Similarity: Numerical Data

Mining Massive Datasets

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Topic 06

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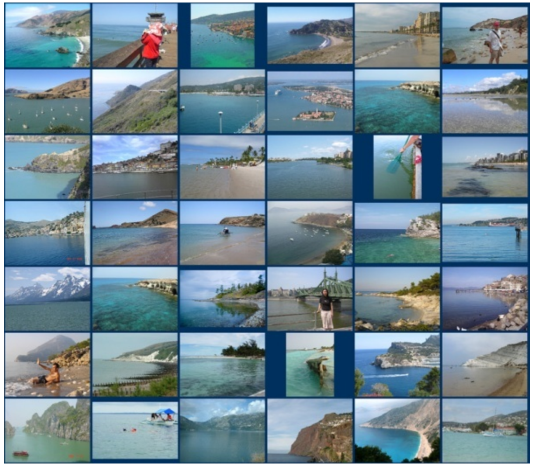
Main Sources

- Data Mining, The Textbook (2015) by Charu Aggarwal (Chapter 3) + slides by Lijun Zhang
- Data Mining Concepts and Techniques, 3rd edition (2011) by Han et al. (Section 2.4)
- Introduction to Data Mining 2nd edition (2019) by Tan et al. (Chapter 2)
- Mining of Massive Datasets 2nd edition (2014) by Leskovec et al. (Chapter 3)

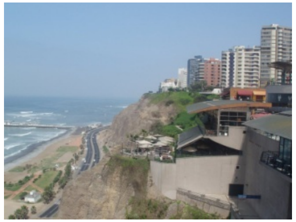
Example: scene completion

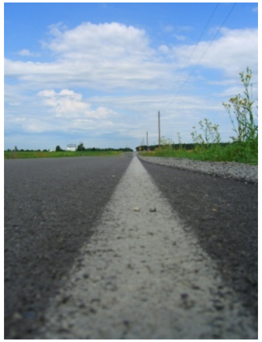
Scene completion problem



[Hays and Efros, SIGGRAPH 2007]

10 closest items in a collection of 20K images





10 closest items in a collection of 2M images











Computing similarity

Computing similarity is important

- Many problems can be expressed as finding “similar” sets:
  - Find near-neighbors in high-dimensional space
- Examples:
  - Pages with similar words
    - For duplicate detection or for classification by topic
  - Customers who purchased similar products
    - Products with similar customer sets
  - Images with similar features
  - Users who visited similar websites

Similarity computation task

- Given two objects u and v, determine the value of:

  similarity(u,v) and distance(u,v)

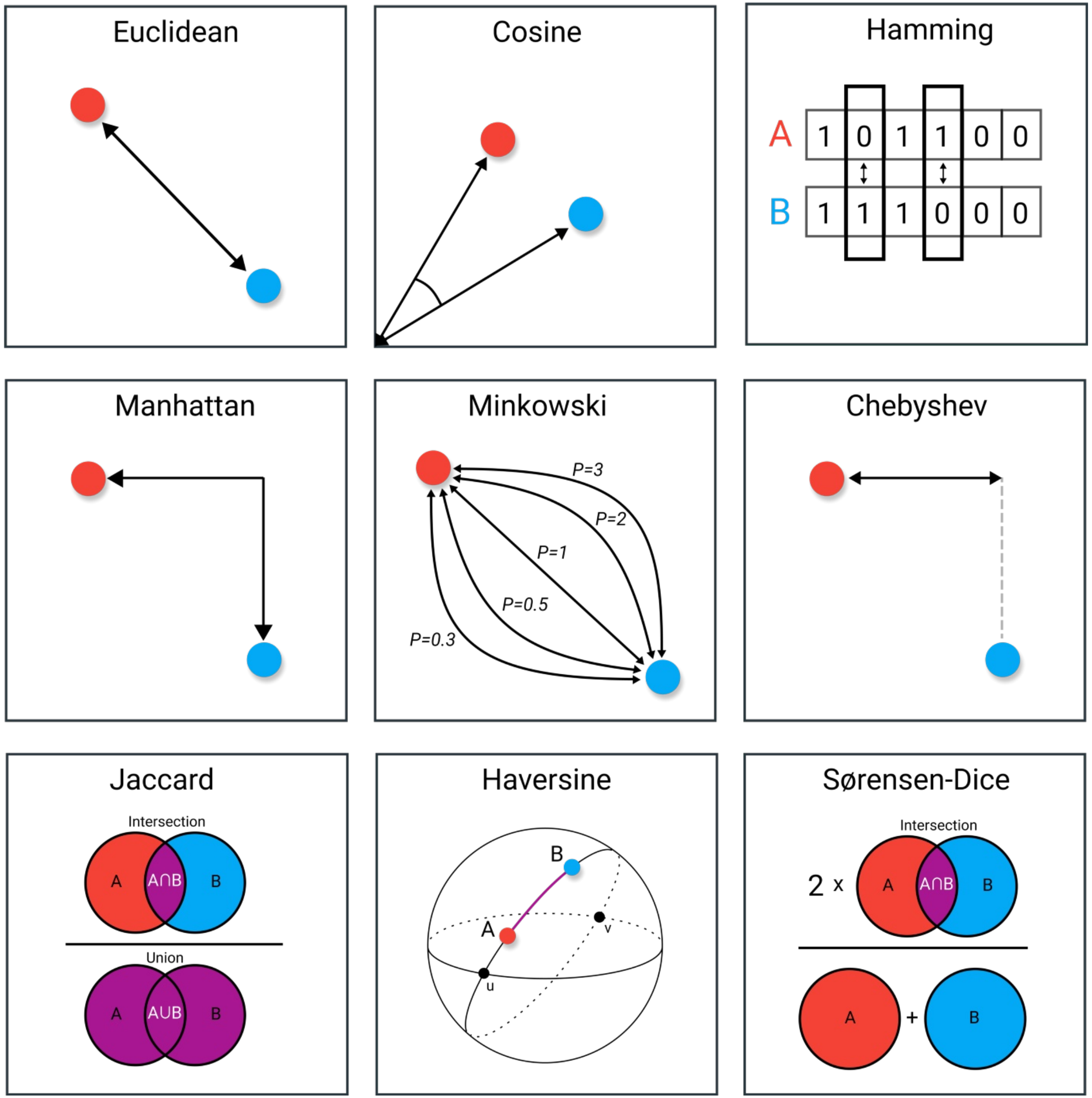
  (Often one is defined in terms of the other)
- Similar objects should have
  large similarity and small distance
- Dissimilar objects should have
  small similarity and large distance
- Closed-form functions (e.g., euclidean distance) or algorithm

