

# Data Mining, Lecture 3: Distance & Similarity Part II

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## Fractional metrics

In many cases metric (or distance) function belongs to the class of  $L_p$  norms

$$S(\bar{X}\bar{Y}) = \left( \sum_{i=1}^d |x_i - y_i|^p \right)^{\frac{1}{p}}$$

$L_p$  norms do not behave in the same way in terms of the impact of irrelevant features or the distance contrast.

Fractional metrics where  $p \in (0, 1)$  is one of the possible solutions. Rule of thumb, larger the dimensionality, smaller the value  $p$ .

# Match-based Similarity Computation

- ▶ How to select (in practice) relevant features for the similarity computations?
  - ▶ For high dimensional data: impact of the noisy variation along individual attributes needs to be de-emphasized while counting the cumulative match across many dimensions.
  - ▶ One of the methods is *proximity thresholding* in a dimensionality-sensitive way.
  - ▶ Perform discretization into  $k_d$  *equidepth buckets*. Each dimension is divided into  $k_d$  equidepth buckets, containing  $1/k_d$  records.  $k_d \propto d$  (proportional).
- ▶ **Definition**
- Two records of dimension  $d$   $\bar{X}$  and  $\bar{Y}$  are said to be in proximity on dimension  $i$  if  $x_i$  and  $y_i$  belong to the same bucket.*

## Match-based Similarity Computation

- ▶ The subset of dimensions where  $\bar{X}$  and  $\bar{Y}$  map to the same bucket is referred as the proximity set, and denoted  $\mathcal{S}(\bar{X}, \bar{Y}, k_d)$ .
- ▶ Let  $m_i$  and  $n_i$  be the upper and lower bounds of the bucket in dimension  $i$
- ▶ Similarity is defined as follows.

$$S_p(\bar{X}, \bar{Y}, k_d) = \left[ \sum_{i \in \mathcal{S}(\bar{X}, \bar{Y}, k_d)} \left( 1 - \frac{|x_i - y_i|}{m_i - n_i} \right)^p \right]^{\frac{1}{p}}$$

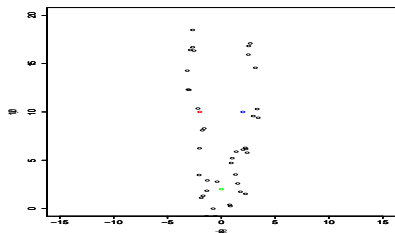
# Impact of Data Distribution

Mahalanobis distance:

$$S_M = \sqrt{(\bar{X} - \bar{Y})\Sigma^{-1}(\bar{X} - \bar{Y})^T}$$

Do not confuse  $\Sigma$  which is covariance matrix with the  $\sum$  which is summation symbol ;)

## Nonlinear distributions ISOMAP



- ▶ Let the data contain nonlinear distributions of arbitrary shape.
- ▶ Consider points  $A$  -blue,  $B$  - red and  $C$  - green. On the basis of the Euclidian distance  $A$  and  $B$  are the closest.
- ▶ According to the *geodesic distance*, where only small "jumps" are allowed  $A$  and  $B$  are not the closest.

## Nonlinear distributions ISOMAP

- ▶ Compute the  $k$ -nearest neighbors of each point. Construct a weighted graph  $G$  with nodes representing data points, and edge weights (costs) representing distances of these  $k$ -nearest neighbors.
- ▶ For any pair of points  $X$  and  $Y$ , find  $S(X, Y)$  as the shortest path between the corresponding nodes in  $G$ .

# Impact of local data distributions

- ▶ Distribution of the data varies significantly with locality.
  - ▶ Density
  - ▶ Orientation
- ▶ Shared Nearest-Neighbor Similarity addresses the first problem.
- ▶ Generic Methods:
  - ▶ Partition the data into a set of local regions.
  - ▶ For any pair of objects, determine the most relevant region for the pair, and compute the pairwise distances using the local statistics of that region. For example, the local Mahalanobis distance may be used in each local region.



## Categorical data



$$S(\bar{X}\bar{Y}) = \sum_{i=1}^d s(x_i, y_i).$$

- ▶ The choice of similarity function  $s(x_i, y_i)$  defines the overall similarity function  $S$ 
  - ▶ The simplest possible function is  $s(x_i, y_i) = \mathbb{I}(x_i, y_i)$
  - ▶ *Inverse occurrence frequency*

$$s(x_i, y_i) = \begin{cases} \frac{1}{p_k(x_i)^2} & \text{if } x_i = y_i \\ 0 & \text{otherwise} \end{cases}$$

here  $p_k(x)$  is the fraction of records where  $x_i = y_i$

- ▶ *Goodall measure*

$$s(x_i, y_i) = \begin{cases} 1 - p_k(x_i)^2 & \text{if } x_i = y_i \\ 0 & \text{otherwise} \end{cases}$$

# Mixed Quantitative and Categorical Data

$$d(x, y) = \lambda d_q(x_q, y_q) + (1 - \lambda)(d_c(x_c, y_c))$$

here index  $q$  denotes quantitative and  $c$  categorical data.

