Proximity and Data Pre-processing

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Outline

- Types of data
- Data quality
- Measurement of proximity
- Data pre-process

Similarity and Dissimilarity

- Dissimilarity (distance)
  - Numerical measure of how different two data objects are
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- Similarity
  - Numerical measure of how alike two data objects are.
  - Is higher when objects are more alike.
  - Often falls in the range [0,1]
- Proximity refers to either a similarity or dissimilarity

Similarity and Dissimilarity (cont.)

- Simple attributes, multiple attributes
  - E.g., Dense data: Euclidean distance
  - E.g., Sparse data: Jaccard and Cosine similarity

Similarity/Dissimilarity for Simple Attributes

- p and q are the attribute values for two data objects.

Attribute type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 \ \textit{if} \ \ p = q \\ 1 \ \textit{if} \ \ p \neq q \end{cases}$	$s = \begin{cases} 1 \ \textit{if} \ \ p = q \\ 0 \ \textit{if} \ \ p \neq q \end{cases}$
Ordinal	$d = \frac{\lvert p-q \rvert}{n-1}$ (values mapped to integers 0 to n-1, where n is the number of values)	$s = 1 - \frac{\lvert p-q \rvert}{n-1}$
Interval or Ratio	$d = \lvert p - q \rvert$	$s = -d$, $s = \frac{1}{d+1}$ or $s = 1 - \frac{d - min_d}{max_d - min_d}$

where *min_d* and *max_d* are the minimum and maximum distances between every two values.

Similarity and Dissimilarity – multiple attributes

- Euclidean, Minkowski, DTW, etc.

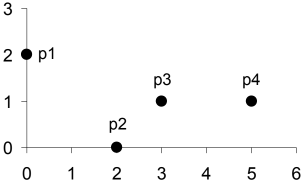
- SMC, Jaccard, Cosine, Hamming, etc.

Euclidean Distance

$$dist = \sqrt{\sum_{i=1}^{n}(q_i - q_i')^2}$$

- n is the number of dimensions (attributes)
- q_i and q_i': the ith attributes (components) of data objects q and q'.
- Standardization is necessary, if scales differ.

Euclidean Distance – Example



point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Distance Matrix

Manhattan Distance

- Considered by Hermann Minkowski in 19th century Germany.

$$dist = (\sum_{i=1}^{n} |q_i - q'_i|)$$

- Taxi cab metric/distance, rectilinear distance, Minkowski's L_1 norm/distance, city block distance, or Manhattan length.
- Parameters
  - n is the number of dimensions (attributes)
  - q_i and q'_i are, respectively, the ith attributes (components) of data objects q and q'.
- Applications
  - In chess, the distance between squares on the chessboard for rooks is measured in Manhattan distance.
  - The length of the shortest path a taxi could take between two intersections equal to the intersections' distance in taxicab geometry.
  - Integrated circuits where wires only run parallel to the X or Y axis.

Minkowski Distance

- The Minkowski distance is a metric on Euclidean space which can be considered as a generalization of both the Euclidean distance and the Manhattan distance.

$$dist = (\sum_{i=1}^{n} |q_i - q_i'|^p)^{\frac{1}{p}}$$

- Parameters
  - p is a parameter
  - n is the number of dimensions (attributes)
  - q_i and q_i' are, respectively, the ith attributes (components) of data objects q and q'.

Minkowski Distance: Illustration

- $p = 1$. Manhattan distance.
- $p = 2$. Euclidean distance.
- $p \to \infty$. Supremum, Chebyshev (L_{max} norm, L_∞ norm) distance.

$$\lim_{p\to\infty}(\sum_{i=1}^{n}|q_i - q_i'|^p)^{\frac{1}{p}} = max_{i=1}^{n}|q_i - q_i'|$$

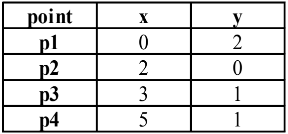
  Kings and queens use Chebyshev distance in Chess.

- L_{min} norm

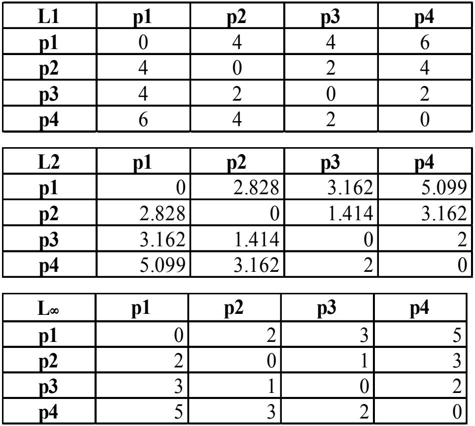
$$\lim_{p\to-\infty}(\sum_{i=1}^{n}|q_i - q_i'|^p)^{\frac{1}{p}} = min_{i=1}^{n}|q_i - q_i'|$$

Note: Do not confuse p with n, i.e., all these distances are defined for all numbers of dimensions.

