Cluster Analysis - Abridged

CS4881 Aritificial Intelligence

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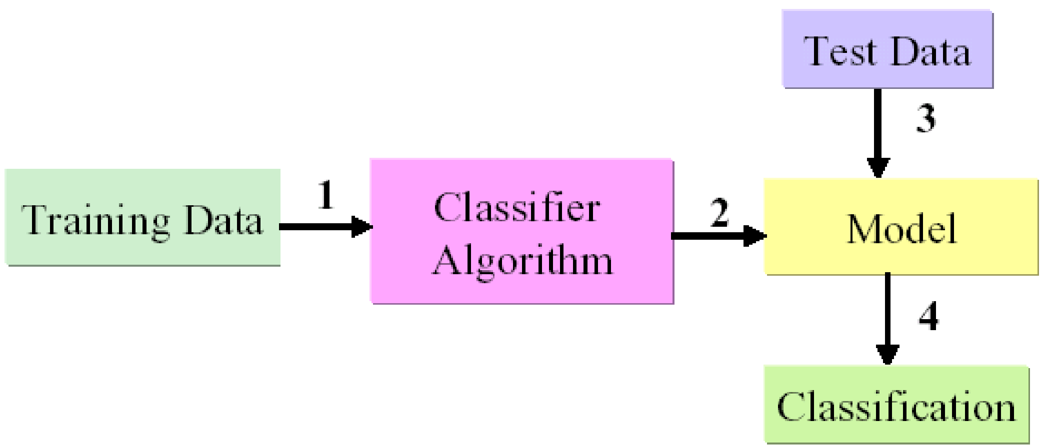
Cluster Analysis

- What is Cluster Analysis?
- Types of Data in Cluster Analysis
- A Categorization of Major Clustering Methods
- Partitioning Methods
- Hierarchical Methods
- Summary

Supervised Learning

Supervised Learning

- Learn by example from training data with a class label
- Create model by running algorithm on training data
- Identify a class label for the incoming new data



Supervised Learning Algorithms

Supervised Learning Algorithms

- Naive Bayes
- Neural Networks
- Decision Trees
- Support Vector Machine
- Bayes Nets

Unsupervised Learning Algorithms

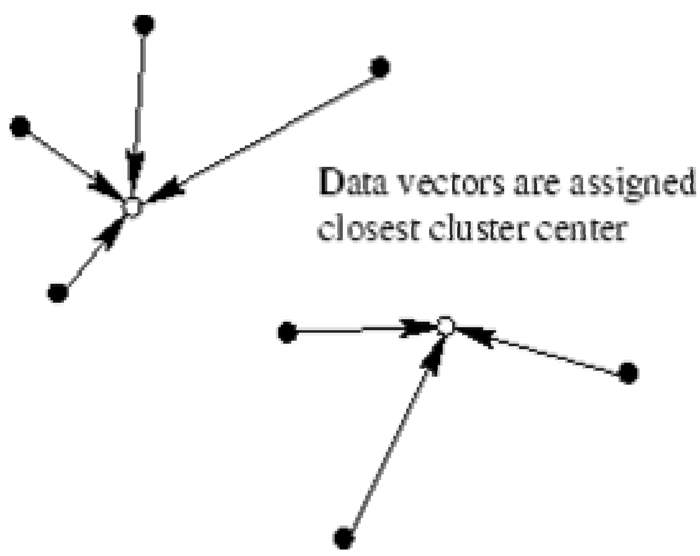
There are many machine learning situations in which class labels are not available, so unsupervised methods are needed.

Unsupervised Learning Algorithms

- Association Rules - Apriori
- Clustering

Clustering

Clustering is a widespread technique that clusters data into groups that reflect distinct regions of the decision space.



One of the first clustering applications?

