Introduction to Data Mining

Chapter 2
Data

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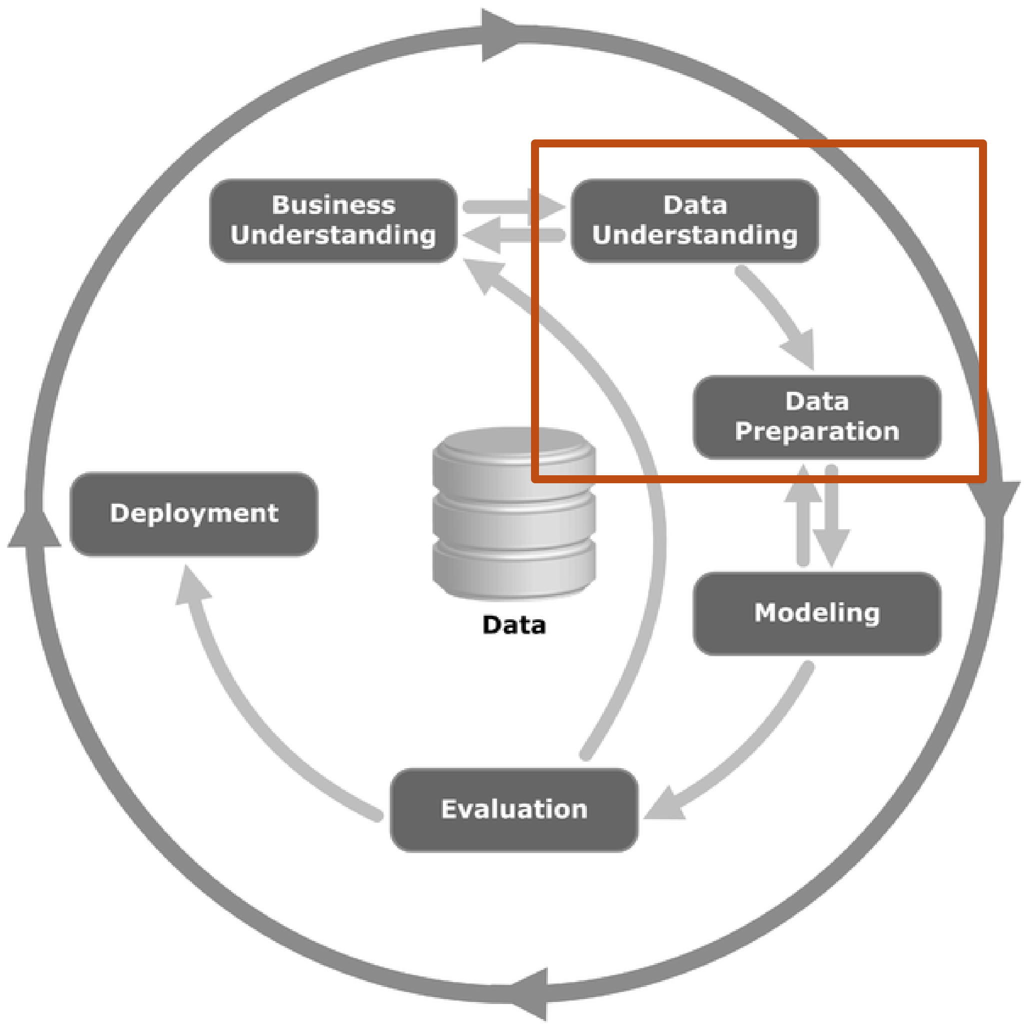
Based in Slides by Tan, Steinbach, Karpatne, Kumar

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

Objects

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}

Categorical, Qualitative

  - Interval
    - Examples: calendar dates, temperatures in Celsius or Fahrenheit.
  - Ratio
    - Examples: temperature in Kelvin, length, time, counts

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}	$=, \neq$ 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	pla y	ball	score	game	wi n	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

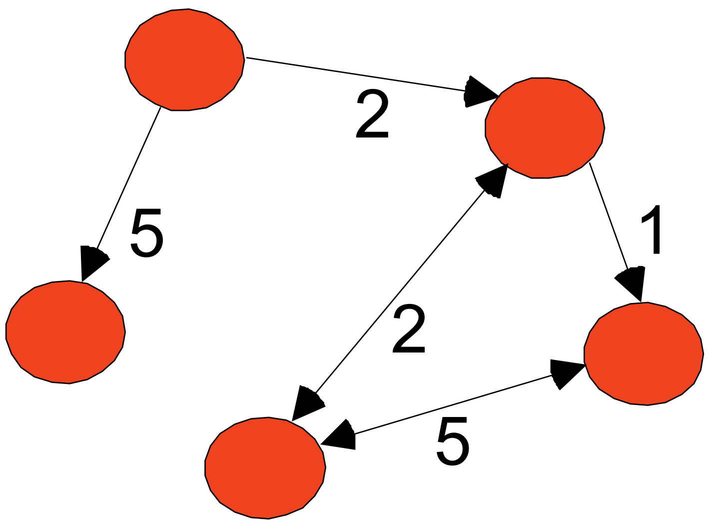
Transaction Data

- 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

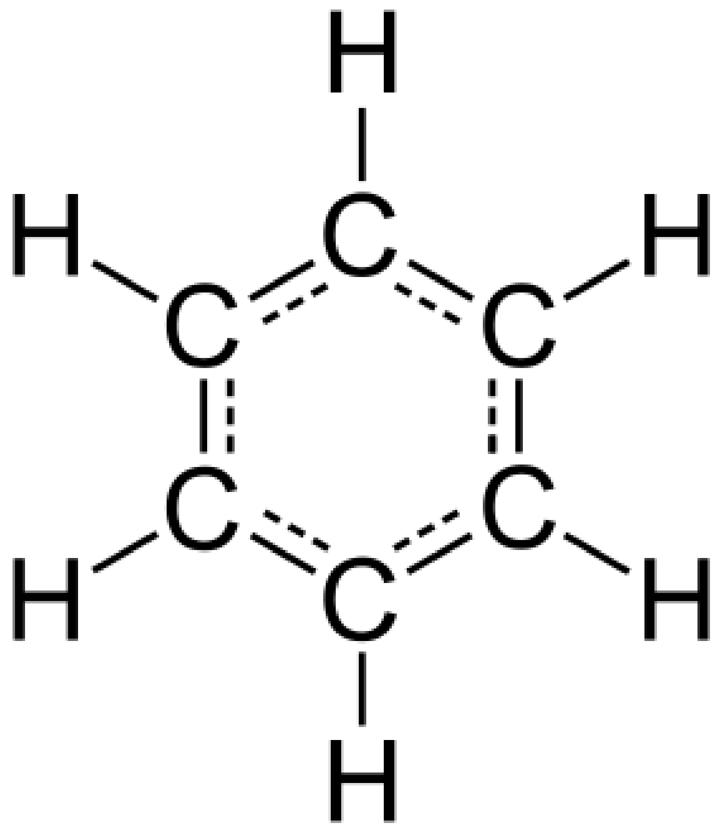
Graph Partitioning

Parallel Solution of Sparse Linear System of Equations

<a href="papers/papers.html#ffff">
N-Body Computation and Dense Linear System Solvers

