Data Mining

Clustering Analysis

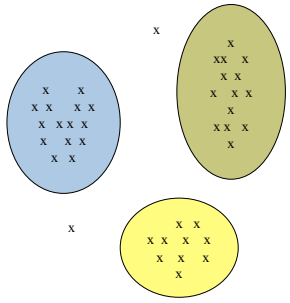
Outline

- What is clustering analysis?
- Types of data in clustering analysis
- A categorization of major clustering methods
  - Partitioning methods
  - Hierarchical methods
  - Model-based clustering methods
- Outlier analysis
- Summary

What Is Clustering Analysis?

- Clustering: a collection of data objects.
  - Similar to one another within the same cluster.
  - Dissimilar to the objects in other clusters.
- Clustering analysis.
  - Grouping a set of data objects into clusters, such that objects within each cluster are similar to each other, objects in different clusters are dissimilar to each other.
- Clustering is unsupervised classification:
  - Objects are not labeled with predefined classes.
  - Different from supervised classification where each training data is labeled with class information

An Example



Problems With Clustering

- Clustering in two dimensions looks easy.
- Clustering small amounts of data looks easy.
- And in most cases, looks are *not* deceiving.

The Curse of Dimensionality

- Many applications involve not 2, but 10 or 10,000 dimensions.
- High-dimensional spaces look different: almost all pairs of points are at about the same distance.

Example: Curse of Dimensionality

- Assume random points within a bounding box, e.g., values between 0 and 1 in each dimension.
- In 2 dimensions: a variety of distances between 0 and 1.41.
- In 10,000 dimensions, the difference in any one dimension is distributed as a triangle.

Curse of Dimensionality – Continued

- The law of large numbers applies.
- Actual distance between two random points is the sqrt of the sum of squares of essentially the same set of differences.

General Applications

- Typical applications.
  - As a stand-alone tool to get insight into data distribution.
  - As a preprocessing step for other algorithms.
- (Spatial) data analysis
- Image processing
- Economic science (especially market research)
- WWW
  - Automatic document categorization
  - Web usage mining: cluster web log data to discover groups of similar access patterns
- Business : customer groups
- Biology: animal and plant taxonomy, Categorize genes by functionality

High-Dimension Application: SkyCat

- A catalog of 2 billion "sky objects" represents objects by their radiation in 7 dimensions (frequency bands).
- Problem: cluster into similar objects, e.g., galaxies, nearby stars, quasars, etc.
- Sloan Sky Survey is a newer, better version.

Clustering CD's (Collaborative Filtering)

- Intuitively: music divides into categories, and customers prefer a few categories.
  - But what are categories really?
- Represent a CD by the customers who bought it.
- Similar CD's have similar sets of customers, and vice-versa.

The Space of CD's

- Think of a space with one dimension for each customer.
  - Values in a dimension may be 0 or 1 only.
- A CD's point in this space is $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ *iff* the i^{th} customer bought the CD.
  - Compare with boolean matrix: rows = customers; cols. = CD's.
- For Amazon, the dimension count is tens of millions.

Clustering Documents

- Represent a document by a vector $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ *iff* the i^{th} word (in some order) appears in the document.
  - It actually doesn't matter if k is infinite; i.e., we don't limit the set of words.
- Documents with similar sets of words may be about the same topic.

Example: DNA Sequences

- Objects are sequences of {C,A,T,G}.
- Distance between sequences is *edit distance*, the minimum number of inserts and deletes needed to turn one into the other.

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 clustering approach used.
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns

Requirements of Clustering in Data Mining

- Scalability
- Ability to deal with different types of attributes
- 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
- Interpretability and usability

Data Structures

- 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

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

Measure the Quality of Clustering

- Dissimilarity/similarity metric: dissimilarity is expressed in terms of a distance function, which is typically metric: d(i, j).
- The definitions of distance functions are usually very different for interval-scaled, boolean, categorical, ordinal variables, and temporal data.
- Weights should be associated with different variables based on applications and data semantics.
- There is a separate "quality" function that measures the "goodness" of a cluster.

