



Introduction to Data Mining

Chapter 2 Data

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Based in Slides by Tan,
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R Code Examples

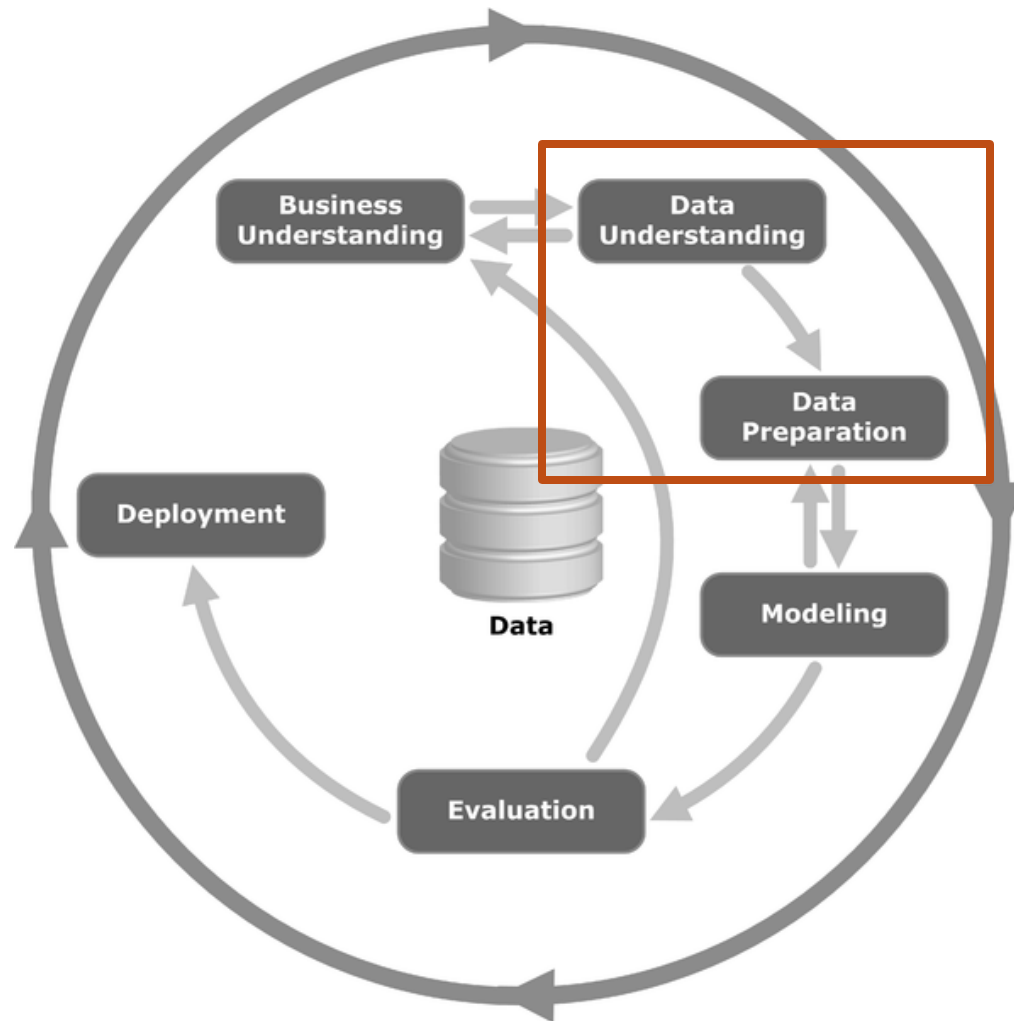
- Available R Code examples are indicated on slides by the R logo



- The Examples are available at https://mhahsler.github.io/Introduction_to_Data_Mining_R_Examples/



Tasks in the CRISP-DM Reference Model





Topics

- **Attributes/Features**
- Types of Data Sets
- Data Quality
- Data Preprocessing
- Similarity and Dissimilarity
- Density



What is Data?

- Collection of data objects and their attributes
- An attribute (in Data Mining and Machine learning often "feature") is a property or characteristic of an object
 - Examples: eye color of a person, temperature, etc.
 - Attribute is also known as variable, field, characteristic
- A collection of attributes describe an object
 - Object is also known as record, point, case, sample, entity, or instance

| Attributes | | | | |
|------------|--------|----------------|----------------|-------|
| Tid | Refund | Marital Status | Taxable Income | Cheat |
| 1 | Yes | Single | 125K | No |
| 2 | No | Married | 100K | No |
| 3 | No | Single | 70K | No |
| 4 | Yes | Married | 120K | No |
| 5 | No | Divorced | 95K | Yes |
| 6 | No | Married | 60K | No |
| 7 | Yes | Divorced | 220K | No |
| 8 | No | Single | 85K | Yes |
| 9 | No | Married | 75K | No |
| 10 | No | Single | 90K | Yes |

Attribute Values

- Attribute values are numbers or symbols assigned to an attribute
- Distinction between attributes and attribute values
 - Same attribute can be mapped to different attribute values
 - Example: height can be measured in feet or meters
 - Different attributes can be mapped to the same set of values
 - Example: Attribute values for ID and age are integers
 - But properties of attribute values can be different
 - ID has no limit but age has a maximum and minimum value

Types of Attributes - Scales

- There are different types of attributes

- Nominal

- Examples: ID numbers, eye color, zip codes

- Ordinal

- Examples: rankings (e.g., taste of potato chips on a scale from 1-10), grades, height in {tall, medium, short}

- Interval

- Examples: calendar dates, temperatures in Celsius or Fahrenheit.

- Ratio

- Examples: temperature in Kelvin, length, time, counts

Categorical,
Qualitative

Quantitative

| Attribute Type | Description | Examples | Operations |
|----------------|--|---|--|
| Nominal | The values of a nominal attribute are just different names or labels , i.e., nominal attributes provide only enough information to distinguish one object from another. | zip codes, employee ID numbers, eye color, sex: {male, female} | =, ≠ mode, entropy, contingency correlation, χ^2 test |
| Ordinal | The values of an ordinal attribute provide enough information to order objects . | zip codes, employee ID numbers, eye color, sex: {male, female} | Nominal + <, > median, percentiles, rank correlation, run tests, sign tests |
| Interval | For interval attributes, the differences between values are meaningful, i.e., a unit of measurement exists. | calendar dates, temperature in Celsius or Fahrenheit | Ordinal + +, - mean, standard deviation, Pearson's correlation, t and F tests |
| Ratio | For ratio variables, both differences and ratios are meaningful . Double the number means twice as much. | temperature in Kelvin, monetary quantities, counts, age, mass, length, electrical current | Interval + *, / geometric mean, harmonic mean, percent variation |

Discrete and Continuous Attributes

- Discrete Attribute

- Has only a finite or countably infinite set of values
- Examples: zip codes, counts, or the set of words in a collection of documents
- Often represented as integer variables.
- Note: binary attributes are a special case of discrete attributes

- Continuous Attribute

- Has real numbers as attribute values
- Examples: temperature, height, or weight.
- Practically, real values can only be measured and represented using a finite number of digits.
- Continuous attributes are typically represented as floating-point variables.

Examples

- What is the scale of measurement of:
 - Number of cars per minute (count data)
 - Age data grouped in:
0-4 years, 5-9, 10-14, ...
 - Age data grouped in:
<20 years, 21-30, 31-40, 41+



Topics

- Attributes/Features
- **Types of Data Sets**
- Data Quality
- Data Preprocessing
- Similarity and Dissimilarity
- Density



Types of data sets

- Record

- Data Matrix
- Document Data
- Transaction Data

- Graph

- World Wide Web
- Molecular Structures

- Ordered

- Spatial Data
- Temporal Data
- Sequential Data
- Genetic Sequence Data

Record Data

- Data that consists of a collection of records, each of which consists of a fixed set of attributes (e.g., from a relational database)

| Tid | Refund | Marital Status | Taxable Income | Cheat |
|-----|--------|----------------|----------------|-------|
| 1 | Yes | Single | 125K | No |
| 2 | No | Married | 100K | No |
| 3 | No | Single | 70K | No |
| 4 | Yes | Married | 120K | No |
| 5 | No | Divorced | 95K | Yes |
| 6 | No | Married | 60K | No |
| 7 | Yes | Divorced | 220K | No |
| 8 | No | Single | 85K | Yes |
| 9 | No | Married | 75K | No |
| 10 | No | Single | 90K | Yes |

Data Matrix

- If data objects have the same fixed set of numeric attributes, then the data objects can be thought of as points in a multi-dimensional space, where each dimension represents a distinct attribute
- Such data set can be represented by an m by n matrix, where there are m rows, one for each object, and n columns, one for each attribute

n attributes

| m objects | Sepal.Length | Sepal.Width | Petal.Length | Petal.Width |
|-----------|--------------|-------------|--------------|-------------|
| | 5.6 | 2.7 | 4.2 | 1.3 |
| | 6.5 | 3.0 | 5.8 | 2.2 |
| | 6.8 | 2.8 | 4.8 | 1.4 |
| | 5.7 | 3.8 | 1.7 | 0.3 |
| | 5.5 | 2.5 | 4.0 | 1.3 |
| | 4.8 | 3.0 | 1.4 | 0.1 |
| | 5.2 | 4.1 | 1.5 | 0.1 |

Document Data

- Each document becomes a 'term' vector,
 - each term is a component (attribute) of the vector,
 - the value of each component is the number of times the corresponding term occurs in the document.