Chemical Data

- Benzene Molecule: C6H6



Ordered Data

- Sequences of transactions

Items/Events

(A B) (D) (C E)
(B D) (C) (E)
(C D) (B) (A E)

An element of the sequence

Ordered Data

- Genomic sequence data

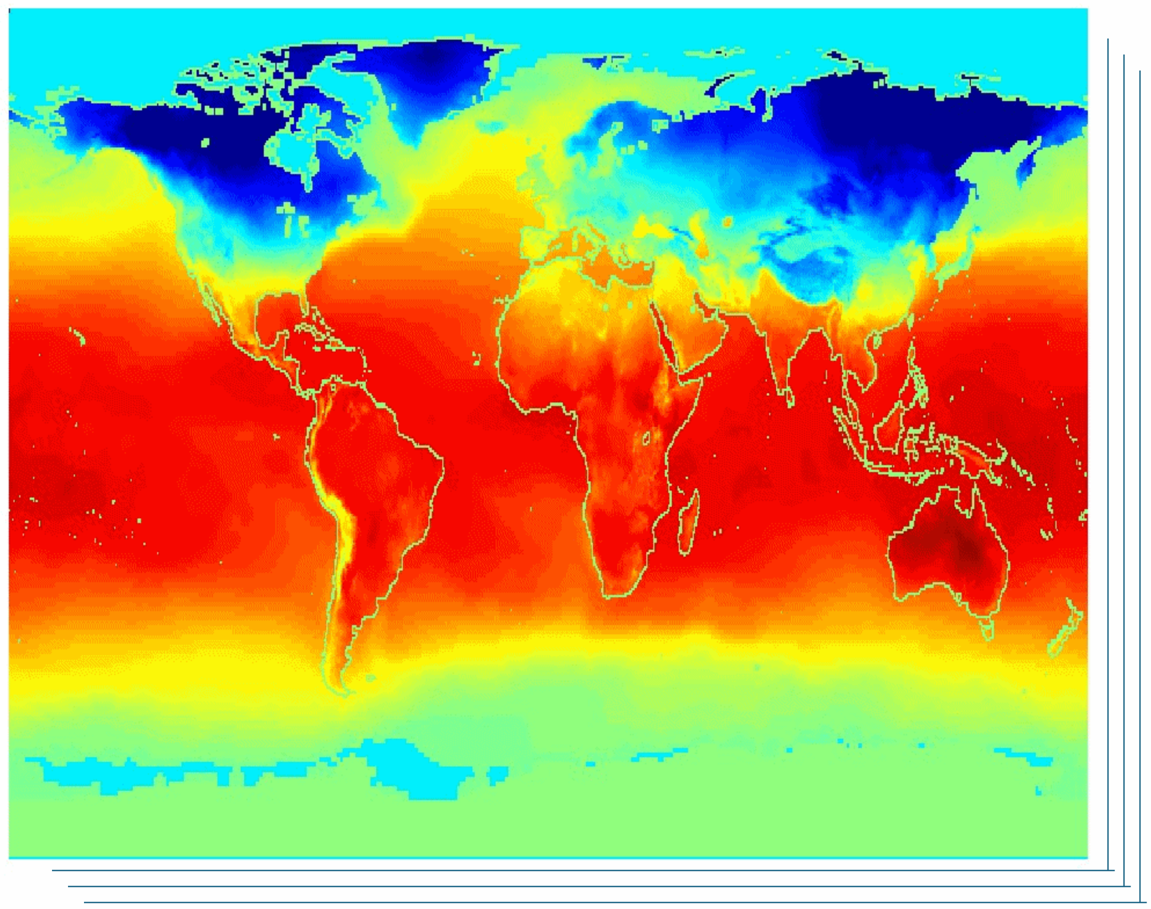
```
GGTTCCGCCTTCAGCCCCGCGCC
CGCAGGGCCCGCCCCGCGCCGTC
GAGAAGGGCCCGCCTGGCGGGCG
GGGGGAGGCGGGGCCGCCCGAGC
CCAACCGAGTCCGACCAGGTGCC
CCCTCTGCTCGGCCTAGACCTGA
GCTCATTAGGCGGCAGCGGACAG
GCCAAGTAGAACACGCGAAGCGC
TGGGCTGCCTGCTGCGACCAGGG
```

Subsequences

Ordered Data: Time Series Data

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

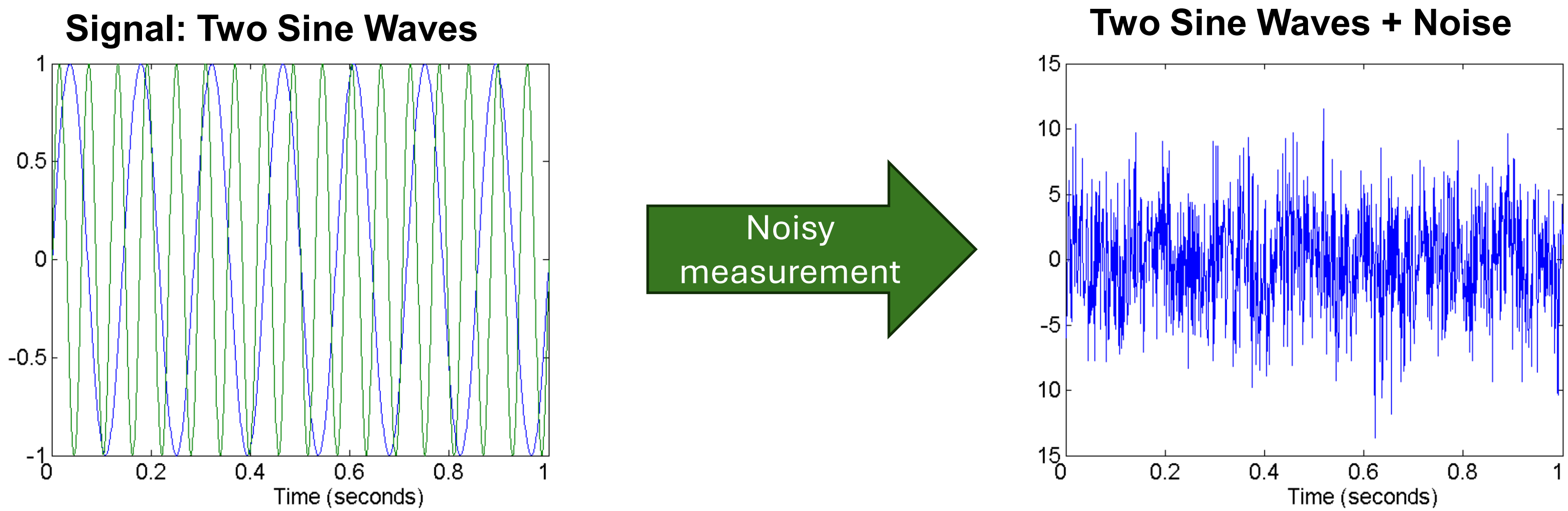
- What kinds of data quality problems exist?
  - Noise and outliers
  - Missing values
  - Duplicate data

- How can we detect problems with the data?
  - Statistics
  - Visualization

- What can we do about these problems?
  - Mark value as missing
  - Remove object