Simple single-attribute similarity

Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } x = y \\ 1 & \text{if } x \neq y \end{cases}$	$s = \begin{cases} 1 & \text{if } x = y \\ 0 & \text{if } x \neq y \end{cases}$
Ordinal	$d = \|x - y\|/(n-1)$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - d$
Interval or Ratio	$d = \|x - y\|$	$s = -d$, $s = \frac{1}{1+d}$, $s = e^{-d}$, $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

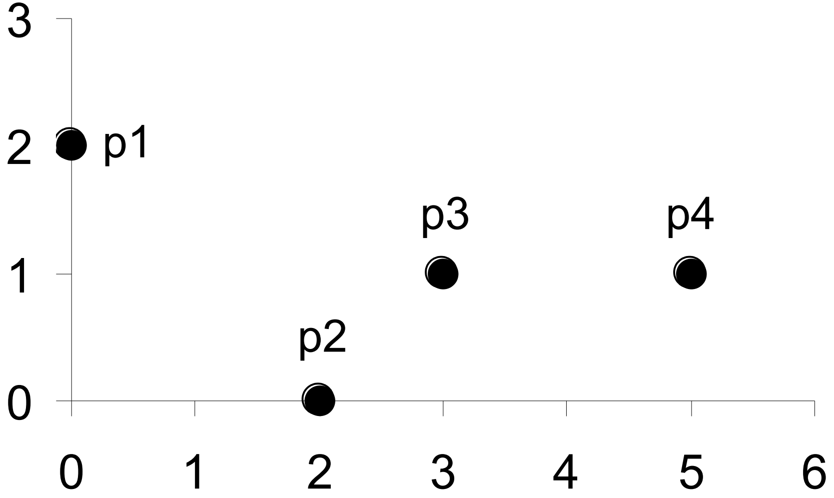
Introduction to Data Mining 2nd edition (2019) by Tan et al. (Chapter 2)

Some distance measures



https://towardsdatascience.com/9-distance-measures-in-data-science-918109d069fa

Euclidean distance: L_2 norm



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

THE CURSE OF DIMENSIONALITY

L_p norm, $p \geq 1$

$$\mathrm{dist}(x,y) = \left(\sum_{i=1}^{d} |x_i - y_i|^p \right)^{\frac{1}{p}}$$

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

Exercise: compute Lp distance

- Given vectors

  $u = (22, 1, 42, 10)$

  $v = (20, 0, 36, 8)$

- Compute:

  L_1 distance

  L_2 distance

  L_∞ distance

Answer in
Nearpod Collaborate
Code to be given in class

Generalized L_p norm, $p \geq 1$

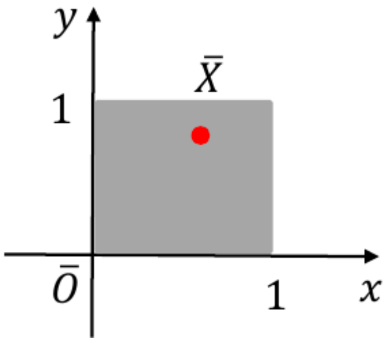
- Useful when some features are more important than others

$$\mathrm{dist}(x, y) = \left(\sum_{i=1}^{d} a_i \left| x_i - y_i \right|^p \right)^{\frac{1}{p}}$$