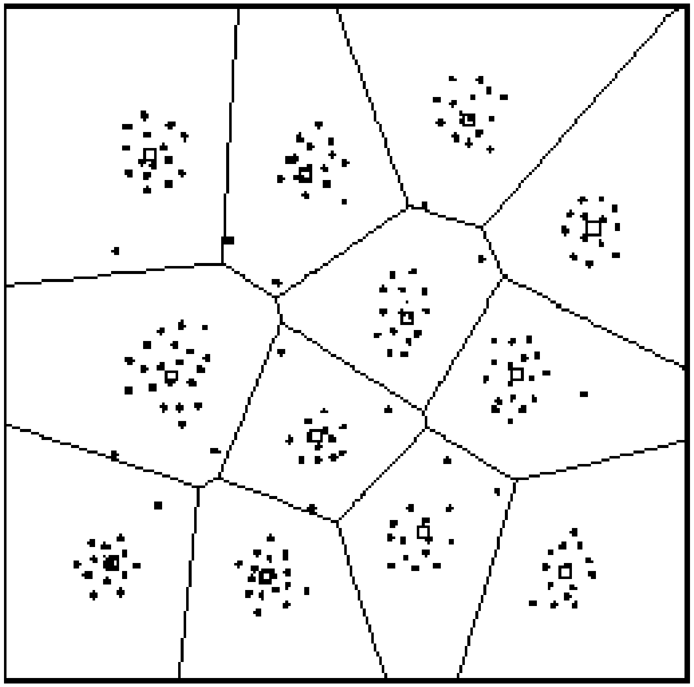
During a cholera outbreak in London in 1854, John Snow used a special map to plot the cases of the disease that were reported.

A key observation, after the creation of the map, was the close association between the density of disease cases and a single well located at a central street.

After this, the well pump was removed putting an end to the epidemic.

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
  - Grouping a set of data objects into clusters
- Clustering is *unsupervised classification*: no predefined classes



General Applications

- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

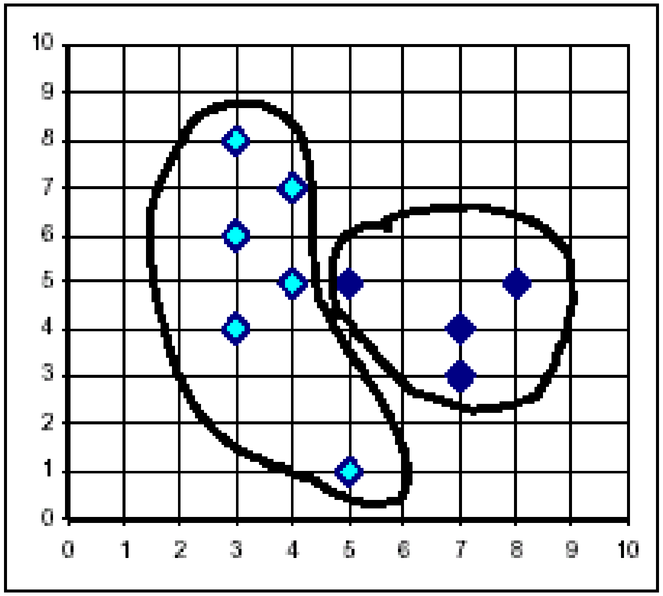
- General Applications
  - Co-expressed genes
  - Pattern Recognition
  - Spatial Data Analysis
  - Image Processing
  - Market research
  - Document/text classification
  - Cluster Weblog data discover search groups

Specific Applications

- Marketing: Discover distinct groups for targeted marketing programs
- Land use: Identification of areas of similar land use
- Insurance: Identifying groups with a high claim cost
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earth-quake studies: Epicenters should be clustered along continent faults.
- Text mining: Identify frequently co-occuring terms for concept identification.

What Is Good Clustering?

- A good clustering method will produce high quality clusters with
  - high intra-class similarity
  - low inter-class similarity
- Dependent on method used, data/domain, and implementation.
- Quality measured by its ability to discover some or all of the hidden patterns.



