Observations:
  - Single link performs well on non-globular data, but it performs poorly in the presence of noise.
  - Average and Complete Linkage performs well on globular data but has mixed results otherwise.
  - Ward is the most effective method for noisy data.

Divisive Clustering

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



- Divisive clustering is a top-down approach
  - The process starts at the root with all the points as one cluster
  - It recursively splits the higher-level clusters to build the dendrogram
  - Can be considered as a global approach
  - More efficient when compared with agglomerative clustering

More on Algorithm Design for Divisive Clustering

- Choosing which cluster to split
  - Check the sums of squared errors of the clusters and choose the one with the largest value
- Splitting criterion: Determining how to split
  - One may use Ward's criterion to chase for greater reduction in the difference in the SSE criterion as a result of a split
  - For categorical data, Gini-index can be used
- Handling the noise
  - Use a threshold to determine the termination criterion (do not generate clusters that are too small because they contain mainly noises)

Extensions to Hierarchical Clustering

- Major weaknesses of hierarchical 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

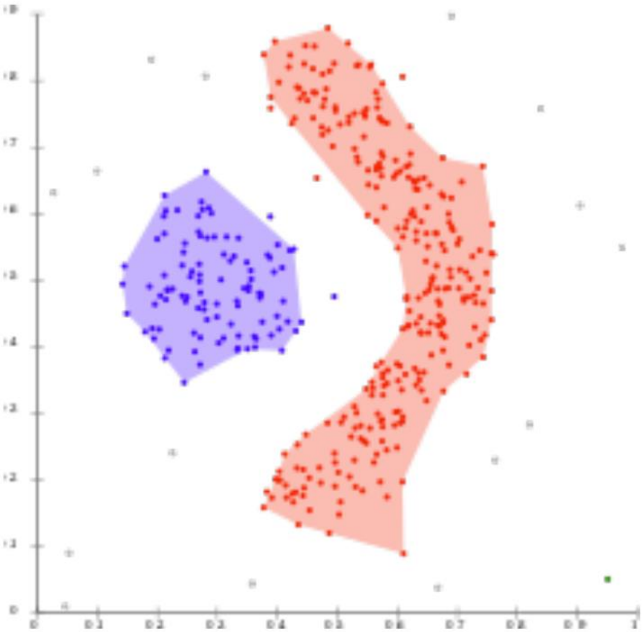
- Other hierarchical clustering algorithms
  - BIRCH (1996): Use CF-tree and incrementally adjust the quality of sub-clusters
  - CURE (1998): Represent a cluster using a set of well-scattered representative points
  - CHAMELEON (1999): Use graph partitioning methods on the K-nearest neighbor graph of the data

Density-Based Methods

Density-based Clustering

- Clustering based on density (a local criterion), such as densely-connected points

- Main Advantages
  - Discover clusters of arbitrary shape
  - Handle noise

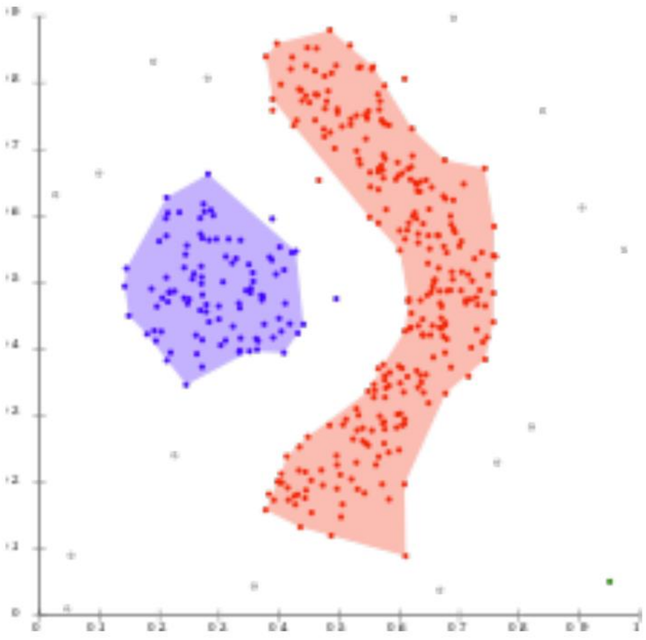


Representative Density-Based Clustering Methods

- Several interesting studies:
  - DBSCAN: Ester, et al. (KDD'96) To be covered in this lecture
  - OPTICS: Ankerst, et al (SIGMOD'99)
  - DENCLUE: Hinneburg & D. Keim (KDD'98)
  - CLIQUE: Agrawal, et al. (SIGMOD'98) (also, grid-based)

