Introduction to Machine Learning

Introduction to Clustering

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Outline

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Supervised Learning vs. Unsupervised Learning

Supervised learning:

- Discover patterns in the data that relate data attributes with a target (class) attribute.

Unsupervised learning:

The data have no target attribute.

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Pattern Recognition

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Search for structure in data

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Elements of Numerical Pattern Recognition

1. Process Description
   - Feature Nomination, Test Data, Design Data
2. Feature Analysis
   - Preprocessing, Extraction, Selection, ...
3. **Cluster Analysis**
   - Labeling, Validity, ...
4. Classifier Design
   - Classification, Estimation, Prediction, Control, ...

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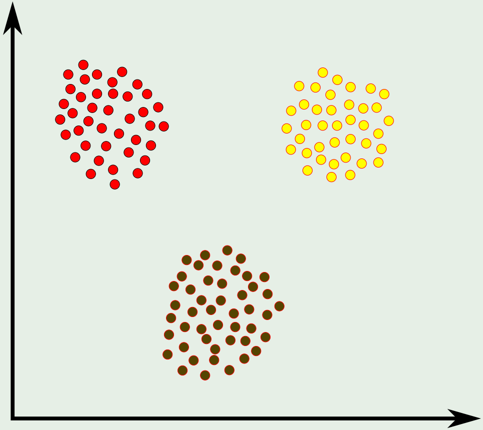
An illustration

The data set has three natural groups of data points, i.e., 3 natural clusters.



Examples

Example 1

Groups people of similar sizes together to make “small”, “medium” and “large” T-Shirts.

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In marketing, segment customers according to their similarities.

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For this, we use the following concept

Clustering!!!

Basically

We want to "reveal" the organization of patterns into "sensible" clusters (groups).

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What is clustering for?

Data Reduction

We can use clustering to reduce the amount of samples in each group to reduce the processing of information.

- Example:
  - In data transmission, a representative for each cluster is defined.
  - Then, instead of transmitting the data samples, we transmit a code number corresponding to the representative.
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Given a set of input patterns $X = \{x_1, x_2, ..., x_N\}$, where $x_j = (x_{1j}, x_{2j}, ..., x_{dj})^T \in \mathbb{R}^d$, with each measure x_{ij} called a feature (attribute, dimension, or variable).

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Hard Partitional Clustering

Definition

Hard partitional clustering attempts to seek a K-partition of $\boldsymbol{X}$, $\boldsymbol{C} = \{C_1, C_2, ..., C_K\}$ with $K \leq N$ such that

1. $C_i \neq \emptyset$ for $i = 1, ..., K$.
2. $\cup_{i=1}^{K} C_i = \boldsymbol{X}$.
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For example, Fuzzy and Possibilistic clustering

Given the membership $A_i(\boldsymbol{x}_j) \in [0,1]$

We can have $\sum_{i=1}^{K} A_i(\boldsymbol{x}_j) = 1, \forall j$ and $\sum_{j=1}^{N} A_i(\boldsymbol{x}_j) < N, \forall i$.

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Features

Usually

A data object is described by a set of features or variables, usually represented as a multidimensional vector.

Thus

We tend to collect all that information as a pattern matrix of dimensionality $N \times d$.

Then

A feature can be classified as continuous, discrete, or binary.

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A continuous feature takes values from an uncountably infinite range set.

Discrete

Discrete features only have finite, or at most, a countably infinite number of values.

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Binary or dichotomous features are a special case of discrete features when they have exactly two values.

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Measurement Level

Meaning

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We have four from lowest to highest

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1. $s\left(\boldsymbol{x}, \boldsymbol{y}\right) \leq s_0$.
2. $s\left(\boldsymbol{x}, \boldsymbol{x}\right) = s_0$ for all $\boldsymbol{x} \in X$.
3. $s\left(\boldsymbol{x}, \boldsymbol{y}\right) = s\left(\boldsymbol{y}, \boldsymbol{x}\right)$ for all $\boldsymbol{x}, \boldsymbol{y} \in X$.
4. If $s\left(\boldsymbol{x}, \boldsymbol{y}\right) = s_0 \iff \boldsymbol{x} = \boldsymbol{y}$.
5. $s\left(\boldsymbol{x}, \boldsymbol{y}\right) s\left(\boldsymbol{y}, \boldsymbol{z}\right) \leq s\left(\boldsymbol{x}, \boldsymbol{z}\right)\left[s\left(\boldsymbol{x}, \boldsymbol{y}\right) + s\left(\boldsymbol{y}, \boldsymbol{z}\right)\right]$ for all $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in X$.