Data Structures

- Data matrix
  - (two modes)

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

- Dissimilarity matrix
  - (one mode)

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ : & : & : & & \\ d(n,1) & d(n,2) & \ldots & \ldots & 0 \end{bmatrix}$$

Measure the Quality of Clustering

- Similarity is expressed in terms of a distance function, which is typically metric: $d(i, j)$
- There is a separate "quality" function that measures the "goodness" of a cluster.
- Distance functions are different for *interval-scaled*, *boolean*, *categorical*, *ordinal* and *ratio* variables.
- Hard to define "similar enough" or "good enough" - subjective

Type of data in clustering analysis

- Nominal
  - ID numbers, eye color, zip codes
- Ordinal
  - Rankings (e.g., taste of potato chips on a scale from 1-10), grades, height in {tall, medium, short}
- Interval
  - Calendar dates, temperatures in Celsius or Fahrenheit.
- Ratio
  - Temperature in Kelvin, length, time, counts

Interval-valued variables

- Standardize data
  - Calculate the *mean absolute deviation*:

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \overline{x})^2}$$

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

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

  - 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

Similarity and Dissimilarity Between Objects

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

- Some popular ones include: Manhattan distance

$$d(i,j) = |x_{i_1} - x_{j_1}| + |x_{i_2} - x_{j_2}| + \dots + |x_{i_p} - x_{j_p}|$$

Similarity and Dissimilarity Between Objects (Cont.)

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

$$d(i,j) = \sqrt{(|x_{i_1} - x_{j_1}|^2 + |x_{i_2} - x_{j_2}|^2 + ... + |x_{i_p} - x_{j_p}|^2)}$$

  - 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, Pearson product correlation, or other disimilarity measures.

Binary Variables

- A contingency table for binary data

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

- Simple matching coefficient (invariant, if the binary variable is *symmetric*):

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

- Jaccard coefficient (noninvariant if the binary variable is *asymmetric*) disregard negative matches:

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

Binary Variables

- Jaccard index is a statistic used for comparing the similarity and diversity of sample sets. Jaccard similarity coefficient:

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|}.$$

- Jaccard distance coefficient:

$$J_\delta(A,B) = 1 - J(A,B) = \frac{|A \cup B| - |A \cap B|}{|A \cup B|}.$$

Binary Variables - Jaccard Index

- Common situation is that objects, *p* and *q*, have only binary attributes
- Compute similarities using the following quantities
  - M01 = the number of attributes where p was 0 and q was 1
  - M10 = the number of attributes where p was 1 and q was 0
  - M00 = the number of attributes where p was 0 and q was 0
  - M11 = the number of attributes where p was 1 and q was 1

SMC vs. Jaccard Index

p = 1 0 0 0 0 0 0 0 0 0

q = 0 0 0 0 0 0 1 0 0 1

M01 = 2 (number of attributes where p was 0 and q was 1)

M10 = 1 (number of attributes where p was 1 and q was 0)

M00 = 7 (number of attributes where p was 0 and q was 0)

M11 = 0 (number of attributes where p was 1 and q was 1)

SMC = (M11 + M00)/(M01 + M10 + M11 + M00)

= (0+7) / (2+1+0+7) = 0.7

J = (M11) / (M01 + M10 + M11)

= 0 / (2 + 1 + 0) = 0

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

Ordinal Variables

- An ordinal variable can be discrete or continuous
- order is important, e.g., rank
- Can be treated like interval-scaled
  - replacing x_{if} by their rank $r_{if} \in \{1, ..., M_f\}$
  - 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

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?)*
  - apply logarithmic transformation

$$y_{if} = log(x_{if})$$

  - treat them as continuous ordinal data treat their rank as interval-scaled.

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.

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

  - *f* is binary or nominal:

    $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$, or $d_{ij}^{(f)} = 1$ o.w.
  - *f* is interval-based: use the normalized distance
  - *f* is ordinal or ratio-scaled

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

    - compute ranks r_{if} and
    - and treat z_{if} as interval-scaled

Major Clustering Approaches

- Partitioning algorithms: Construct various partitions and then evaluate them by some criterion
- Hierarchy algorithms: Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Density-based: based on connectivity and density functions
- Grid-based: based on a multiple-level granularity structure
- Model-based: A model is hypothesized for each of the clusters and the idea is to find the best fit of that model to each other