Noise

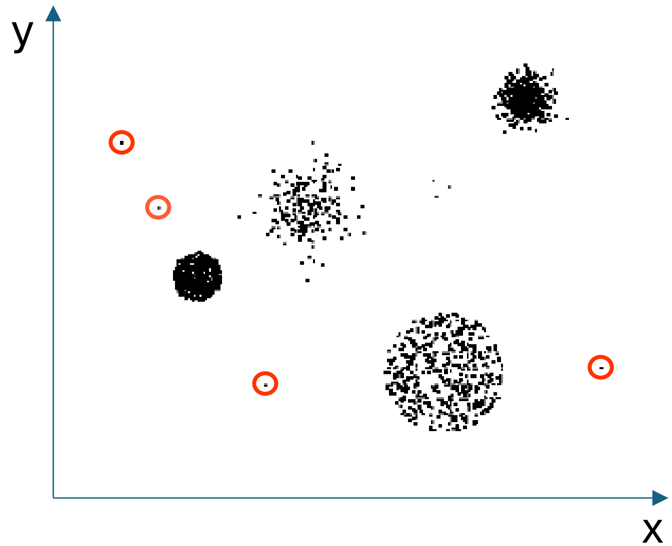
- Noise refers to modification of original values
  - Examples: distortion of a person’s voice when talking on a poor phone, “snow” on television screen, measurement errors.



- Find less noisy data
- Sometimes we can de-noise (signal processing)

Outliers

- Outliers are data objects with feature values that are considerably different than most of the other data objects in the data set.
- Reasons:
  - A true outlier is a special object (e.g., a genius' IQ score).
  - May be the result of a measurement mistake.



- Typical treatment: Statistical outlier detection +
  - Make outlying feature missing, or
  - Remove outlier object

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)
  - Value was a mistake and set to missing.

- 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

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- **Data Preprocessing**
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Data Preprocessing

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

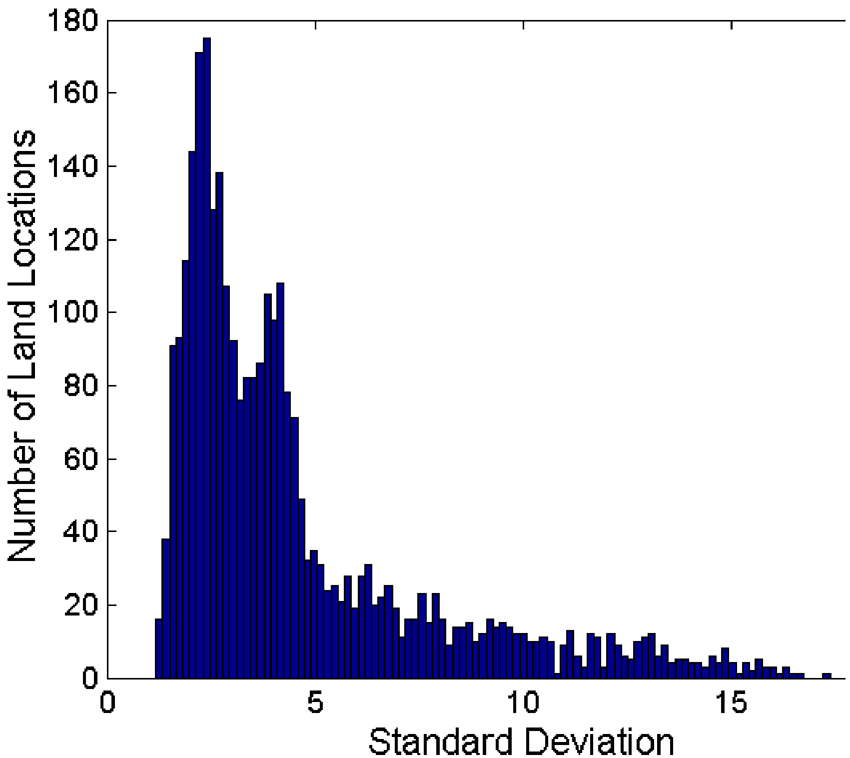
Aggregation

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

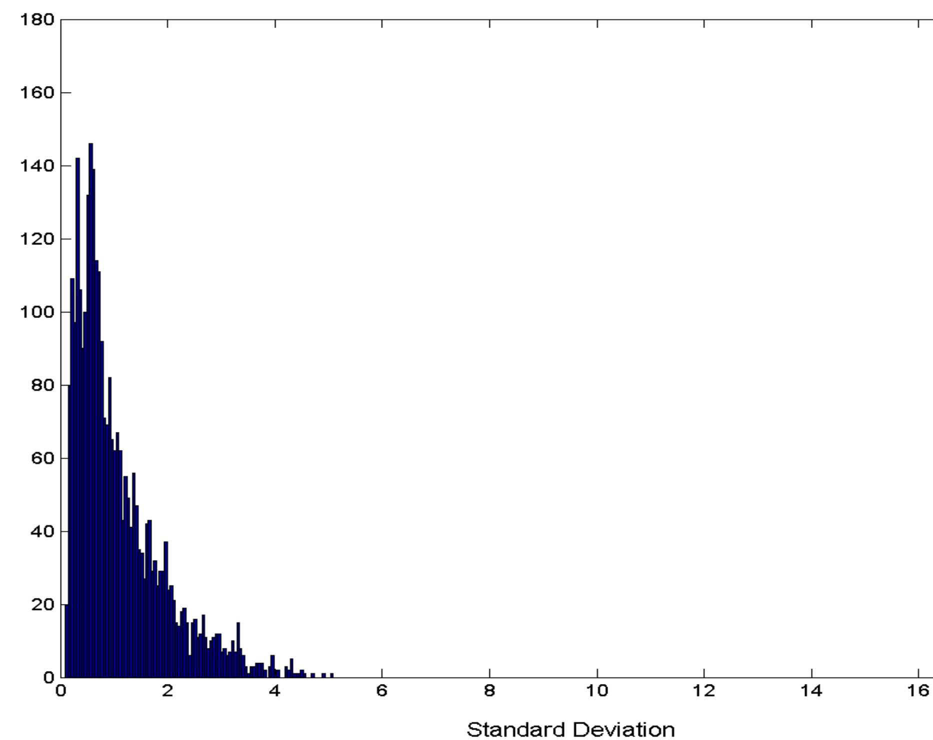
- Purpose
  - Data reduction
    - Reduce the number of attributes or objects
  - Change of scale
    - Cities aggregated into regions, states, countries, etc
  - More "stable" data
    - Aggregated data tends to have less variability (e.g., reduce seasonality by aggregation to yearly data)

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.

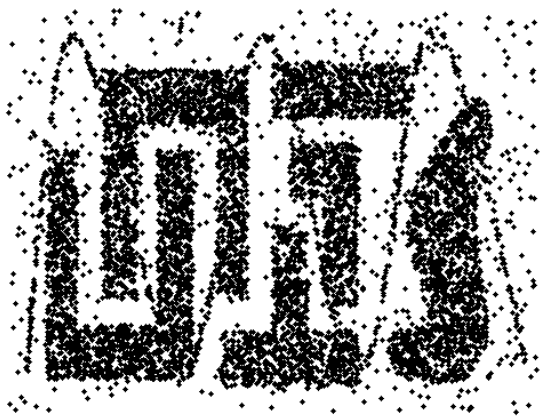
- **Sampling with replacement**
  Objects are not removed from the population as they are selected for the sample. Note: the same object can be picked up more than once.

