Week1

2021年1月16日 11:25

1.1. 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*)

1.2. Applications of Cluster Analysis

- 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

1.4 A Multi-Dimensional Categorization

- **Technique-Centered**
  - Distance-based methods
  - Density-based and grid-based methods
  - Probabilistic and generative models
  - Leveraging dimensionality reduction methods
  - High-dimensional clustering
  - Scalable techniques for cluster analysis
- **Data Type-Centered**
  - Clustering numerical data, categorical data, text data, multimedia data, time-series data, sequences, stream data, networked data, uncertain data

1.5 An Overview of Typical Clustering Methodologies

- **Distance-based methods**
  - Partitioning algorithms: K-Means, K-Medians, K-Medoids
  - Hierarchical algorithms: Agglomerative vs. divisive methods
- **Density-based and grid-based methods**
  - Density-based: Data space is explored at a high-level of granularity and then post-processing to put together dense regions into an arbitrary shape
  - Grid-based: Individual regions of the data space are formed into a grid-like structure
- **Probabilistic and generative models:** Modeling data from a generative process
  - Assume a specific form of the generative model (e.g., mixture of Gaussians)
  - Model parameters are estimated with the Expectation-Maximization (EM) algorithm (using the available dataset, for a maximum likelihood fit)
  - Then estimate the generative probability of the underlying data points

- **High-dimensional clustering**
  - Subspace clustering: Find cluster on various subspaces
    - Bottom-up, top-down, correlation-based methods vs. δ-cluster methods
  - Dimensionality reduction: A vertical form (i.e., columns) of clustering
    - Columns are clustered; may cluster rows and columns together (co-clustering)
    - Probabilistic latent semantic indexing (PLSI) then LDA: Topic modeling of text data
      - A cluster (i.e., topic) is associated with a set of words (i.e., dimensions) and a set of documents (i.e., rows) simultaneously
    - Nonnegative matrix factorization (NMF) (as one kind of co-clustering)
      - A nonnegative matrix A (e.g., word frequencies in documents) can be approximately factorized two non-negative low rank matrices U and V

1.6 An Overview of Clustering Different Types of Data

- **Numerical data**
  - Most earliest clustering algorithms were designed for numerical data
- **Categorical data** (including binary data)
  - Discrete data, no natural order (e.g., sex, race, zip-code, and market-basket)
- **Text data**: Popular in social media, Web, and social networks
  - Features: High-dimensional, sparse, value corresponding to word frequencies
  - Methods: Combination of k-means and agglomerative; topic modeling; co-clustering
- **Multimedia data**: Image, audio, video (e.g., on Flickr, YouTube)
  - Multi-modal (often combined with text data)
  - Contextual: Containing both behavioral and contextual attributes
    - Images: Position of a pixel represents its context, value represents its behavior
    - Video and music data: Temporal ordering of records represents its meaning

- **Time-series data**: Sensor data, stock markets, temporal tracking, forecasting, etc.
  - Data are temporally dependent
  - Time: contextual attribute; data value: behavioral attribute
  - Correlation-based online analysis (e.g., online clustering of stock to find stock tickers)
  - Shape-based offline analysis (e.g., cluster ECG based on overall shapes)
- **Sequence data**: Weblogs, biological sequences, system command sequences
  - Contextual attribute: Placement (rather than time)
  - Similarity functions: Hamming distance, edit distance, longest common subsequence
  - Sequence clustering: Suffix tree; generative model (e.g., Hidden Markov Model)

