Similarity and Distances

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Outline

☐ **Introduction**

☐ Multidimensional Data

☐ Text Similarity Measures

☐ Temporal Similarity Measures

☐ Graph Similarity Measures

☐ Supervised Similarity Functions

☐ Summary

Introduction

☐ Motivation

"*Love is the power to see similarity in the dissimilar.*"—Theodor Adorno

☐ Definition

Given two objects O_1 *and* O_2, *determine a value of the similarity* $Sim(O_1, O_2)$ *(or distance* $Dist(O_1, O_2)$*) between the two objects.*

- Distance functions for spatial data
- Similarity functions for text

☐ Representation

- Closed-form, such as Euclidean distance
- Defined algorithmically

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- ☐ **Multidimensional Data**
- ☐ Text Similarity Measures
- ☐ Temporal Similarity Measures
- ☐ Graph Similarity Measures
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- ☐ Summary

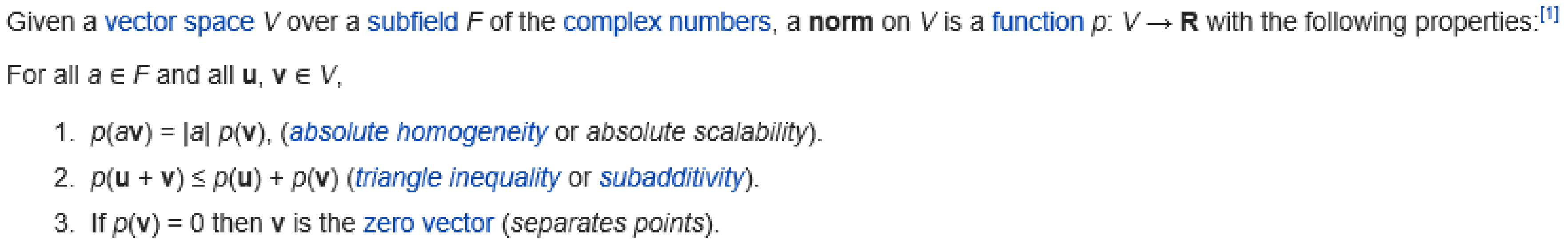
Multidimensional Data (Vectors)

- **Quantitative Data**
- Categorical Data
- Mixed Quantitative and Categorical Data

Quantitative Data (1)

- L_p-Norm $(p \geq 1)$
  - Given $\overline{X} = (x_1 \ldots x_d)$ and $\overline{Y} = (y_1 \ldots y_d)$

$$Dist(\overline{X}, \overline{Y}) = \left(\sum_{i=1}^{d} |x_i - y_i|^p \right)^{1/p}$$



Given a vector space *V* over a subfield *F* of the complex numbers, a **norm** on *V* is a function *p*: *V* → **R** with the following properties:[1]

For all *a* ∈ *F* and all **u**, **v** ∈ *V*,

1. *p*(*a***v**) = |*a*| *p*(**v**), (*absolute homogeneity* or *absolute scalability*).
2. *p*(**u** + **v**) ≤ *p*(**u**) + *p*(**v**) (*triangle inequality* or *subadditivity*).
3. If *p*(**v**) = 0 then **v** is the zero vector (*separates points*).

https://en.wikipedia.org/wiki/Norm_(mathematics)

Quantitative Data (2)

- ☐ L_p-Norm $(p \geq 1)$
  - Given $\overline{X} = (x_1 \ldots x_d)$ and $\overline{Y} = (y_1 \ldots y_d)$

$$Dist(\overline{X}, \overline{Y}) = \left(\sum_{i=1}^{d} |x_i - y_i|^p \right)^{1/p}$$

  - $p = 1$: Manhattan norm
    - ✓ Sum of absolute values
  - $p = 2$: Euclidean norm
    - ✓ Square root of sum of squares
    - ✓ Rotation-invariant
  - $p = \infty$: Infinity norm
    - ✓ Largest absolute value

Quantitative Data (3)

- “L_p-Norm” $(p < 1)$
  - Given $\overline{X} = (x_1 \ldots x_d)$ and $\overline{Y} = (y_1 \ldots y_d)$

$$Dist(\overline{X}, \overline{Y}) = \left(\sum_{i=1}^{d} |x_i - y_i|^p \right)^{1/p}$$

  - $p = 0$: Zero norm
    - ✓ Number of nonzero elements
    - ✓ Nonconvex
  - $0 < p < 1$: Fractional-norm
    - ✓ Nonconvex

Impact of Domain-Specific Relevance

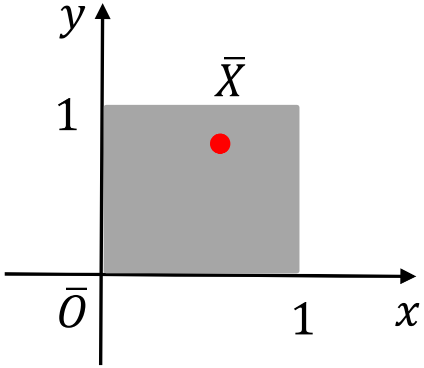
- Some Features are more Important
  - Credit-scoring
    - ✓ Salary is more important than Gender
- Generalized L_p-Norm

$$Dist(\overline{X},\overline{Y}) = \left(\sum_{i=1}^{d} a_i \cdot |x_i - y_i|^p \right)^{1/p}.$$

  - $a_1, \ldots, a_d$ are nonnegative coefficients
  - Generalized Minkowski distance

Impact of High Dimensionality (1)

- Curse of Dimensionality
  - Distance-based algorithms lose their effectiveness as the dimensionality increases
- An Example
  - A unit cube of dimensionality d in the nonnegative quadrant
  - $\bar{X}$ is a random point in the cube
  - Manhattan distance between $\bar{O}$ and $\bar{X}$

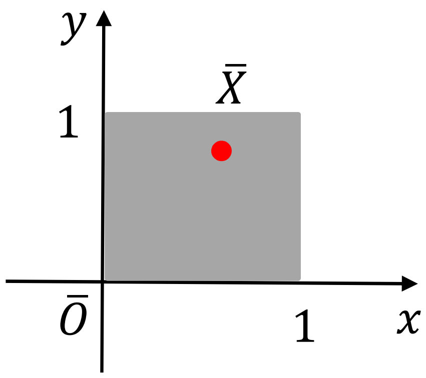


Impact of High Dimensionality (2)

- Manhattan distance between $\bar{O}$ and $\bar{X}$

$$Dist(\overline{O},\overline{X}) = \sum_{i=1}^{d}(Y_i - 0).$$

where $\bar{X} = [Y_1, \ldots, Y_d]$



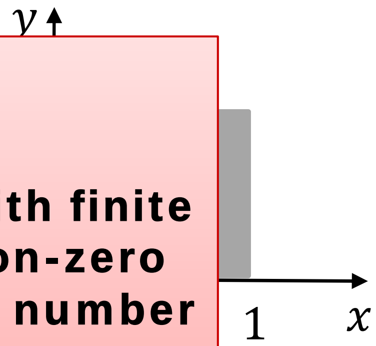
- $Dist(\bar{O},\bar{X})$ is a random variable
    - Since $\bar{X}$ is a random variable
    - Mean is $\mu = d/2$
    - Standard deviation $\sigma = \sqrt{d/12}$
- With a probability at least 8/9

$$Dist(\bar{O},\bar{X}) \in [\underbrace{\mu - 3\sigma}_{D_{min}}, \underbrace{\mu + 3\sigma}_{D_{max}}]$$