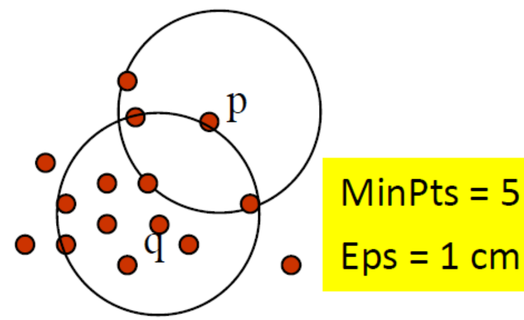
DBSCAN: High-Level Idea

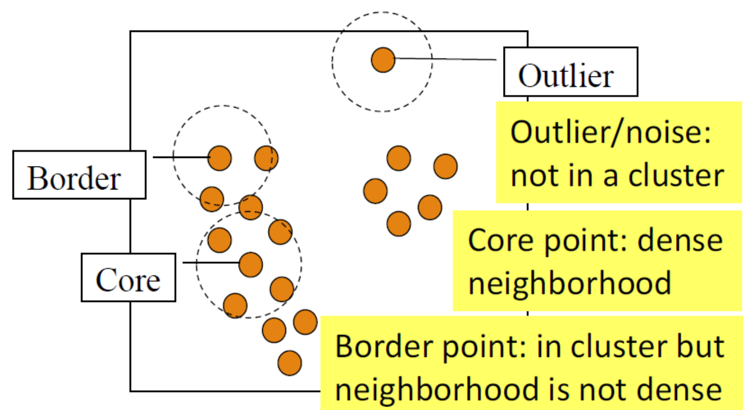
- DBSCAN
  - Discovers clusters of arbitrary shape: Density-Based Spatial Clustering of Applications with Noise
- A density-based notion of cluster
  - A cluster is defined as a maximal set of density-connected points



DBSCAN: Core Concepts

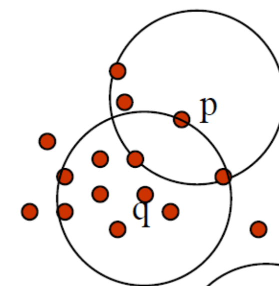
- **DBSCAN**: A cluster is defined as a maximal set of density connected points
- Two parameters:
  - **Eps(ε)**: Maximum radius of the neighborhood
  - **MinPts**: Minimum number of points in the Eps-neighborhood of a point
- The Eps(ε)-neighborhood of a point q:
  - NEps(q): {p belongs to D | dist(p, q) ≤ Eps}





DBSCAN: Density-Reachable and Density-Connected

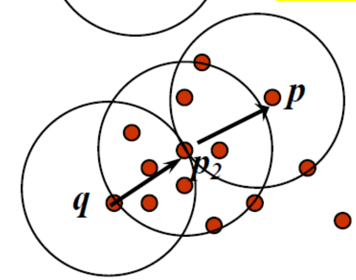
- **Directly density-reachable:**
  - A point p is directly density-reachable from a point q w.r.t. Eps(ε), MinPts if
    - p belongs to N_{Eps}(q)
    - **core point** condition: $|N_{Eps}$ (q)$|$ ≥ MinPts



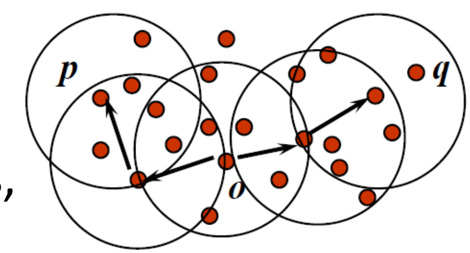
MinPts = 5

Eps = 1 cm

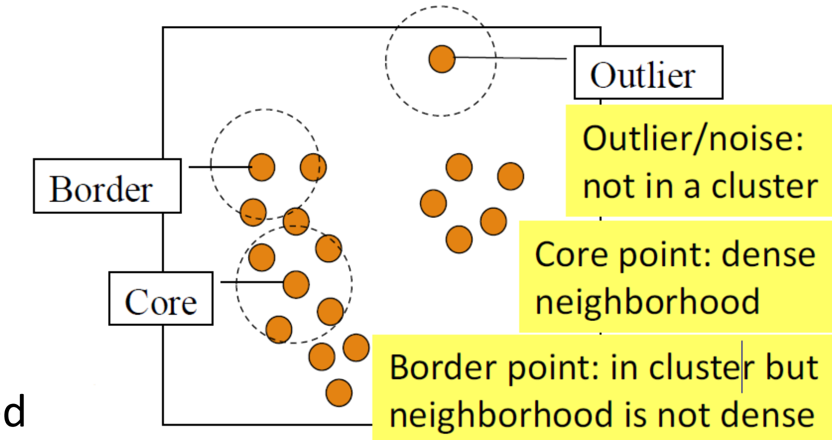
- **Density-reachable**: (asymmetric)
  - A point p is density-reachable from a point q w.r.t. Eps, MinPts if there is a chain of points $p_1, \ldots, p_n$, $p_1 = q, p_n = p$ such that p_{i+1} is directly density-reachable from p_i



