

Machines will be capable, within twenty years, of doing any work that a man can do.

- Herbert Simon, 1965

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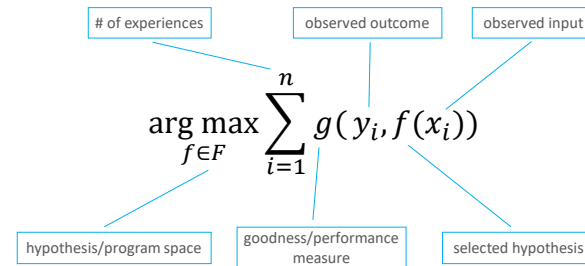
2024-2025 Spring Semester

Clustering

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Supervised Machine Learning



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What is Cluster Analysis?

- **Cluster**: a collection of data objects
 - Similar to one another within the same cluster
 - Dissimilar to the objects in other clusters
- **Cluster analysis**
 - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- **Unsupervised learning**: no predefined classes
- **Typical applications**
 - As a **stand-alone tool** to get insight into data distribution
 - As a **preprocessing step** for other algorithms

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Examples of Clustering Applications

- **Marketing**: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- **Land use**: Identification of areas of similar land use in an earth observation database
- **Insurance**: Identifying groups of motor insurance policy holders with a high average claim cost
- **City-planning**: Identifying groups of houses according to their house type, value, and geographical location
- **Earth-quake studies**: Observed earth quake epicenters should be clustered along continent faults

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Quality: What Is Good Clustering?

- A good clustering method will produce high quality clusters with
 - high intra-class similarity
 - low inter-class similarity
- The quality of a clustering result depends on both the similarity measure used by the method and its implementation
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns

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Measure the Quality of Clustering

- Dissimilarity/Similarity metric: Similarity is expressed in terms of a distance function, typically metric: $d(i, j)$
- There is a separate “quality” function that measures the “goodness” of a cluster.
- The definitions of distance functions are usually very different for interval-scaled, boolean, categorical, ordinal ratio, and vector variables.
- Weights should be associated with different variables based on applications and data semantics.
- It is hard to define “similar enough” or “good enough”
 - the answer is typically highly subjective.

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Requirements of Clustering

- Scalability
- Ability to deal with different types of attributes
- Ability to handle dynamic data
- Discovery of clusters with arbitrary shape
- Minimal requirements for domain knowledge to determine input parameters
- Able to deal with noise and outliers
- Insensitive to order of input records
- High dimensionality
- Incorporation of user-specified constraints
- Interpretability and usability


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12. Summary

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Data Structures

- Data matrix
 - (two modes)

$$\begin{bmatrix} x_{11} & \dots & x_{1f} & \dots & x_{1p} \\ \dots & \dots & \dots & \dots & \dots \\ x_{i1} & \dots & x_{if} & \dots & x_{ip} \\ \dots & \dots & \dots & \dots & \dots \\ x_{n1} & \dots & x_{nf} & \dots & x_{np} \end{bmatrix}$$

- Dissimilarity matrix
 - (one mode)

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & \ddots & \\ d(n,1) & d(n,2) & \dots & \dots & 0 \end{bmatrix}$$

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Type of Data in Clustering Analysis

- Interval-scaled variables
- Binary variables
- Nominal, ordinal, and ratio variables
- Variables of mixed types

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Interval-valued Variables

- Standardize data

- Calculate the mean absolute deviation:

$$s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + \dots + |x_{nf} - m_f|)$$

where

$$m_f = \frac{1}{n}(x_{1f} + x_{2f} + \dots + x_{nf})$$

- Calculate the standardized measurement (z-score)

$$z_{if} = \frac{x_{if} - m_f}{s_f}$$

- Using mean absolute deviation is more robust than using standard deviation

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Similarity and Dissimilarity Between Objects

- Distances are normally used to measure the similarity or dissimilarity between two data objects

- Some popular ones include: *Minkowski distance*:

$$d(i, j) = \sqrt[q]{(|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + \dots + |x_{ip} - x_{jp}|^q)}$$

where $i = (x_{i1}, x_{i2}, \dots, x_{ip})$ and $j = (x_{j1}, x_{j2}, \dots, x_{jp})$ are two p -dimensional data objects, and q is a positive integer

- If $q = 1$, d is Manhattan distance

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ip} - x_{jp}|$$

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Similarity and Dissimilarity Between Objects

- If $q = 2$, d is Euclidean distance:

$$d(i, j) = \sqrt{(|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \dots + |x_{ip} - x_{jp}|^2)}$$