- ▶ how to choose  $\lambda$ ?
- ▶ data normalization ?

# Text Similarity Measures

- ▶ Levenshtein or SED distance. SED - minimal number of single-character edits required to change one string into another. Edit operations are as follows:
  - ▶ insertions
  - ▶ deletions
  - ▶ substitutions
- ▶  $SED(\text{delta}, \text{delata})=1$  delete "a" or  $SED(\text{kitten}, \text{sitting})=3$  : substitute "k" with "s", substitute "e" with "i", insert "g".
- ▶ Hamming distance Similar to Levenshtein but with substitution operation only. Frequently used with categorical and binary data.

## Text Similarity Measures

- ▶ Text may be considered as the multidimensional data if it treated as the bag of words. Lexicon can be treated as the full set of attributes and word frequencies as the quantitative attributes.
- ▶ Many attributes would take the value "0",  $L_p$  norms do not adjust well to the different lengths of the documents.
- ▶ The cosine measure computes the *angle* between two documents. Let  $\bar{X} = (x_1, \dots, x_d)$  and  $\bar{Y} = (y_1, \dots, y_d)$  will be two documents on a lexicon of size  $d$ . Then cosine measure is defines as follows:

$$\cos(\bar{X}, \bar{Y}) = \frac{\sum_{i=1}^d x_i \cdot y_i}{\sum_{i=1}^d x_i^2 \cdot \sum_{i=1}^d y_i^2}$$

This measure uses the raw frequencies between attributes.

## Text Similarity Measures

- ▶ If two documents match in a uncommon word it is more indicative than if two documents match on a word that occurs very commonly.
- ▶ The *inverse document frequency* is defined as

$$id_i = \log(n/n_i).$$

- ▶ Sometimes a dumping function  $f(\cdot)$  which is either logarithm or square root is used.
- ▶ The normalized frequency for the  $i$ th word is defined as follows

$$h(x_i) = f(x_i) \cdot id_i$$

- ▶ Combined together with the cosine distance this leads

$$\cos(\bar{X}, \bar{Y}) = \frac{\sum_{i=1}^d h(x_i) \cdot h(y_i)}{\sum_{i=1}^d h(x_i)^2 \cdot \sum_{i=1}^d h(y_i)^2}$$

## Binary and Sparse Data

- ▶ Already known to you Jaccard distance may be rewritten in the following way

$$J(\bar{X}, \bar{Y}) = \frac{\sum_{i=1}^d h(x_i) \cdot h(y_i)}{\sum_{i=1}^d h(x_i)^2 + \sum_{i=1}^d h(y_i)^2 - \sum_{i=1}^d h(x_i) \cdot h(y_i)}$$

- ▶ Let  $\bar{X}, \bar{Y}$  are binary representations of the two sets  $H_X$  and  $H_Y$  respectively. Then

$$J(\bar{X}, \bar{Y}) = \frac{\sum_{i=1}^d x_i \cdot y_i}{\sum_{i=1}^d x_i^2 + \sum_{i=1}^d y_i^2 - \sum_{i=1}^d x_i \cdot y_i}$$

## Temporal Similarity Measures

- ▶ Temporal data contain a single contextual attribute representing time and one or more behavioral attributes that measure the properties varying along a particular time period.
- ▶ Temporal data shares some similarities with discrete sequences *strings*.
- ▶ Temporal data is usually represented by continuous or discrete time-series.
- ▶ Time-series similarity measures
  - ▶ Behavioral attribute scaling and translation.
  - ▶ Temporal (contextual) attribute translation.
  - ▶ Temporal (contextual) attribute scaling.
  - ▶ Noncontiguity in matching.
- ▶  $L_p$  norms may be used to measure similarities of time series of equal length. But can not address distortions on temporal (contextual) attributes.

# Dynamic Time Wrapping DTW

- ▶ DTW stretches the series along the time axis in a varying (or dynamic) way over different portions to enable more effective matching.
- ▶ Unlike  $L_p$  norms it allows many-to-one mappings. In turn allows to artificial creation of two equal length series.
- ▶ Temporal data is usually represented by continuous or discrete time-series.