- E.g., in credit scoring, salary is more important than gender
- a_i are domain-specific non-negative coefficients

THE CURSE OF DIMENSIONALITY

- When the dimensionality is high, all points are at similar L_p distances from each other
- 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 $\bar{X}$



THE CURSE OF DIMENSIONALITY

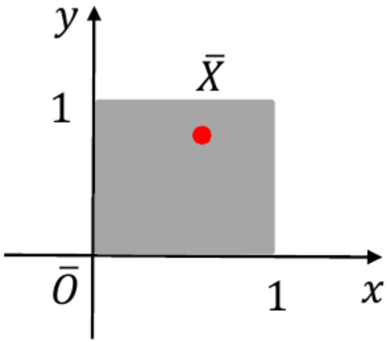
- Example (cont.):

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

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

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

$Dist(\bar{O}, \bar{X})$ is a random variable



- ✓ Since $\bar{X}$ is a random variable
- ✓ Mean is $\mu = d/2$
- ✓ Standard deviation $\sigma = \sqrt{d/12}$

The Curse of Dimensionality

Applying Chebyshev's inequality:

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

$$Pr(|\operatorname{Dist}(\overline{O}, \overline{X}) - \mu| \geq 3\sigma) \leq \frac{1}{3^2}$$

$$Pr(\operatorname{Dist}(\overline{O}, \overline{X}) \in [\mu - 3\sigma, \mu + 3\sigma]) > 8/9$$

THE CURSE OF DIMENSIONALITY

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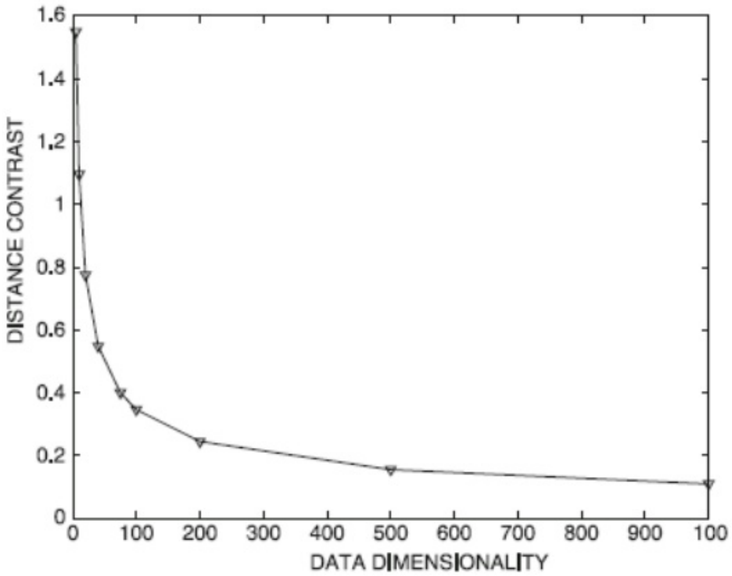
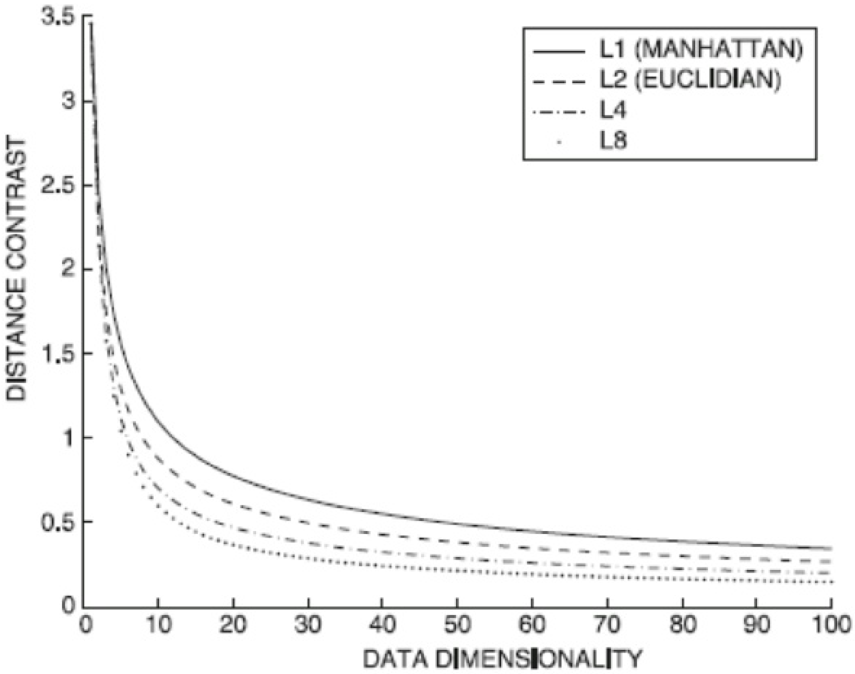


$$\operatorname{Contrast(d)} = \frac{D_{\max}-D_{\min}}{\mu} = \sqrt{12/d}$$

Irrelevant features

- Many features are probably irrelevant for your purposes, specially in high-dimensional data
- L_p norm suffers from irrelevant features
- Contrast worsens for large p