- Properties

- $d(i, j) \geq 0$
- $d(i, i) = 0$
- $d(i, j) = d(j, i)$
- $d(i, j) \leq d(i, k) + d(k, j)$

- Also, one can use weighted distance, parametric Pearson product moment correlation, or other dissimilarity measures

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Binary Variables

- A contingency table for binary data
- Distance measure for symmetric binary variables:
- Distance measure for asymmetric binary variables:
- Jaccard coefficient (*similarity* measure for *asymmetric* binary variables):

		Object j		
		1	0	sum
Object i	1	a	b	$a+b$
	0	c	d	$c+d$
sum		$a+c$	$b+d$	p

$$d(i, j) = \frac{b + c}{a + b + c + d}$$

$$d(i, j) = \frac{b + c}{a + b + c}$$

$$\text{sim}_{\text{Jaccard}}(i, j) = \frac{a}{a + b + c}$$

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Symmetry

- A binary variable is symmetric if both of its states are equally valuable, that is, there is no preference on which outcome should be coded as 1
- A binary variable is asymmetric if the outcome of the states are not equally important, such as positive or negative outcomes of a disease test

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Dissimilarity between Binary Variables

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	Y	N	P	N	N	N
Mary	F	Y	N	P	N	P	N
Jim	M	Y	P	N	N	N	N

- gender is a symmetric attribute
- the remaining attributes are asymmetric binary
- let the values Y and P be set to 1, and the value N be set to 0

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Dissimilarity between Binary Variables

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	Y 1	N 0	P 1	N 0	N 0	N 0
Mary	F	Y 1	N 0	P 1	N 0	P 1	N 0
Jim	M	Y 1	P 1	N 0	N 0	N 0	N 0

$$d(\text{jack}, \text{mary}) = \frac{0 + 1}{2 + 0 + 1} = 0.33$$

		Object <i>j</i>		
		1	0	sum
Object <i>i</i>	1	<i>a</i>	<i>b</i>	<i>a + b</i>
	0	<i>c</i>	<i>d</i>	<i>c + d</i>
	sum	<i>a + c</i>	<i>b + d</i>	<i>p</i>

$$d(i, j) = \frac{b + c}{a + b + c}$$

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Dissimilarity between Binary Variables

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	Y 1	N 0	P 1	N 0	N 0	N 0
Mary	F	Y 1	N 0	P 1	N 0	P 1	N 0
Jim	M	Y 1	P 1	N 0	N 0	N 0	N 0

$$d(\text{jack}, \text{mary}) = \frac{0 + 1}{2 + 0 + 1} = 0.33$$

$$d(\text{jack}, \text{jim}) = \frac{1 + 1}{1 + 1 + 1} = 0.67$$

$$d(\text{jim}, \text{mary}) = \frac{1 + 2}{1 + 1 + 2} = 0.75$$

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Nominal Variables

- A generalization of the binary variable in that it can take more than 2 states, e.g., red, yellow, blue, green
- Method 1: Simple matching
 - m : # of matches, p : total # of variables

$$d(i, j) = \frac{p - m}{p}$$

- Method 2: use a large number of binary variables
 - creating a new binary variable for each of the M nominal states

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Ordinal Variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank $r_{if} \in \{1, \dots, M_f\}$
- Can be treated like interval-scaled
 - replace x_{if} by their rank
 - map the range of each variable onto $[0, 1]$ by replacing i -th object in the f -th variable by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

- compute the dissimilarity using methods for interval-scaled variables

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Ratio-Scaled Variables

- Ratio-scaled variable: a positive measurement on a nonlinear scale, approximately at exponential scale, such as Ae^{Bt} or Ae^{-Bt}
- Methods:
 - treat them like interval-scaled variables—*not a good choice!* (why?—the scale can be distorted)
 - apply logarithmic transformation

$$y_{ij} = \log(x_{ij})$$
 - treat them as continuous ordinal data treat their rank as interval-scaled

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Variables of Mixed Types

- A database may contain all the six types of variables
 - symmetric binary, asymmetric binary, nominal, ordinal, interval and ratio
- One may use a weighted formula to combine their effects

$$d(i, j) = \frac{\sum_{f=1}^p \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^p \delta_{ij}^{(f)}}$$

- f is binary or nominal:
 - $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$, or $d_{ij}^{(f)} = 1$ otherwise
- f is interval-based: use the normalized distance
- f is ordinal or ratio-scaled
 - compute ranks r_{if} and
 - and treat z_{if} as interval-scaled