- **Density-connected**: (symmetric)
  - A point p is density-connected to a point q w.r.t. Eps, MinPts if there is a point o such that both p and q are density-reachable from o w.r.t. Eps and MinPts



DBSCAN: the Algorithm



- Algorithm
  - Arbitrarily select a point p
  - Retrieve all points density-reachable from p w.r.t. Eps and MinPts
    - If p is a core point, a cluster is formed
    - If p is a border point, no points are density-reachable from p, and DBSCAN visits the next point of the database
  - Continue the process until all of the points have been processed
- Computational complexity
  - If a spatial index is used, the computational complexity of DBSCAN is $O(nlogn)$, where n is the number of database objects
  - Otherwise, the complexity is $O(n^2)$

DBSCAN Is Sensitive to the Setting of Parameters

Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.

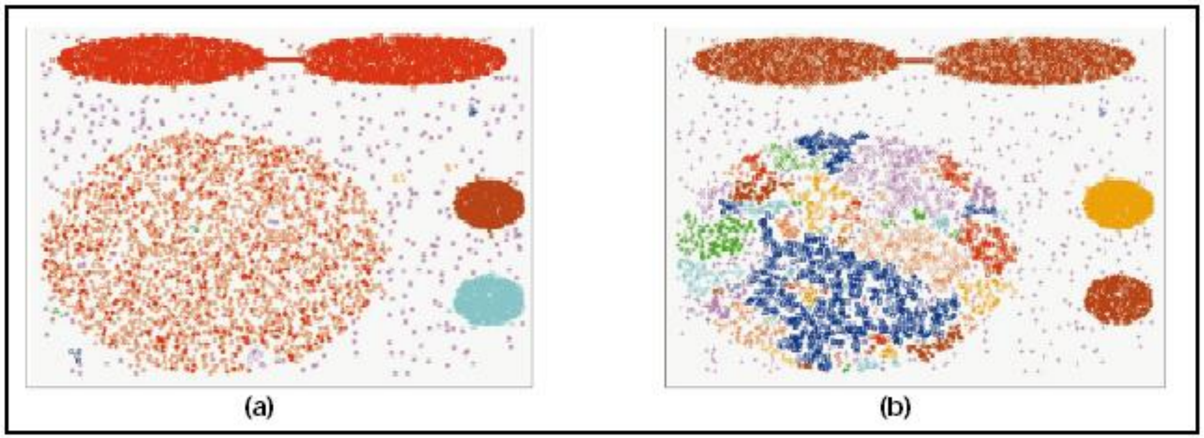
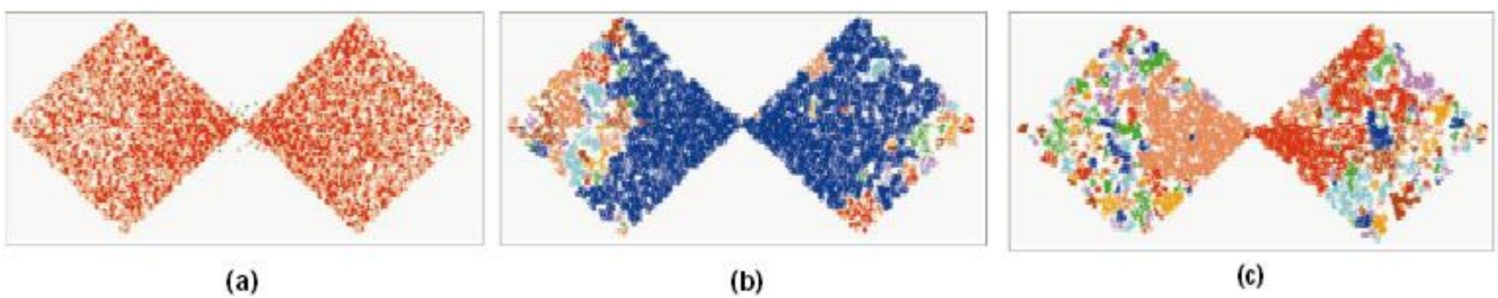


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



Ack. Figures from G. Karypis, E.-H. Han, and V. Kumar, *COMPUTER*, 32(8), 1999

Evaluation of Clustering

Clustering Validation and Assessment

- Major issues on clustering validation and assessment
  - Clustering evaluation
    - Evaluating the goodness of the clustering
  - Clustering stability
    - To understand the sensitivity of the clustering result to various algorithm parameters, e.g., # of clusters
  - Clustering tendency
    - Assess the suitability of clustering, i.e., whether the data has any inherent grouping structure