Match-based similarity

Idea: to compute similarity(u,v) ignore dimensions in which they are “too far apart”

1) Discretize each dimension into k_d equi-depth buckets
2) For two objects u, v, determine the dimensions in which they map to the same bucket
3) Compute L_p norm on those dimensions only

Match-based similarity (cont.)

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

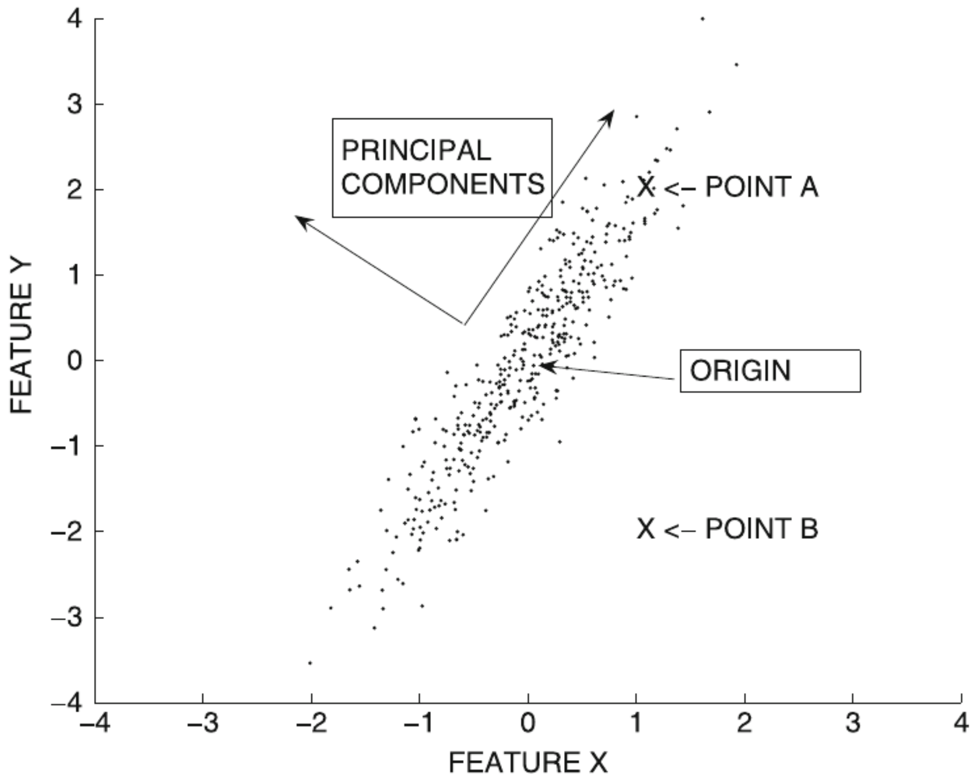
- $S(\overline{X}, \overline{Y}, k_d)$ is the set of features for which $\overline{X}$ and $\overline{Y}$ map to the same bucket
- m_i, n_i are the max and min value of that bucket
- $k_d \propto d$ achieves a constant level of contrast in high dimensions for certain data distributions

Distances and orientation

Useful distances, in general, depend on data distributions

Points A and B are equidistant from the origin

However, point A should be considered closer to the origin than point B (think of a perfectly circular cloud of points)