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

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Vector Objects

- Vector objects: keywords in documents, gene features in micro-arrays, etc.
- Broad applications: information retrieval, biologic taxonomy, etc.
- Cosine measure

$$s(\vec{X}, \vec{Y}) = \frac{\vec{X}^t \cdot \vec{Y}}{|\vec{X}| |\vec{Y}|},$$

\vec{X}^t is a transposition of vector \vec{X} , $|\vec{X}|$ is the Euclidean normal of vector \vec{X} ,
- A variant: Tanimoto coefficient


$$s(\vec{X}, \vec{Y}) = \frac{\vec{X}^t \cdot \vec{Y}}{\vec{X}^t \cdot \vec{X} + \vec{Y}^t \cdot \vec{Y} - \vec{X}^t \cdot \vec{Y}}$$

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Major Clustering Approaches (I)

- Partitioning approach:
 - Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
 - Typical methods: k-means, k-medoids, CLARANS
- Hierarchical approach:
 - Create a hierarchical decomposition of the set of data (or objects) using some criterion
 - Typical methods: Diana, Agnes, BIRCH, ROCK, CAMELEON
- Density-based approach:
 - Based on connectivity and density functions
 - Typical methods: DBSACN, OPTICS, DenClue

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Major Clustering Approaches (II)

- Grid-based approach:
 - based on a multiple-level granularity structure
 - Typical methods: STING, WaveCluster, CLIQUE
- Model-based:
 - A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
 - Typical methods: EM, SOM, COBWEB
- Frequent pattern-based:
 - Based on the analysis of frequent patterns
 - Typical methods: pCluster
- User-guided or constraint-based:
 - Clustering by considering user-specified or application-specific constraints
 - Typical methods: COD (obstacles), constrained clustering

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Calculating the Distance between Clusters

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

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

- **Centroid:** the "middle" of a cluster
- **Radius:** square root of average distance from any point of the cluster to its centroid

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

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

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

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


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Partitioning Algorithms: Basic Concept

- **Partitioning method:** Construct a partition of a database D of n objects into a set of k clusters, s.t., min sum of squared distance

$$\sum_{m=1}^k \sum_{t_{mi} \in K_m} (C_m - t_{mi})^2$$

- Given a k , find a partition of k clusters that optimizes the chosen partitioning criterion
 - Global optimal: exhaustively enumerate all partitions
 - Heuristic methods: k -means and k -medoids algorithms
 - k -means (MacQueen'67): Each cluster is represented by the center of the cluster
 - k -medoids or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

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The K -Means Clustering Method

- Given k , the k -means algorithm is implemented in four steps:
 - Partition objects into k nonempty subsets
 - Compute seed points as the centroids of the clusters of the current partition (the centroid is the center, i.e., *mean point*, of the cluster)
 - Assign each object to the cluster with the nearest seed point
 - Go back to Step 2, stop when no more new assignment

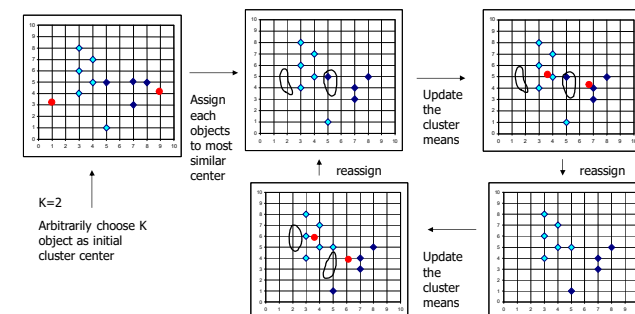
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The K -Means Clustering Method



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Comments on the *K-Means* Method

- Strength: *Relatively efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, $k, t \ll n$.
 - Comparing: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$
- Comment: Often terminates at a *local optimum*. The *global optimum* may be found using techniques such as: *deterministic annealing* and *genetic algorithms*
- Weakness
 - Applicable only when *mean* is defined, then what about categorical data?
 - Need to specify k , the *number* of clusters, in advance
 - Unable to handle noisy data and *outliers*
 - Not suitable to discover clusters with *non-convex shapes*

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Variations of the *K-Means* Method

- A few variants of the *k-means* which differ in
 - Selection of the initial k means
 - Dissimilarity calculations
 - Strategies to calculate cluster means
- Handling categorical data: *k-modes* (Huang'98)
 - Replacing means of clusters with modes
 - Using new dissimilarity measures to deal with categorical objects
 - Using a frequency-based method to update modes of clusters
 - A mixture of categorical and numerical data: *k-prototype* method

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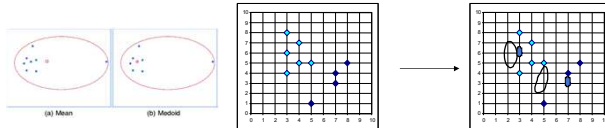
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What Is the Problem of the K-Means Method?