Impact of High Dimensionality (2)

- Manhattan distance between $\bar{O}$ and $\bar{X}$

$$Dist(\overline{O},\overline{X}) \quad \sum^{d}(X \quad 0)$$



where $\bar{X}$ =

- $Dist(\bar{O},\bar{X})$
  - ✓ Since $\bar{X}$
  - ✓ Mean is
  - ✓ Standa
- With a probabi least 8/9

Chebyshev's inequality

Let X be a random variable with finite expected value μ and finite non-zero variance σ^2. Then for any real number $k > 0$,

$$\Pr(|X - \mu| \geq k\sigma) \leq \frac{1}{k^2}$$

$$Dist(\bar{O},\bar{X}) \in [\underbrace{\mu - 3\sigma}_{D_{min}}, \underbrace{\mu + 3\sigma}_{D_{max}}]$$

Impact of High Dimensionality (3)

- Manhattan distance between $\bar{O}$ and $\bar{X}$

$$Dist(\overline{O}, \overline{X}) = \sum_{i=1}^{d} (Y_i - 0).$$

- $Dist(\bar{O}, \bar{X})$ is a random variable
  - ✓ Mean is $\mu = d/2$
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- With a probability at least 8/9

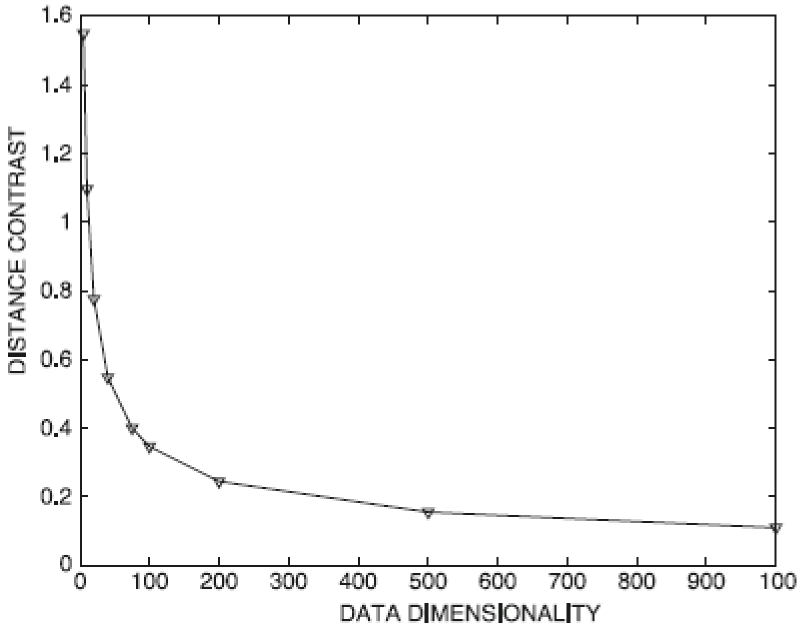
$$Dist(\bar{O}, \bar{X}) \in [\underbrace{\mu - 3\sigma}_{D_{min}}, \underbrace{\mu + 3\sigma}_{D_{max}}]$$

- Contrast

$$\text{Contrast}(d) = \frac{D_{max} - D_{min}}{\mu} = \sqrt{12/d}.$$

Impact of High Dimensionality (4)

- Contrast→ 0, as $d \to \infty$
  - As d increases, variation become neglectable



(a) Contrasts with dimensionality

Impact of Locally Irrelevant Features

- Many features are likely to be irrelevant
  - Especially in high-dimensional data
- An Example
  - A cluster containing diabetic patients
    - ✓ Blood glucose level are more important
- L_p-Norm
  - Suffer from the additive noise effects of the irrelevant features

Impact of Different L_p-Norms (1)

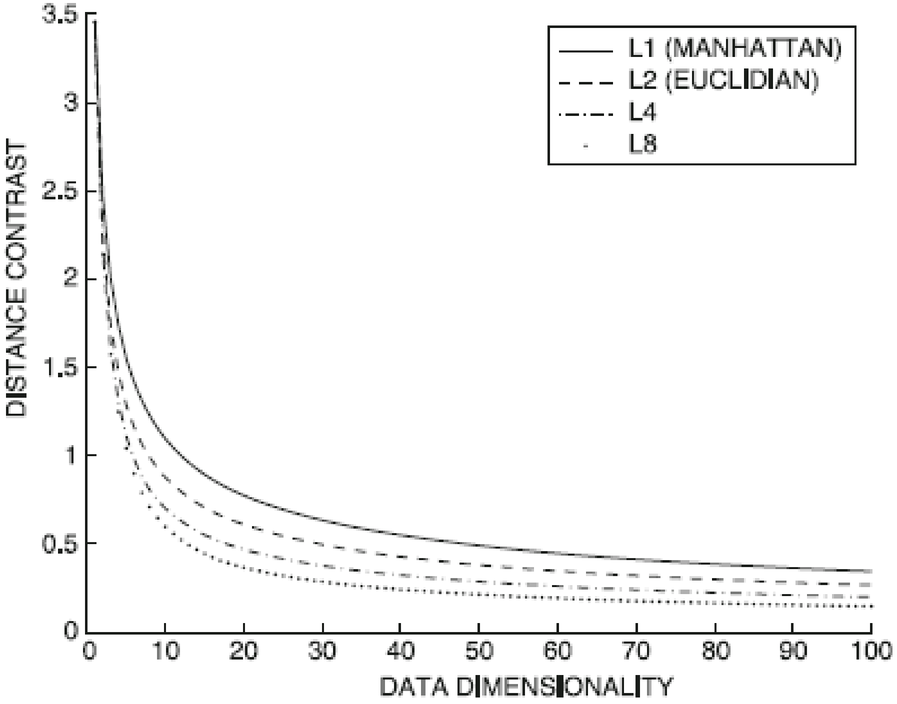
- Different L_p-Norms do not behave in a similar way
  - When the dimensionality is high
  - When there exist irrelevant features
- L_∞-Norms

$$dist(\bar{X}, \bar{Y}) = \max_i |x_i - y_i|$$

  - Sensitive to noise
- Irrelevant attributes are emphasized for large values of p

Impact of Different L_p-Norms (2)