Minkowski Distance– Example



point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1



L1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

L∞	p1	p2	p3	p4
p1	0	2	3	5
p2	2	0	1	3
p3	3	1	0	2
p4	5	3	2	0

Distance Matrix

Issues to Consider in Calculating Distance

- Attributes have different scales
- Attributes are correlated
- Objects are composed of different types of attributes (Qualitative vs. quantitative)
- Attributes have different weights

Common Properties of a Distance

- Distances, such as the Euclidean distance, have some well known properties.
    - Positivity:
      $d(p, q) \geq 0$ for all p and q;
      $d(p, q) = 0$ only if $p = q$.
    - Symmetry: $d(p, q) = d(q, p)$ for all p and q.
    - Triangle Inequality: $d(p, r) \leq d(p, q) + d(q, r)$ for all points p, q, and r.
- A distance that satisfies these properties is a metric.

Elastic distances

- Dynamic Time Warping (DTW)
- Edit distance based measure
  - Longest Common SubSequence (LCSS)
  - Edit Distance on Real Sequence (EDR)

Elastic distances - DTW

- In time series analysis, Dynamic Time Warping (DTW) is an algorithm for measuring similarity between two temporal sequences which may vary in time or speed.
- DTW is a technique to find an optimal alignment[1] between time series if one time series can be "warped" non-linearly by stretching or shrinking it.
- Applications: similarities in walking patterns, video, audio, etc.
- Calculates an optimal match between two given sequences (e.g., time series) with certain restrictions

[1] M. Müller, Information Retrieval for Music and Motion, Springer, 2007, ISBN: 978-3-540-74047-6, http://www.springer.com/978-3-540-74047-6

Elastic distances - DTW - Problem definition

- Given a reference sequence $s[1, \cdots, n]$ and a query sequence $t[1, \cdots, m]$ and local distance measure $dist(s[i], t[j])$

- Goal: find an alignment between s and t having minimal overall cost

- An (n,m)-warping path (or simply referred to as warping path if n and m are clear from the context) is a sequence $p{=}(p_1, \cdots, p_L)$ with $p_i = (n_i, m_i) \in [1 : n] \times [1 : m]$ for i $(1 \leq i \leq L)$ satisfying the following three conditions
    - Boundary condition: $p_1{=}(1{,}1)$ and $p_L{=}$(n,m)
    - Monotonicity condition: $n_1 \leq n_2 \leq \cdots \leq n_L$ and $m_1 \leq m_2 \leq \cdots \leq m_L$
    - Step size condition: $p_{i+1} - p_i$ is in {(1,0),(0,1),(1,1)} for i $(1 \leq i \leq L-1)$

Elastic distances - DTW - Distance

- Total cost of a warping path $p{=}(p_1, \cdots, p_L)$ between s and t is

$$cost_p(s,t) = \sum_{i=1}^{L} dist(p_i) = \sum_{i=1}^{L} dist(s[n_i], t[m_i])$$

where $p_i = (n_i, m_i)$.

- Let p^* be an optimal warping path between s and t

- The DTW distance DTW(s,t) between s and t is defined as the total cost of p^*.

$$\begin{aligned} DTW(s,t) &= cost_{p^*}(s,t) \\ &= min\ \{cost_p(s,t) | p \text{ is an (n,m)-warping path}\} \end{aligned}$$

Check algorithm.

DTW calculation using Python

Reference

```
import numpy as np
from fastdtw import fastdtw
from scipy.spatial.distance import euclidean

x = np.array([1, 2, 3, 3, 7])
y = np.array([1, 2, 2, 2, 2, 2, 2, 4])

distance, path = fastdtw(x, y, dist=euclidean)

print(distance)
print(path)

# 5.0
# [(0, 0), (1, 1), (1, 2), (1, 3), (1, 4), (2, 5), (3, 6), (4, 7)]
```

Another good library:

https://pyts.readthedocs.io/en/stable/generated/pyts.metrics.dtw.html

Common Properties of a Similarity

- Similarities also have some well known properties.
  - Maximum similarity: $s(p, q) = 1$ only if $p = q$
  - Symmetry: $s(p, q) = s(q, p)$ for all p and q
- $s(p, q)$ is the similarity between points (data objects) p and q.