| | Terms | | | | | | | | | |
|------------|-------|-------|------|------|-------|------|-----|------|---------|--------|
| | team | coach | play | ball | score | game | win | lost | timeout | season |
| Document 1 | 3 | 0 | 5 | 0 | 2 | 6 | 0 | 2 | 0 | 2 |
| Document 2 | 0 | 7 | 0 | 2 | 1 | 0 | 0 | 3 | 0 | 0 |
| Document 3 | 0 | 1 | 0 | 0 | 1 | 2 | 2 | 0 | 3 | 0 |

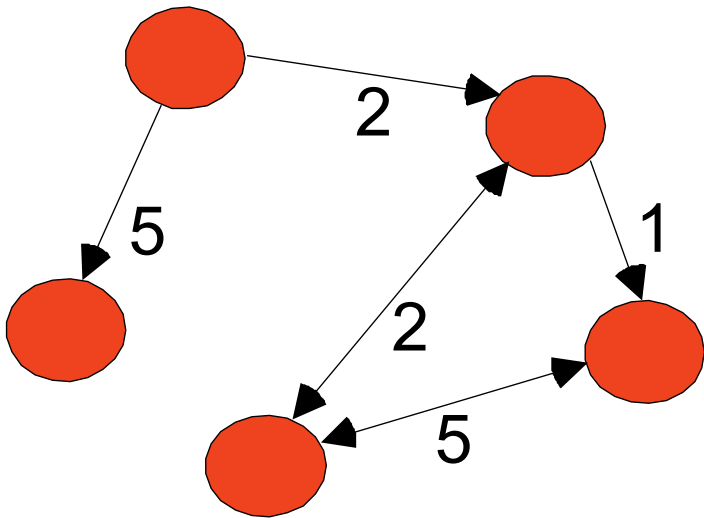
Transaction Data

- A special type of record data, where
 - each record (transaction) involves a set of items.
 - For example, consider a grocery store. The set of products purchased by a customer during one shopping trip constitute a transaction, while the individual products that were purchased are the items.

| TID | Items |
|-----|---------------------------|
| 1 | Bread, Coke, Milk |
| 2 | Beer, Bread |
| 3 | Beer, Coke, Diaper, Milk |
| 4 | Beer, Bread, Diaper, Milk |
| 5 | Coke, Diaper, Milk |

Graph Data

- Examples: Generic graph and HTML Links



``
Data Mining ``

``

``
Graph Partitioning ``

``

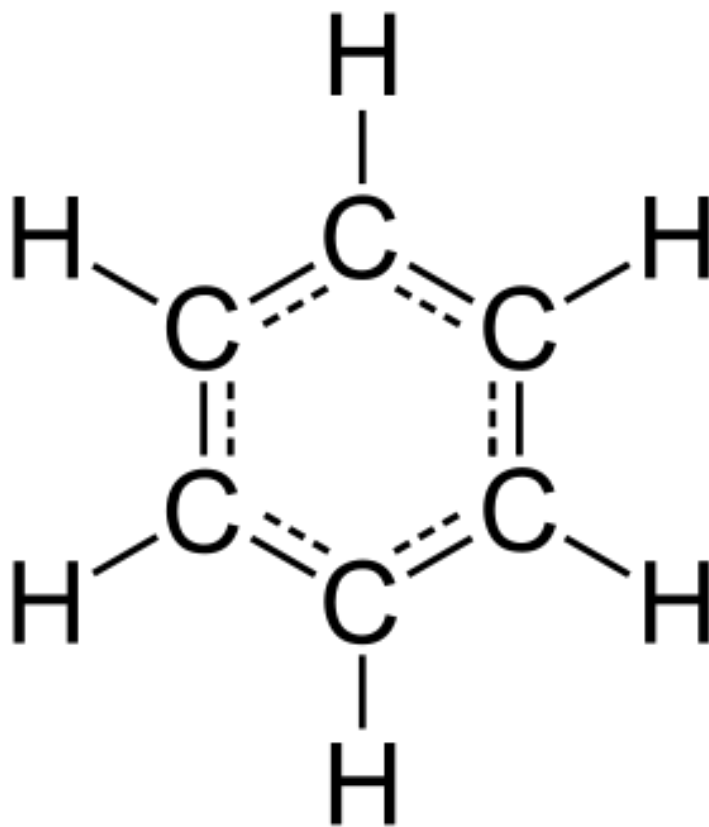
``
Parallel Solution of Sparse Linear System of Equations ``

``

``
N-Body Computation and Dense Linear System Solvers

Chemical Data

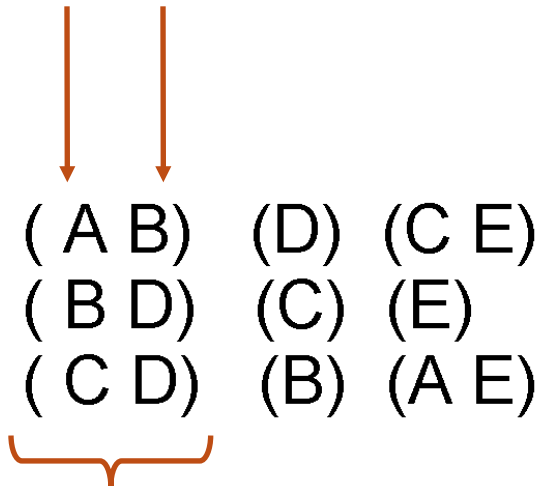
- Benzene Molecule: C₆H₆



Ordered Data

- Sequences of transactions

Items/Events



**An element of
the sequence**

Ordered Data

- Genomic sequence data

GGTTCCGCCTTCAGCCCCGCGCC
CGCAGGGCCCGCCCCGCGCCGTC
GAGAAGGGCCCGCCTGGCGGGCG
GGGGGAGGCGGGGGCCGCCCGAGC
CCAACCGAGTCCGACCAGGTGCC
CCCTCTGCTCGGCCTAGACCTGA
GCTCATTAGGCGGCAGCGGACAG
GCCAAGTAGAACACGCGAAGCGC
TGGGCTGCCTGCTGCGACCAGGG

Subsequences

Ordered Data: Time Series Data

S&P 500 Index

April 1, 2016 – March 31, 2017

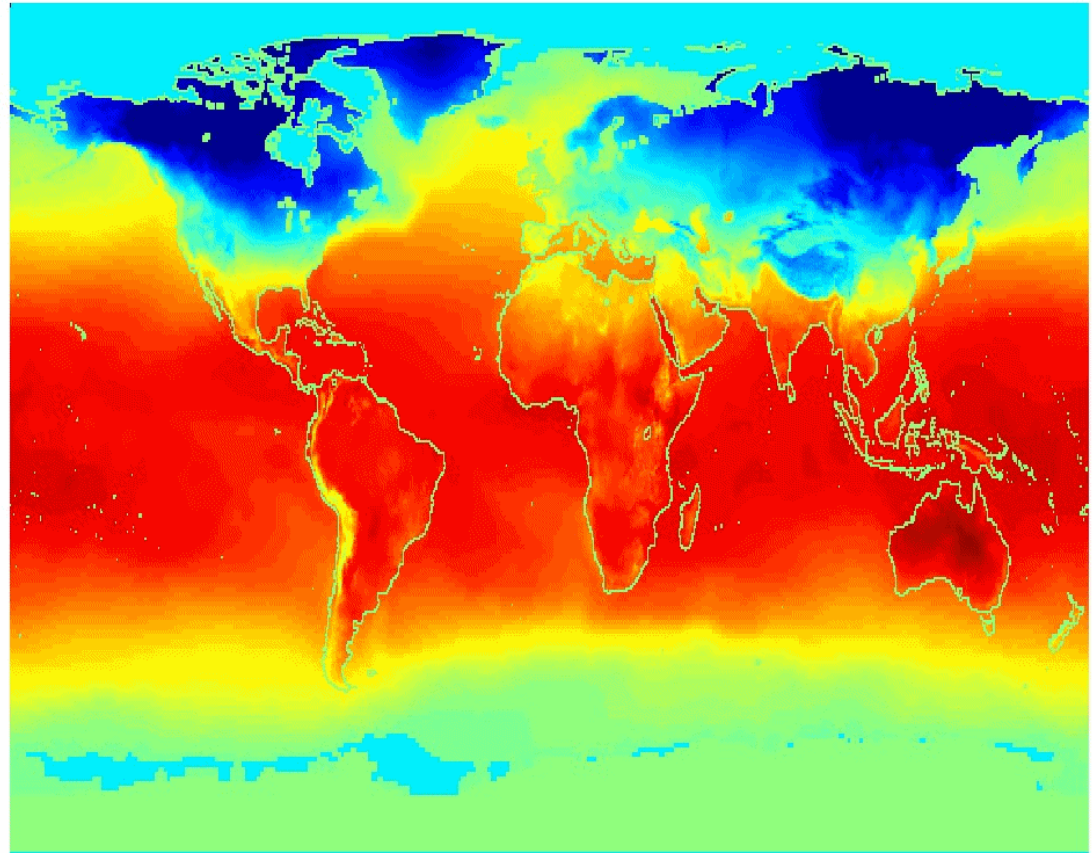


Source: FactSet

Ordered Data: Spatio-Temporal

Jan, Feb, Mar, ...