Partitioning Algorithms: Basic Concept

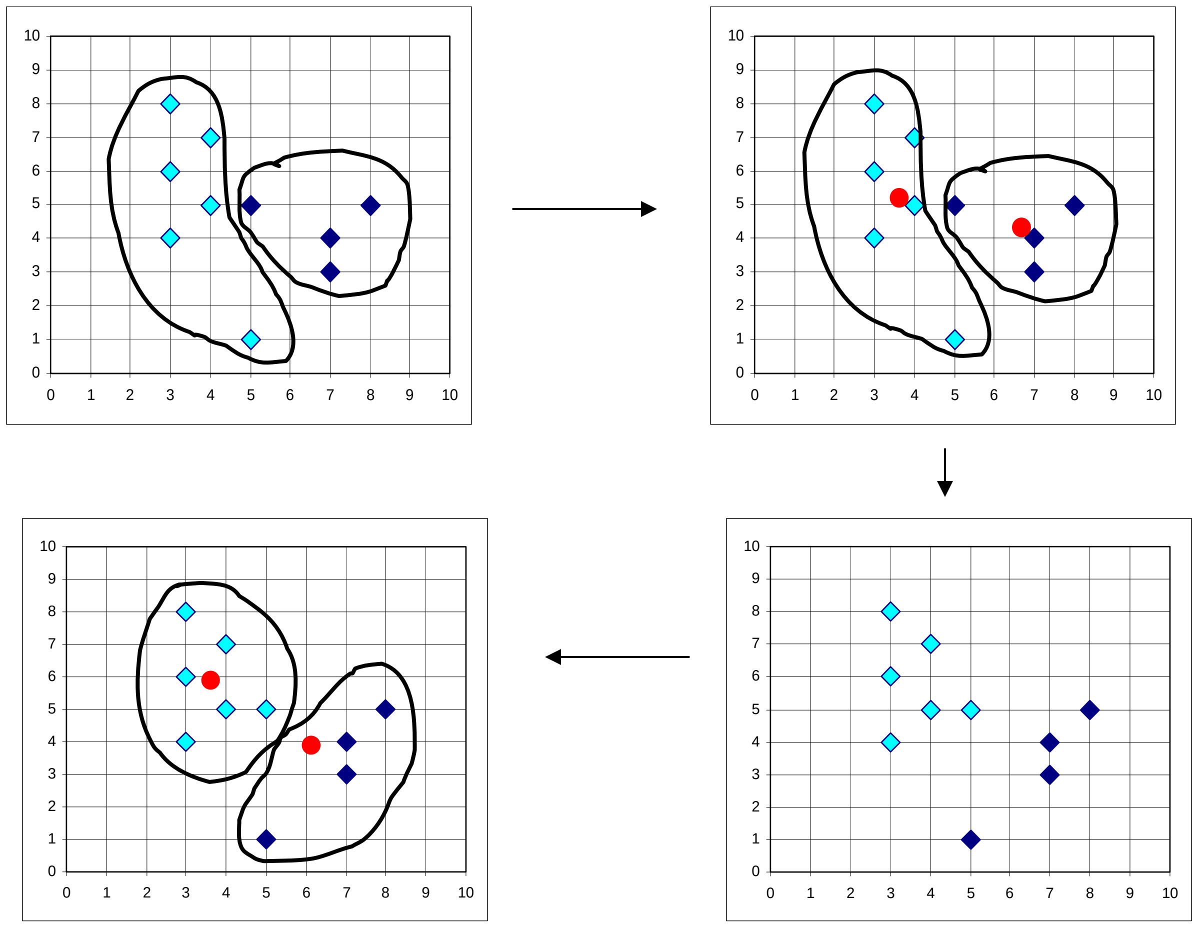
- <u>Partitioning method:</u> Construct a partition of a database ***D*** of ***n*** objects into a set of ***k*** clusters
- Given a *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - <u>*k-means*</u> (MacQueen'67): Each cluster is represented by the center of the cluster
  - <u>*k-medoids*</u> or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

The *K-Means* Clustering Method

- Given *k*, the *k-means* algorithm is implemented in 4 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 (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.