Clustering Validation

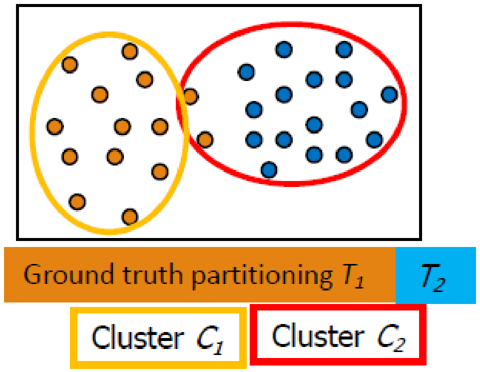
- Clustering Validation: Basic Concepts
- External Measures for Clustering Validation
  - I: Matching-Based Measures
  - II: Entropy-Based Measures
  - III: Pairwise Measures
- Internal Measures for Clustering Validation (optional)
- Relative Measures (optional)
- Cluster Stability (optional)
- Clustering Tendency (optional)

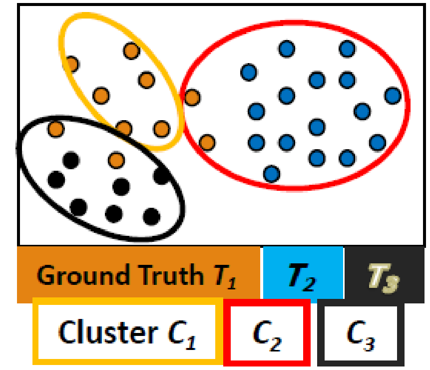
Measuring Clustering Quality

- **Clustering Evaluation**: Evaluating the goodness of clustering results
  - No commonly recognized best suitable measure in practice
- **Three categorization of measures**: External, Internal, and Relative
  - **External**: Supervised, employ criteria not inherent to the dataset
    - Compare a clustering against prior or expert-specified knowledge (i.e., the ground truth) using certain clustering quality measure
  - **Internal**: Unsupervised, criteria derived from data itself
    - Evaluate the goodness of a clustering by considering how well the clusters are separated and how compact the clusters are, e.g., silhouette coefficient
  - **Relative**: Directly compare different clusterings, usually those obtained via different parameter settings for the same algorithm

Commonly Used External Measures

- **Matching-based measures**
  - Purity, maximum matching, F-measure
- **Entropy-Based Measures**
  - Conditional entropy
  - Normalized mutual information (NMI)
- **Pairwise measures**
  - Four possibilities: True positive (TP), FN, FP, TN
  - Jaccard coefficient, Rand statistic, Fowlkes-Mallow measure





Matching-Based Measures (I): Purity vs. Maximum Matching

$C\backslash T$	T_1	T_2	T_3	Sum
C_1	0	20	30	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	40	35	100

$C\backslash T$	T_1	T_2	T_3	Sum
C_1	0	30	20	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	50	25	100

- **Purity**: Quantifies the extent that cluster Ci contains points only from one (ground truth) partition: $purity_i = \frac{1}{n_i} \max_{j=1}^{k} \{n_{ij}\}$
  - Total purity of clustering C: $purity = \sum_{i=1}^{r} \frac{n_i}{n} purity_i = \frac{1}{n} \sum_{i=1}^{r} \max_{j=1}^{k} \{n_{ij}\}$
  - Perfect clustering if purity = 1 and r = k (the number of clusters obtained is the same as that in the ground truth)
  - Ex. 1 (green or orange): $purity_1 = 30/50$; $purity_2 = 20/25$; $purity_3 = 25/25$; purity = (30 + 20 + 25)/100 = 0.75
  - Two clusters may share the same majority partition

Problem?
High purity is easy to achieve when the number of clusters is large - in particular, purity is 1 if each document gets its own cluster.

Matching-Based Measures (I): Purity vs. Maximum Matching

- **Maximum matching:** Only one cluster can match one partition
  - Match: Pairwise matching, weight w(e_{ij}) = n_{ij}
  - Maximum weight matching: $match = \arg\max_M\{\frac{w(M)}{n}\}$
  - Ex2. (green) match = purity = 0.75; (orange) match = 0.65 > 0.6

$C\backslash T$	T_1	T_2	T_3	Sum
C_1	0	30	20	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	50	25	100

- **Maximum matching:** Only one cluster can match one partition
  - Match: Pairwise matching, weight w(e_{ij}) = n_{ij} $\quad w(M) = \sum_{e \in M} w(e)$
  - Maximum weight matching: $match = \arg\max_M\{\frac{w(M)}{n}\}$
  - Ex2. (green) match = purity = 0.75; (orange) match = 0.65 > 0.6