Type of Data in Clustering Analysis

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

Standardize Numeric Data

- Standardize data
  - Calculate the mean absolute deviation:

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

  Where

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

  - Calculate the standardized measurement (*z-score*)

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

- Normalizing data

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

Similarity/Dissimilarity Between Objects

- Distances are normally used to measure the similarity or dissimilarity between two data objects
- Some popular ones include: *Minkowski distance*:

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

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

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

Similarity/Dissimilarity Between Objects

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

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

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

Triangular inequality

Other Similarity/Distance measures

- Sets as vectors: measure similarity by the cosine distance.

$$x_i = [x_{i1}, x_{i2}, ... x_{ip}]$$

$$x_j = [x_{j1}, x_{j2}, ... x_{jp}]$$

$$\cos(x_i, x_j) = \frac{x_i \bullet x_j}{|x_i| * |x_j|} = \hat{x}_i \bullet \hat{x}_j$$

Other Similarity/Distance measures

- Measure distance between words/address/ query, or between DNA sequences by edit distance
  - Given two strings S_1 and S_2, the minimum number of operations to convert one to the other
  - Operations are typically character-level
    - Insert, Delete, Replace, (Transposition)
  - E.g., the edit distance from ***dof*** to ***dog*** is 1
    - From ***cat*** to ***act*** is 2 (Just 1 with transpose.)
    - from ***cat*** to ***dog*** is 3.
- Generally found by dynamic programming.

Similarity/Dissimilarity for Binary Data

- A contingency table for binary data

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

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

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

- Jaccard coefficient (if the binary variable is *asymmetric*):

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

Dissimilarity between Binary Variables

- Example

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

Jaccard coefficient

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

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

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

Nominal Attributes

- A generalization of the binary attribute 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 attributes
  - creating a new binary variable for each of the M nominal states

Ordinal Attributes

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

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

  - compute the dissimilarity using methods for interval-scaled attributes

Attributes of Mixed Types

- A database may contain different types of attributes
  - symmetric binary, asymmetric binary, nominal, ordinal, and interval.

Attributes of Mixed Types

- Use weighted formula to combine their effects.
  - Feature value missing, or asymmetric binary with $x_{if} = x_{jf} = 0$ ➔ $\delta_{ij}(f) = 0$
  - Otherwise ➔ $\delta_{ij}(f) = 1$
  - feature is interval-based: use the normalized distance ($\delta_{ij}^{(f)}$ is weight on feature f)

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

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

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

Practice Question

- Compute the distance between (obj1, obj2),

	Gender	Age	Heart Rate	Fever	Cough	Category
Obj1	F	18	120	N	N	Severe-1
Obj2	M	36	89	N	N	Normal

For Age: m=42, s=3.5,
For heart rate: m=95, s=10
Possible values for Category include : Normal, Severe-1, Severe-2, Dying

For simplicity in demonstration, use Manhattan distance for interval data.

Practice Question

- Compute the distance between (obj1, obj2), (obj3, obj4)

	Gender	Age	Time	Fever	Cough
Obj1	F	23	2	Y	N
Obj2	M	2	0.5	N	N
Obj3	F	15	3	Y	Y
Obj4	F	18	0.5	Y	N
Obj5	M	58	4	N	Y
Obj6	F	44	14	N	Y

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
- 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

- Partitioning method: 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
  - *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

The *K-Means* Clustering Method

- **Objective**: to form a set of clusters that are as compact and separated as possible
- **Distance Measure**: Euclidean distance between data object and cluster center
- **Clustering criterion function**:
  mean squared error (MSE)