**Average Monthly
Temperature of
land and ocean**





Topics

- Attributes/Features
- Types of Data Sets
- **Data Quality**
- Data Preprocessing
- Similarity and Dissimilarity
- Density



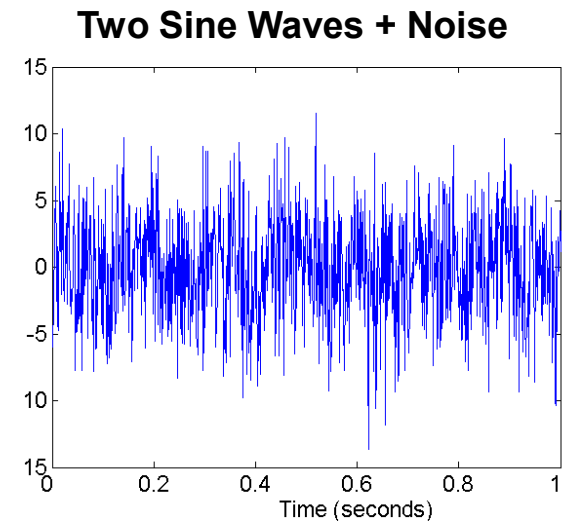
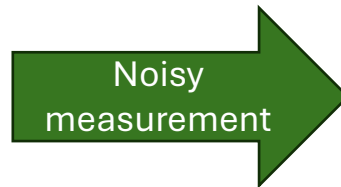
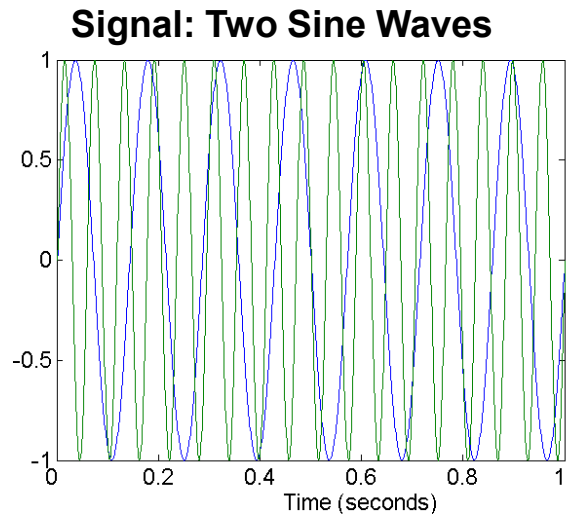
Data Quality

- What kinds of data quality problems?
- How can we detect problems with the data?
- What can we do about these problems?

- Examples of data quality problems:
 - Noise and outliers
 - missing values
 - duplicate data

Noise

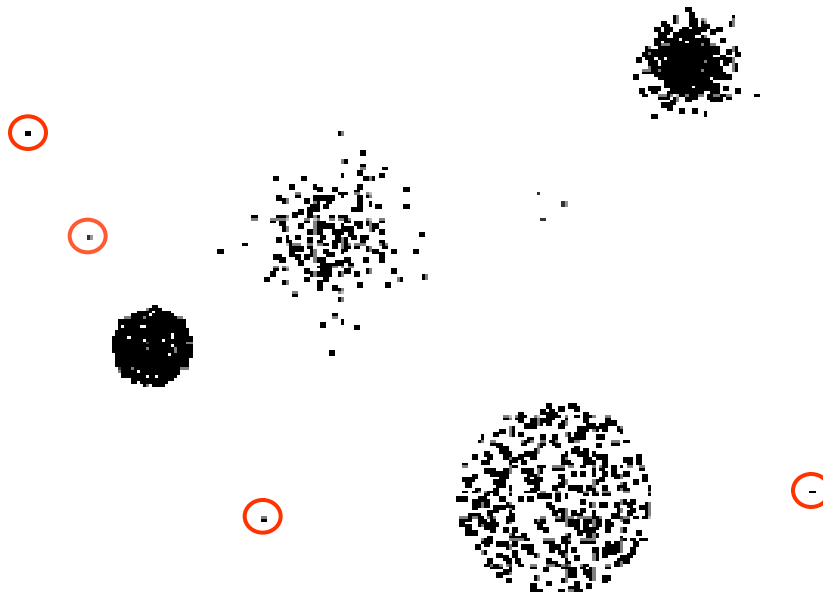
- Noise refers to modification of original values
 - Examples: distortion of a person's voice when talking on a poor phone, “snow” on television screen, measurement errors.



- Find less noisy data
- De-noise (signal processing)

Outliers

- Outliers are data objects with characteristics that are considerably different than most of the other data objects in the data set



- Outlier detection + remove outliers

Missing Values

- Reasons for missing values

- Information is not collected
(e.g., people decline to give their age and weight)
- Attributes may not be applicable to all cases
(e.g., annual income is not applicable to children)

- Handling missing values

- Eliminate data objects with missing value
- Eliminate feature with missing values
- Ignore the missing value during analysis
- Estimate missing values = Imputation
(e.g., replace with mean or weighted mean where all possible values are weighted by their probabilities)

Duplicate Data

- Data set may include data objects that are duplicates, or "close duplicates" of one another
 - Major issue when merging data from heterogeneous sources
- Examples:
 - Same person with multiple email addresses
- Data cleaning
 - Process of dealing with duplicate data issues
 - ETL tools typically support deduplication





Topics

- Attributes/Features
- Types of Data Sets
- Data Quality
- **Data Preprocessing**
- Similarity and Dissimilarity
- Density



Data Preprocessing

- Aggregation
- Sampling
- Dimensionality Reduction
- Feature subset selection
- Feature creation
- Discretization and Binarization
- Attribute Transformation

Aggregation

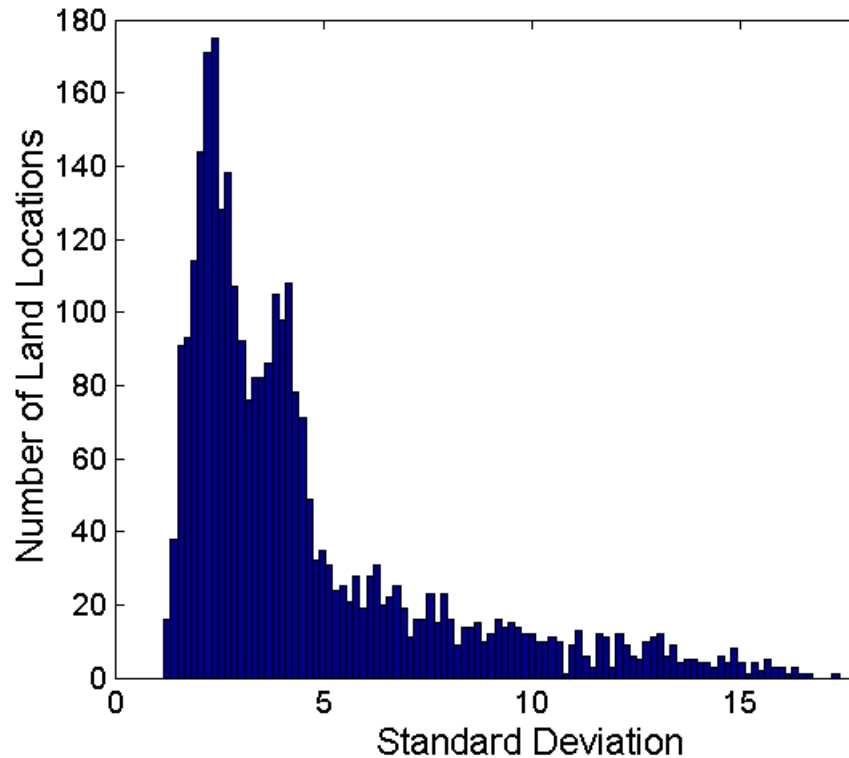
- Combining two or more attributes (or objects) into a single attribute (or object)

- Purpose
 - Data reduction
 - Reduce the number of attributes or objects
 - Change of scale
 - Cities aggregated into regions, states, countries, etc
 - More “stable” data
 - Aggregated data tends to have less variability (e.g., reduce seasonality by aggregation to yearly data)

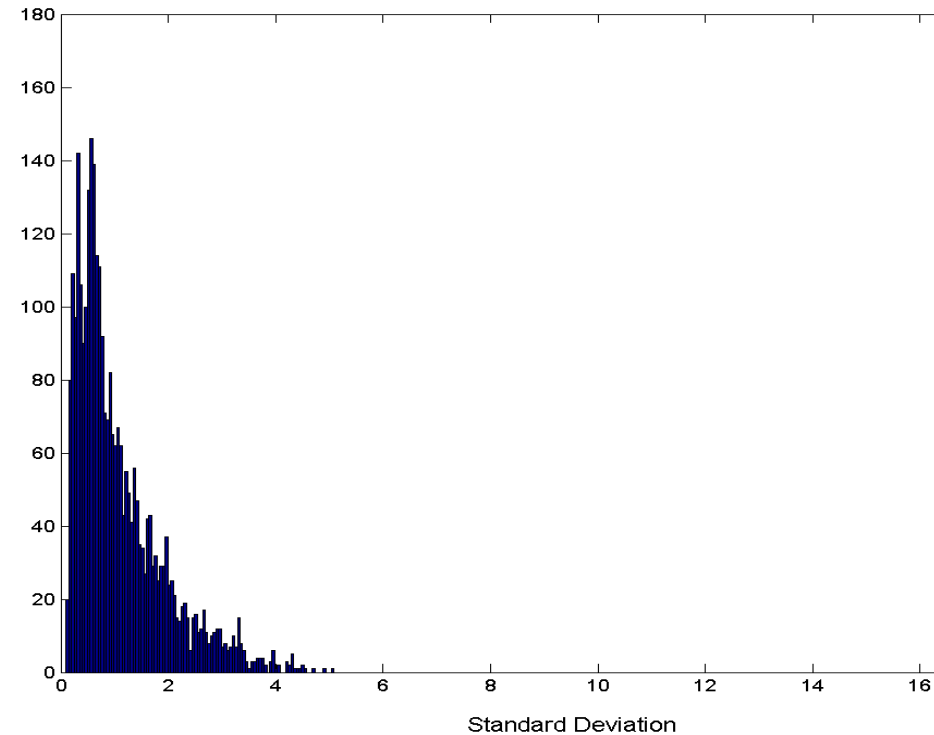


Aggregation

Variation of Precipitation in Australia



**Standard Deviation of Average
Monthly Precipitation**



**Standard Deviation of Average
Yearly Precipitation**

Sampling

- Sampling is the main technique employed for data selection.
 - 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 (e.g., does not fit into memory or is too slow).