Matching-Based Measures (II): F-Measure

- **Precision**: The fraction of points in C_i from the majority partition T_{j_i} (i.e., the same as purity), where j_i is the partition that contains the maximum # of points from C_i

$$prec_i = \frac{1}{n_i}\max_{j=1}^{k}\{n_{ij}\} = \frac{n_{ij_i}}{n_i}$$

  - Ex. For the green table
    - $prec_1$ = 30/50; $prec_2$ = 20/25; $prec_3$ = 25/25
- **Recall**: The fraction of point in partition T_{j_i} shared in common with cluster C_i , where $m_{j_i} = |T_{j_i}|$

$$recall_i = \frac{n_{ij_i}}{|T_{j_i}|} = \frac{n_{ij_i}}{m_{j_i}}$$

  - Ex. For the green table
    - $recall_1$ = 30/35; $recall_2$ = 20/40; $recall_3$ = 25/25
- **F-measure** for C_i : The harmonic means of $prec_i$ and $recall_i$:

$$F_i = \frac{2n_{ij_i}}{n_i + m_{j_i}}$$

- F-measure for clustering C: average of all clusters:

$$F = \frac{1}{r}\sum_{i=1}^{r} F_i$$

  - Ex. For the green table
    - F_1 = 60/85; F_2 = 40/65; F_3 = 1; F = 0.774

C\T	T_1	T_2	T_3	Sum
C_1	0	20	30	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	40	35	100

Matching-Based Measures (II): F-Measure

- **Precision**: The fraction of points in C_i from the majority partition T_{j_i} (i.e., the same as purity), where j_i is the partition that contains the maximum # of points from C_i

$$prec_i = \frac{1}{n_i} \max_{j=1}^{k} \{n_{ij}\} = \frac{n_{ij_i}}{n_i}$$

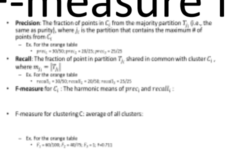
  - Ex. For the orange table
    - $prec_1$ = 30/50; $prec_2$ = 20/25; $prec_3$ = 25/25
- **Recall**: The fraction of point in partition T_{j_i} shared in common with cluster C_i , where $m_{j_i} = |T_{j_i}|$

$$recall_i = \frac{n_{ij_i}}{|T_{j_i}|} = \frac{n_{ij_i}}{m_{j_i}}$$

  - Ex. For the orange table
    - $recall_1$ = 30/50; $recall_2$ = 20/50; $recall_3$ = 25/25
- **F-measure** for C_i : The harmonic means of $prec_i$ and $recall_i$:

$$F_i = \frac{2n_{ij_i}}{n_i + m_{j_i}}$$

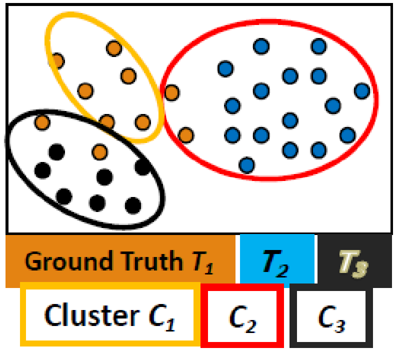
- F-measure for clustering C: average of all clusters:



  - Ex. For the orange table
    - F_1 = 60/100; F_2 = 40/75; F_3 = 1; F=0.711

C\T	T_1	T_2	T_3	Sum
C_1	0	30	20	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	50	25	100

Entropy-Based Measures (I): Conditional Entropy



- **Entropy of clustering C**:

$$H(\mathcal{C}) = -\sum_{i=1}^{r} p_{C_i} \log p_{C_i} \qquad p_{C_i} = \frac{n_i}{n} \text{ (i.e., the probability of cluster } C_i\text{)}$$

- **Entropy of partitioning T**: $H(\mathcal{T}) = -\sum_{j=1}^{k} p_{T_j} \log p_{T_j}$
- **Entropy of T with respect to cluster C_i**: $H(\mathcal{T}|C_i) = -\sum_{j=1}^{k} (\frac{n_{ij}}{n_i}) \log(\frac{n_{ij}}{n_i})$
- **Conditional entropy of T with respect to clustering C**:

$$H(\mathcal{T}|\mathcal{C}) = -\sum_{i=1}^{r} (\frac{n_i}{n}) H(\mathcal{T}|C_i) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log(\frac{p_{ij}}{p_{C_i}})$$

  - The more a cluster's members are split into different partitions, the higher the conditional entropy
  - For a perfect clustering, the conditional entropy value is 0

C\T	T_1	T_2	T_3	Sum
C_1	0	30	20	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	50	25	100

$$H(\mathcal{T}|\mathcal{C}) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij}(\log p_{ij} - \log p_{C_i}) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij}\log p_{ij} + \sum_{i=1}^{r}(\log p_{C_i} \sum_{j=1}^{k} p_{ij})$$

$$= -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij}\log p_{ij} + \sum_{i=1}^{r}(p_{C_i}\log p_{C_i}) = H(\mathcal{C},\mathcal{T}) - H(\mathcal{C})$$

Entropy-Based Measures (II): Normalized Mutual Information (NMI)