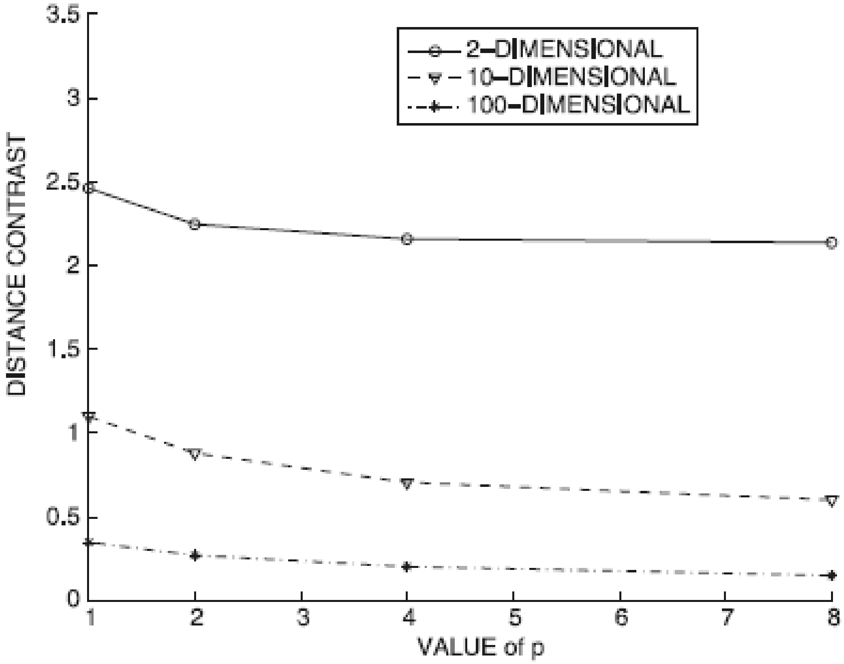
- ☐ Distance contrasts are also poorer for large values of p



(b) Contrasts with norms

Impact of Different L_p-Norms (3)

- ☐ Distance contrasts are also poorer for large values of p



(a) Contrast

Match-Based Similarity Computation

- ☐ The Key Idea
  - De-emphasize irrelevant features
- ☐ Proximity Thresholding
  - Discretized each feature into k_d equidepth buckets
- ☐ Similarity Evaluation

$$\begin{aligned}\bar{X} &= [x_1, x_2, \cdots, x_d] \Longrightarrow [1,\boxed{3,}\cdots,\boxed{k_d}]\\ \bar{Y} &= [y_1, y_2, \cdots, y_d] \Longrightarrow [5,\boxed{3,}\cdots,\boxed{k_d}]\end{aligned}$$

  - $S(\bar{X}, \bar{Y}, k_d)$ is the set of features mapped to the same bucket

Match-Based Similarity Computation

- The Key Idea
  - De-emphasize irrelevant features
- Proximity Thresholding
  - Discretized each feature into k_d equidepth buckets
- Similarity Evaluation

$$PSelect(\overline{X},\overline{Y},k_d) = \left[\sum_{i\in S(\overline{X},\overline{Y},k_d)} \left(1-\frac{|x_i-y_i|}{m_i-n_i}\right)^p\right]^{1/p} \in [0, S(\bar{X},\bar{Y},k_d)]$$

  - $S(\bar{X},\bar{Y},k_d)$ is the set of features mapped to the same bucket

Match-Based Similarity Computation

- ☐ The Key Idea
  - De-emph res
- ☐ Proxim
  - Disc
    equide

Picking $k_d \propto d$ achieves a constant level of contrast in high dimensional space for certain data distributions.

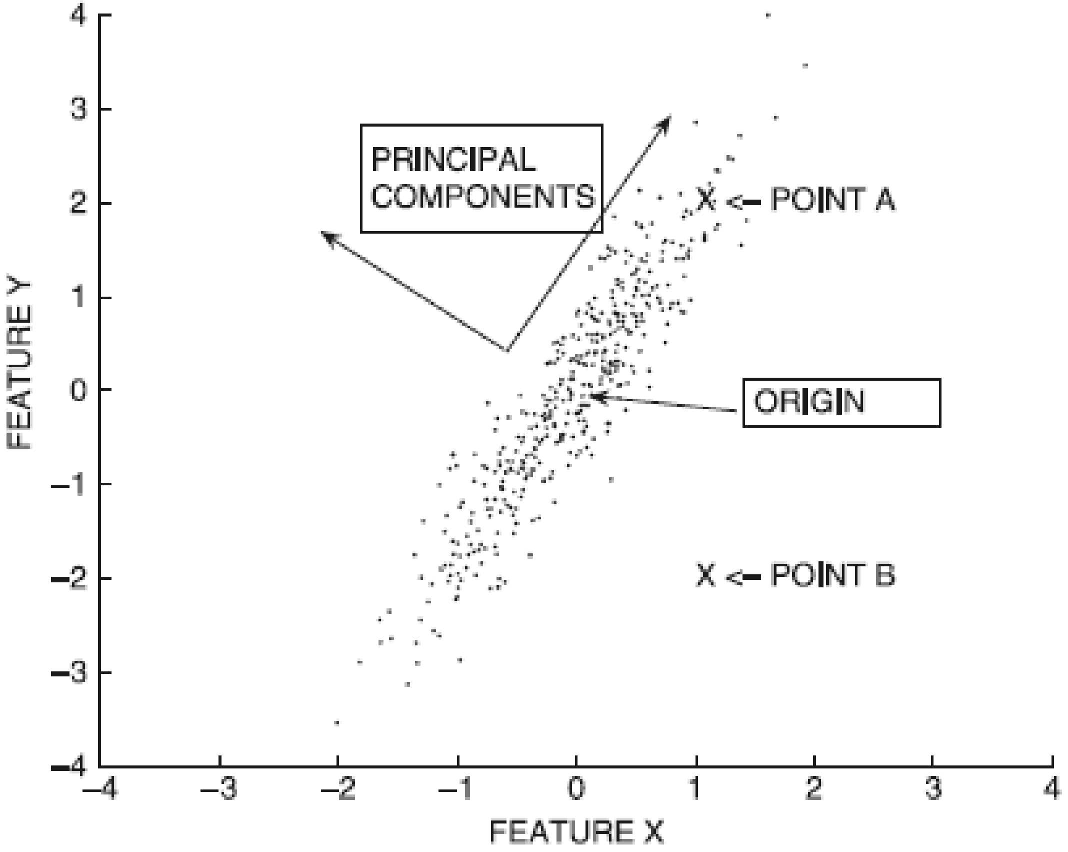
- ☐ Similarity Eva ion

$$PSelect(\overline{X},\overline{Y},k_d) = \left[\sum_{i \in S(\overline{X},\overline{Y},k_d)} \left(1 - \frac{|x_i - y_i|}{m_i - n_i}\right)^p \right]^{1/p} \in [0, S(\bar{X},\bar{Y},k_d)]$$