The *K-Means* Clustering Method

- Example



Comments on the *K-Means* Method

- Strength
  - *Relatively efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, k, $t << n$.
  - 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*

Variations of the *K-Means* Method

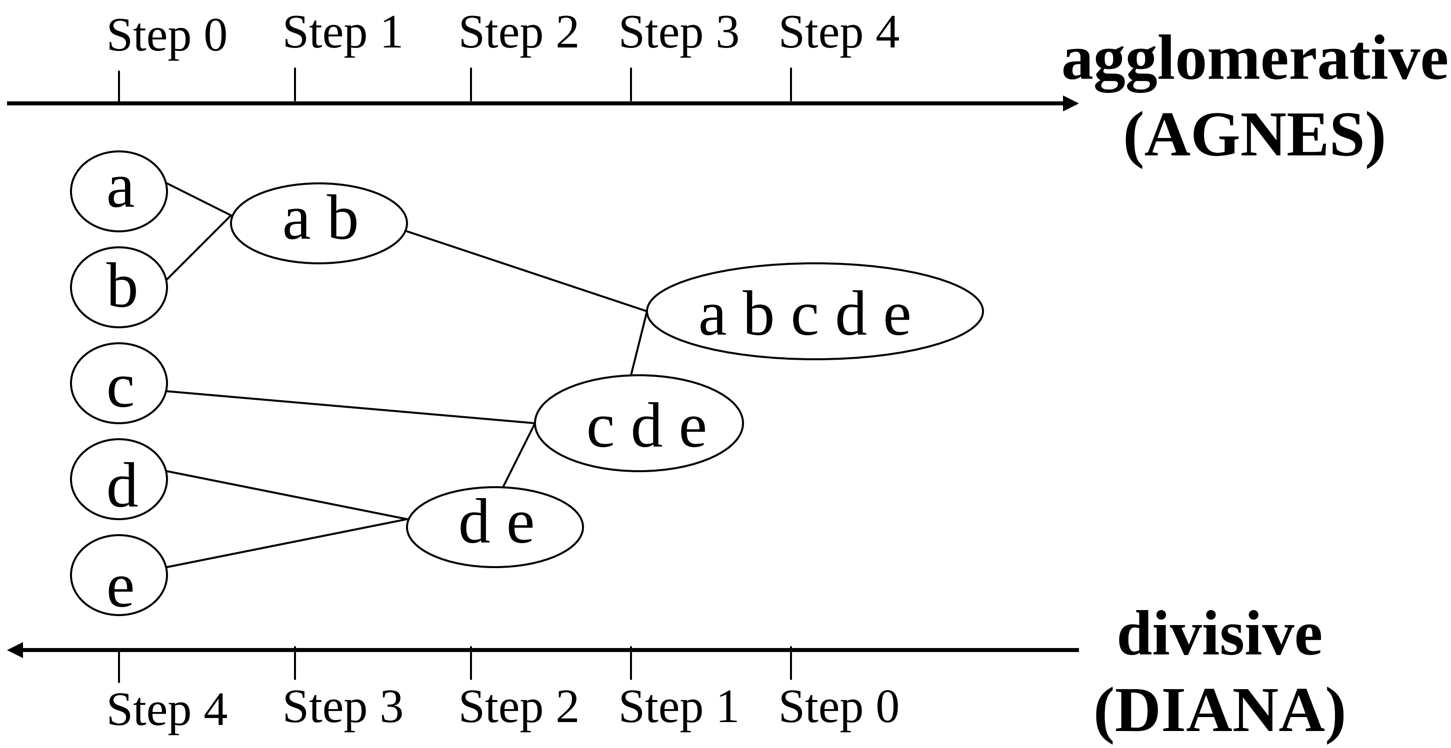
- A few variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means
- Handling categorical data: *k-modes* (Huang'98)
  - Replacing means of clusters with <u>modes</u>
  - Using new dissimilarity measures to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

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)