Selection?

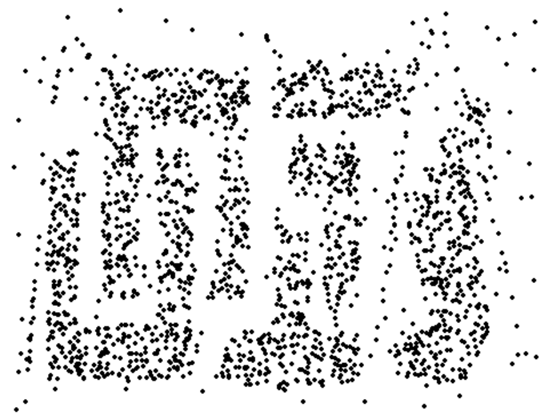
- **Simple random sampling**
  There is an equal probability of selecting any particular item.

- **Stratified sampling**
  Split the data into several partitions; then draw random samples from each partition.

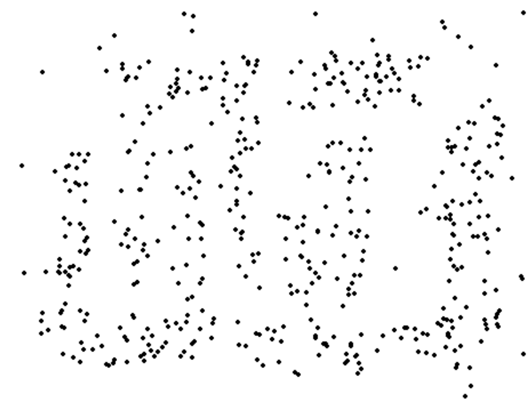
Sample Size



8000 points



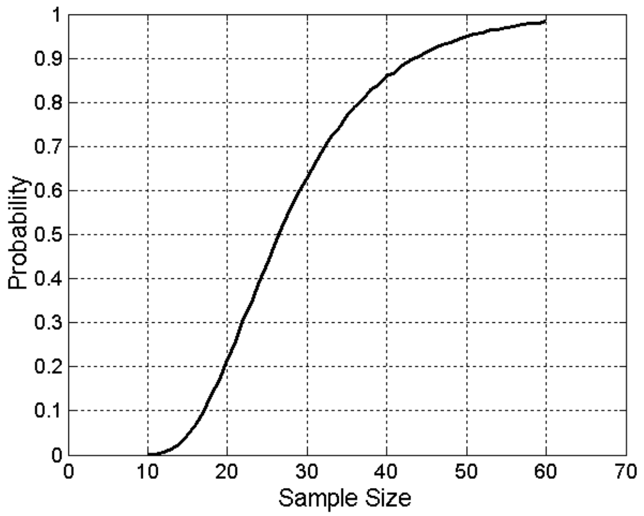
2000 Points



500 Points

Sample Size

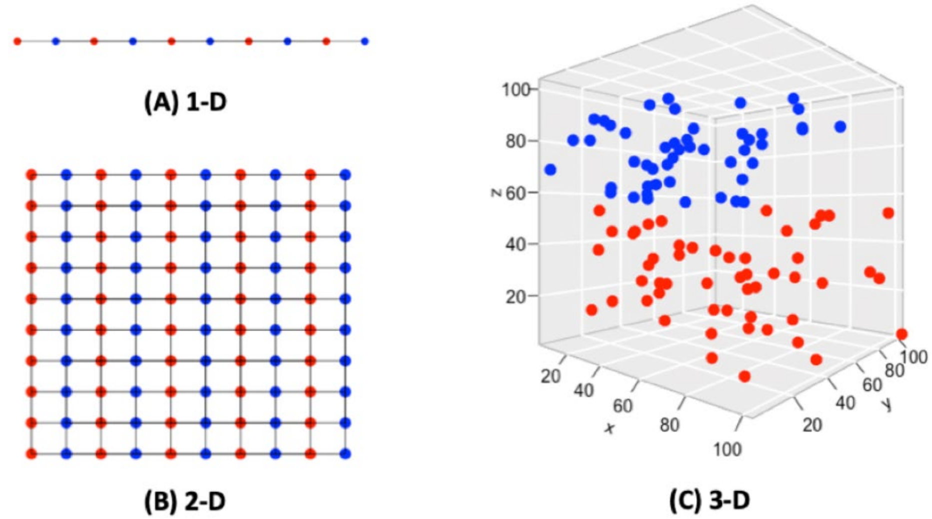
- What sample size is necessary to get at least one object from each of 10 groups.



- 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

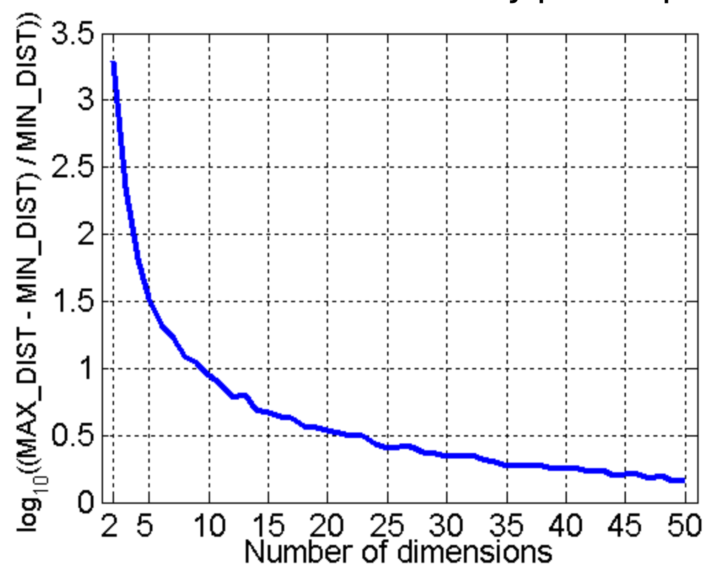
- When dimensionality increases, the size of the data space grows exponentially.