  - $S(\bar{X},\bar{Y},k_d)$ is the set of features mapped to the same bucket

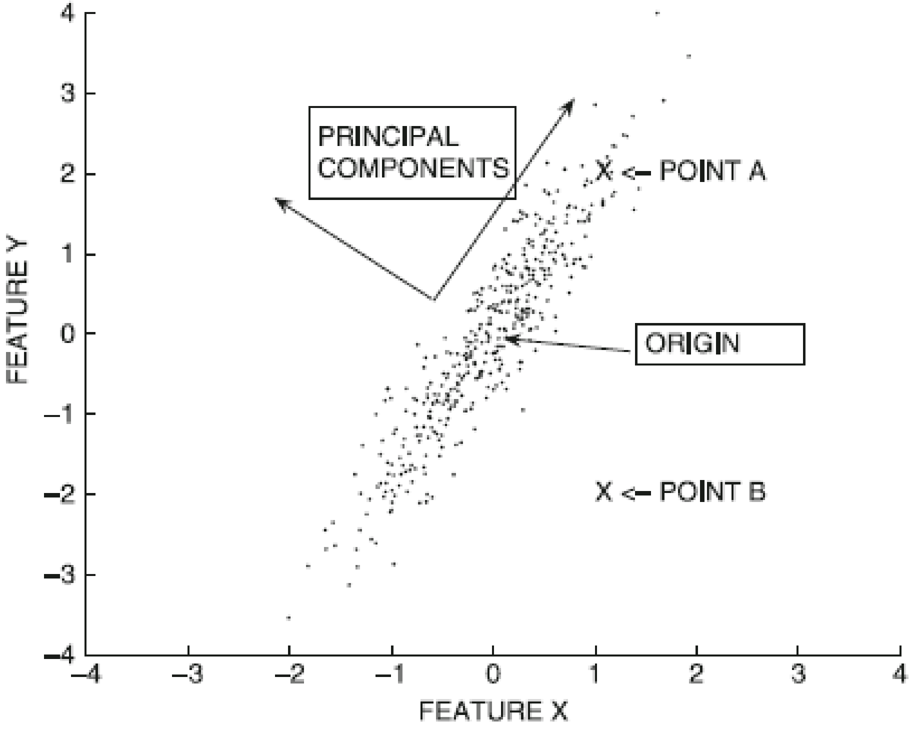
Impact of Data Distribution (1)

☐ $A = (1,2)$ and $B = (1,-2)$



Impact of Data Distribution (2)

- $A = (1,2)$ and $B = (1,-2)$
  - O—A is aligned with a high-variance direction
  - O—B is aligned with a low-variance direction
  - O—A ought to be less than O—B



Impact of Data Distribution (3)

- ☐ The Mahalanobis distance
  - Let Σ be the covariance matrix

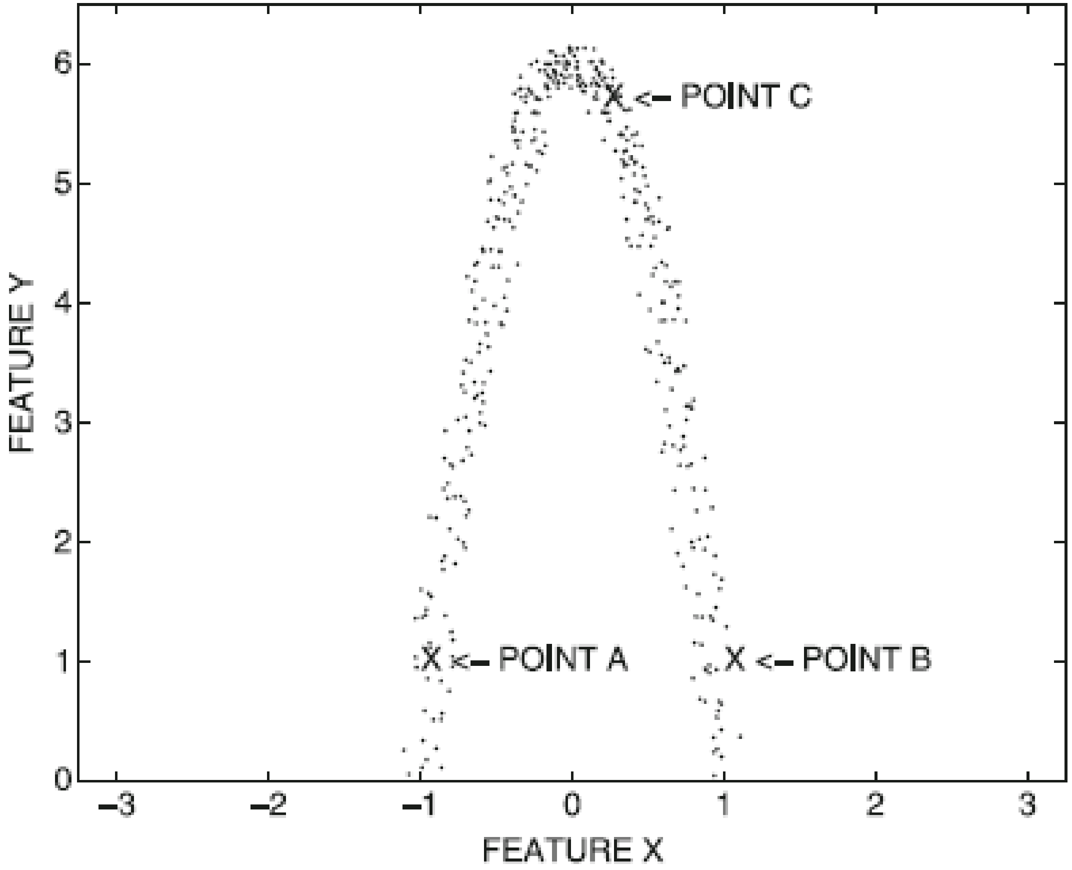
$$Maha(\overline{X},\overline{Y}) = \sqrt{(\overline{X}-\overline{Y})\Sigma^{-1}(\overline{X}-\overline{Y})^{T}}.$$

  - Projection+Normalization
    - ✓ Let $\Sigma = U\Lambda U^\top = \sum_{i=1}^{d} \sigma_i \mathbf{u}_i \mathbf{u}_i^\top$
    - ✓ Then, $\Sigma^{-1} = U\Lambda^{-1}U^\top = \sum_{i=1}^{d} \sigma_i^{-1} \mathbf{u}_i \mathbf{u}_i^\top$

$$Maha(\bar{X},\bar{Y}) = \sqrt{(\bar{X}-\bar{Y})\left(\sum_{i=1}^{d} \sigma_i^{-1}\mathbf{u}_i\mathbf{u}_i^\top\right)(\bar{X}-\bar{Y})^\top} = \sqrt{\sum_{i=1}^{d} \frac{\left((\bar{X}-\bar{Y})\mathbf{u}_i\right)^2}{\sigma_i}}$$

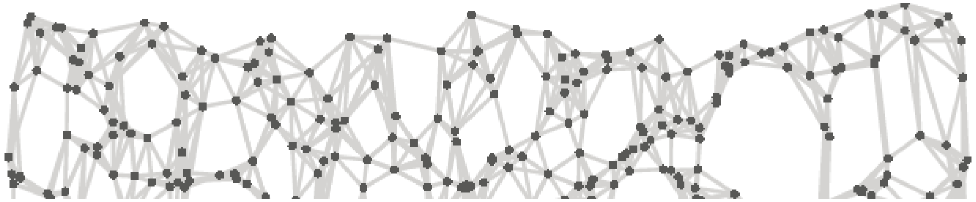
Nonlinear Distributions: ISOMAP (1)

☐ Which one of B and C is closer to A?