Similarity Between Binary Vectors

- Compute similarities using the following quantities
  - M_{01} = the number of attributes where p was 0 and q was 1
  - M_{10} = the number of attributes where p was 1 and q was 0
  - M_{00} = the number of attributes where p was 0 and q was 0
  - M_{11} = the number of attributes where p was 1 and q was 1
- Similarity coefficient
- In the range of [0,1]

Distance

- Simple Matching Coefficient (SMC)
- Jaccard Coefficient
- Cosine Similarity
- Hamming distance
- Correlation
- Mutual information (MI)

Simple Matching Coefficient (SMC)

$$\text{SMC} = \frac{\text{number of matches}}{\text{number of attributes}} = \frac{M_{11} + M_{00}}{M_{01} + M_{10} + M_{11} + M_{00}}$$

Example:

- $p = 1\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0$
- $q = 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 0\ 1$
- $M_{01} = 2,\ M_{10} = 1,\ M_{00} = 7,\ M_{11} = 0$
- $SMC = \frac{7+0}{10} = 0.7$

Jaccard Coefficient

$$J = \frac{\text{\# of 11 matches}}{\text{total \# of attributes - \# of 00 matches}} = \frac{M_{11}}{M_{01} + M_{10} + M_{11}}$$

- Handle asymmetric binary attributes
- Example:
  - $p = 1\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0$
  - $q = 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 0\ 1$
  - $M_{01} = 2,\ M_{10} = 1,\ M_{00} = 7,\ M_{11} = 0$
  - $J = \frac{0}{2+1+0} = 0$

Cosine Similarity

- If d_1 and d_2 are two document vectors, then

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

  - $\cdot$ indicates vector dot product
  - $||d||$ is the length of vector d

- $d_1 = 3\ 2\ 0\ 5\ 0\ 0\ 0\ 2\ 0\ 0$
- $d_2 = 1\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 0\ 2$
- $d_1 \cdot d_2 = 3 + 2 = 5$
- $||d_1|| = \sqrt{42} = 6.481$
- $||d_2|| = \sqrt{7} = 2.646$
- $cos(d1, d2) = \frac{5}{6.481 * 2.646} = 0.2916$

Hamming distance

- Measure distance among vectors of equal length with nominal values.
- The number of positions at which the corresponding symbols are different.
- Example
  - “toned” and “roses” is 3.
  - 1011101 and 1001001 is 2.
  - 2173896 and 2233796 is 3.
- Named after *Richard Hamming*. It is used in telecommunication to count the number of flipped bits in a fixed-length binary word as an estimate of error, and therefore is sometimes called the signal distance.
- Not suitable for comparing strings of different lengths, or strings where not just substitutions but also insertions or deletions have to be expected

Correlation

- Correlation measures the linear relationship between objects
- To compute correlation, we standardize data objects, p and q, and then take their dot product

$$corr(p,q) = \frac{covariance(p,q)}{std(p) * std(q)} = \frac{s_{pq}}{s_p * s_q}$$

$$covariance(p,q) = s_{pq} = \frac{1}{n-1}\sum_{i=1}^{n}(p_i - \bar{p})(q_i - \bar{q})$$

$$std(p) = s_p = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(p_i - \bar{p})^2}$$

$$std(q) = s_q = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(q_i - \bar{q})^2}$$

$$\bar{p} = \frac{1}{n}\sum_{i=1}^{n} p_i, \bar{q} = \frac{1}{n}\sum_{i=1}^{n} q_i$$

Correlation - Example 1

```
x = (-3, 6, 0, 3, -6)
y = (1, -2, 0, -1, 2)
```

Compute the Pearson's correlation

$corr(x, y) = -1$, $x = -3y$

Correlation - Example 2

```
x = (-3, -2, -1, 0, 1, 2, 3)
y = (9, 4, 1, 0, 1, 4, 9)
```

- Compute the Pearson's correlation $corr(x, y) = 0$, $y = x^2$
- No linear relationship, but nonlinear relationships can still exist.
- Pearson's correlation only measures linear correlation.

Correlation - Python Example

```
from scipy.stats import pearsonr

p = np.array([1,3,5])
q = np.array([2,3,5])

corr, _ = pearsonr(p, q)
print(’Pearsons correlation: %.3f’ % corr)

#Pearsons correlation: 0.982
```

Mutual information

- For measuring nonlinear correlation
- Come from information theory

$$I(X, Y) = H(X) + H(Y) - H(X, Y)$$

where

- $H(X) = -\sum_{j=1}^{m} P(X = u_j) log_2 P(X = u_j)$, the entropy (average information) of X
- $H(Y) = -\sum_{k=1}^{n} P(Y = v_k) log_2 P(Y = v_k)$, the entropy (average information) of X
- $H(X, Y) = -\sum_{j=1}^{m} \sum_{k=1}^{n} P(X = u_j, Y = v_k) log_2 P(X = u_j, Y = v_k)$, the joint entropy of X and Y

- Minimum value is 0, representing that the value of one variable tells us nothing about the another.
- Maximum value (no fixed value), representing that one variable completely depend on another.