Points and space

- Definitions of density and distance between points, which is critical for clustering and outlier detection, become less meaningful
  - Density → 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

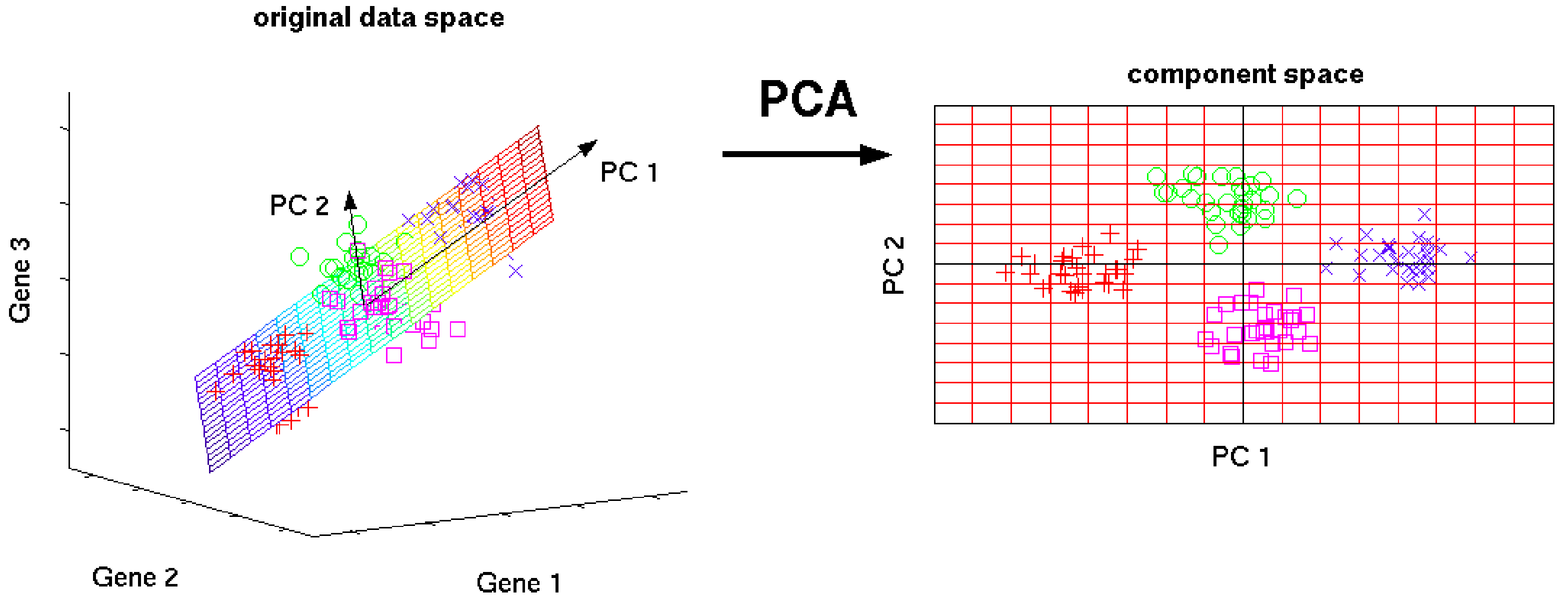


Dimensionality Reduction

- 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

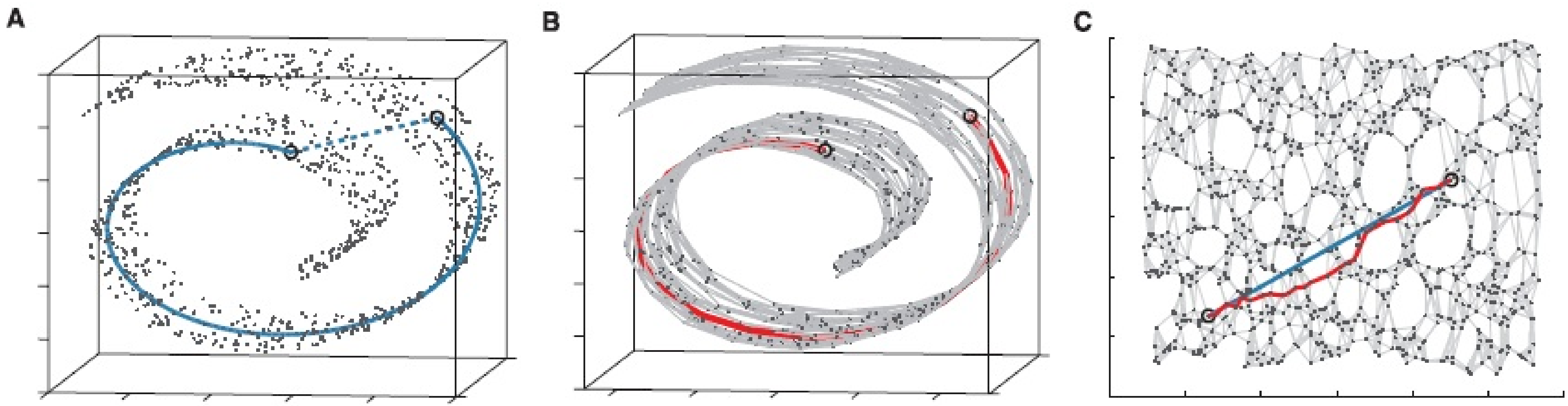
Dimensionality Reduction: Principal Components Analysis (PCA)

- **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

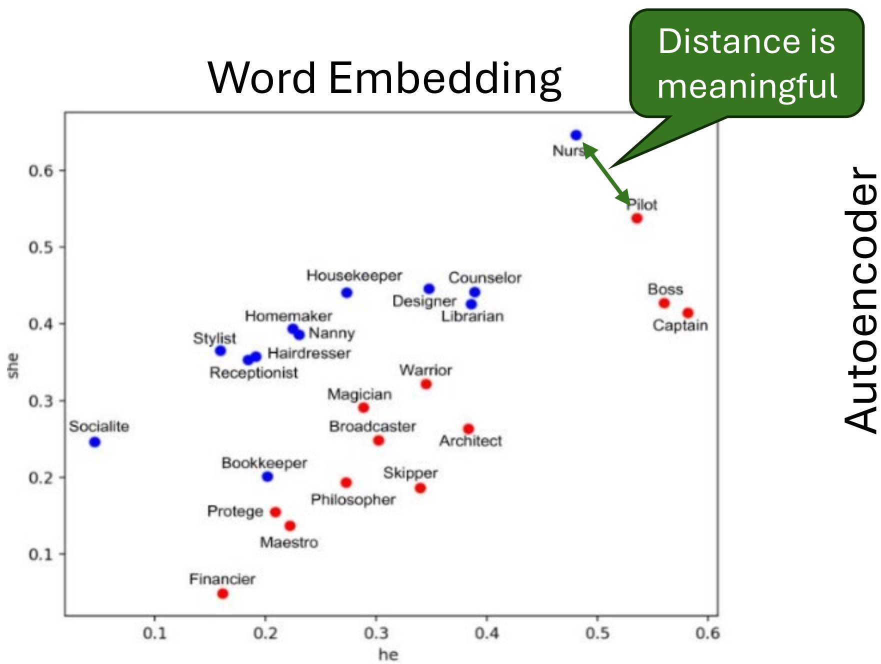


- **Goal**: Unroll the "swiss roll!" (i.e., preserve distances on the roll)
- **Method**: Use a non-metric space, i.e., distances are not measured by Euclidean distance, but along the surface of the roll (geodesic distances).
  1. Construct a neighbourhood graph (k-nearest neighbors or within a radius).
  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)