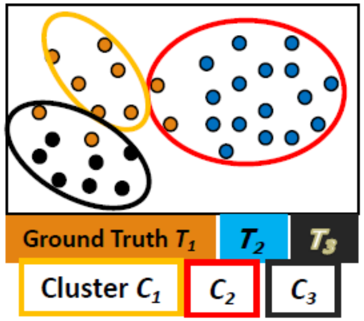
- **Mutual information**:
  - Quantifies the amount of shared info between the clustering C and partitioning T
  - Measures the dependency between the observed joint probability p_{ij} of C and T, and the expected joint probability $p_{Ci} \cdot p_{Tj}$ under the independence assumption
  - When C and T are independent, $p_{ij} = p_{Ci} \cdot p_{Tj}$, I(C, T) = 0.

$$I(C,T)=\sum_{i=1}^{r}\sum_{j=1}^{k}p_{ij}\log(\frac{p_{ij}}{p_{C_i}\cdot p_{T_j}})$$

- **Normalized mutual information** (NMI)

$$NMI(\mathcal{C},\mathcal{T})=\sqrt{\frac{I(\mathcal{C},\mathcal{T})}{H(\mathcal{C})}\cdot\frac{I(\mathcal{C},\mathcal{T})}{H(\mathcal{T})}}=\frac{I(\mathcal{C},\mathcal{T})}{\sqrt{H(\mathcal{C})\cdot H(\mathcal{T})}}$$

  - Value range of NMI: [0,1]
  - Value close to 1: a good clustering



C\T	T_1	T_2	T_3	Sum
C_1	0	30	20	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	50	25	100

Pairwise Measures

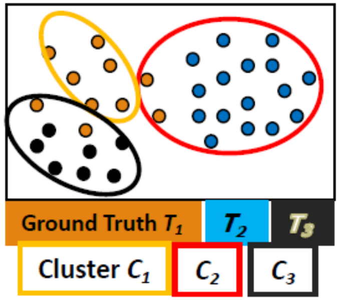
Data points	Output clustering	Ground truth (class)
A	1	2
B	1	2
C	2	2
D	2	1

- # pairs of data points: 6
  - (a, b): same class, same cluster
  - (a, c): same class, different cluster
  - (a, d): different class, different cluster
  - (b, c): same class, different cluster
  - (b, d): different class, different cluster
  - (c, d): different class, same cluster

TP = 1
FP = 1
FN = 2
TN = 2

RI = 0.5
Precision= ½, Recall= 1/3
F = 0.4

Pairwise Measures: Four Possibilities for Truth Assignment



- **Four possibilities** based on the agreement between cluster label and partition label
  - TP: true positive—Two points x_i and x_j belong to the same partition T, and they also in the same cluster C

    $$TP = \left|\left\{\left(x_i, x_j\right):\ y_i = y_j\ and\ \hat{y_i} = \hat{y_j}\right\}\right|$$

    where y_i: the true partition label , and $\hat{y_i}$: the cluster label for point x_i
  - FN: false negative $FN = \left|\left\{\left(x_i, x_j\right):\ y_i = y_j\ and\ \hat{y_i} \neq \hat{y_j}\right\}\right|$
  - FP: false positive $FP = \left|\left\{\left(x_i, x_j\right):\ y_i \neq y_j\ and\ \hat{y_i} = \hat{y_j}\right\}\right|$
  - TN: true negative $TN = \left|\left\{\left(x_i, x_j\right):\ y_i \neq y_j\ and\ \hat{y_i} \neq \hat{y_j}\right\}\right|$

TP	***FN***	***P***
FP	***TN***	***N***
P'	***N'***	***All***

$$P = Precision = \frac{TP}{TP + FP}$$

$$R = Recall = \frac{TP}{TP + FN}$$

$$F_1 = F_1\ Measure = \frac{2P * R}{P + R}$$

Pairwise Measures: Jaccard Coefficient and Rand Statistic

- **Jaccard coefficient**: Fraction of true positive point pairs, but after ignoring the true negatives (thus asymmetric)
  - Jaccard = TP/(TP + FN + FP) [i.e., denominator ignores TN]
  - Perfect clustering: Jaccard = 1
- **Rand Statistic**:
  - Rand = (TP + TN)/All
  - Symmetric; perfect clustering: Rand = 1
- **Fowlkes-Mallow Measure**:
  - Geometric mean of precision and recall

$$FM = \sqrt{prec \times recall} = \frac{TP}{\sqrt{(TP + FN)(TP + FP)}}$$

Summary

Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: An Introduction
- Partitioning Methods
- Gaussian Mixture Models and E-M algorithm
- Evaluation of Clustering
- More on Clustering (not covered)
  - Hierarchical Methods
  - Density- and Grid-Based Methods
  - Spectral Methods
  - …

Clustering Validation (Optional)

- Clustering Validation: Basic Concepts
- External Measures for Clustering Validation
  - I: Matching-Based Measures
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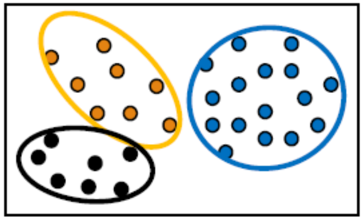
- Clustering Tendency (optional)

