POLITECNICO DI MILANO

Clustering: Introduction

Data Mining and Text Mining (UIC 583 @ Politecnico di Milano)

Prof. Pier Luca Lanzi (Spring 2009)

Lecture outline

- What is cluster analysis?
- Why clustering?
- What is good clustering?
- How to manage data types?
- What are the major clustering approaches?

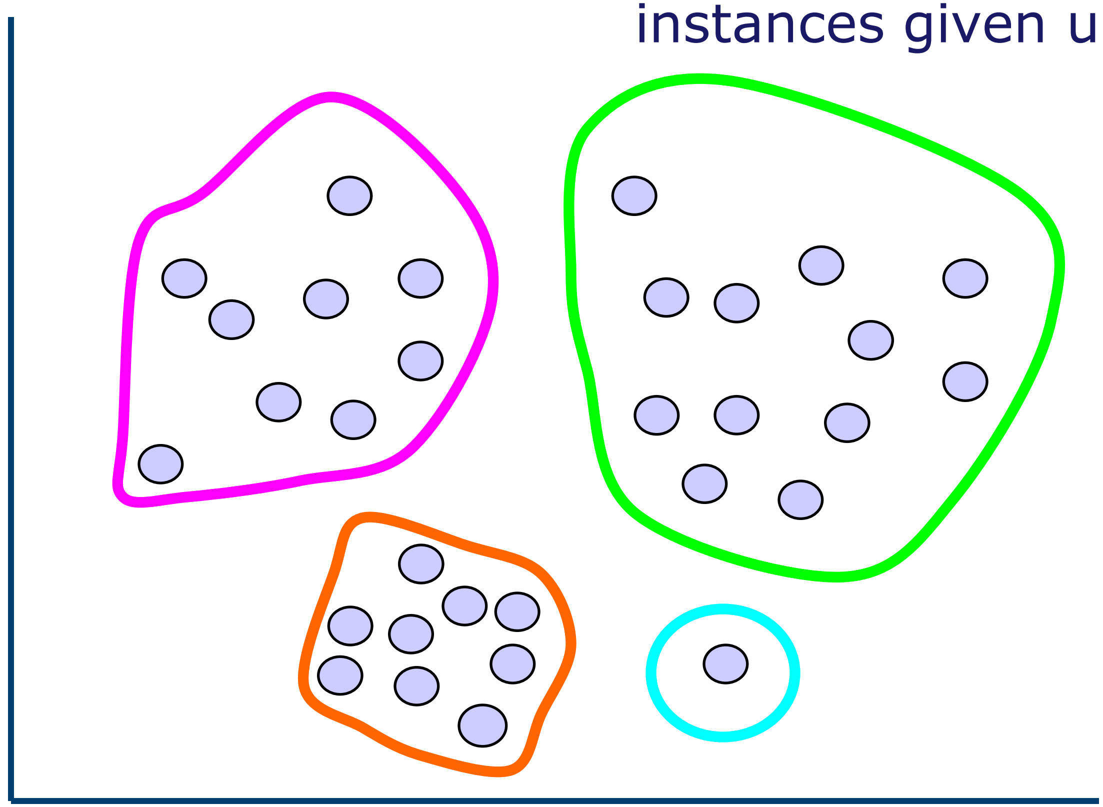
What is Cluster Analysis?

- A cluster is 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

Data Mining Tasks: clustering

Clustering = Unsupervised learning:

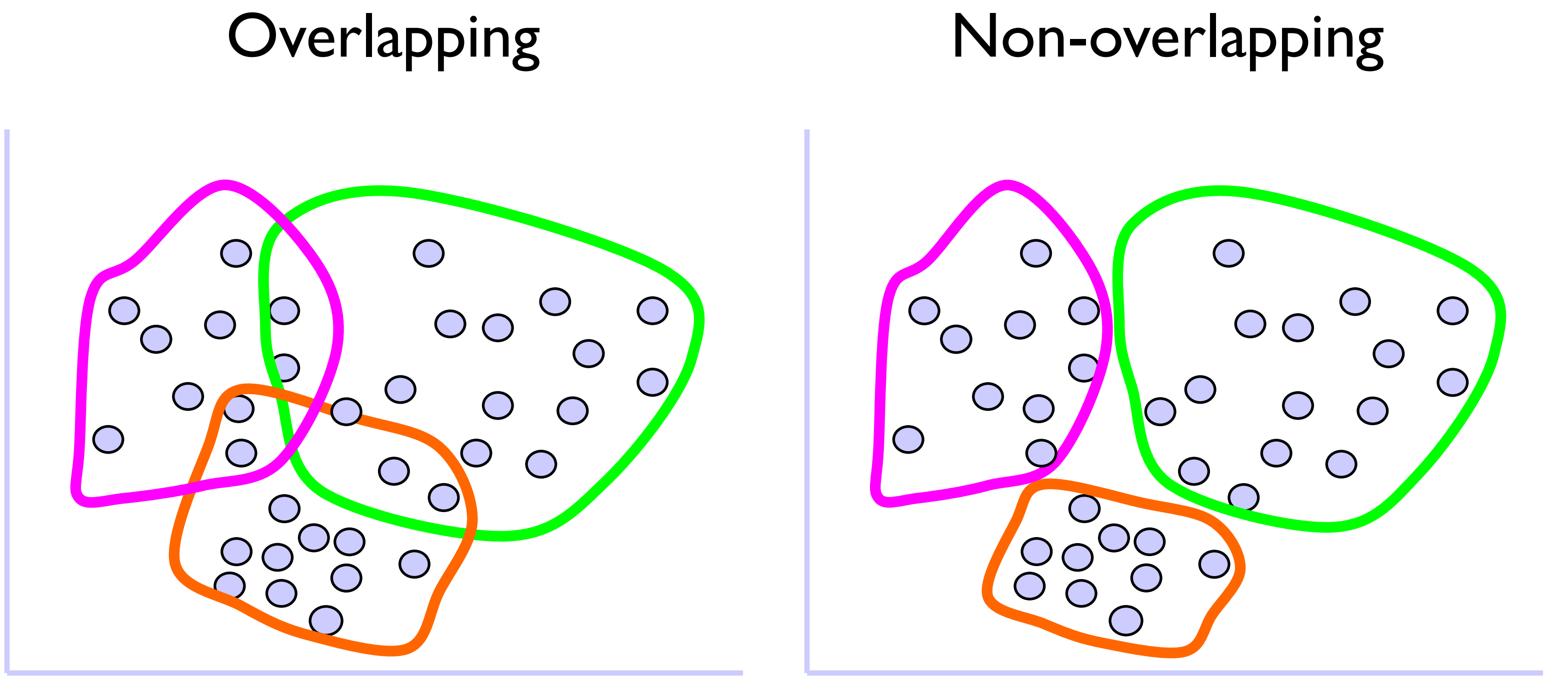
Finds "natural" grouping of instances given un-labeled data



Clustering Methods

- Many different method and algorithms:
  - For numeric and/or symbolic data
  - Deterministic vs. probabilistic
  - Exclusive vs. overlapping
  - Hierarchical vs. flat
  - Top-down vs. bottom-up

Clusters: exclusive vs. overlapping



Clustering: Evaluation

- Manual inspection
- Benchmarking on existing labels
- Cluster quality measures
  - distance measures
  - high similarity within a cluster, low across clusters

Clustering: Rich Applications and Multidisciplinary Efforts

- Pattern Recognition
- Spatial Data Analysis
  - Create thematic maps in GIS by clustering feature spaces
  - Detect spatial clusters or for other spatial mining tasks
- Image Processing
- Economic Science (especially market research)
- WWW
  - Document classification
  - Cluster Weblog data to discover groups of similar access patterns

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

What is Good Clustering?

- A good clustering consists of 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

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.

Requirements of Clustering in Data Mining

- 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

Data Structures

- Data

Outlook	Temperature	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	Normal	False	Yes
…	…	…	…	…

- Dissimilarity matrix

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

- Data matrix

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

- Dissimilarity matrix

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

Type of data in clustering analysis

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

- Standardize data
  - Calculate the mean absolute deviation,

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

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

  - 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: Minkowski distance:

$$d(i,j)=\sqrt[q]{(|x_{i_1}-x_{j_1}|^q+|x_{i_2}-x_{j_2}|^q+\ldots+|x_{i_p}-x_{j_p}|^q)}$$

- where i = (x_{i1}, x_{i2}, …, x_{ip}) and j = (x_{j1}, x_{j2}, …, x_{jp}) are two p-dimensional data objects, and q is a positive integer
- If q = 1, d is Manhattan distance

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

Similarity and Dissimilarity Between Objects (Cont.)

- If q = 2, d is Euclidean distance:

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

  - 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, parametric Pearson product moment correlation, or other disimilarity measures

Binary Variables

- Contingency table for binary data:

	1	0	sum
1	a	b	a+b
0	c	d	c+d
sum	a+c	b+d	p

- Distance measure for symmetric binary variables:

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

- Distance measure for asymmetric binary variables:

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

- Jaccard coefficient (similarity measure for asymmetric binary variables):

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

Example of Dissimilarity in 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
- Remaining attributes are asymmetric binary
- Let the values Y and P be set to 1, and the value N be set to 0

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

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

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

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
  - replace xif by their rank

$$r_{if} \in \{1, \ldots, M_f\}$$

  - 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?—the scale can be distorted)
  - 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

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

  - 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 rif and
    - and treat z_{if} as interval-scaled $z_{if} = \frac{r_{if} - 1}{M_f - 1}$

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

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

- A variant: Tanimoto coefficient

$\vec{X}^t$ is a transposition of vector $\vec{X}$, $|\vec{X}|$ is the Euclidean normal of vector $\vec{X}$,

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

Major Clustering Approaches

- 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

Major Clustering Approaches

- 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

Summary

- Clusters are collection of data objects
- Objects should be
  - Similar to one another within the same cluster
  - Dissimilar to the objects in other clusters
- Cluster analysis searches for similarities between data according to the characteristics found in the data and groups similar data objects into clusters
- Similarity is defined in terms of distance between objects and between clusters
- Several approaches: partition-based, hierarchical, density-based, model-based, etc.