2.1 Basic Concepts: Measuring Similarity between Objects

- 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

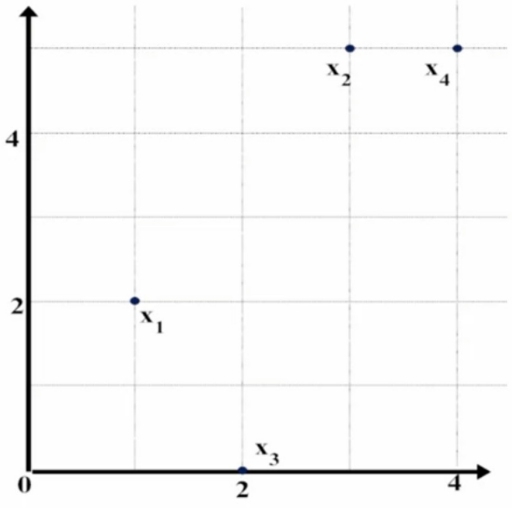
2.2 Distance on Numeric Data Minkowski Distance

- Data matrix
  - A data matrix of n data points with *l* dimensions

$$D = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1l} \\ x_{21} & x_{22} & \dots & x_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nl} \end{pmatrix}$$

- Dissimilarity (distance) matrix
  - n data points, but registers only the distance $d(i, j)$ (typically metric)
  - Usually symmetric, thus a triangular matrix
  - Distance functions are usually different for real, boolean, categorical, ordinal, ratio, and vector variables
  - Weights can be associated with different variables based on applications and data semantics

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



Data Matrix

point	attribute1	attribute2
x1	1	2
x2	3	5
x3	2	0
x4	4	5

Dissimilarity Matrix (by Euclidean Distance)

	x1	*x2*	*x3*	*x4*
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

- Minkowski distance: A popular distance measure

$$d(i,j) = \sqrt[p]{|x_{i1}-x_{j1}|^p + |x_{i2}-x_{j2}|^p + \cdots + |x_{il}-x_{jl}|^p}$$

where $i = (x_{i1}, x_{i2}, \ldots, x_{il})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jl})$ are two l-dimensional data objects, and p is the order (the distance so defined is also called L-p norm)

- Properties
  - d(i, j) > 0 if i ≠ j, and d(i, i) = 0 (Positivity)
  - d(i, j) = d(j, i) (Symmetry)
  - d(i, j) ≤ d(i, k) + d(k, j) (Triangle Inequality)

- p = 1: (L_1 norm) Manhattan (or city block) distance
  - E.g., the Hamming distance: the number of bits that are different between two binary vectors

$$d(i,j) = |x_{i1}-x_{j1}| + |x_{i2}-x_{j2}| + \cdots + |x_{il}-x_{jl}|$$

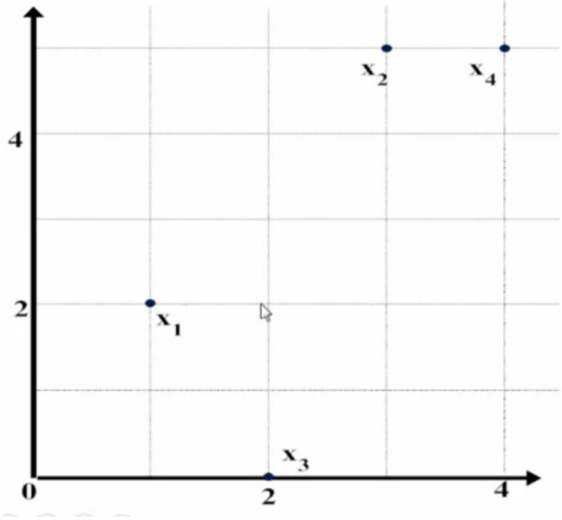
- p = 2: (L_2 norm) Euclidean distance

$$d(i,j) = \sqrt{|x_{i1}-x_{j1}|^2 + |x_{i2}-x_{j2}|^2 + \cdots + |x_{il}-x_{jl}|^2}$$

- $p \to \infty$: (L_{max} norm, L_∞ norm) "supremum" distance
  - The maximum difference between any component (attribute) of the vectors

$$d(i,j) = \lim_{p\to\infty} \sqrt[p]{|x_{i1}-x_{j1}|^p + |x_{i2}-x_{j2}|^p + \cdots + |x_{il}-x_{jl}|^p} = \max_{f=1}^{l} |x_{if}-x_{jf}|$$

point	attribute 1	attribute 2
x1	1	2
x2	3	5
x3	2	0
x4	4	5



Manhattan (L_1)