Sampling ...

- The key principle for effective sampling is the following:
 - 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

Replacement?

- **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. Note: the same object can be picked up more than once.

Selection?

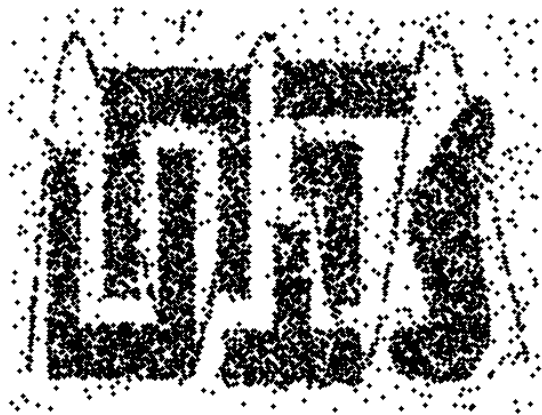
- **Simple random sampling**

There is an equal probability of selecting any particular item.

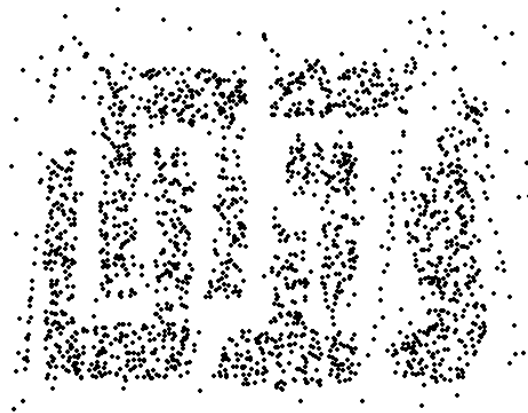
- **Stratified sampling**

Split the data into several partitions; then draw random samples from each partition.

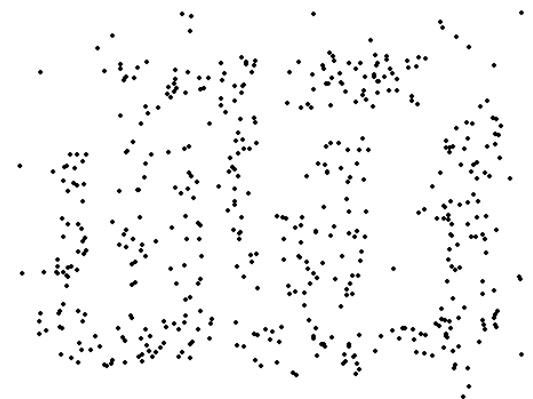
Sample Size



8000 points



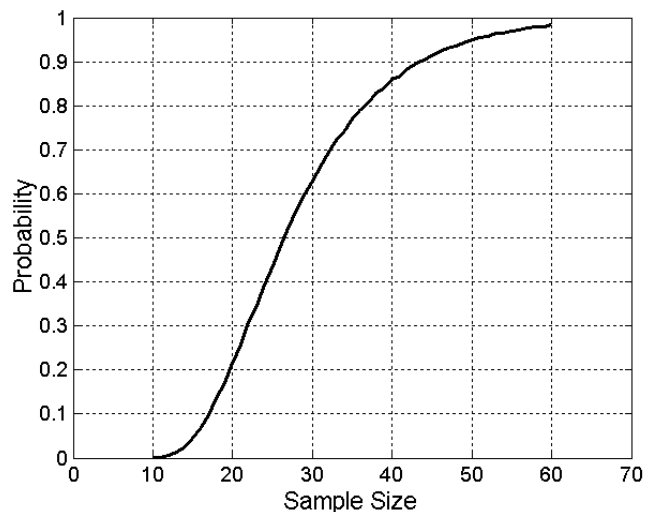
2000 Points



500 Points

Sample Size

- What sample size is necessary to get at least one object from each of 10 groups.

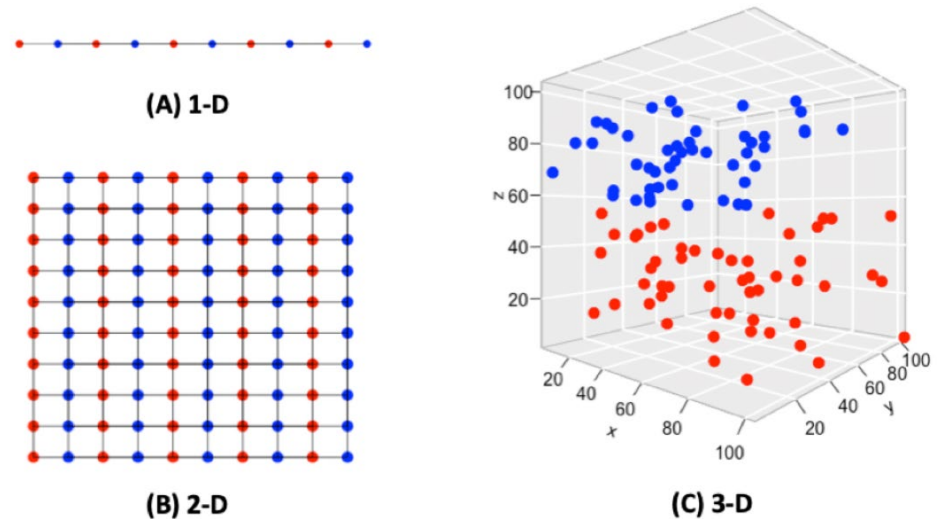


- Sample size determination:
 - Statistics: confidence interval for parameter estimate or desired statistical power of test.
 - Machine learning: often more is better, cross-validated accuracy.



Curse of Dimensionality

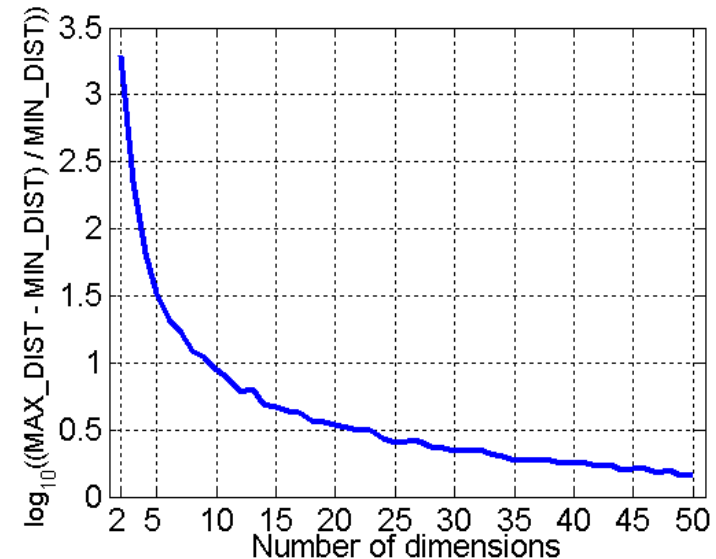
- When dimensionality increases, the size of the data space grows exponentially.



Points and space

- Definitions of density and distance between points, which is critical for clustering and outlier detection, become less meaningful
 - Density $\rightarrow 0$
 - All points tend to have the same Euclidean distance to each other.

Experiment: Randomly generate 500 points. Compute difference between max and min distance between any pair of points



Dimensionality Reduction

- Purpose:

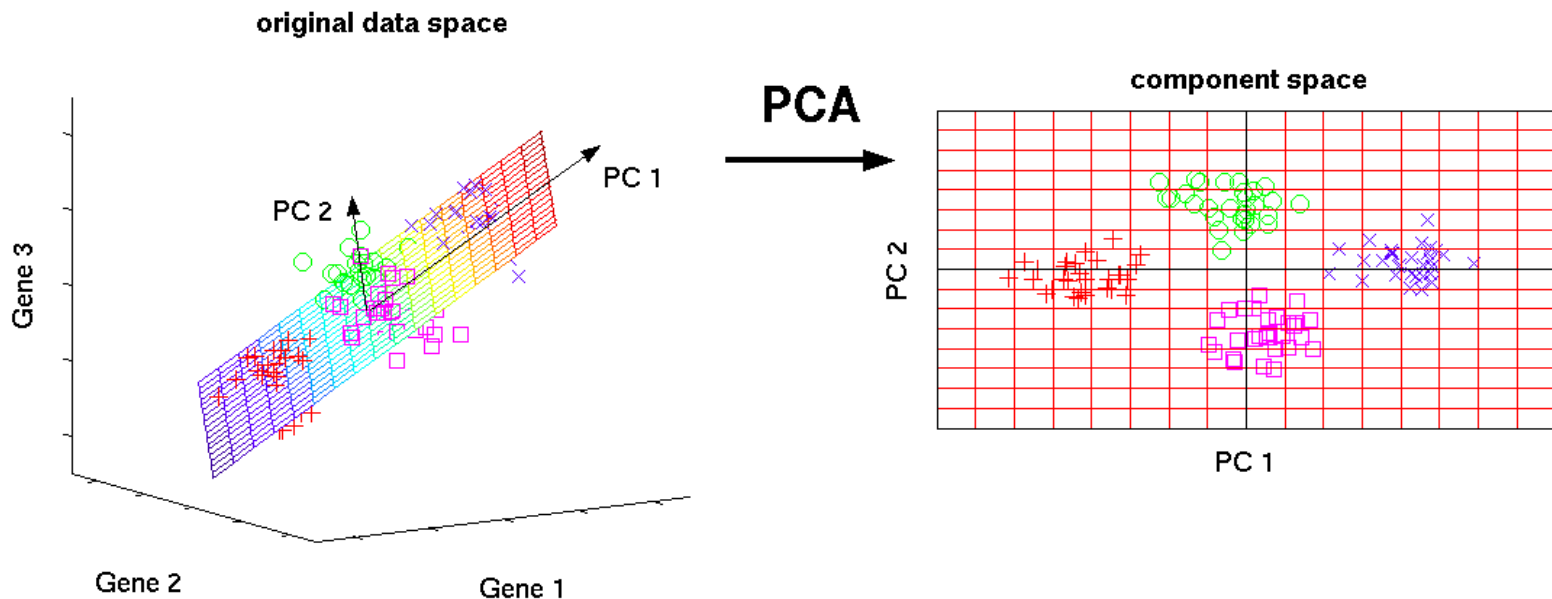
- Avoid curse of dimensionality
- Reduce amount of time and memory required by data mining algorithms
- Allow data to be more easily visualized
- May help to eliminate irrelevant features or reduce noise