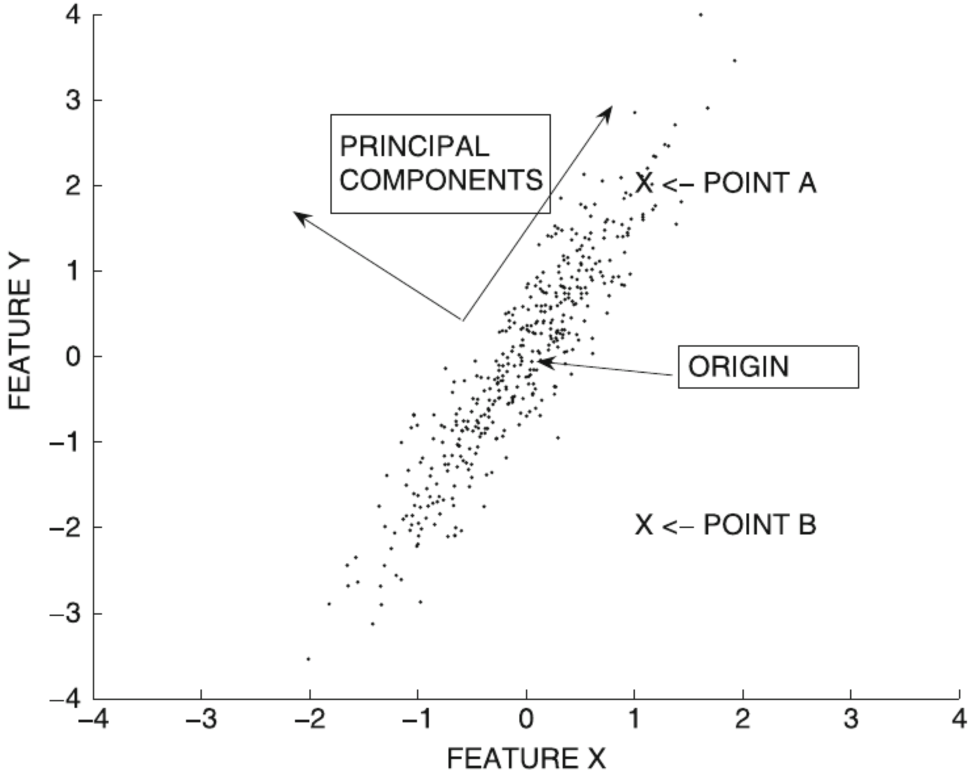


Useful distances, in general, depend on data distributions (cont.)

The Mahalanobis distance, with Σ covariance matrix

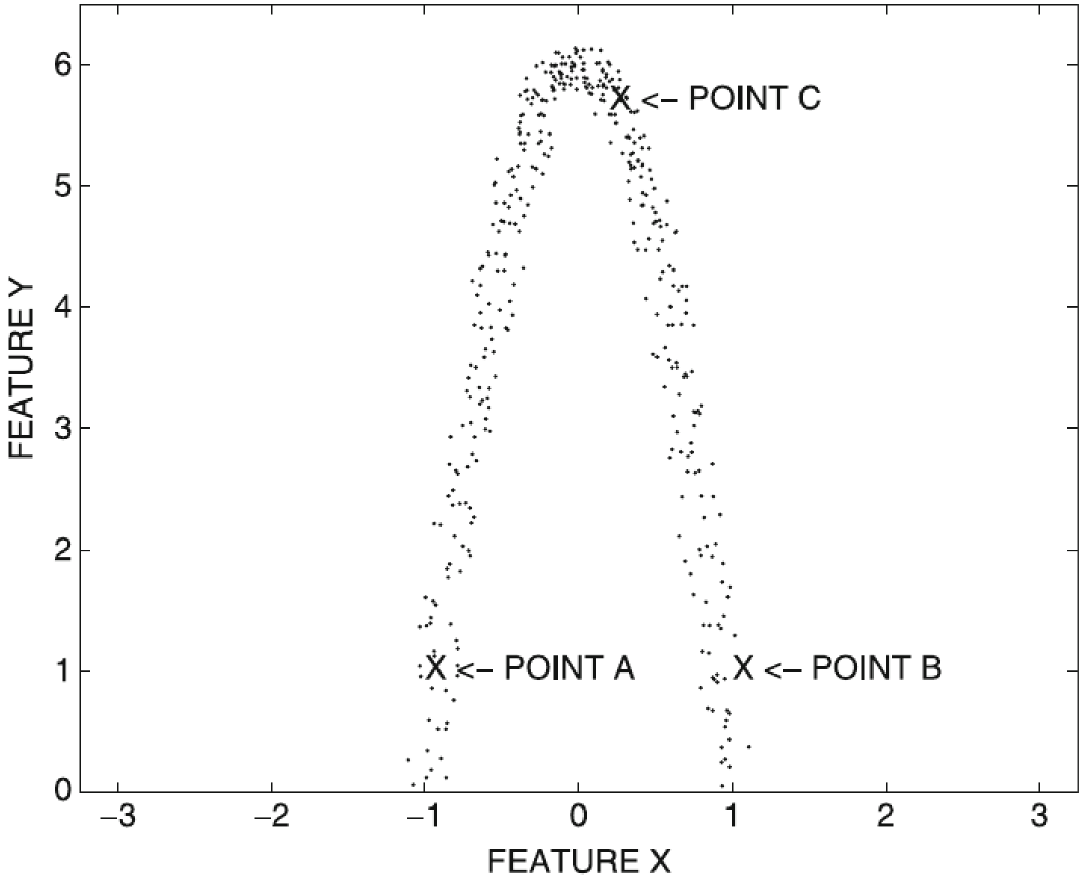
$$Maha(\overline{X}, \overline{Y}) = \sqrt{(\overline{X} - \overline{Y})\Sigma^{-1}(\overline{X} - \overline{Y})^T}.$$

is equivalent to applying PCA, dividing each coordinate by the standard deviation of that feature, and computing Euclidean distance