L	x1	x2	x3	x4
x1	0			
x2	5	0		
x3	3	6	0	
x4	6	1	7	0

Euclidean (L_2)

L2	x1	x2	x3	x4
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

Supremum (L_∞)

L_∞	x1	x2	x3	x4
x1	0			
x2	3	0		
x3	2	5	0	
x4	3	1	5	0

2.3 Proximity Measure for Symetric vs Asymmetric Binary Variables

- A contingency table for binary data

Object *i* \ Object *j*	1	0	sum
1	q	r	$q+r$
0	s	t	$s+t$
sum	$q+s$	$r+t$	p

- Distance measure for symmetric binary variables: $$d(i,j) = \frac{r+s}{q+r+s+t}$$
- Distance measure for asymmetric binary variables: $$d(i,j) = \frac{r+s}{q+r+s}$$
- Jaccard coefficient (*similarity* measure for *asymmetric* binary variables): $$sim_{Jaccard}(i,j) = \frac{q}{q+r+s}$$

Example (usually, the asymmetric attributes are more important)

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 (not counted in)
- The remaining attributes are asymmetric binary
- Let the values Y and P be 1, and the value N be 0
- Distance: $d(i, j) = \frac{r + s}{q + r + s}$

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

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

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

Mary

Jack	1	0	$\sum_{row}$
1	2	0	2
0	1	3	4
$\sum_{col}$	3	3	6

Jim

Jack	1	0	$\sum_{row}$
1	1	1	2
0	1	3	4
$\sum_{col}$	2	4	6

Mary

Jim	1	0	$\sum_{row}$
1	1	1	2
0	2	2	4
$\sum_{col}$	3	3	6

2.4 Distance between Categorical Attributes Ordinal Attributes and Mixed Types

- Categorical data, also called nominal attributes
  - Example: Color (red, yellow, blue, green), profession, etc.
- 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 attribute for each of the *M* nominal states

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank (e.g., freshman, sophomore, junior, senior)
- Can be treated like interval-scaled
  - Replace *an ordinal variable value* by its 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

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

    - Example: freshman: 0; sophomore: 1/3; junior: 2/3; senior 1
      - Then distance: d(freshman, senior) = 1, d(junior, senior) = 1/3
  - Compute the dissimilarity using methods for interval-scaled variables

2.5 Proximity Measure between Two Vectors Cosine Similarity

Example: Calculating Cosine Similarity

- Calculating Cosine Similarity:

$$cos(d_1, d_2) = \frac{d_1 \bullet d_2}{\| d_1 \| \times \| d_2 \|}$$

  where • indicates vector dot product, ||*d*||: the length of vector *d*

- Ex: Find the **similarity** between documents 1 and 2.

  d_1 = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0) d_2 = (3, 0, 2, 0, 1, 1, 0, 1, 0, 1)

  - First, calculate vector dot product

    $d_1 \bullet d_2$ = 5 X 3 + 0 X 0 + 3 X 2 + 0 X 0 + 2 X 1 + 0 X 1 + 0 X 1 + 2 X 1 + 0 X 0 + 0 X 1 = 25

  - Then, calculate ||d_1|| and ||d_2||

$$\| d_1 \| = \sqrt{5 \times 5 + 0 \times 0 + 3 \times 3 + 0 \times 0 + 2 \times 2 + 0 \times 0 + 0 \times 0 + 2 \times 2 + 0 \times 0 + 0 \times 0} = 6.481$$

$$\| d_2 \| = \sqrt{3 \times 3 + 0 \times 0 + 2 \times 2 + 0 \times 0 + 1 \times 1 + 1 \times 1 + 0 \times 0 + 1 \times 1 + 0 \times 0 + 1 \times 1} = 4.12$$