- Techniques

- Principle Component Analysis
- Singular Value Decomposition
- Others: supervised and non-linear techniques

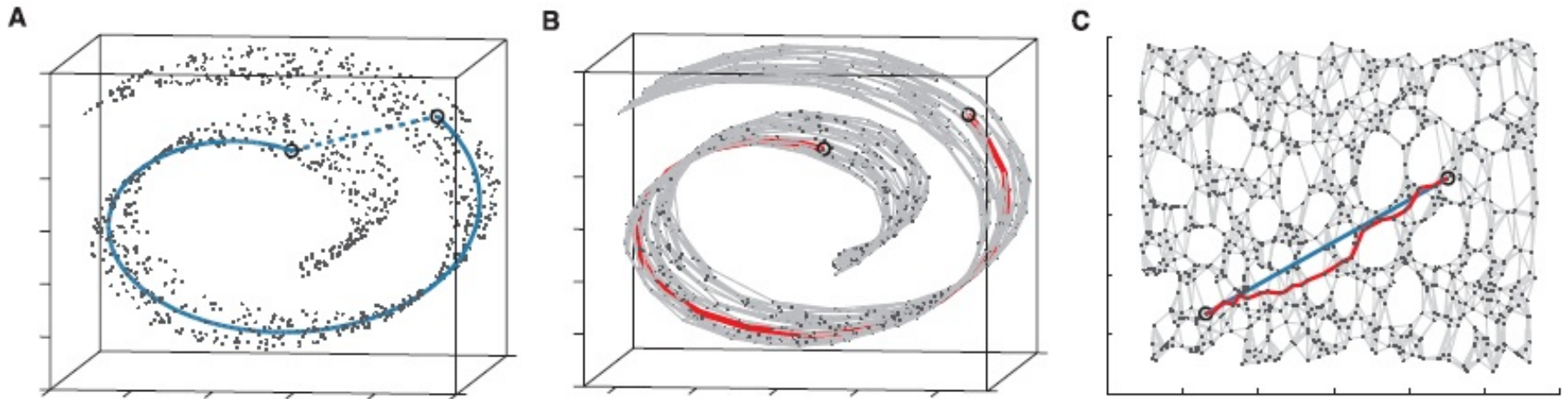
Dimensionality Reduction: Principal Components Analysis (PCA)

- **Goal:** Map points to a lower dimensional space while preserving distance information.



- **Method:** Find a projection (new axes) that captures the largest amount of variation in data. This can be done using eigenvectors of the covariance matrix or SVD (singular value decomposition).

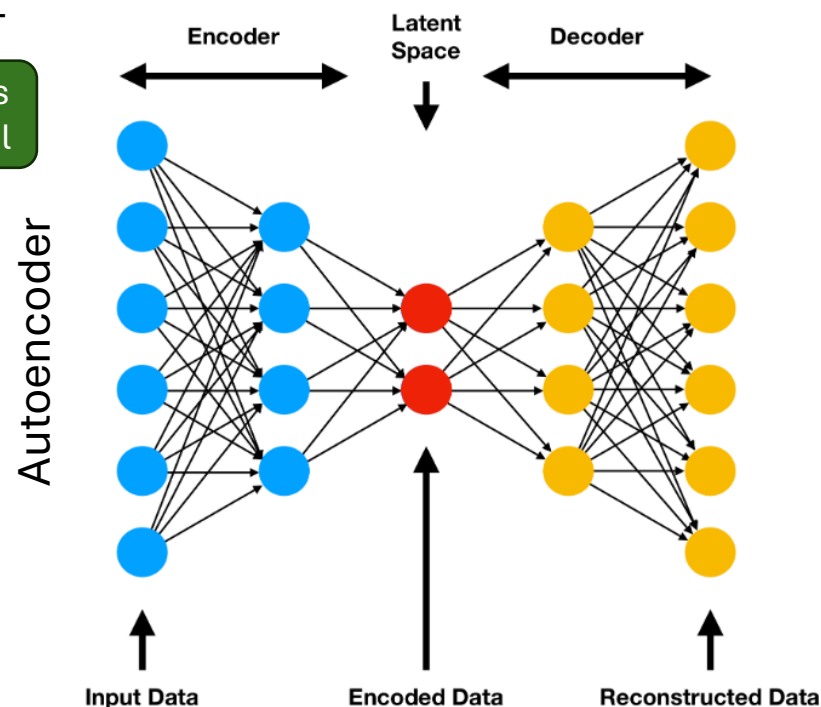
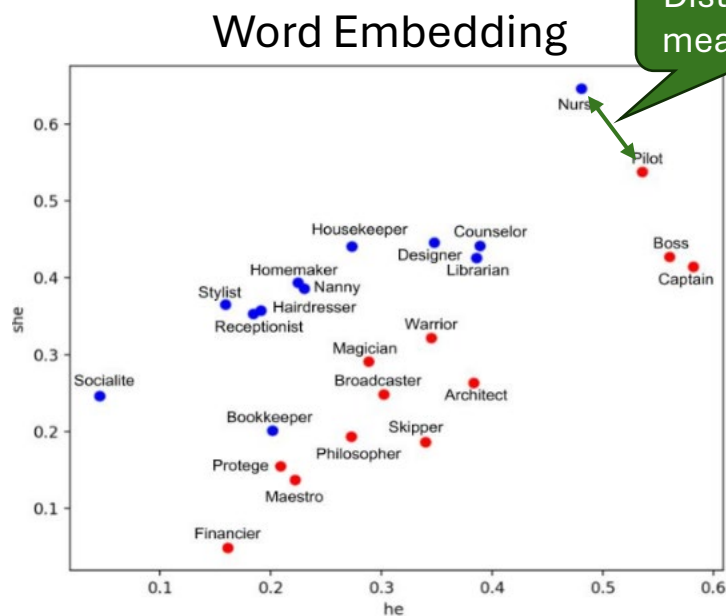
Dimensionality Reduction: ISOMAP



- **Goal:** Unroll the “swiss roll!” (i.e., preserve distances on the roll)
- **Method:** Use a non-metric space, i.e., distances are not measured by Euclidean distance, but along the surface of the roll (geodesic distances).
 1. Construct a neighbourhood graph (k-nearest neighbors or within a radius).
 2. For each pair of points in the graph, compute the shortest path distances = geodesic distances.
 3. Create a lower dimensional embedding using the geodesic distances (multi-dimensional scaling; MDS)

Low-dimensional Embedding

- General notion of representing objects described in one space (i.e., set of features) in a different space using a map $f : X \rightarrow Y$
- PCA is an example where Y is the space spanned by the principal components and objects close in the original space X are embedded in space Y .
- Low-dimensional embeddings can be produced with various other methods:
 - T-SNE: T-distributed Stochastic Neighbor Embedding; non-linear for visualization of high-dimensional datasets.
 - Autoencoders (deep learning): non-linear
 - Word embedding: Word2vec, GloVe, BERT



Feature Subset Selection

= Remove features (columns):

- Redundant features
 - duplicate information contained in multiple features (are correlated)
 - 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
 - Example: students' ID is often irrelevant to the task of predicting students' GPA

Methods

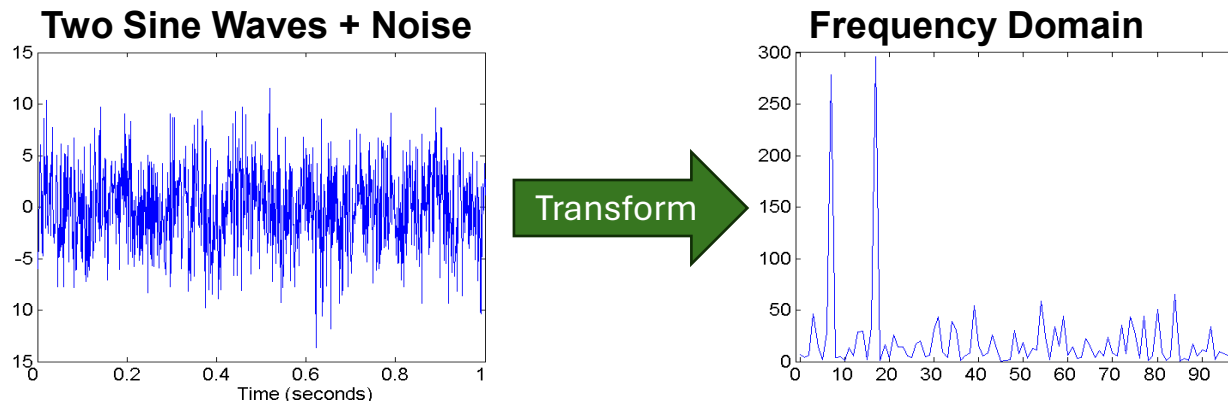
- Embedded approaches:
 - Feature selection occurs naturally as part of the data mining algorithm (e.g., regression, decision trees).
- Filter approaches:
 - Features are selected before data mining algorithm is run
 - (e.g., highly correlated features)
- Brute-force approach:
 - Try all possible feature subsets as input to data mining algorithm and choose the best.
- Wrapper approaches:
 - Use the data mining algorithm as a black box to find best subset of attributes (often using greedy search)