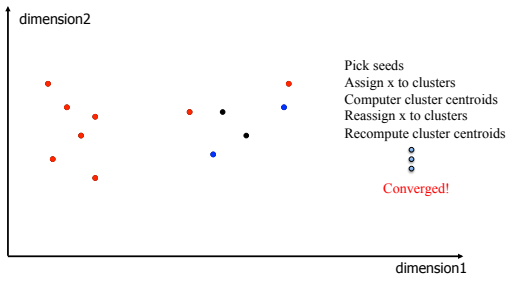
$$MSE = \sum_{i=1}^{k} \sum_{p \subseteq C_i} | x - m_i |^2$$

x: a data object
C_i: cluster i
m_i: center of cluster i
k: number of clusters

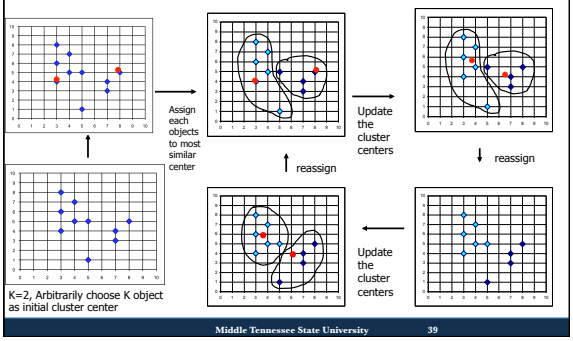
The *K-Means* Clustering Method

- **Approach**: Given *k*, the *k-means* algorithm is implemented as the following:
  - arbitrarily choose *K* objects as the initial cluster centers.
  - Repeat:
    - **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.**
  - stop when no more new assignment, or when clustering criterion function (mean squared error) converges.

K Means Example (*K*=2)



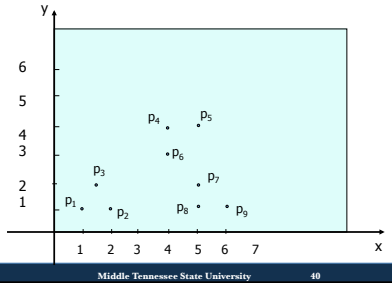
K-Means



Practice Question

Apply K-means clustering algorithm to partition the following data with 9 data objects:

P1(1, 1)
P2(2,1)
P3(1.5,2)
P4(4, 4)
P5(5,4)
P6(4,3)
P7(5,2)
P8(5,1)
P9(6,1)



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
  - Sensitive to initial seed selection
  - Unable to handle noisy data and *outliers*

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

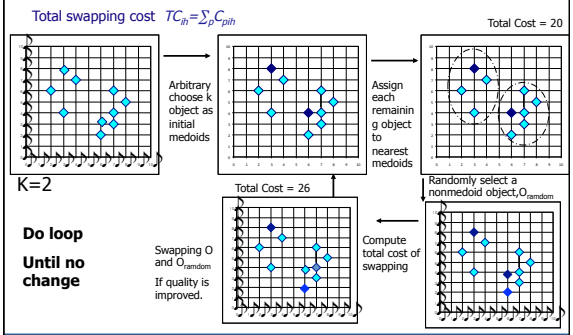
The *K-Medoids* Clustering Method

- 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

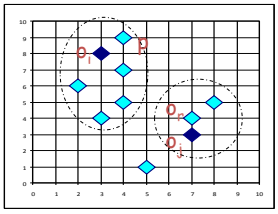
K-Medoids

- Arbitrarily choose K objects as the initial medoids;
- Repeat:
  - Assign each remaining object to the cluster with the nearest medoids;
  - Randomly select a nonmedoid object O_{random};
  - Compute the total cost, S, of swapping O_j with O_{random};
  - If S<0, then swap O_j with O_{random} to form the new set of k medoids;
- Until no change

k-Medoids



Four Cases – Case C



Replace o_j with o_r

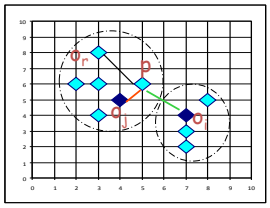
$p \in o_i$; $i \neq j$;