Nonlinear Distributions: ISOMAP (2)

- Geodesic Distances
  - Compute the k-nearest neighbors of each point
  - Construct a weighted graph G with nodes representing data points, and edge weights representing (Euclidean) distance of these k-nearest neighbors



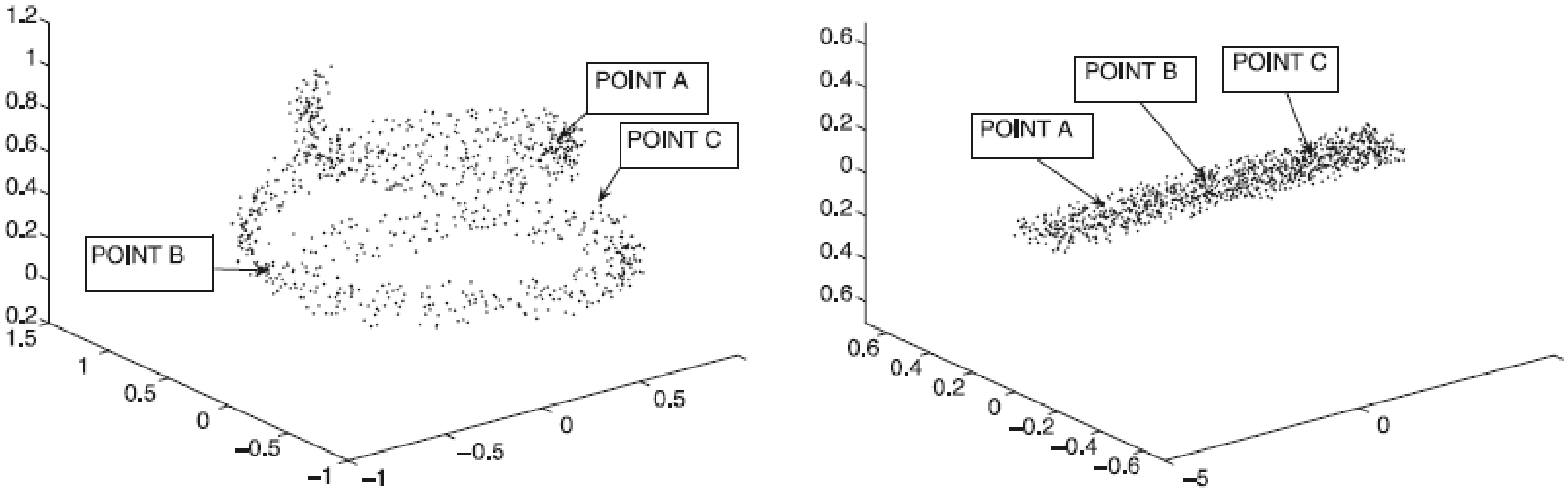
  - $Dist(\bar{X}, \bar{Y})$ is the shortest path between $\bar{X}$ and $\bar{Y}$ in the graph

Nonlinear Distributions: ISOMAP (3)

- ☐ Nonlinear Dimensionality Reduction by ISOMAP
  - Compute the k-nearest ...
  - Construct a weighted graph G ...
  - Compute the distances between all pairs of data points
    - ✓ A $d \times d$ distance matrix
  - Find vector representations by multidimensional scaling (MDS)
  - $Dist(\bar{X}, \bar{Y})$ is the Euclidean distance of the new representations

Nonlinear Distributions: ISOMAP (4)

- An Example of ISOMAP



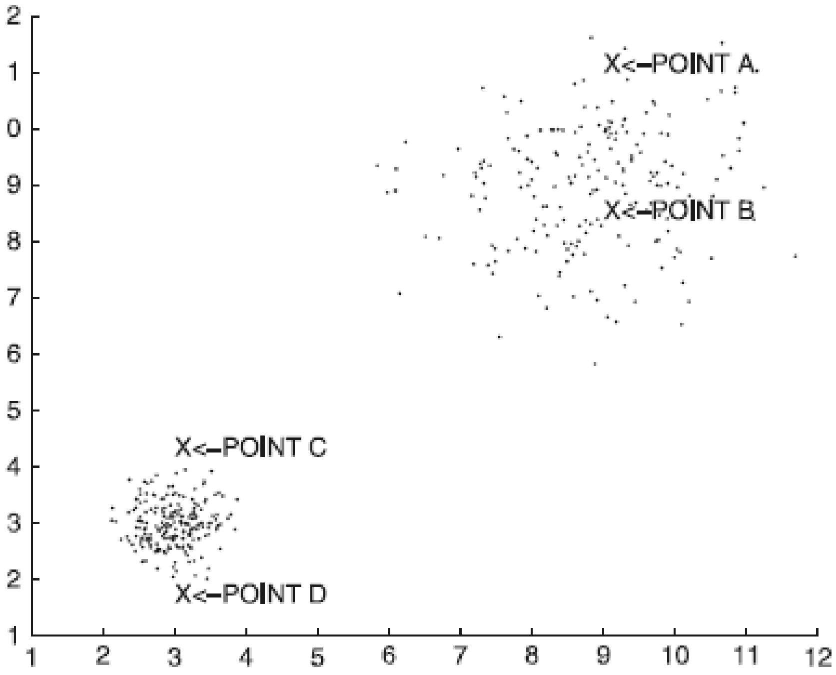
(a) A and C seem close
(original data)

(b) A and C are actually far away
(*ISOMAP* embedding)

- Manifold Learning (ISOMAP, LLE, LE)

Impact of Local Data Distribution (1)

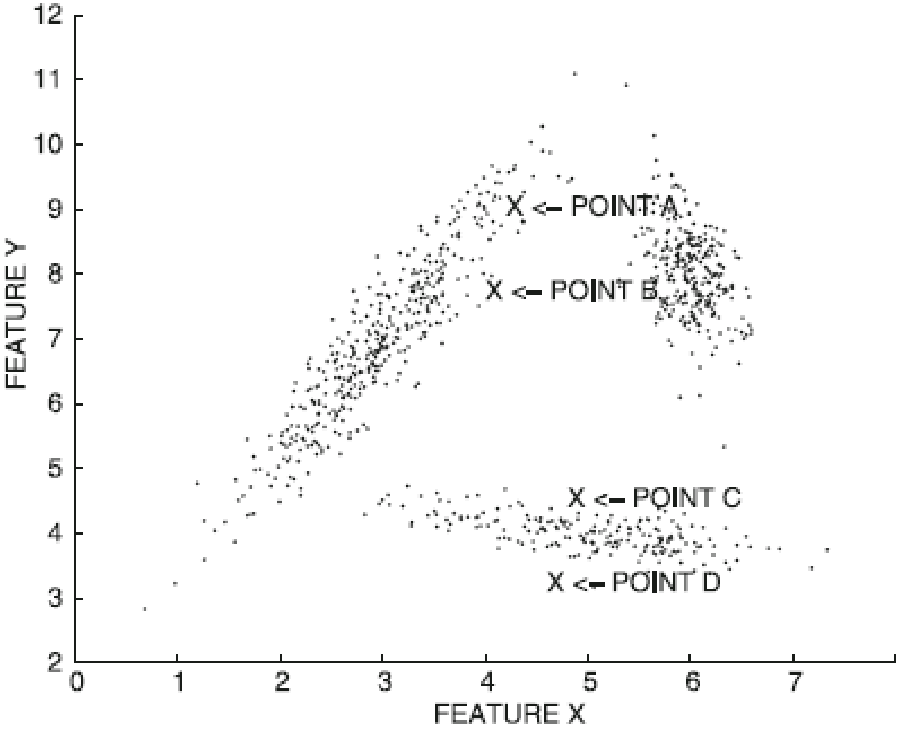
- Local Density Variation
  - $C — D$ should be longer than $A — B$