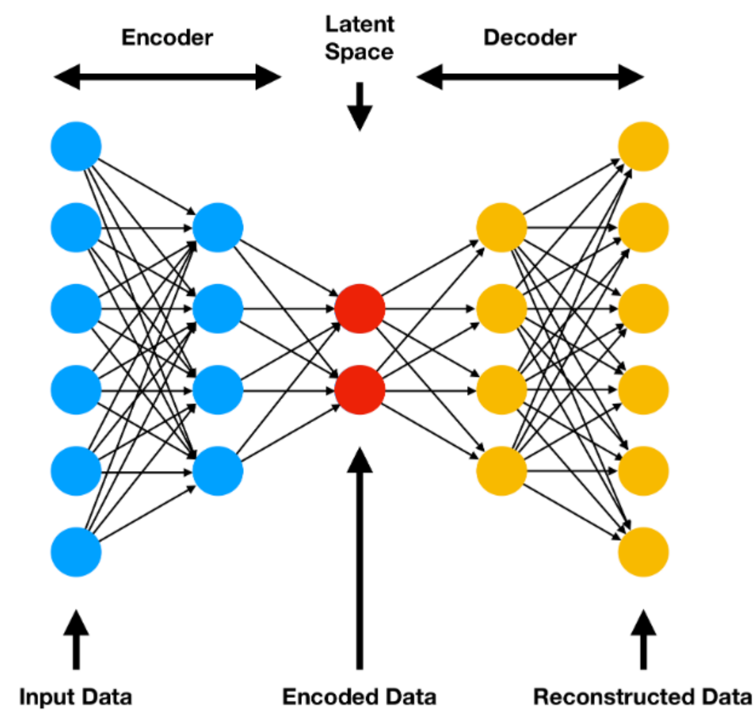
Low-dimensional Embedding

- General notion of representing objects described in one space (i.e., set of features) in a different space using a map $f : X \to Y$
- 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-SNA: T-distributed Stochastic Neighbor Embedding; non-linear for visualization of high-dimensional datasets.
  - —Autoencoders (deep learning): non-linear
  - —Word embedding: Word2vec, GloVe, BERT

Word Embedding



Autoencoder



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

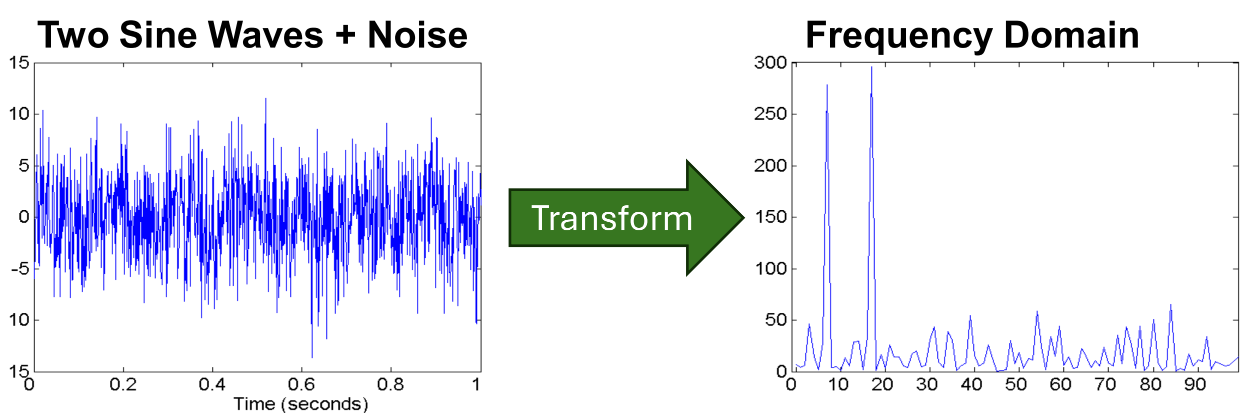
- Embedded approaches:
  - Feature selection occurs naturally as part of the data mining algorithm (e.g., regression, decision trees).
- Filter approaches:
  - Features are selected before data mining algorithm is run
  - (e.g., highly correlated features)
- Brute-force approach:
  - Try all possible 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

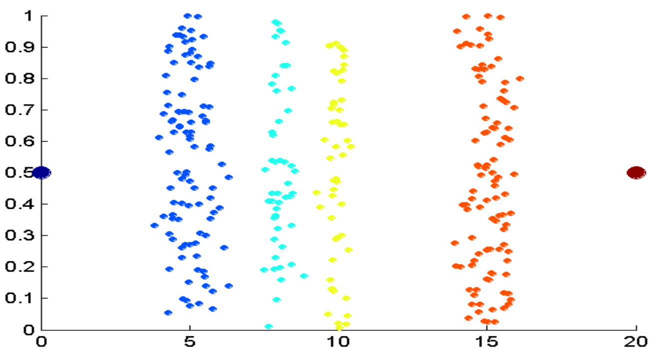
Create new attributes that can capture the important information in a data set much more efficiently than the original attributes

Three general methodologies

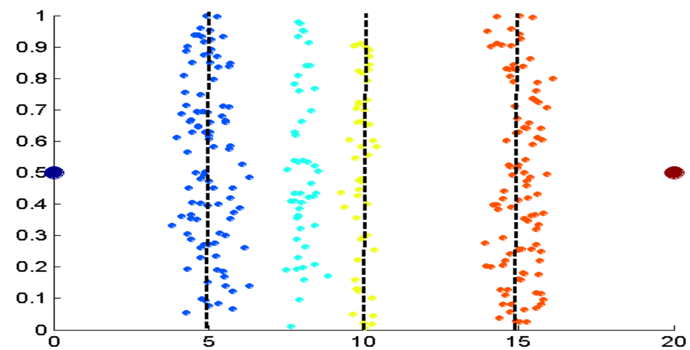
- Feature Extraction
  - Domain-specific (e.g., face recognition in image mining)
- Feature Construction / Feature Engineering
  - combining features (interactions: multiply features)
  - Example: Calculate the body mass index from height and weight
- Mapping Data to New Space
  - Example: Fourier transform/Wavelet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



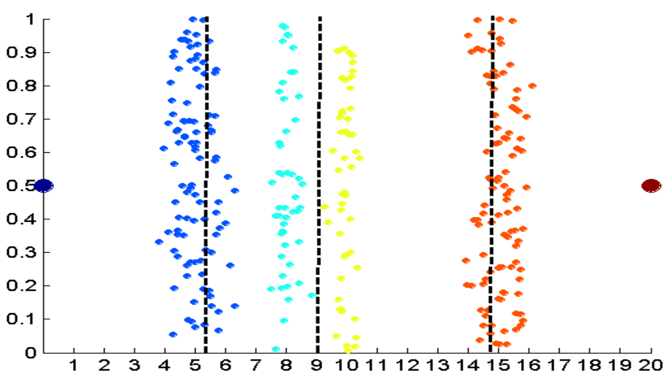
Unsupervised Discretization



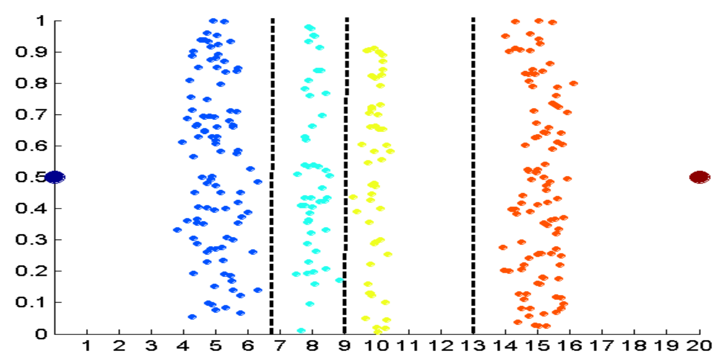
Data



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

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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	$d = \frac{\lvert p-q \rvert}{n-1}$ (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	$d = \lvert p - q \rvert$	$s = -d$, $s = \frac{1}{1+d}$ 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