Outline

Dissimilarity Measures

Defintion

A Dissimilarity Measure d on X is a function

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Dissimilarity Measures

The Hamming distance for $\{0,1\}$

The vectors here are collections of zeros and ones. Thus,

$$d_H(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{d} (x_i - y_i)^2 \tag{3}$$

Euclidean distance

$$d(\boldsymbol{x},\boldsymbol{y}) = \left(\sum_{i=1}^{d} |x_i - y_i|^{\frac{1}{2}} \right)^2 \tag{4}$$

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Dissimilarity Measures

The weighted l_p metric DMs

$$d_p\left(\boldsymbol{x},\boldsymbol{y}\right)=\left(\sum_{i=1}^{d} w_i\left|x_i-y_i\right|^p\right)^{\frac{1}{p}} \tag{5}$$

Where

Where x_i, y_i are the ith coordinates of x and y, $i = 1, \ldots, d$ and $w_i \geq 0$ is the ith weight coefficient.

Important

A well-known representative of the latter category of measures is the Euclidean distance.

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The weighted l_2 metric DM can be further generalized as follows

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{(\boldsymbol{x} - \boldsymbol{y})^T B (\boldsymbol{x} - \boldsymbol{y})} \tag{6}$$

Where B is a symmetric, positive definite matrix

A special case

This includes the Mahalanobis distance as a special case

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Special l_p metric DMs that are also encountered in practice are

$$d_1(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{d} w_i |x_i - y_i| \quad \text{(Weighted Manhattan Norm)}$$

$$d_\infty(\boldsymbol{x}, \boldsymbol{y}) = \max_{1 \le i \le d} w_i |x_i - y_i| \quad \text{(Weighted } l_\infty \text{ Norm)}$$

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Outline

Similarity Measures

The inner product

$$s_{inner}\left(\boldsymbol{x},\boldsymbol{y}\right)=\boldsymbol{x}^{T}\boldsymbol{y}=\sum_{i=1}^{d}x_i y_i \tag{7}$$

Closely related to the inner product is the cosine similarity measure

$$s_{cosine}\left(\boldsymbol{x},\boldsymbol{y}\right)=\frac{\boldsymbol{x}^{T}\boldsymbol{y}}{\left\Vert \boldsymbol{x}\right\Vert \left\Vert \boldsymbol{y}\right\Vert} \tag{8}$$

Where $\left\Vert \boldsymbol{x}\right\Vert=\sqrt{\sum_{i=1}^{d}x_i^2}$ and $\left\Vert \boldsymbol{y}\right\Vert=\sqrt{\sum_{i=1}^{d}y_i^2}$, the length of the vectors!!!

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Similarity Measures

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$$r_{\text{Pearson}}\left(\boldsymbol{x},\boldsymbol{y}\right) = \frac{\boldsymbol{x}^T\boldsymbol{y}}{\|\boldsymbol{x}\|\,\|\boldsymbol{y}\|} \tag{9}$$

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Where $\boldsymbol{x} = \left(x_1 - \overline{\boldsymbol{x}}, ..., x_d - \overline{\boldsymbol{x}}\right)^T$ and $\boldsymbol{y} = \left(y_1 - \overline{\boldsymbol{y}}, ..., y_d - \overline{\boldsymbol{y}}\right)^T$

$$\overline{\boldsymbol{x}} = \frac{1}{d}\sum_{i=1}^{d} x_i \text{ and } \overline{\boldsymbol{y}} = \frac{1}{d}\sum_{i=1}^{d} y_i \tag{10}$$

- The difference between r_{cosine} and r_{Pearson} does not depend directly on $\boldsymbol{x}$ and $\boldsymbol{y}$ but on their corresponding difference vectors.

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Properties

- It is clear that $r_{\text{Pearson}}\left(\boldsymbol{x}, \boldsymbol{y}\right)$ takes values between -1 and +1.
- The difference between s_{inner} and r_{Pearson} does not depend directly on x and y but on their corresponding difference vectors.

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Similarity Measures

The Tanimoto measure or distance

$$s_T(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x}^T \boldsymbol{y}}{\|\boldsymbol{x}\|^2 + \|\boldsymbol{y}\|^2 - \boldsymbol{x}^T \boldsymbol{y}} \tag{11}$$

Something Notable

$$s_T(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{1 + \frac{(\boldsymbol{x}-\boldsymbol{y})^T(\boldsymbol{x}-\boldsymbol{y})}{\boldsymbol{x}^T \boldsymbol{y}}} \tag{12}$$

Meaning

The Tanimoto measure is inversely proportional to the squared Euclidean distance.