Internal Measures (I): BetaCV Measure (Optional)

- A trade-off in maximizing intra-cluster compactness and inter-cluster separation
- Given a clustering C = $\{C_1, . . ., C_k\}$ with k clusters, cluster C_i containing n_i = | C_i | points
  - Let W(S, R) be sum of weights on all edges with one vertex in S and the other in R
  - The sum of all the intra-cluster weights over all clusters: $W_{in} = \frac{1}{2}\sum_{i=1}^{k} W(C_i, C_i)$
  - The sum of all the inter-cluster weights:

$$W_{out} = \frac{1}{2}\sum_{i=1}^{k} W(C_i, \overline{C_i}) = \sum_{i=1}^{k-1}\sum_{j>i} W(C_i, C_j)$$



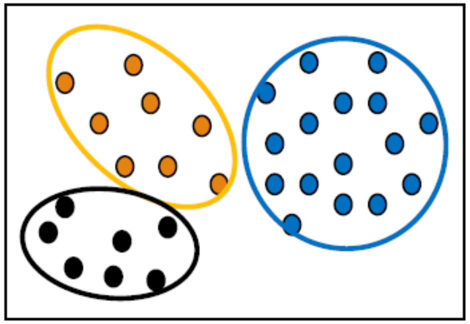
  - The number of distinct intra-cluster edges: $N_{in} = \sum_{i=1}^{k}\binom{n_i}{2}$
  - The number of distinct inter-cluster edges: $N_{out} = \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} n_i n_j$
- **Beta-CV measure**: $BetaCV = \frac{W_{in}/N_{in}}{W_{out}/N_{out}}$
  - The ratio of the mean intra-cluster distance to the mean inter-cluster distance
  - The smaller, the better the clustering

Internal Measures (II): Normalized Cut (Optional)

- **Normalized cut**:

$$NC = \sum_{i=1}^{k} \frac{W(C_i, \overline{C_i})}{vol(C_i)} = \sum_{i=1}^{k} \frac{W(C_i, \overline{C_i})}{W(C_i, V)} = \sum_{i=1}^{k} \frac{W(C_i, \overline{C_i})}{W(C_i, C_i) + W(C_i, \overline{C_i})} = \sum_{i=1}^{k} \frac{1}{\frac{W(C_i, C_i)}{W(C_i, \overline{C_i})} + 1}$$

  - where $vol(C_i) = W(C_i, V)$ is the volume of cluster C_i
  - The higher normalized cut value, the better the clustering



Clustering Validation (Optional)

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Relative Measure (Optional)

- Relative measure: Directly compare different clusterings, usually those obtained via different parameter settings for the same algorithm
- **Silhouette coefficient** as an **internal measure**: Check cluster cohesion and separation
  - For each point x_i, its silhouette coefficient s_i is: $s_i = \frac{\mu_{out}^{\min}(\mathbf{x}_i) - \mu_{in}(\mathbf{x}_i)}{\max\{\mu_{out}^{\min}(\mathbf{x}_i), \mu_{in}(\mathbf{x}_i)\}}$

    where $\mu_{in}(\mathbf{x}_i)$ is the mean distance from x_i to points in its own cluster
    $\mu_{out}^{\min}(\mathbf{x}_i)$ is the mean distance from x_i to points in its closest cluster
  - Silhouette coefficient (*SC*) is the mean values of s_i across all the points: $SC = \frac{1}{n}\sum_{i=1}^{n} s_i$
  - *SC* close to +1 implies good clustering
    - Points are close to their own clusters but far from other clusters
- **Silhouette coefficient** as a **relative measure**: Estimate the # of clusters in the data
  - $SC_i = \frac{1}{n_i}\sum_{x_j \in C_i} s_j$
  - Pick the k value that yields the best clustering, i.e., yielding high values for SC and SC_i (1 ≤ i ≤ k)

Silhouette Coefficient (Optional)

- Advantages
  - The score is bounded between -1 for incorrect clustering and +1 for highly dense clustering. Scores around zero indicate overlapping clusters.
  - The score is higher when clusters are dense and well separated, which relates to a standard concept of a cluster.
- Drawbacks
  - The Silhouette Coefficient is generally higher for convex clusters than other concepts of clusters, such as density-based clusters like those obtained through DBSCAN.