- 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.



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Example: Hand Image vs Background

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Example: Text Documents

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The K -Medoids Clustering Method

- Find *representative* objects, called medoids, in clusters
- PAM (Partitioning Around Medoids, 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 distance of the resulting clustering
 - PAM works effectively for small data sets, but does not scale well for large data sets
- CLARA (Kaufmann & Rousseeuw, 1990)
- CLARANS (Ng & Han, 1994): Randomized sampling
- Focusing + spatial data structure (Ester et al., 1995)

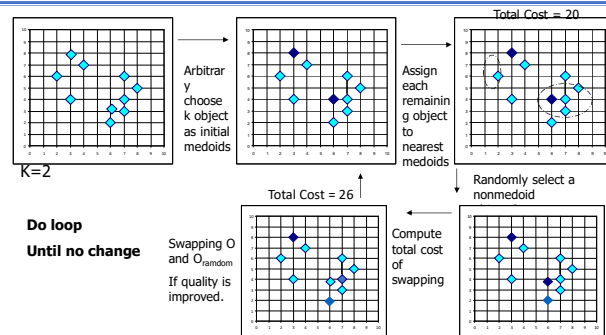
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A Typical K -Medoids Algorithm (PAM)



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PAM (Partitioning Around Medoids) (1987)

- PAM (Kaufman and Rousseeuw, 1987), built in Splus
- Use real object to represent the cluster
 - Select k representative objects arbitrarily
 - For each pair of non-selected object h and selected object i , calculate the total swapping cost TC_{ih}
 - For each pair of i and h ,
 - If $TC_{ih} < 0$, i is replaced by h
 - Then assign each non-selected object to the most similar representative object
 - repeat steps 2-3 until there is no change

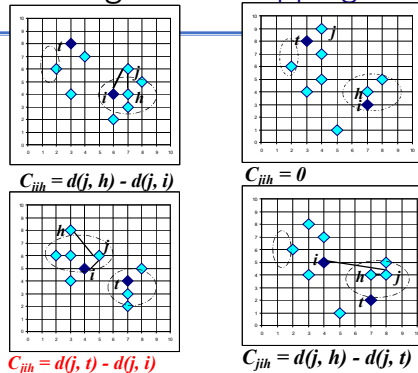
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PAM Clustering: Total swapping cost $TC_{ih} = \sum_j C_{jih}$



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What Is the Problem with PAM?

- Pam is more robust than k-means in the presence of noise and outliers because a medoid is less influenced by outliers or other extreme values than a mean
 - Pam works efficiently for small data sets but does not **scale well** for large data sets.
 - $O(k(n-k)^2)$ for each iteration
 - where n is # of data, k is # of clusters
- Sampling based method,
CLARA (Clustering LARge Applications)

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CLARA (Clustering Large Applications)

- CLARA (Kaufmann and Rousseeuw in 1990)
 - Built in statistical analysis packages, such as S+
- It draws *multiple samples* of the data set, applies PAM on each sample, and gives the best clustering as the output
- Strength:** deals with larger data sets than PAM
- Weakness:**
 - Efficiency depends on the sample size
 - A good clustering based on samples will not necessarily represent a good clustering of the whole data set if the sample is biased

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CLARANS ("Randomized" CLARA)

- CLARANS (A Clustering Algorithm based on Randomized Search) (Ng and Han'94)
- CLARANS draws sample of neighbors dynamically
- The clustering process can be presented as searching a graph where every node is a potential solution, that is, a set of k medoids
- If the local optimum is found, CLARANS starts with new randomly selected node in search for a new local optimum
- It is more efficient and scalable than both PAM and CLARA
- Focusing techniques and spatial access structures may further improve its performance (Ester et al.'95)