p still closest to o_i

no change

$$C_{p,j,r} = 0$$

Four Cases – Case A



Replace o_j with o_r

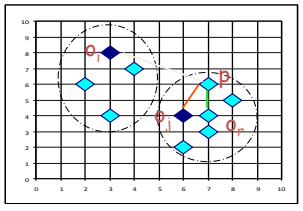
$p \in o_j$

p is now closer to o_i $i \neq j$

Reassign p to O_i

$$C_{p,j,r} = d(p - o_i) - d(p - o_j)$$

Four Cases – Case B



Replace o_j with o_r

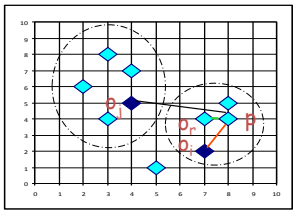
$p \in o_j$

p closest to o_r

Reassign p to O_r

$$C_{p,j,r} = d(p - o_r) - d(p - o_j)$$

Four Cases – Case D



Replace o_j with o_r

$p \in o_i$; $i \neq j$;

p closest to o_r

Reassign p to O_r

$$C_{p,j,r} = d(p - o_r) - d(p - o_i)$$

Practice Question

- Apply PAM on the following data, K=2

	Gender	Age	Time	Fever	Cough
Obj1	F	2	2	Y	N
Obj2	M	2	0.5	N	N
Obj3	F	15	3	Y	Y
Obj4	F	18	0.5	Y	N
Obj5	M	58	4	N	Y
Obj6	F	44	14	N	Y

Practice Question

Assume this is the distance table

	O1	O2	O3	O4	O5	O6
O1	--					
O2	0.94	--				
O3	0.36	0.91	--			
O4	0.19	0.75	0.39	--		
O5	1.15	1.38	0.99	1.3	--	
O6	1.38	2.16	1.22	1.5	1.2	--

PAM Complexity Analysis

- Total k*(n-k) pairs of (O_i, O_h)
- For each pair of (O_i, O_h):
  - compute Tc_{ih} require the examination of (n-k) non-selected objects.
- Total complexity:

  $O(k*(n-k)^2)$

Compare K-means and PAM

- K-means is computationally more efficient
- K-means only handles numeric data
- PAM can handle different types of data
- PAM is better in terms of handling outliers in data

The CLARA algorithm

- Objective: to improve the computational efficiency of PAM, through sampling
- Basic idea:
  - draw a sample of the original data set, applies PAM on the sample, and finds the medoids of the sample.
  - Repeat the process a fixed number of times and return the medoids that generate the lowest average dissimilarity from the data objects
- Complexity: $O(k*(40+k)^2 + k*(n-k))$

The CLARA Algorithm

For I=1 to 5, repeat the following steps:

- Draw a sample of 40+2k objects randomly from the entire data set, and call algorithm PAM to find the *k* medoids of the sample
- For each object O_j in the entire data set, determine which of the *k* medoids is the most similar to O_j.
- Calculate the average dissimilarity of the clustering obtained in the previous step. If this value is < current minimum, set current minimum to this value, and retain the current set of *k* medoids
- Return to step 1 to start the next iteration

CLARANS ("Randomized" CLARA)

- *CLARANS* (A Clustering Algorithm based on Randomized Search)
- 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*

The CLARANS Algorithm

1. Input *numlocal* and *maxneighbor*
   i=1, mincost=FLT_MAX, bestnode=NULL
2. *current* = an arbitrary *k* modiods
3. j=1
4. Pick random neighbor *S* of *current*, compute the cost difference between *S* and *current*
5. If S has lower cost, set *current* = S, goto 3
   else
      j=j+1;
      if (j <=*maxneighbor*) goto 4
      else
            if (cost(*current*) < *mincost*)
             mincost = cost(*current*)
             bestnode = *current*
6. i= i+1;
7. If (i <= *numlocal*)
      goto step 2
   else
      output *bestnode* and halt