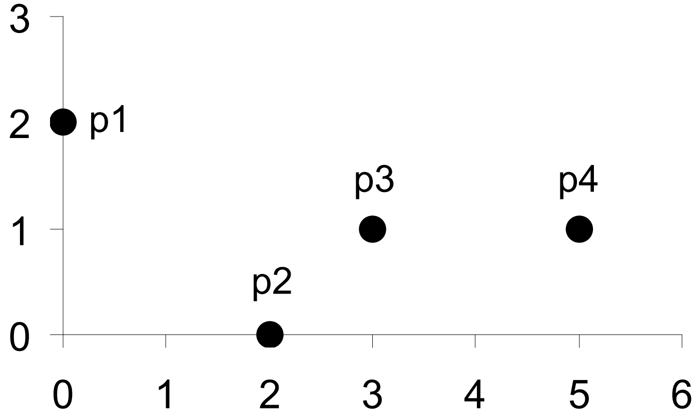
- Euclidean Distance (for quantitative attribute vectors)

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

  - Where $\boldsymbol{p}$ and $\boldsymbol{q}$ 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 kth 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 $\boldsymbol{p}$ 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

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

  — Where $\boldsymbol{p}$ and $\boldsymbol{q}$ 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 kth attributes (components) or 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

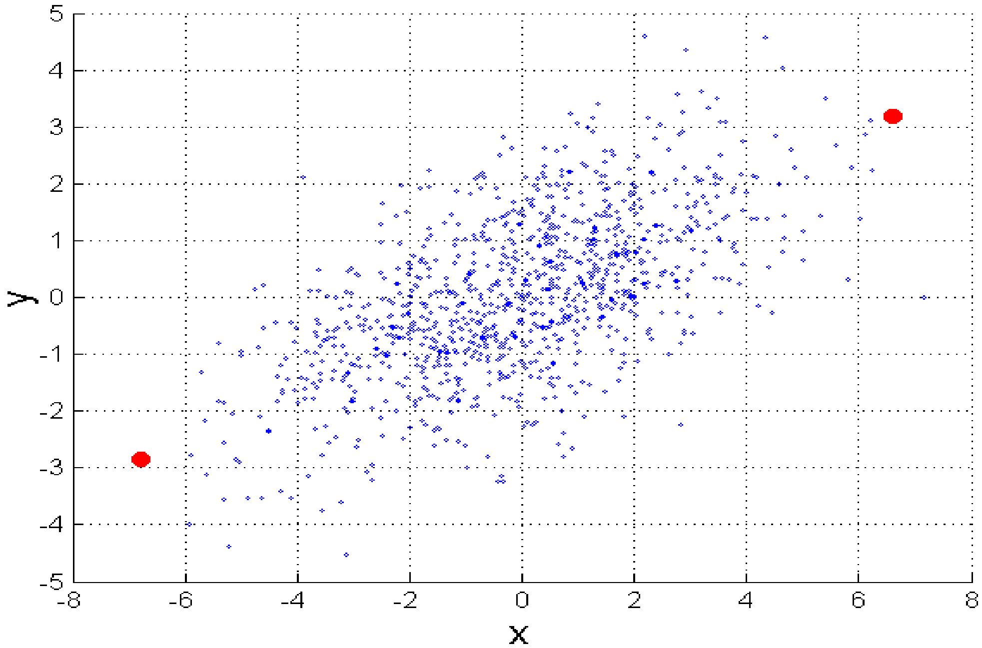
L^1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

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

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

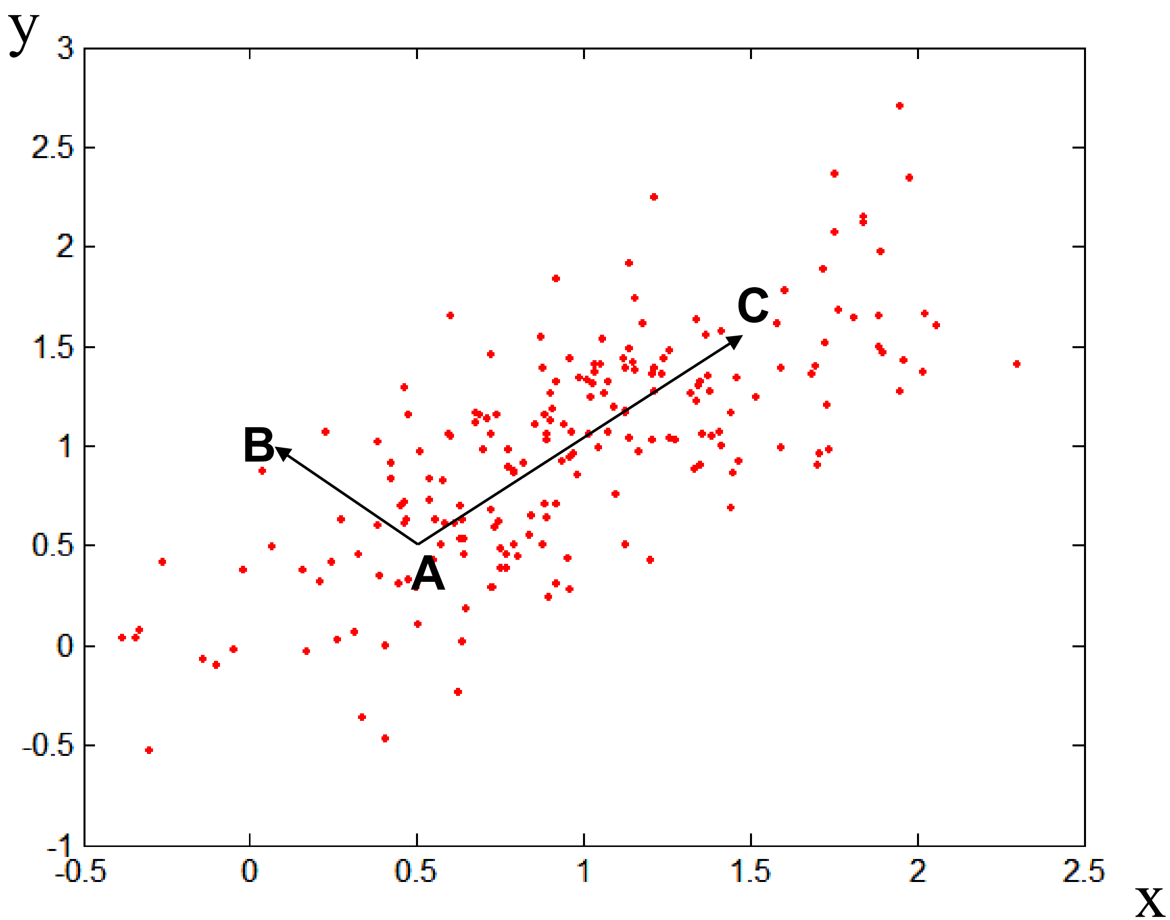


S^{-1} is the inverse of the covariance matrix of the input data

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)