(a) local density variation

Impact of Local Data Distribution (2)

- Local Density Variation
  - $C—D$ should be longer than $A—B$



(b) local orientation variation

Impact of Local Data Distribution (3)

- Generic Methods
  - Partition the data into a set of local regions (Nontrivial)
  - For any pair of objects, determine the most relevant region for the pair
  - If they belong to the same region
    - ✓ Compute the pairwise distances using the local statistics of that region
    - ✓ Local Mahalanobis distance
  - If they belong to different regions
    - ✓ Global statistics or averaged statistics

Multidimensional Data (Vectors)

- Quantitative Data
- **Categorical Data**
- Mixed Quantitative and Categorical Data

Categorical Data (1)

- Given $\overline{X} = (x_1 \dots x_d)$ and $\overline{Y} = (y_1 \dots y_d)$
  - Sum of similarities on the individual features

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

  - The simplest $S(x_i, y_i)$

$$S(x_i, y_i) = \begin{cases} 1, & x_i = y_i \\ 0, & x_i \neq y_i \end{cases}$$

    - ✓ Ignore the relative frequencies
      - Two documents containing “Science” is less similar than two documents containing “Data Mining”

Categorical Data (2)

- ☐ Given $\overline{X} = (x_1 \dots x_d)$ and $\overline{Y} = (y_1 \dots y_d)$
  - Sum of similarities on the individual features

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

  - Inverse occurrence frequency

$$S(x_i, y_i) = \begin{cases} 1/p_i(x_i)^2, & x_i = y_i \\ 0, & x_i \neq y_i \end{cases}$$

    - ✓ $p_i(x_i)$ is the fraction of records in which the i-th feature takes on the value of x_i

Categorical Data (3)

- Given $\overline{X} = (x_1 \dots x_d)$ and $\overline{Y} = (y_1 \dots y_d)$
  - Sum of similarities on the individual features

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

  - Goodall measure

$$S(x_i, y_i) = \begin{cases} 1 - p_i(x_i)^2, & x_i = y_i \\ 0, & x_i \neq y_i \end{cases}$$

    - ✓ $p_i(x_i)$ is the fraction of records in which the i-th feature takes on the value of x_i

Multidimensional Data (Vectors)

- Quantitative Data
- Categorical Data
- **Mixed Quantitative and Categorical Data**

Mixed Quantitative and Categorical Data

- Given $\overline{X} = (\overline{X_n}, \overline{X_c})$ and $\overline{Y} = (\overline{Y_n}, \overline{Y_c})$
  - Where $\overline{X_n}$, $\overline{Y_n}$ are the subsets of numerical attributes and $\overline{X_c}$, $\overline{Y_c}$ are the subsets of categorical attributes
  - Weighted Average

$$Sim(\overline{X}, \overline{Y}) = \lambda \cdot NumSim(\overline{X_n}, \overline{Y_n}) + (1 - \lambda) \cdot CatSim(\overline{X_c}, \overline{Y_c})$$

    - ✓ λ is difficult to decide
  - Normalized Weighted Average

$$Sim(\overline{X}, \overline{Y}) = \lambda \cdot NumSim(\overline{X_n}, \overline{Y_n})/\sigma_n + (1 - \lambda) \cdot CatSim(\overline{X_c}, \overline{Y_c})/\sigma_c.$$

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Text Similarity Measures (1)

- ☐ As Quantitative Multidimensional Data
  - Bag of words model
  - It is very sparse
  - L_p-norm does not work well
    - ✓ Long documents have long distance
- ☐ Dimensionality Reduction (A Possible Solution)
  - Latent Semantic Analysis (SVD)
  - L_p-norm in the new space

Text Similarity Measures (2)

- Cosine Similarity
  - The angle between two documents

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

  - Ignore the relative frequencies
    - ✓ Two documents containing “Science” is less similar than two documents containing “Data Mining”

Text Similarity Measures (3)

- Cosine Similarity with TF-IDF
  - Inverse document frequency

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

where n_i is number of documents in which the i-th word occurs

  - A damping function may be applied to term frequencies

$$f(x_i) = \sqrt{x_i}$$
$$f(x_i) = \log(x_i)$$

    - ✓ The excessive presence of single word does not throw off the similarity measure

Text Similarity Measures (4)

- Cosine Similarity with TF-IDF
  - Normalized frequency for the i-th word

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

  - Then, we define

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

- Jaccard coefficient

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

Binary and Set Data

- ☐ Given $\bar{X} = (x_1, \dots, x_d)$ and $\bar{Y} = (y_1, \dots, y_d)$ with $x_i, y_i \in (0,1)$
  - They can be treated as vector representations of two sets

$$S_X = \{i | x_i = 1\}$$

$$S_Y = \{i | y_i = 1\}$$

  - Jaccard coefficient

$$J(\overline{X}, \overline{Y}) = \frac{\sum_{i=1}^{d} x_i \cdot y_i}{\sum_{i=1}^{d} x_i^2 + \sum_{i=1}^{d} y_i^2 - \sum_{i=1}^{d} x_i \cdot y_i} = \frac{|S_X \cap S_Y|}{|S_X \cup S_Y|}.$$

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Temporal Similarity Measures