Feature Creation

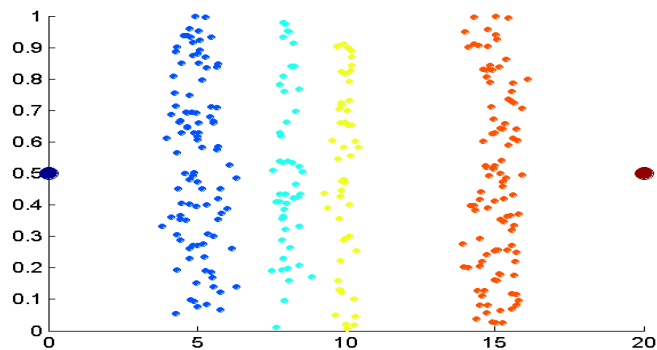
Create new attributes that can capture the important information in a data set much more efficiently than the original attributes

Three general methodologies

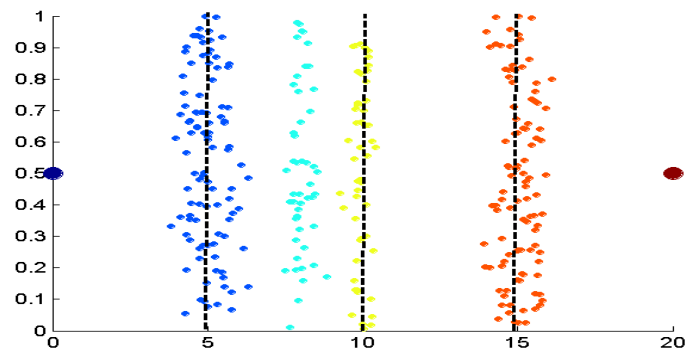
- Feature Extraction
 - Domain-specific (e.g., face recognition in image mining)
- Feature Construction / Feature Engineering
 - combining features (interactions: multiply features)
 - Example: Calculate the body mass index from height and weight
- Mapping Data to New Space
 - Example: Fourier transform/Wavelet transform



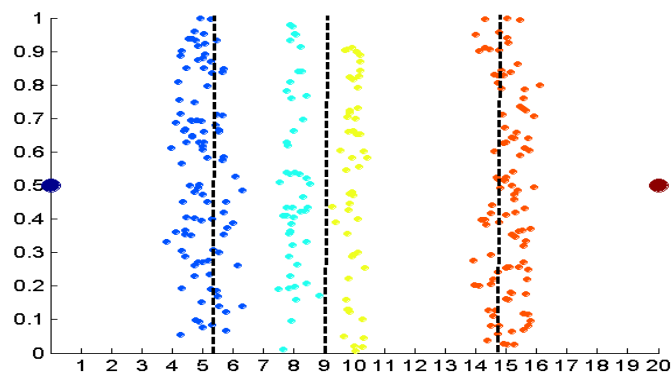
Unsupervised Discretization



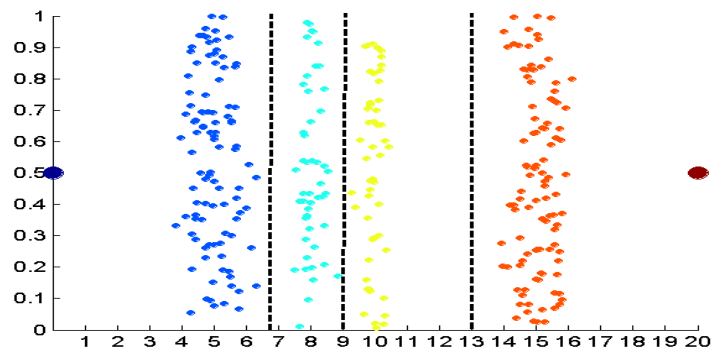
Data



Equal interval width



Equal frequency



K-means



Attribute Transformation

- A function that maps the entire set of values of a given attribute to a new set of replacement values such that each old value can be identified with one of the new values
 - Simple functions: x^k , $\log(x)$, e^x , $|x|$
 - Standardization and Normalization
 - The z-score normalizes data roughly to an interval of $[-3,3]$.

$$x' = \frac{x - \bar{x}}{s_x}$$

\bar{x} ... column (attribute) mean

s_x ... column (attribute) standard deviation





Topics

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- Types of Data Sets
- Data Quality
- Data Preprocessing
- **Similarity and Dissimilarity**
- Density



Similarity and Dissimilarity

- Similarity

- Numerical measure of how alike two data objects are.
- Is higher when objects are more alike.
- Often falls in the range $[0,1]$

- Dissimilarity

- Numerical measure of how different are two data objects
- Lower when objects are more alike
- Minimum dissimilarity is often 0
- Upper limit varies

- Proximity refers to a similarity or dissimilarity

Similarity/Dissimilarity for Simple Attributes

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

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

$$s = f(d)$$

f can be any strictly decreasing function.

Euclidean Distance

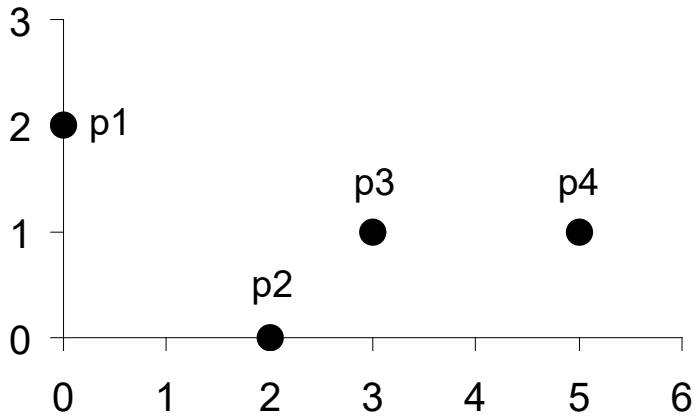
| point | x | y |
|-------|---|---|
| p | 0 | 2 |
| q | 2 | 0 |

- Euclidean Distance (for quantitative attribute vectors)

$$d_E = \sqrt{\sum_{k=1}^n (p_k - q_k)^2} = \|\mathbf{p} - \mathbf{q}\|_2$$

- Where \mathbf{p} and \mathbf{q} are two objects represented by vectors. n is the number of dimensions (attributes) of the vectors and p_k and q_k are, respectively, the k th attributes (components) or data objects p and q .
 - $\|\cdot\|_2$ is the L^2 vector norm (i.e., length of a vector in Euclidean space).
- **Note:** If ranges differ between components of \mathbf{p} then standardization (z-scores) is necessary to avoid one variable to dominate the distance.

Euclidean Distance



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

| | p1 | p2 | p3 | p4 |
|----|------|------|------|------|
| p1 | 0.00 | 2.83 | 3.16 | 5.10 |
| p2 | 2.83 | 0.00 | 1.41 | 3.16 |
| p3 | 3.16 | 1.41 | 0.00 | 2.00 |
| p4 | 5.10 | 3.16 | 2.00 | 0.00 |

Distance Matrix

Minkowski Distance

| point | x | y |
|-------|---|---|
| p | 0 | 2 |
| q | 2 | 0 |

- Minkowski Distance is a generalization of Euclidean Distance

$$d_M = \left(\sum_{k=1}^n |p_k - q_k|^r \right)^{\frac{1}{r}} = \| \mathbf{p} - \mathbf{q} \|_r$$

- Where \mathbf{p} and \mathbf{q} are two objects represented by vectors. n is the number of dimensions (attributes) of the vectors and p_k and q_k are, respectively, the k th attributes (components) of data objects p and q .
- **Note:** If ranges differ then standardization (z-scores) is necessary to avoid one variable to dominate the distance.

Minkowski Distance: Examples

- $r = 1$. City block (Manhattan, taxicab, L^1 norm) distance.
 - A common example of this is the Hamming distance, which is just the number of bits that are different between two binary vectors
- $r = 2$. Euclidean distance (L^2 norm)
- $r = \infty$. “supremum” (maximum norm, L^∞ norm) distance.
 - This is the maximum difference between any component of the vectors
- Do not confuse r with n , i.e., all these distances are defined for all numbers of dimensions.