Mutual information - Example

```
x = (-3, -2, -1, 0, 1, 2, 3)
y = (9, 4, 1, 0, 1, 4, 9)
```

- Compute the mutual information $I(X, Y) = 1.9502$

General Approach for Combining Similarities

- Situation: attributes are of different types, an overall similarity is needed
- For the ith attribute, compute a similarity $s_i \in [0, 1]$
- Define δ_i for the ith attribute
  - $\delta_i = 0$ (i.e., do not count this attribute)
    if the ith attribute is an asymmetric attribute and both objects have a value of 0
    or if one of the objects has a missing value for the ith attribute
  - $\delta_i = 1$ otherwise
- Compute the overall similarity

$$similarity(p, q) = \frac{\sum_{i=1}^{n} \delta_i s_i}{\sum_{i=1}^{n} \delta_i}$$

Using Weights to Combine Similarities

- May not want to treat all attributes the same.

- Use weights $w_i \in [0, 1]$ and $\sum_{i=1}^{n} w_i = 1$.

$$similarity(p, q) = \frac{\sum_{i=1}^{n} w_i \delta_i s_i}{\sum_{i=1}^{n} \delta_i}$$

Sampling

- It is often used for both the preliminary investigation of the data and the final data analysis.
- Statisticians sample because obtaining the entire set of data of interest is too expensive or time consuming.
- Sampling is used in data mining because processing the entire set of data of interest is too expensive or time consuming.

Key Principle for Effective Sampling

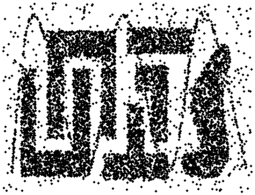
- Using a sample will work almost as well as using the entire data sets, if the sample is representative

- A sample is representative if it has approximately the same property (of interest) as the original set of data

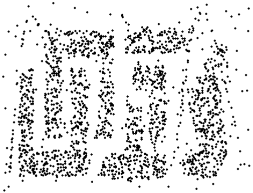
Types of Sampling

- Simple Random Sampling: there is an equal probability of selecting any particular item
- Variations
  - Sampling without replacement: As each item is selected, it is removed from the population
  - Sampling with replacement: Objects are not removed from the population as they are selected for the sample.
    - In sampling with replacement, the same object can be picked up more than once
- Stratified sampling: Split the data into several partitions; then draw random samples from each partition

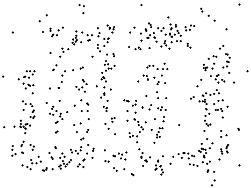
Sample Size



8000 points



2000 Points



500 Points

Curse of Dimensionality

- Data analysis becomes significantly harder as the dimensionality of the data increases.

- Data becomes increasingly sparse in the space that it occupies

Dimensionality Reduction

- Purpose:
  - Avoid curse of dimensionality
  - Reduce amount of time and memory required by data mining algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise
- Techniques
  - Principle Component Analysis (PCA)
  - Singular Value Decomposition (SVD)
  - Others: supervised and non-linear techniques

Feature Subset Selection

- Another way to reduce dimensionality of data
- Redundant features
  - Duplicate much or all of the information contained in one or more other attributes
  - Example: purchase price of a product and the amount of sales tax paid
- Irrelevant features
  - Contain no information that is useful for the data mining task at hand
  - Example: students' ID is often irrelevant to the task of predicting students' GPA

Feature Subset Selection–Techniques (S.S.)

- Brute-force approach:
  - Try all possible feature subsets as input to data mining algorithm
- Embedded approaches:
  - Feature selection occurs naturally as part of the data mining algorithm
- Filter approaches
  - Features are selected before data mining algorithm is run
- Wrapper approaches:
  - Use the data mining algorithm as a black box to find best subset of attributes

Feature Creation (S.S.)

- Create new attributes that can capture the important information in a data set much more efficiently than the original attributes
- Three general methodologies
  - Feature extraction: domain-specific
  - Mapping data to new space
    - Fourier transform
    - Wavelet transform
  - Feature construction: combining features. E.g., Density in cluster analysis.

- Chapter 2: Introduction to Data Mining (2nd Edition) by Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, and Vipin Kumar.

- Textbook website: `https://www-users.cse.umn.edu/~kumar001/dmbook/index.php`

- `https://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics.pairwise`