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Outline

We consider now vectors whose coordinates belong to a finite set

Given $F = \{0, 1, 2, ..., k-1\}$ where k is a positive integer

There are exactly k^d vectors $\boldsymbol{x} \in F^d$

Now consider $\boldsymbol{x}, \boldsymbol{y} \in F^d$

With $A(\boldsymbol{x}, \boldsymbol{y}) = [a_{ij}]$, $i, j = 0, 1, ..., k-1$ be a $k \times k$ matrix

Where

The element a_{ij} is the number of places where the first vector has the i symbol and the corresponding element of the second vector has the j symbol.

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Using Indicator functions

We can think of each element a_{ij}

$$a_{ij} = \sum_{r=1}^{d} I\left[(i,j) == (x_r, y_r)\right] \quad (13)$$

Thanks to Ricardo Llamas and Gibran Felix!!! Class Summer 2015.

Contingency Matrix

Thus

This matrix is called a **contingency table.**

For example if $d = 6$ and $k = 3$

With $\boldsymbol{x} = [0, 1, 2, 1, 2, 1]^T$ and $\boldsymbol{y} = [1, 0, 2, 1, 0, 1]^T$

Then

$$A(\boldsymbol{x}, \boldsymbol{y}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{14}$$

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Thus, we have that

Easy to verify that

$$\sum_{i=0}^{k-1}\sum_{j=0}^{k-1} a_{ij} = d \tag{15}$$

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Most of the proximity measures between two discrete-valued vectors may be expressed as combinations of elements of matrix $A(x, y)$.

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Dissimilarity Measures

The Hamming distance

It is defined as the number of places where two vectors differ:

$$d\left(\boldsymbol{x},\boldsymbol{y}\right)=\sum_{i=0}^{k-1}\sum_{j=0,j\neq i}^{k-1}a_{ij} \tag{16}$$

The summation of all the off-diagonal elements of A, which indicate the positions where $\boldsymbol{x}$ and $\boldsymbol{y}$ differ.

Special case $k=2$, thus vectors are binary valued

The vectors $\boldsymbol{x}\in F^{d}$ are binary valued and the Hamming distance becomes

$$\begin{aligned}d_H\left(\boldsymbol{x},\boldsymbol{y}\right)&=\sum_{i=1}^{d}\left(x_i+y_i-2x_iy_i\right)\\&=\sum_{i=1}^{d}\left(x_i-y_i\right)^2\end{aligned}$$

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Dissimilarity Measures

The l_1 distance

It is defined as in the case of the continuous-valued vectors,

$$d_1(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{d} w_i |x_i - y_i| \tag{17}$$

Outline

Similarity Measures

The Tanimoto measure

Given two sets X and Y, we have that

$$s_T(X, Y) = \frac{n_{X \cap Y}}{n_X + n_Y - n_{X \cap Y}} \tag{18}$$

where $n_X = |X|$, $n_Y = |Y|$, $n_{X \cap Y} = |X \cap Y|$.

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Thus, if x, y are discrete-valued vectors

The measure takes into account all pairs of corresponding coordinates, except those whose corresponding coordinates (x_i, y_i) are both 0.

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We now define

$n_x = \sum_{i=1}^{k-1} \sum_{j=0}^{k-1} a_{ij}$ and $n_y = \sum_{i=0}^{k-1} \sum_{j=1}^{k-1} a_{ij}$

In other words

n_x and n_y denotes the number of the nonzero coordinate of x and y.

Thus, we have

$$s_T(\boldsymbol{x}, \boldsymbol{y}) = \frac{\sum_{i=1}^{k-1} \sum_{j=i}^{k-1} a_{ii}}{n_X + n_Y - \sum_{i=1}^{k-1} \sum_{j=i}^{k-1} a_{ij}} \quad (19)$$

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Outline

Between Sets

Jaccard Similarity

Given two sets X and Y, we have that

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Given two sets X and Y, we have that

$$J(X, Y) = \frac{|X \cap Y|}{|X \cup Y|} \tag{20}$$

Although there are more stuff to look for

Please Refer to

1. Theodoridis' Book Chapter 11.
2. Rui Xu and Don Wunsch. 2009. *Clustering*. Wiley-IEEE Press.