  - Calculate cosine similarity: cos(d_1, d_2) = 26/ (6.481 X 4.12) = 0.94

Covariance Matrix

- The variance and covariance information for the two variables X_1 and X_2 can be summarized as 2 X 2 covariance matrix as

$$\Sigma = E[(\mathbf{X}-\mu)(\mathbf{X}-\mu)^T] = E[\begin{pmatrix} X_1-\mu_1 \\ X_2-\mu_2 \end{pmatrix}(X_1-\mu_1 \quad X_2-\mu_2)]$$

$$= \begin{pmatrix} E[(X_1-\mu_1)(X_1-\mu_1)] & E[(X_1-\mu_1)(X_2-\mu_2)] \\ E[(X_2-\mu_2)(X_1-\mu_1)] & E[(X_2-\mu_2)(X_2-\mu_2)] \end{pmatrix}$$

$$= \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{pmatrix}$$

- Generalizing it to *d* dimensions, we have,

$$D = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{d1} & x_{d2} & \cdots & x_{dd} \end{pmatrix} \qquad \Sigma = E[(\mathbf{X}-\mu)(\mathbf{X}-\mu)^T] = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1d} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{d1} & \sigma_{d2} & \cdots & \sigma_d^2 \end{pmatrix}$$

Week1-Quiz

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1. Answer : 4.6

1. The following real dataset contains information about two different flowers: Iris setosa and Iris versicolor.

Species	Sepal length	Sepal width	Petal length	Petal width
Iris setosa	4.9	3.0	1.4	0.2
Iris versicolor	5.6	2.5	3.9	1.1

What is the Manhattan distance between these two objects?

2. Answer: 1/4

2. The following real dataset contains two samples from the dataset for Prediction of Molecular Bioactivity for Drug Design – Binding to Thrombin, with sampled features. For each activity (F1, F2, ..., F10), the class value (0/1) indicates if the activity is active or inactive.

Cases	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10
1	0	1	1	0	0	0	1	1	1	1
2	0	1	0	0	1	0	1	0	0	1

Assume all the activities are *asymmetric* binary variables. What is the Jaccard coefficient between case 1 and case 2?

3. Answer: 8/21

3. The following real world dataset contains two samples from Car Evaluation Database, which was derived from a simple hierarchical decision model originally developed for the demonstration of DEX (Bohanec, M., & Rajkovic, V. (1990). Expert system for decision making. *Sistemica 1*(1), 145-157.). The model evaluates cars according to the following concept structure: **1 / 1 point**

CAR	car acceptability
.PRICE	overall price
. . buying	buying price
. . maint	price of the maintenance
. TECH	technical characteristics
. . COMFORT	comfort
. . . doors	number of doors
. . . persons	capacity in terms of persons to carry
. . . lug_boot	the size of luggage boot
. . safety	estimated

The attribute values are as follows:

Attribute	Values (categorical)
buying	v-high, high, med, low
maint	v-high, high, med, low
doors	2, 3, 4, 5 - more
persons	2, 4, more
lug_boot	small, med, big
safety	low, med, high

Case	buying	maint	doors	persons	lug_boot	safety
Car 1	med	v-high	3	more	small	med
Car 2	high	v-high	4	4	big	med

To calculate the distance between objects with categorical attributes, we use a set of binary attributes to represent each categorical attribute. Assume all the binary attributes are **symmetric**. What is the distance between Car 1 and Car 2?

5. Answer : 0.4

5. Given the following two short texts with punctuation removed, calculate the cosine similarity between them based on the bag of words model. 1 / 1 point

Text1: all grown-ups were once children but only few of them remember it

Text2: all children should be very understanding of grown-ups

6. Answer 0.882

6. With regard to the species of Iris versicolor, we have sampled data on the features of sepal length and sepal width, as follows. 1 / 1 point

Feature	Sepal length	Petal length
Case 1	7.0	3.2
Case 2	6.4	3.2
Case 3	6.9	3.1
Case 4	5.5	2.3
Case 5	6.5	2.8

What is the correlation coefficient between sepal length and sepal width?