Minkowski Distances

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

Distance Matrix

| L^1 | p1 | p2 | p3 | p4 |
|-------|----|----|----|----|
| p1 | 0 | 4 | 4 | 6 |
| p2 | 4 | 0 | 2 | 4 |
| p3 | 4 | 2 | 0 | 2 |
| p4 | 6 | 4 | 2 | 0 |

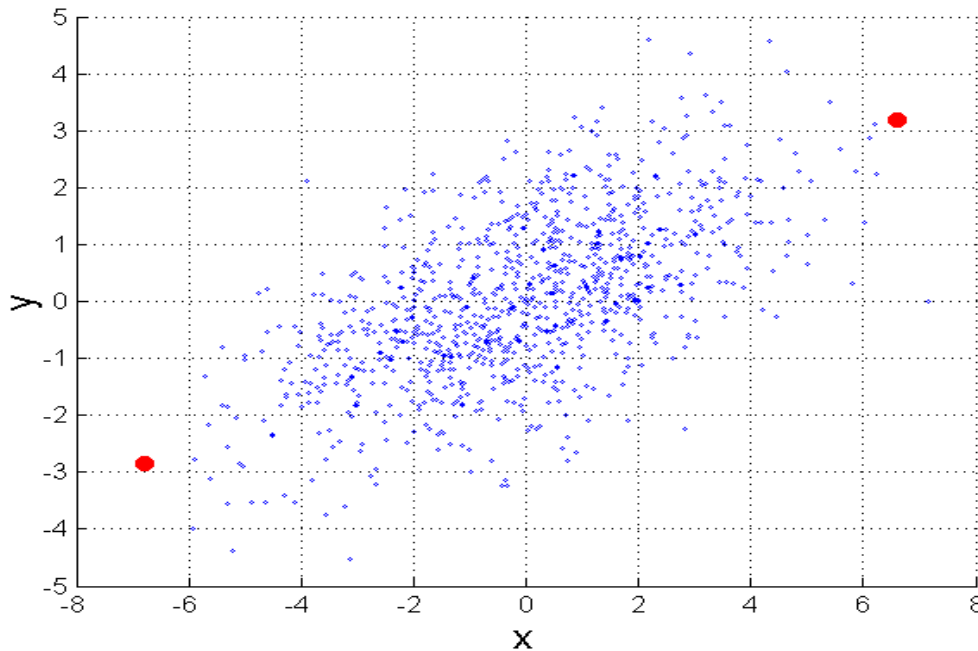
| L^2 | p1 | p2 | p3 | p4 |
|-------|------|------|------|------|
| p1 | 0.00 | 2.83 | 3.16 | 5.10 |
| p2 | 2.83 | 0.00 | 1.41 | 3.16 |
| p3 | 3.16 | 1.41 | 0.00 | 2.00 |
| p4 | 5.10 | 3.16 | 2.00 | 0.00 |

| 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 |



Mahalanobis Distance

$$d_{mahalanobis}(\mathbf{p}, \mathbf{q}) = \sqrt{(\mathbf{p} - \mathbf{q})^T \mathbf{S}^{-1} (\mathbf{p} - \mathbf{q})}$$

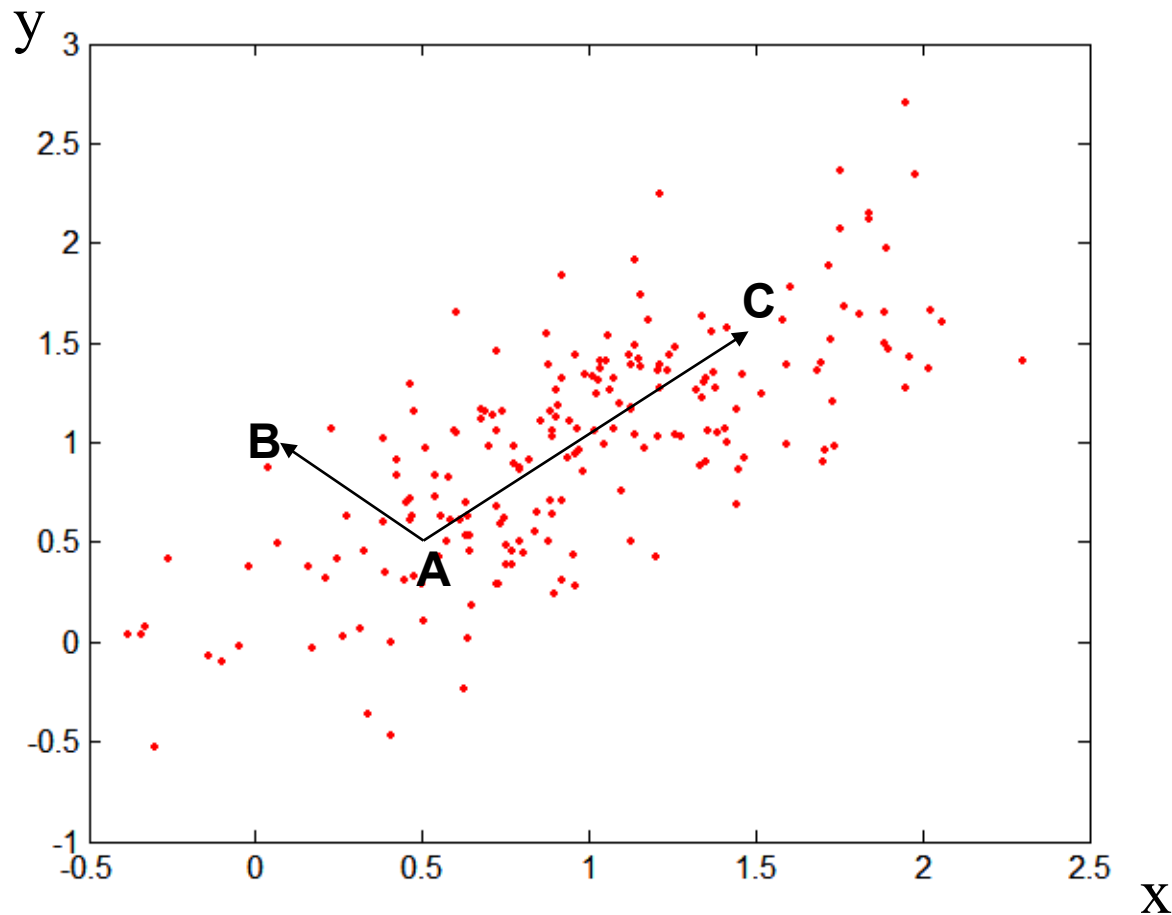


\mathbf{S}^{-1} is the inverse of the covariance matrix of the input data

Measures how many standard deviations two points are away from each other → scale invariant measure

Example: For red points, the Euclidean distance is 14.7, Mahalanobis distance is 6.

Mahalanobis Distance



Covariance Matrix:

$$S = \begin{bmatrix} .3 & .2 \\ .2 & .3 \end{bmatrix}$$

A: (0.5, 0.5)

B: (0, 1)

C: (1.5, 1.5)

$$d_{mahal}(A, B) = 5$$

$$d_{mahal}(A, C) = 4$$

Data varies in direction A-C more than in A-B!

Cosine Similarity

For two vector A and B, the cosine similarity is defined as

$$\cos(\theta) = \frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|} = \frac{\sum_{i=1}^n A_i B_i}{\sqrt{\sum_{i=1}^n A_i^2} \sqrt{\sum_{i=1}^n B_i^2}}$$

Example:

A = 3 2 0 5 0 0 0 2 0 0

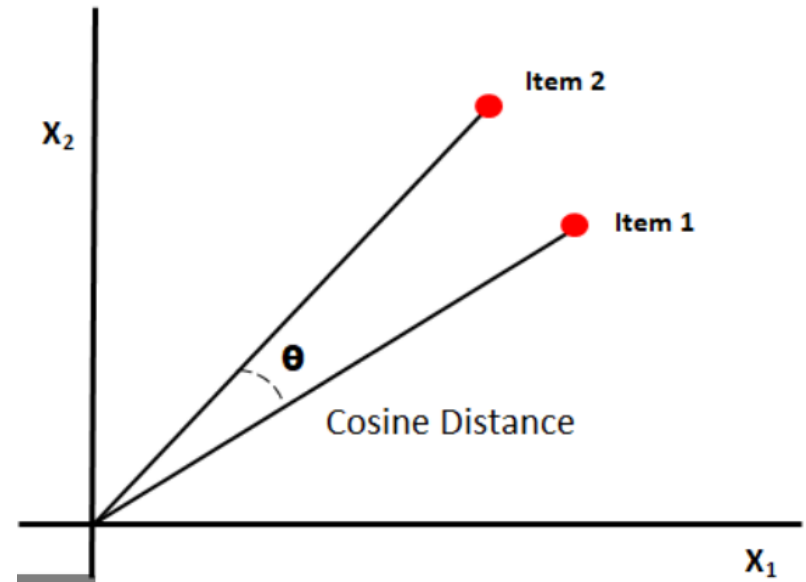
B = 1 0 0 0 0 0 0 1 0 2

$$\mathbf{A} \cdot \mathbf{B} = 3 * 1 + 2 * 0 + 0 * 0 + 5 * 0 + 0 * 0 + 0 * 0 + 0 * 0 + 2 * 1 + 0 * 0 + 0 * 2 = 5$$

$$\|\mathbf{A}\| = (3 * 3 + 2 * 2 + 0 * 0 + 5 * 5 + 0 * 0 + 0 * 0 + 0 * 0 + 2 * 2 + 0 * 0 + 0 * 0)^{0.5} = 6.481$$

$$\|\mathbf{B}\| = (1 * 1 + 0 * 0 + 0 * 0 + 0 * 0 + 0 * 0 + 0 * 0 + 0 * 0 + 1 * 1 + 0 * 0 + 2 * 2)^{0.5} = 2.245$$

$$s_{\cosine} = .3150$$



Cosine similarity is often used for word count vectors to compare documents.

Similarity Between Binary Vectors

- Common situation is that objects, p and q, have only binary attributes

- Compute similarities using the following quantities

M01 = the number of attributes where p was 0 and q was 1

M10 = the number of attributes where p was 1 and q was 0

M00 = the number of attributes where p was 0 and q was 0

M11 = the number of attributes where p was 1 and q was 1

- Simple Matching and Jaccard Coefficients

s_{SMC} = number of matches / number of attributes

$$= (M11 + M00) / (M01 + M10 + M11 + M00)$$

s_J = number of 11 matches / number of not-both-zero attribute values

$$= (M11) / (M01 + M10 + M11)$$

Note: Jaccard ignores 0s!