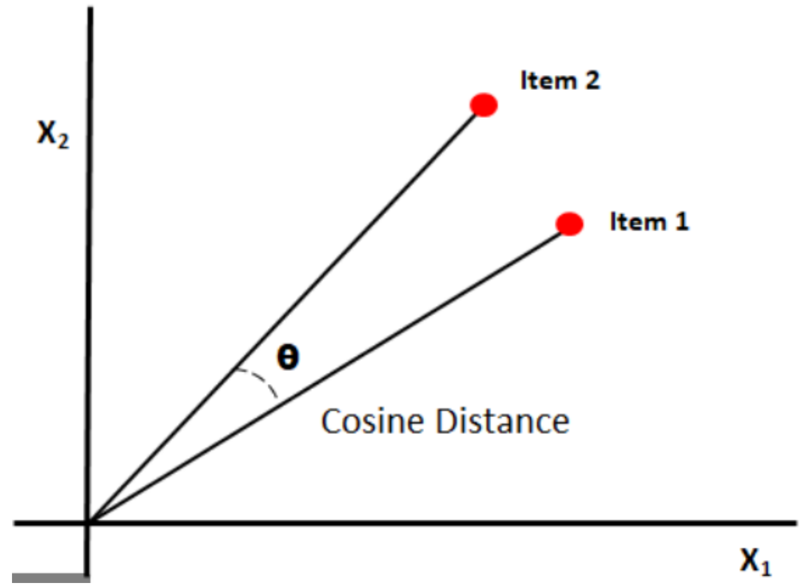
$$d_{mahal}(A, B) = 5$$
$$d_{mahal}(A, C) = 4$$

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

$$\boldsymbol{A} \cdot \boldsymbol{B} = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$$
$$\|\boldsymbol{A}\| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)0.5 = 6.481$$
$$\|\boldsymbol{B}\| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)\,0.5 = 2.245$$

$$s_{cosine} = .3150$$

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

$$p = 1\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0$$
$$q = 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 0\ 1$$

$M01 = 2$ (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:

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

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

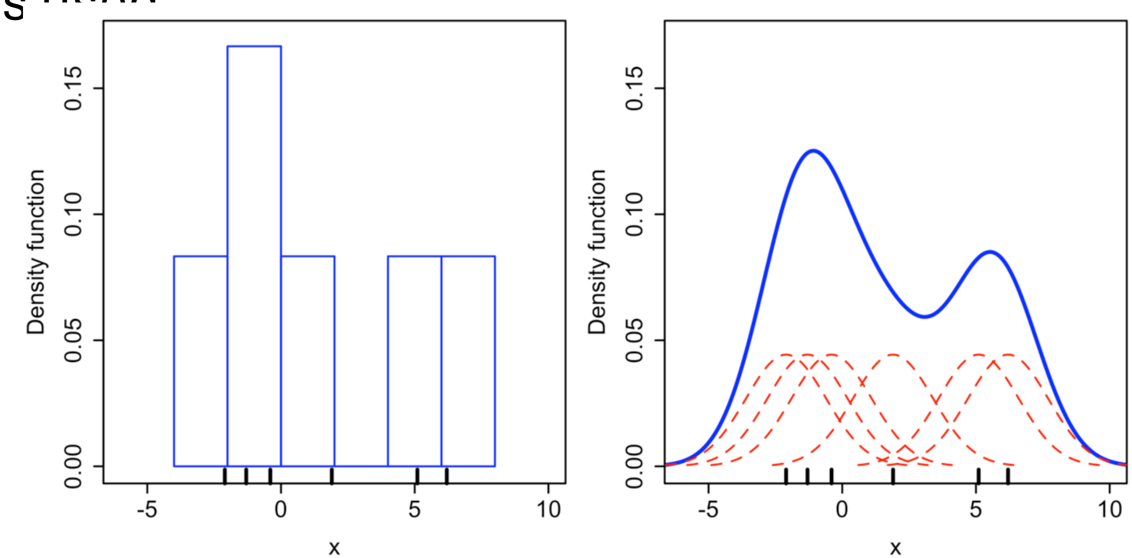
- Examples:
  - Probability density (function) = describes the likelihood of a random variable taking a given value
  - Euclidean density = number of points per unit volume
  - ~~Graph-based density = number of edges compared to a complete graph~~
  - ~~Density of a matrix = proportion of non-zero entries.~~

Kernel Density Estimation (KDE)

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

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

- 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.

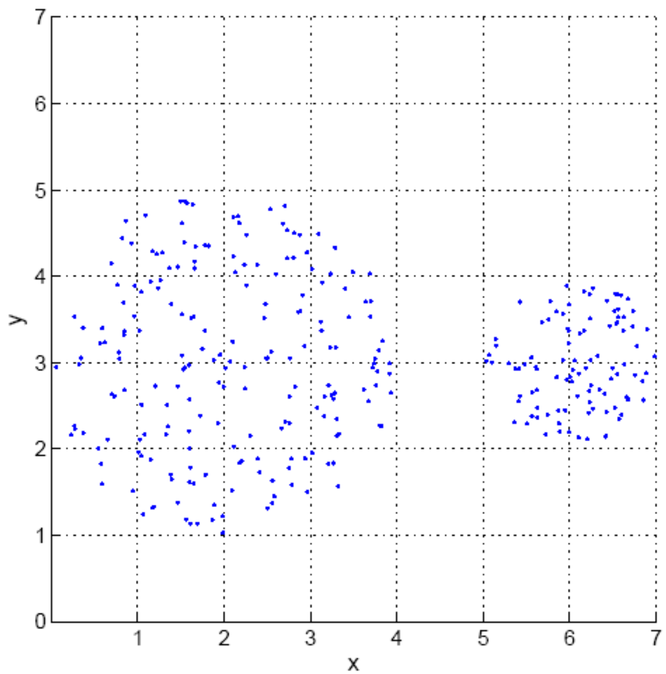


Figure 7.13. Cell-based density.

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

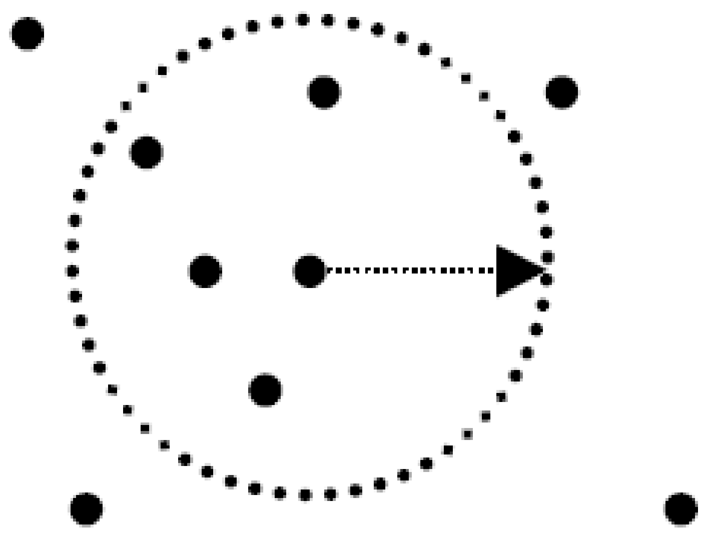


Figure 7.14. Illustration of center-based density.

See Data Exploration

You should know now about…

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