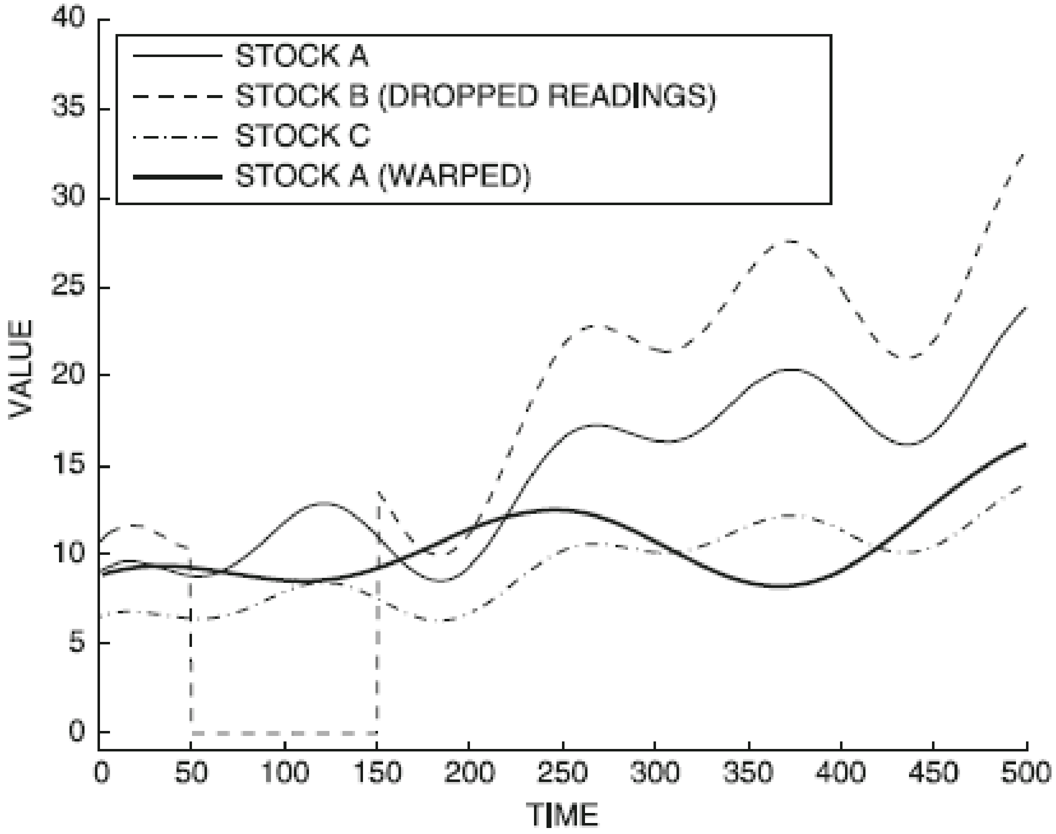
- Temporal data
  - **Continuous time series**
  - Discrete sequences

Time-Series Similarity Measures (1)

- Distortion Factors
  - Behavioral attribute scaling and translation
  - Temporal (contextual) attribute translation
  - Temporal (contextual) attribute scaling
  - Noncontiguity in matching

Time-Series Similarity Measures (2)

- ☐ Impact of scaling, translation, and noise



Time-Series Similarity Measures (3)

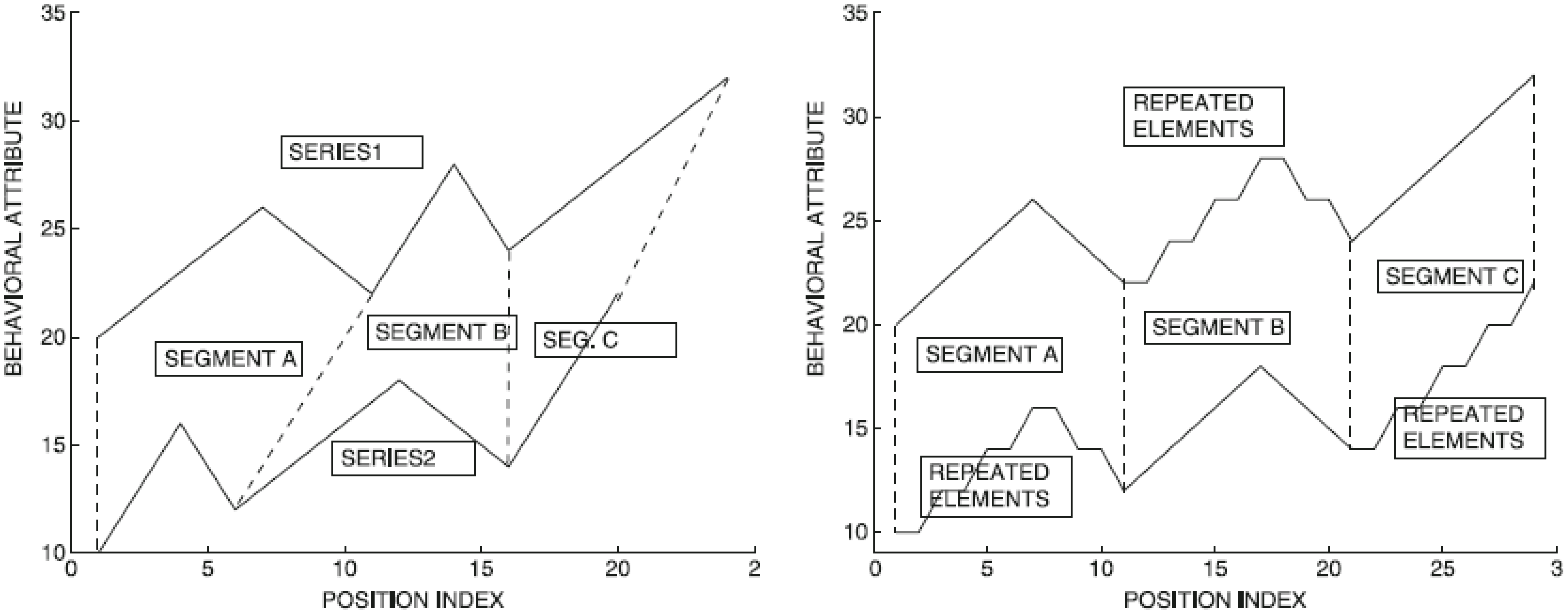
- ☐ Impact of Behavioral Attribute Normalization
  - Behavioral attribute translation
    - ✓ The behavioral attribute is mean centered
  - Behavioral attribute scaling
    - ✓ The standard deviation is scaled to 1
- ☐ L_p-Norm

$$Dist(\overline{X},\overline{Y}) = \left(\sum_{i=1}^{n} |x_i - y_i|^p\right)^{1/p}$$

  - Combined with wavelet transformations

Dynamic Time Warping Distance (1)

☐ Address contextual attribute scaling



☐ Can be used either for time-series or sequence data

Dynamic Time Warping Distance (2)

- Given $\overline{X} = (x_1 \ldots x_m)$ and $\overline{Y} = (y_1 \ldots y_n)$
  - The two series have different lengths
- $DTW(i,j)$
  - The distance between the first i elements of $\bar{X}$ and the first j elements of $\bar{Y}$
- An Recursive Definition

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

Dynamic Time Warping Distance (3)