SMC versus Jaccard: Example

$$\begin{array}{rcl} p & = & 1\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0 \\ q & = & 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 0\ 1 \end{array}$$

$M01 = 2$ (the number of attributes where p was 0 and q was 1)

$M10 = 1$ (the number of attributes where p was 1 and q was 0)

$M00 = 7$ (the number of attributes where p was 0 and q was 0)

$M11 = 0$ (the number of attributes where p was 1 and q was 1)

$$s_{SMC} = \frac{M11 + M00}{M01 + M10 + M11 + M00} = (0 + 7) / (2 + 1 + 0 + 7) = 0.7$$

$$s_J = \frac{M11}{M01 + M10 + M11} = 0 / (2 + 1 + 0) = 0$$

Extended Jaccard Coefficient (Tanimoto)

- Variation of Jaccard for continuous or count attributes:

$$T(p, q) = \frac{p \cdot q}{\|p\|^2 + \|q\|^2 - p \cdot q}$$

where \cdot is the dot product between two vectors and $\|\cdot\|^2$ is the Euclidean norm (length of the vector).

Reduces to Jaccard for binary attributes

Dis(similarities) With Mixed Types

- Sometimes attributes are of many different types (nominal, ordinal, ratio, etc.), but an overall similarity is needed.
 - Gower's (dis)similarity:
 - Ignores missing values
 - Final (dis)similarity is a weighted sum of variable-wise (dis)similarities
1. For the k^{th} attribute, compute a similarity, s_k , in the range $[0, 1]$.
 2. Define an indicator variable, δ_k , for the k_{th} attribute as follows:

$$\delta_k = \begin{cases} 0 & \text{if the } k^{th} \text{ attribute is a binary asymmetric attribute and both objects have} \\ & \text{a value of 0, or if one of the objects has a missing values for the } k^{th} \text{ attribute} \\ 1 & \text{otherwise} \end{cases}$$

3. Compute the overall similarity between the two objects using the following formula:

$$similarity(p, q) = \frac{\sum_{k=1}^n \delta_k s_k}{\sum_{k=1}^n \delta_k}$$



Common Properties of a Distance

- Distances, such as the Euclidean distance, have some well-known properties.

1. $d(p, q) \geq 0$ for all p and q and $d(p, q) = 0$ only if $p = q$. (Positive definiteness)
2. $d(p, q) = d(q, p)$ for all p and q . (Symmetry)
3. $d(p, r) \leq d(p, q) + d(q, r)$ for all points p, q , and r . (Triangle Inequality)

where $d(p, q)$ is the distance (dissimilarity) between points (data objects), p and q .

- A distance that satisfies these properties is a **metric** and forms a **metric space**.

Common Properties of a Similarity

- Similarities, also have some well-known properties.

$s(p, q) = 1$ (or maximum similarity) only if $p = q$.

$s(p, q) = s(q, p)$ for all p and q . (Symmetry)

where $s(p, q)$ is the similarity between points (data objects), p and q .

Exercise

| | x | y |
|---|---|---|
| A | 2 | 1 |
| B | 4 | 3 |
| C | 1 | 1 |

- Calculate the Euclidean and the Manhattan distances between A and C and A and B
- Calculate the Cosine similarity between A and C and A and B



Topics

- Attributes/Features
- Types of Data Sets
- Data Quality
- Data Preprocessing
- Similarity and Dissimilarity
- **Density**



Density

- Density-based clustering require a notion of density
- Examples:
 - Probability density (function) = describes the likelihood of a random variable taking a given value
 - Euclidean density = number of points per unit volume
 - ~~— Graph-based density = number of edges compared to a complete graph~~
 - ~~— Density of a matrix = proportion of non-zero entries.~~

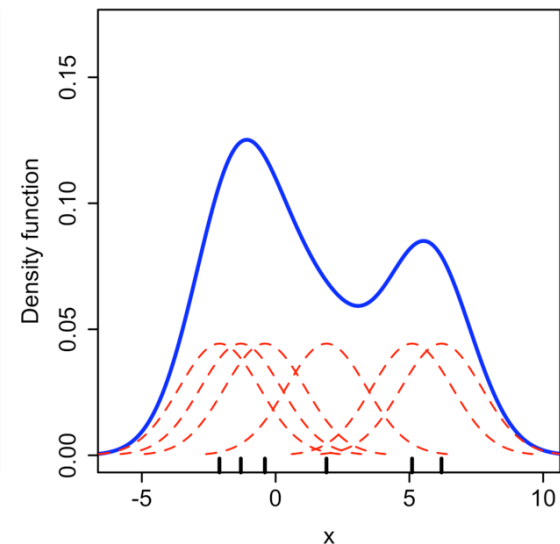
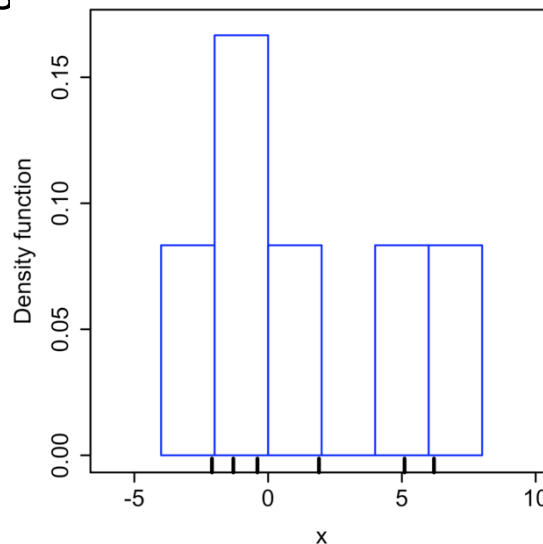
Kernel Density Estimation (KDE)

- KDE is a non-parametric way to estimate the probability density function of a random variable.

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^n K_h(x - x_i) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{x - x_i}{h}\right),$$

- K is the kernel (a non-negative function that integrates to one) and $h > 0$ is a smoothing parameter called the bandwidth. Often a Gaussian kernel is used

- Example:



Euclidean Density – Cell-based

- Simplest approach is to divide region into a number of rectangular cells of equal volume and define density as # of points the cell contains.

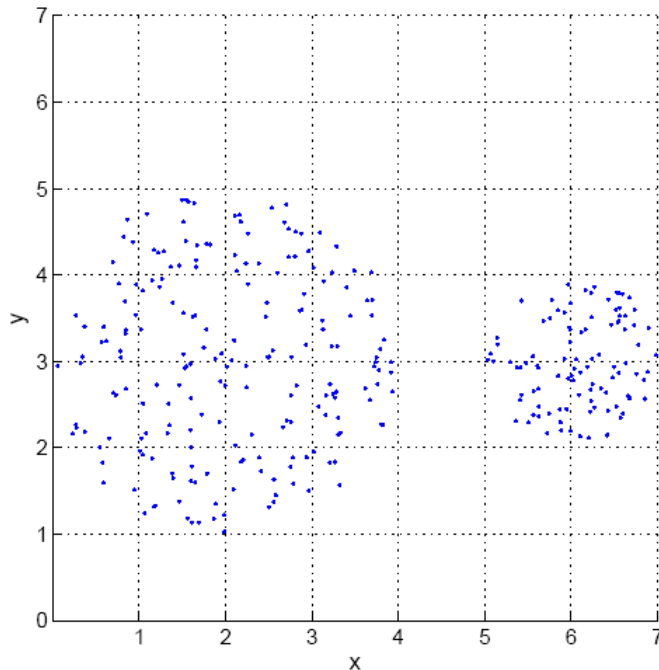


Figure 7.13. Cell-based density.

| | | | | | | |
|----|----|----|----|---|----|----|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | 17 | 18 | 6 | 0 | 0 | 0 |
| 14 | 14 | 13 | 13 | 0 | 18 | 27 |
| 11 | 18 | 10 | 21 | 0 | 24 | 31 |
| 3 | 20 | 14 | 4 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Table 7.6. Point counts for each grid cell.

Euclidean Density – Center-based

- Euclidean density is the number of points within a specified radius of the point

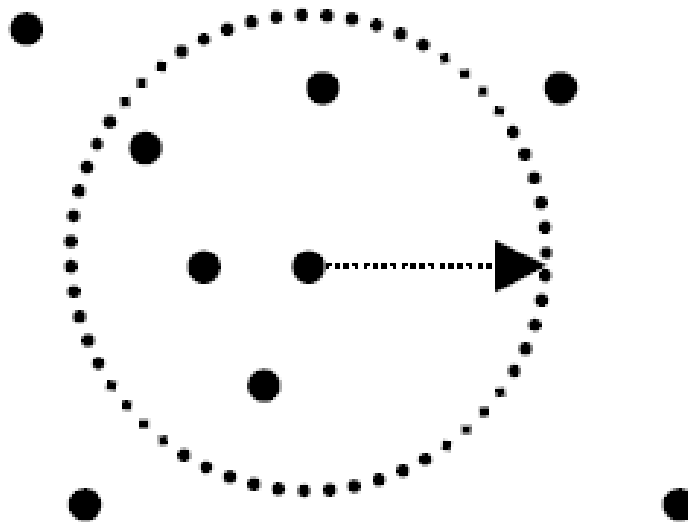


Figure 7.14. Illustration of center-based density.



You should know now about...

- Attributes/Features
- Types of Data Sets
- Data Quality
- Data Preprocessing
- Similarity and Dissimilarity
- Density