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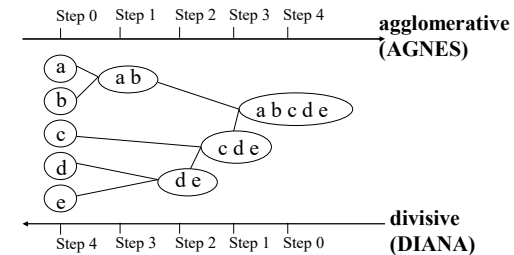
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Hierarchical Clustering

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



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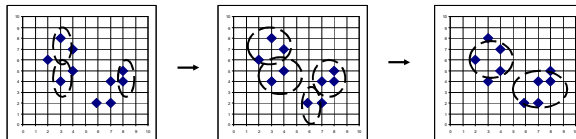
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AGNES (Agglomerative Nesting)

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



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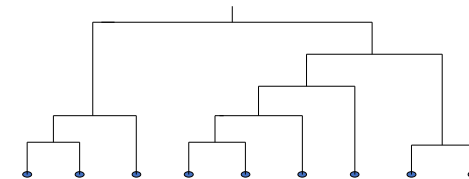
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Dendrogram: Shows How the Clusters are Merged

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

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



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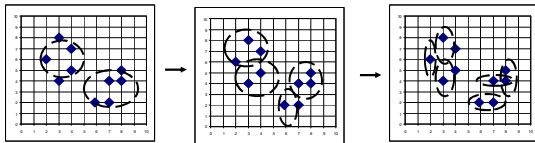
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DIANA (Divisive Analysis)

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



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Other Hierarchical Clustering Methods

- Major weakness of agglomerative clustering methods
 - do not scale well: time complexity of at least $O(n^2)$, where n is the number of total objects
 - can never undo what was done previously
- Integration of hierarchical with distance-based clustering
 - BIRCH (1996): uses CF-tree and incrementally adjusts the quality of sub-clusters
 - ROCK (1999): clustering categorical data by neighbor and link analysis
 - CHAMELEON (1999): hierarchical clustering using dynamic modeling


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Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
 - Discover clusters of arbitrary shape
 - Handle noise
 - One scan
 - Need density parameters as termination condition
- Several interesting studies:
 - DBSCAN: Ester, et al. (KDD'96)
 - OPTICS: Ankerst, et al (SIGMOD'99).
 - DENCLUE: Hinneburg & D. Keim (KDD'98)
 - CLIQUE: Agrawal, et al. (SIGMOD'98) (more grid-based)

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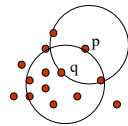
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Density-Based Clustering: Basic Concepts

- Two parameters:
 - Eps**: Maximum radius of the neighbourhood
 - MinPts**: Minimum number of points in an Eps-neighbourhood of that point
- $N_{Eps}(p)$: $\{q \text{ belongs to } D \mid \text{dist}(p, q) \leq Eps\}$
- 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

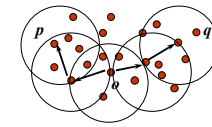
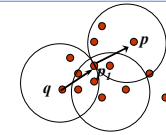
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Density-Reachable and Density-Connected

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



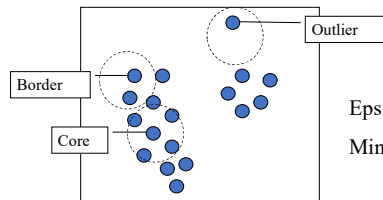
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DBSCAN: Density Based Spatial Clustering of Applications with Noise

- Relies on a *density-based* notion of cluster: A *cluster* is defined as a maximal set of density-connected points
- Discovers clusters of arbitrary shape in spatial databases with noise



Eps = 1cm
MinPts = 5

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DBSCAN: The Algorithm

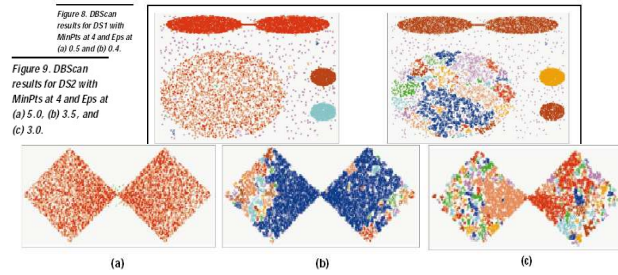
- Arbitrary select a point p
- Retrieve all points density-reachable from p w.r.t. Eps and $MinPts$.
- If p is a core point, a cluster is formed.
- If p is a border point, no points are density-reachable from p and DBSCAN visits the next point of the database.
- Continue the process until all of the points have been processed.

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DBSCAN: Sensitive to Parameters



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Thanks for listening!

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