- ☐ Implementation
  - Recursive computer program

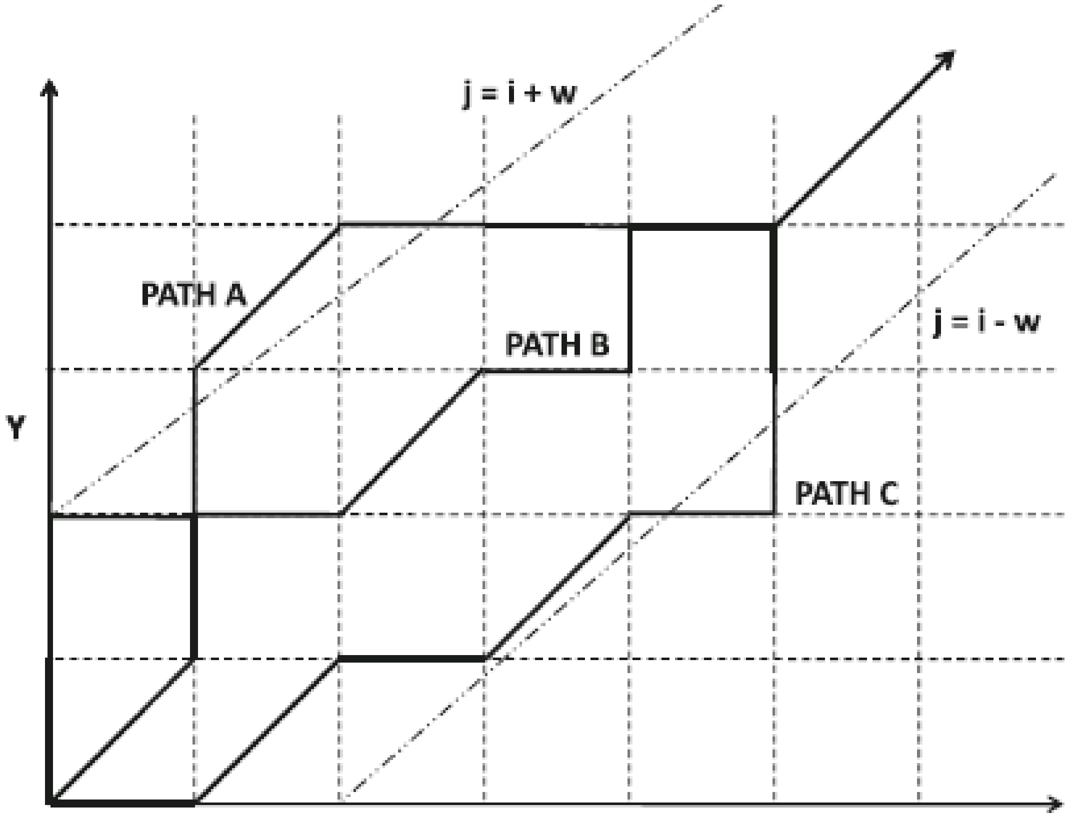
$$DTW(i,j) = distance(x_i, y_j) + \min \begin{cases} DTW(i, j-1) & \text{repeat } x_i \\ DTW(i-1, j) & \text{repeat } y_j \\ DTW(i-1, j-1) & \text{repeat neither} \end{cases}$$

  - Nested Loop

```
for $i = 1$ to $m$
  for $j = 1$ to $n$
    compute $DTW(i,j)$ using Eq. 3.18
```

Dynamic Time Warping Distance (3)

- Optimal Warping = Optimal Path



Temporal Similarity Measures

- Temporal data
  - Continuous time series
  - **Discrete sequences**

Edit Distance (1)

- Edit Distance of Two Sequences
    - The cost of “edits” to transfer the first one to the second one
- Edits
    - Insertions
    - Deletions
    - Replacements
- Sequence abababab to babababa
    - 8 Replacements
    - 1 Deletion+1 Insertion

Edit Distance (2)

- Two Sequences $\overline{X} = (x_1 \dots x_m)$ and $\overline{Y} = (y_1 \dots y_n)$
  - $Edit(\bar{X}, \bar{Y})$ may not be the same as $Edit(\bar{Y}, \bar{X})$
- $Edit(i, j)$
  - The edit distance between the first i symbols of $\bar{X}$ and the first j symbols of $\bar{Y}$
- An Recursive Definition

$$Edit(i,j) = \min \begin{cases} Edit(i-1,j) + \text{Deletion Cost} \\ Edit(i,j-1) + \text{Insertion Cost} \\ Edit(i-1,j-1) + I_{ij} \cdot (\text{Replacement Cost}) \end{cases}$$

Longest Common Subsequence (LCSS)

- LCSS of $\overline{X} = (x_1 \ldots x_m)$ and $\overline{Y} = (y_1 \ldots y_n)$;
  - Length of the longest common subsequence
- $LCSS\ (i, j)$
  - The LCSS between the first i symbols of $\bar{X}$ and the first j symbols of $\bar{Y}$
- An Recursive Definition

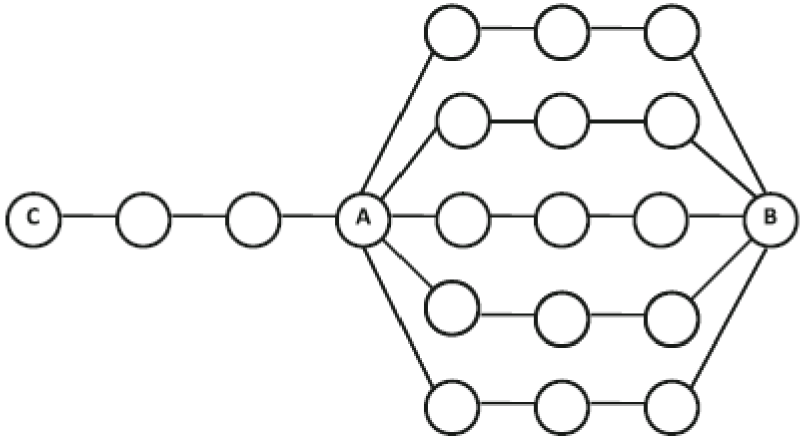
$$LCSS(i,j) = \max \begin{cases} LCSS(i-1, j-1) + 1 & \text{only if } x_i = y_j \\ LCSS(i-1, j) & \text{otherwise (no match on } x_i) \\ LCSS(i, j-1) & \text{otherwise (no match on } y_j) \end{cases}$$

Outline

- ☐ Introduction
- ☐ Multidimensional Data
- ☐ Text Similarity Measures
- ☐ Temporal Similarity Measures
- ☐ **Graph Similarity Measures**
- ☐ Supervised Similarity Functions
- ☐ Summary

Similarity between Two Nodes in a Single Graph

- ☐ Structural Distance-Based Measure
  - Shortest-path on the graph
  - Dijkstra algorithm
- ☐ Random Walk-Based Similarity
  - Accounts for multiplicity in paths during similarity computation



Similarity Between Two Graphs

- Extremely Challenging
  - Even the graph isomorphism problem is NP-hard
- Possible Solutions
  - Maximum common subgraph distance
  - Substructure-based similarity
  - Graph-edit distance
  - Graph kernels

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Supervised Similarity Functions

- User Feedback

$$\mathcal{S} = \{(O_i, O_j) : O_i \text{ is similar to } O_j\}$$
$$\mathcal{D} = \{(O_i, O_j) : O_i \text{ is dissimilar to } O_j\}.$$

- Learn a distance function that fits the feedback
  - Find parameter Θ to minimize

$$E = \sum_{(O_i,O_j)\in\mathcal{S}} (f(O_i, O_j, \Theta) - 0)^2 + \sum_{(O_i,O_j)\in\mathcal{D}} (f(O_i, O_j, \Theta) - 1)^2$$

where $f(O_i, O_j, \Theta)$ is a distance function with parameter Θ

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Summary

- Multidimensional Data
  - L_p-Norm, Generalized Minkowski distance
  - Match-Based Similarity Computation
  - Mahalanobis distance, Geodesic distances
  - Inverse Occurrence Frequency
- Text Similarity Measures
  - Cosine, TF-IDF
- Temporal Similarity Measures
  - Dynamic Time Warping
  - Edit Distance, Longest Common Subsequence
- Graph Similarity Measures
  - Shortest-path, Random Walk
- Supervised Similarity Functions