Clustering Validation (Optional)

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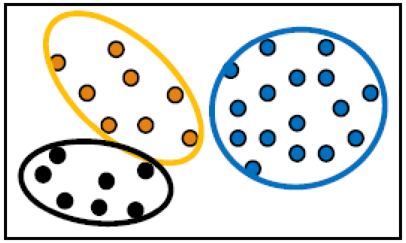
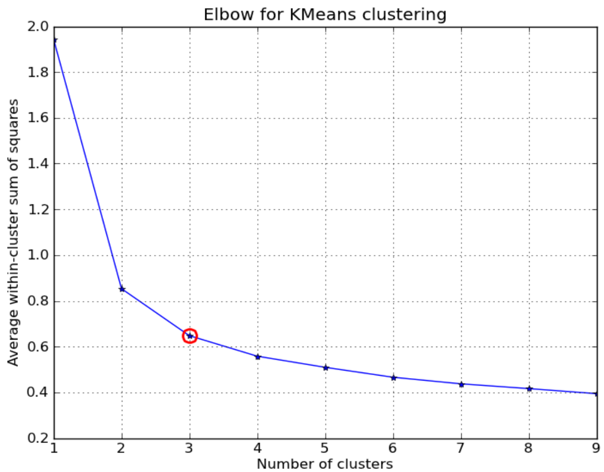
Cluster Stability (Optional)



- Clusters obtained from several datasets sampled from the same underlying distribution as **D** should be similar or "stable"
- Typical approach:
  - Find good parameter values for a given clustering algorithm
- Example: Find a good value of k, the correct number of clusters
- A **bootstrapping approach** to find the best value of k (judged on stability)
  - Generate t samples of size n by sampling from D with replacement
  - For each sample D_i, run the same clustering algorithm with k values from 2 to k_{max}
  - Compare the distance between all pairs of clusterings $C_k(D_i)$ and $C_k(D_j)$ via some distance function
    - Compute the expected pairwise distance for each value of k
  - The value k* that exhibits the least deviation between the clusters obtained from the resampled datasets is the best choice for k since it exhibits the most stability

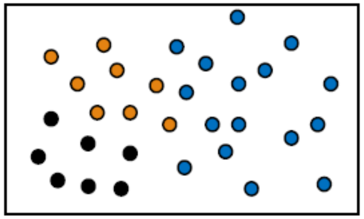
Other Methods for Finding K, the Number of Clusters (Optional)

- **Empirical method**
  - # of clusters $k \approx \sqrt{n/2}$ for a dataset of n points (e.g., n = 200, k = 10)
- **Elbow method**: Use the turning point in the curve of the sum of within cluster variance with respect to 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
    - For example, 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

Clustering Tendency: Whether the Data Contains Inherent Grouping Structure (Optional)



- Assessing the **suitability of clustering**
  - i.e., whether the data has any inherent grouping structure
- Determining **clustering tendency** or **clusterability**
  - **A hard task** because there are so many different definitions of clusters
    - E.g., partitioning, hierarchical, density-based, graph-based, etc.
  - Even fixing cluster type, still hard to define an appropriate null model for a data set
- Still, there are some **clusterability assessment methods**, such as
  - **Spatial histogram**: Contrast the histogram of the data with that generated from random samples To be covered here
  - **Distance distribution**: Compare the pairwise point distance from the data with those from the randomly generated samples
  - **Hopkins Statistic**: A sparse sampling test for spatial randomness

Clustering Validation (Optional)

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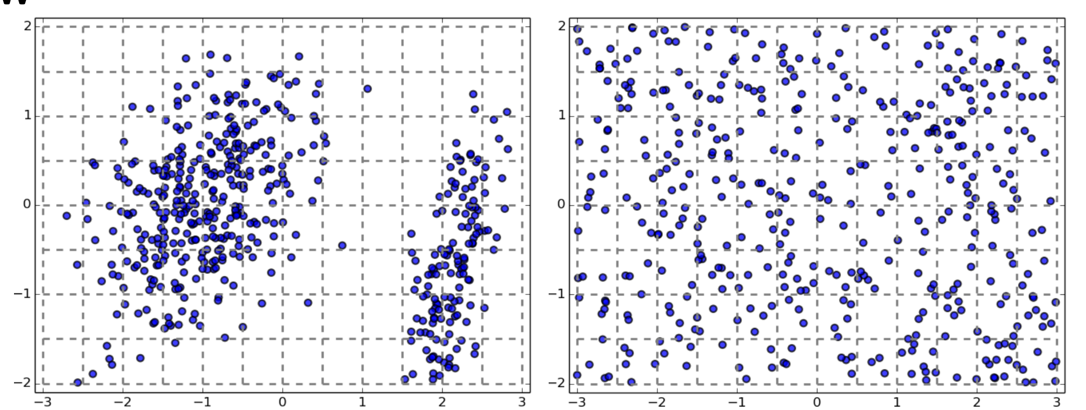
Testing Clustering Tendency: A Spatial Histogram Approach (Optional)

- **Spatial Histogram Approach**: Contrast the d-dimensional histogram of the input dataset **D** with the histogram generated from random samples
  - Dataset D is clusterable if the distributions of two histograms are rather different
- Method outline
  - Divide each dimension into equi-width bins, count how many points lie in each cells, and obtain the empirical joint probability mass function (EPMF)
  - Do the same for the randomly sampled data
  - Compute how much they differ using the Kullback-Leibler (KL) divergence value



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