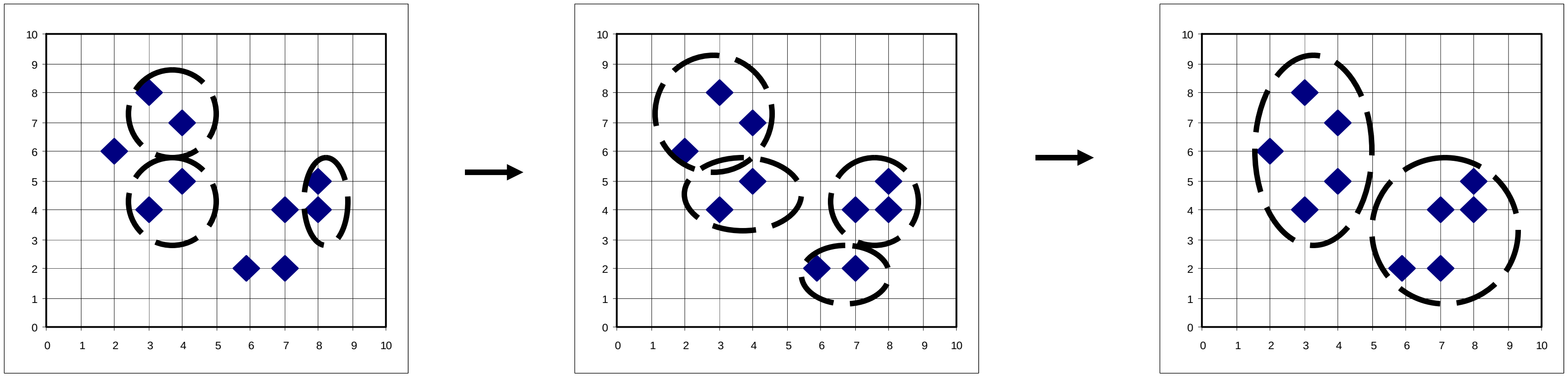
Hierarchical Clustering

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



AGNES (Agglomerative Nesting)

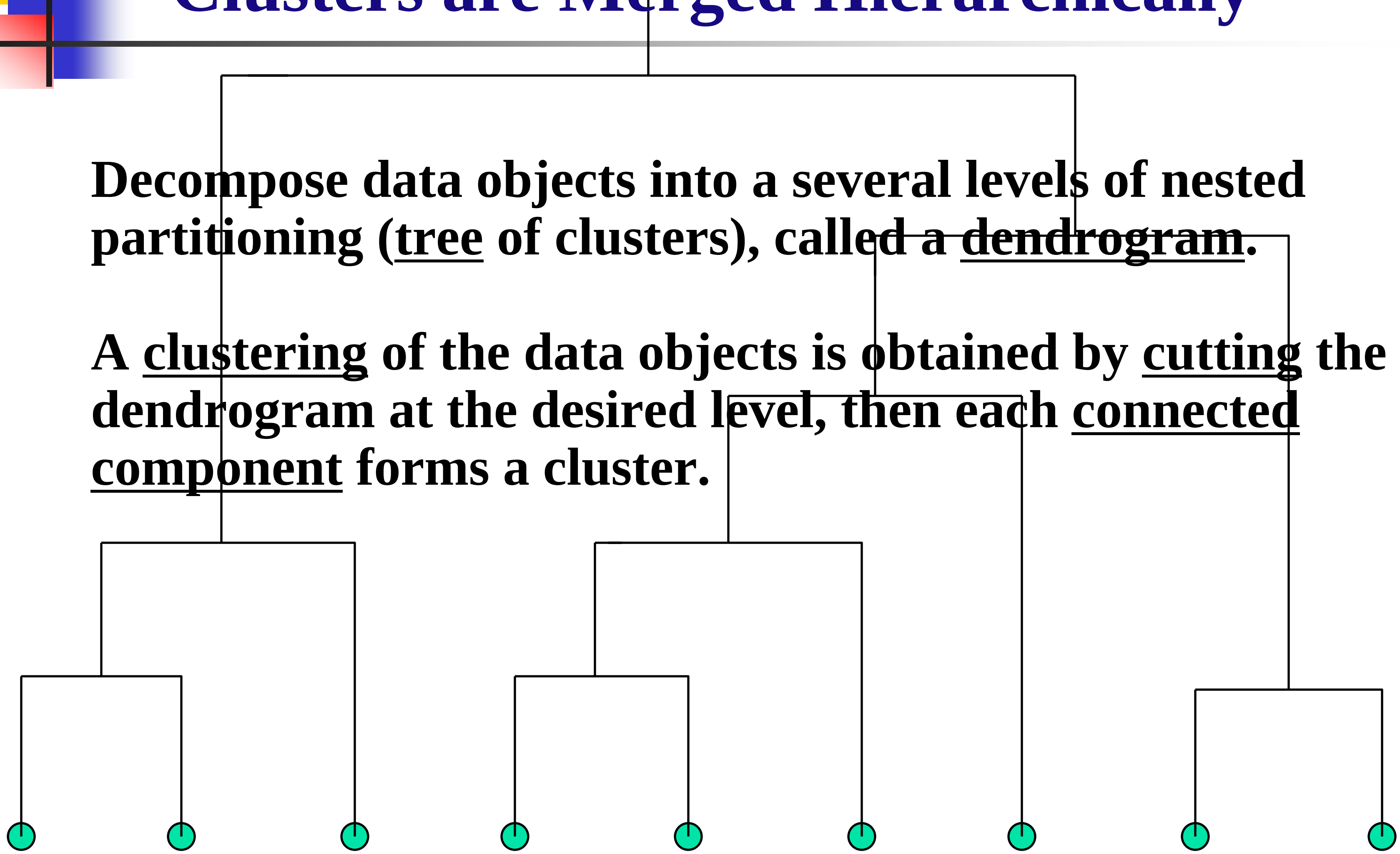
- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical analysis packages, e.g., Splus
- Use the Single-Link method and the dissimilarity matrix.
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster



A *Dendrogram* Shows How the Clusters are Merged Hierarchically

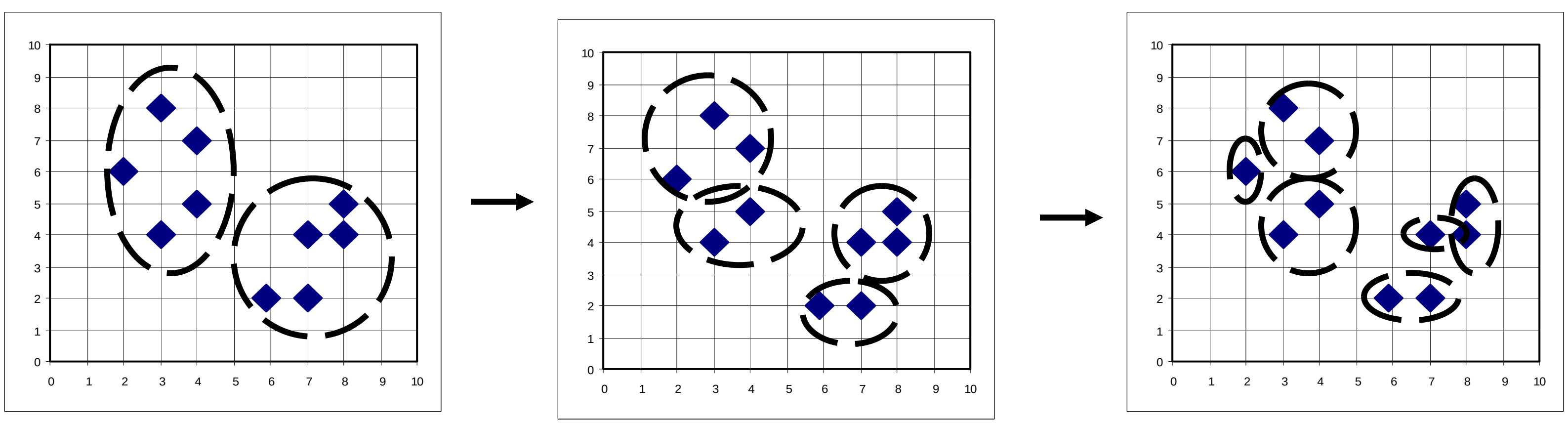
Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram.

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



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



More on 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
  - CURE (1998): selects well-scattered points from the cluster and then shrinks them towards the center of the cluster by a specified fraction
  - CHAMELEON (1999): hierarchical clustering using dynamic modeling

Summary

- Cluster analysis groups objects based on their similarity and has wide applications
- Measure of similarity can be computed for various types of data
- Clustering algorithms can be categorized into partitioning methods, hierarchical methods, density-based methods, grid-based methods, and model-based methods
- Outlier detection and analysis are very useful for fraud detection, etc. and can be performed by statistical, distance-based or deviation-based approaches
- There are still lots of research issues on cluster analysis, such as constraint-based clustering

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