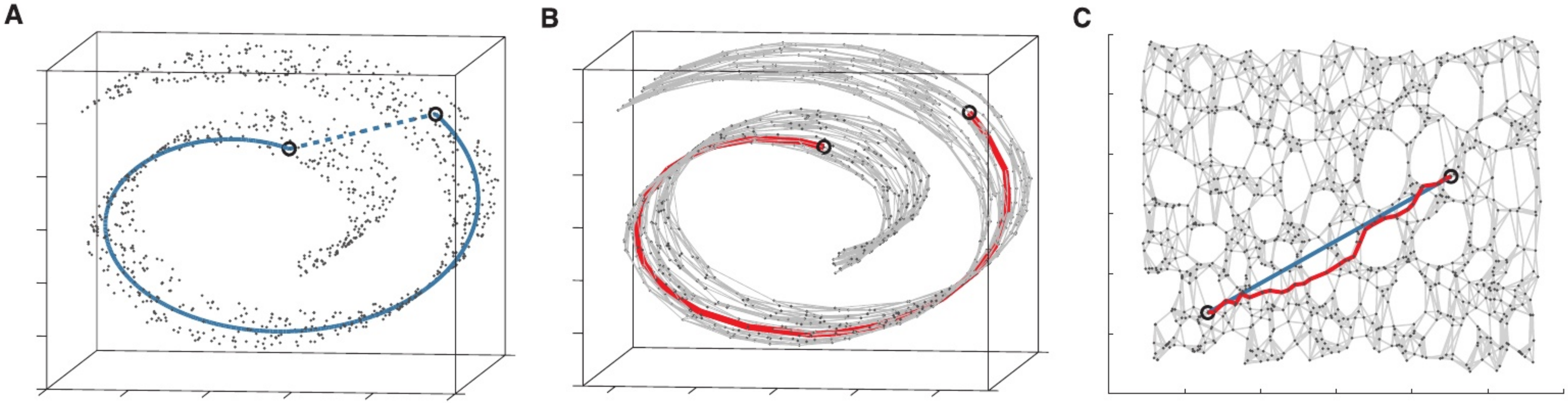
Non-linear distributions

Which point would you consider as closer to A?



(Blackboard collaborate poll)

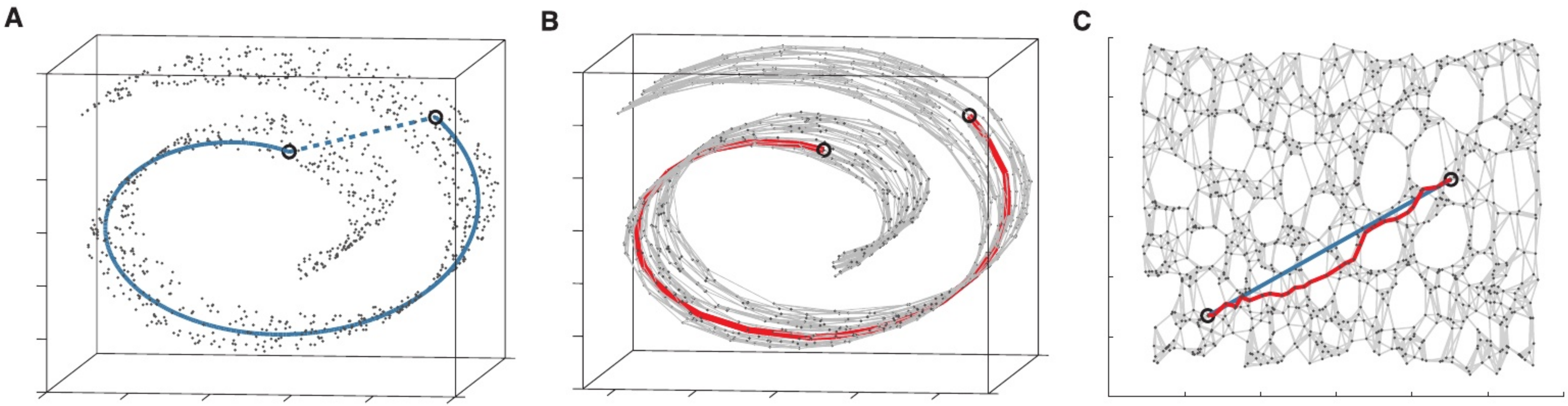
ISOMAP (general idea)



Original data Nearest neighbors graph Graph projection

Tenenbaum, Joshua B., Vin De Silva, and John C. Langford. "A global geometric framework for nonlinear dimensionality reduction." Science 2000.