## DTW Example

- ▶ Consider  $L_1$  Manhattan metric computed on the first  $n$  elements of two time series  $\bar{X} = (x_1, \dots, x_n)$  and  $\bar{Y} = (y_1, \dots, y_n)$ .
- ▶ The value of Manhattan metric may be written recursively as follows

$$M(\bar{X}_i, \bar{Y}_i) = |x_i - y_i| + M(\bar{X}_{i-1}, \bar{Y}_{i-1})$$

- ▶ Let DTW will be optimal distance between the first  $i$  and the first  $j$  elements of two time series  $\bar{X} = (x_1, \dots, x_n)$  and  $\bar{Y} = (y_1, \dots, y_m)$ . Then DTW is defined as follows

$$DTW(i, j) = s(x_i, y_i) + \min \begin{cases} DTW(i, j-1) & \text{repeat } x_i \\ DTW(i-1, j) & \text{repeat } y_i \\ DTW(i-1, j-1) & \text{repeat neither} \end{cases}$$

## Window-based methods

- ▶ Dropped readings (observation points) may cause a gap in the matching.
- ▶ If two sequences have contiguous matching segments, they should be considered similar.
- ▶ Let  $\bar{X}$  and  $\bar{Y}$  are two series, and let  $\bar{X}_1, \dots, \bar{X}_r$  and  $\bar{Y}_1, \dots, \bar{Y}_r$  be temporally ordered and nonoverlapping windows extracted from the respective series. Then overall similarity function may be defines as follows

$$S(\bar{X}\bar{Y}) = \sum_{i=1}^r M(\bar{X}_i\bar{Y}_i)$$

where  $M(\bar{X}_i\bar{Y}_i)$  is some suitable matching function.

## Discrete Sequence Similarity Measures: Edit distance

- ▶ Let us consider Levenshtein distance in a more detailed way.
- ▶ *Edit* distance defines the similarity between the two strings in terms of cost (effort) of transforming one sequence into another.
- ▶ Let  $\bar{X} = (x_1, \dots, x_m)$ ,  $\bar{Y} = (y_1, \dots, y_n)$  be the two sequences and let the edit is performed to transform  $X$  into  $Y$ .
- ▶ the optimal matching is defined as follows

$$E(i, j) = \min \begin{cases} E(i-1, j) + C_D \\ E(i-1, j) + C_I \\ E(i-1, j-1) + I_{i,j} \cdot C_R \end{cases}$$

where  $C_D$  denotes deletion cost,  $C_I$  -insertion cost and  $C_R$  -replacement cost.

# Discrete Sequence Similarity Measures: Longest Common Subsequence

- ▶ Optimal matching based on the longest common subsequence LCSS is defined as follows.

$$LCSS(i, j) = \max \begin{cases} LCSS(i-1, j-1) & \text{if } x_i = y_i \\ LCSS(i-1, j) & \text{otherwise no match on } x_i \\ LCSS(i, j-1) & \text{otherwise no match on } y_i \end{cases}$$

## Graph Similarity Measures: Similarity between two nodes

- ▶ Let  $G = (N, A)$  is undirected network with node set  $N$  and edge set  $A$ .
- ▶ Assume that either weights are associated with nodes or costs are associated with edges. (Distance functions are usually work with costs and similarity functions -with weights).
- ▶ Heuristic kernel functions  $K(x) = e^{x^2/t^2}$  are used to convert between costs and weights.
- ▶ Nodes similarity is based on the principal of *homophily*
- ▶ Structural Distance-Based Measure
- ▶ Random Walk-Based Similarity

# Graph Similarity Measures: Similarity between two graphs

- ▶ Maximum common subgraph distance
- ▶ Substructure-based similarity
- ▶ Graph-edit distance
- ▶ Graph kernels

## Supervised Similarity Functions

$$\mathcal{S} = \{(\mathcal{O}_i, \mathcal{O}_j) : \mathcal{O}_i \text{ is similar } \mathcal{O}_j\} \quad \mathcal{D} = \{(\mathcal{O}_i, \mathcal{O}_j) : \mathcal{O}_i \text{ is dissimilar } \mathcal{O}_j\}$$

Distance function

$$f_i(\mathcal{O}_i, \mathcal{O}_j; \Theta) = \begin{cases} 0 & \text{if } (\mathcal{O}_i, \mathcal{O}_j) \in \mathcal{S} \\ 1 & \text{if } (\mathcal{O}_i, \mathcal{O}_j) \in \mathcal{D} \end{cases}$$

It may be optimized with respect to the following error function

$$\mathcal{E} = \sum_{(\mathcal{O}_i, \mathcal{O}_j) \in \mathcal{S}} \left(f_i(\mathcal{O}_i, \mathcal{O}_j; \Theta) - 0\right)^2 + \sum_{(\mathcal{O}_i, \mathcal{O}_j) \in \mathcal{D}} \left(f_i(\mathcal{O}_i, \mathcal{O}_j; \Theta) - 1\right)^2$$