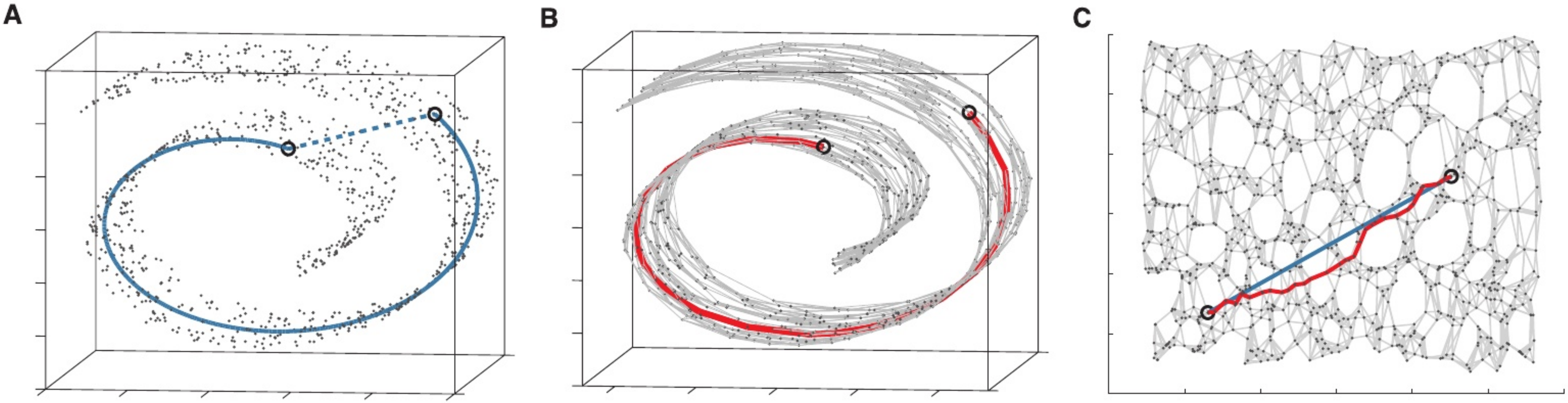
ISOMAP (1/3)



The first step is to connect each point to its k nearest neighbors (here k=7)

Tenenbaum, Joshua B., Vin De Silva, and John C. Langford. "A global geometric framework for nonlinear dimensionality reduction." Science 2000.

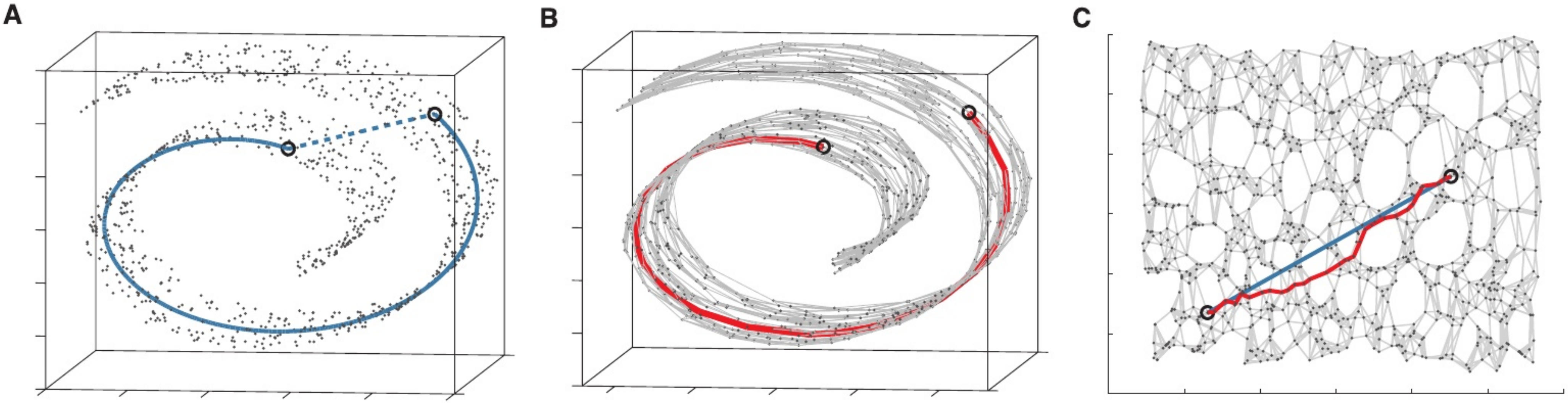
ISOMAP (2/3)



Now, shortest path or *geodesic* distances can be computed on the graph (red color)

Tenenbaum, Joshua B., Vin De Silva, and John C. Langford. "A global geometric framework for nonlinear dimensionality reduction." Science 2000.

ISOMAP (3/3)



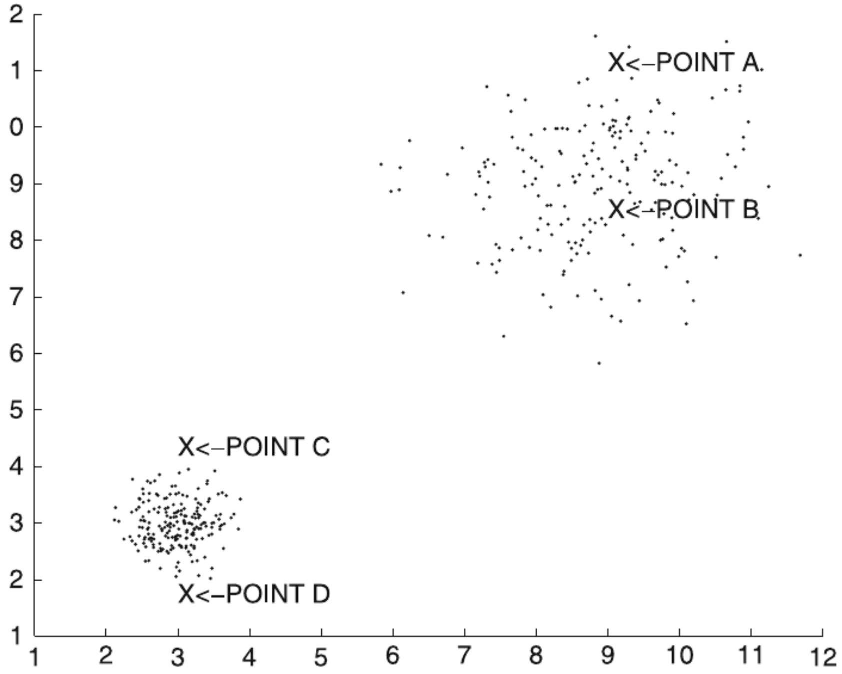
It is, however, more effective to project the graph and compute Euclidean distances in the projected graph (blue color)

Tenenbaum, Joshua B., Vin De Silva, and John C. Langford. "A global geometric framework for nonlinear dimensionality reduction." Science 2000.

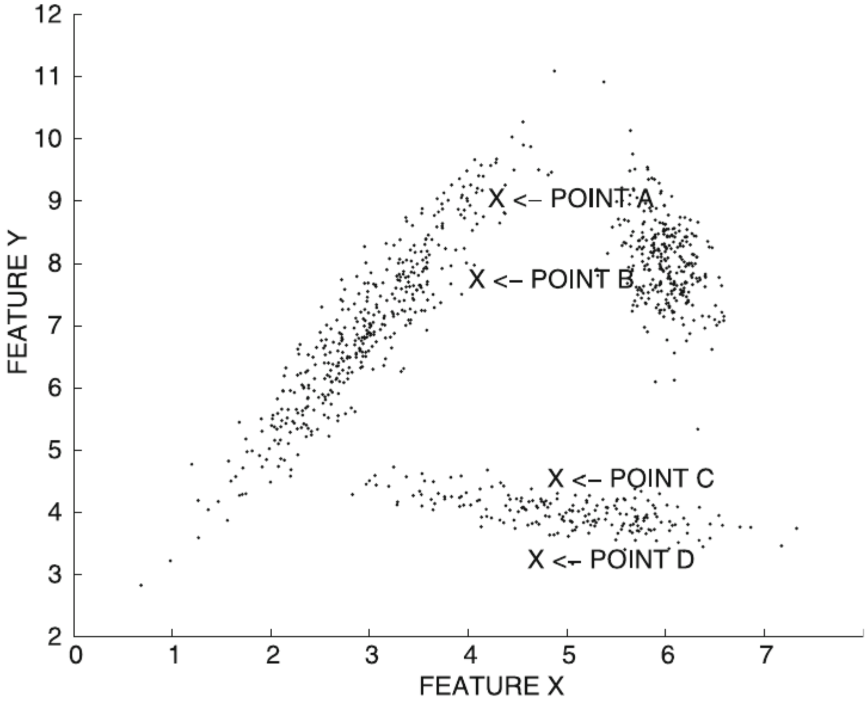
Local variations

Which distance should be larger? A-B or C-D?

Which distance should be larger? A-B or C-D?



(a) local density variation



(b) local orientation variation

Solution for local variations

- Partition the data into a set of local regions
  - (Nontrivial, which distance to use?)
- 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
  - E.g., local Mahalanobis distance
- If they belong to different regions
  - Global statistics or averaged statistics

Summary

Things to remember

- Distance/similarity is a key component of many data mining algorithms
- Sensitive to dimensionality, global/local nature of data distribution

Exercises for TT06-TT07

- **Data Mining, The Textbook (2015) by Charu Aggarwal**
  - **Exercises 3.9 on similarity measures**
- Introduction to Data Mining 2^{nd} edition (2019) by Tan et al.
  - Exercises 2.6 → 14-28
- Mining of Massive Datasets 2^{nd} edition (2014) by Leskovec et al.
  - Exercises 3.5.7 on distance measures
- Data Mining Concepts and Techniques, 3^{rd} ed. (2011) by Han et al.
  - Exercises 2.6 → 2.5-2.8