



# Introduction to Data Mining

## Chapter 2 Data

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Based in Slides by Tan,  
Steinbach, Karpatne, Kumar



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# R Code Examples

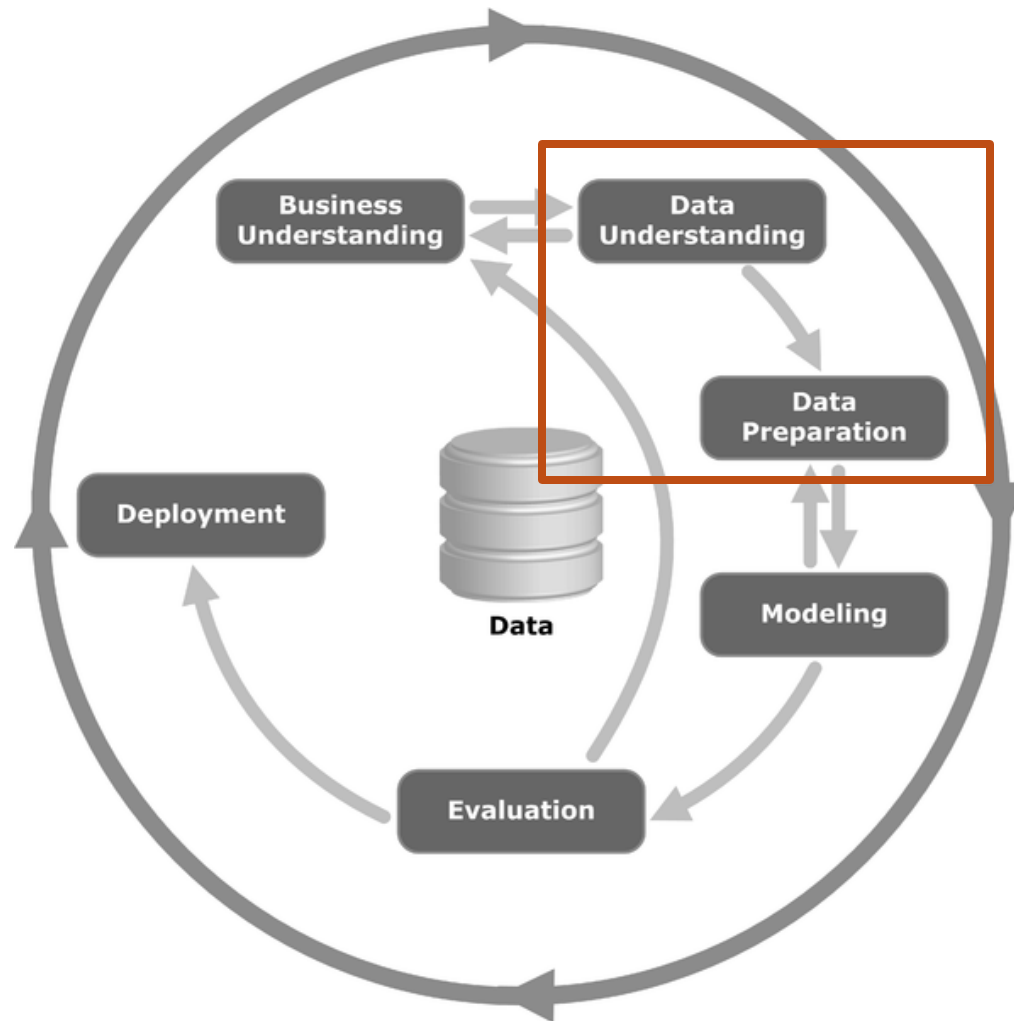
- Available R Code examples are indicated on slides by the R logo



- The Examples are available at [https://mhahsler.github.io/Introduction\\_to\\_Data\\_Mining\\_R\\_Examples/](https://mhahsler.github.io/Introduction_to_Data_Mining_R_Examples/)



# Tasks in the CRISP-DM Reference Model





## Topics

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- **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 <b>names or labels</b> , 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, $\chi^2$ test
Ordinal	The values of an ordinal attribute provide enough information to <b>order objects</b> .	zip codes, employee ID numbers, eye color, sex: {male, female}	Nominal + <, >  median, percentiles, rank correlation, run tests, sign tests
Interval	For interval attributes, the <b>differences between values</b> 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 <b>ratios are meaningful</b> . 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

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- 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

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
$m$ objects	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

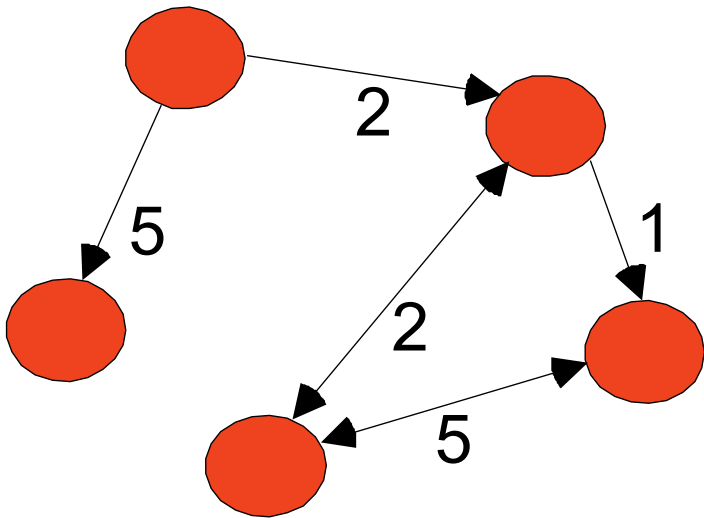
- A special type of record data, where
  - each record (transaction) involves a set of items.
  - For example, consider a grocery store. The set of products purchased by a customer during one shopping trip constitute a transaction, while the individual products that were purchased are the items.

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



```
<a href="papers/papers.html#bbbb">
```

```
Data Mining </a>
```

```
<li>
```

```
<a href="papers/papers.html#aaaa">
```

```
Graph Partitioning </a>
```

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<li>
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<a href="papers/papers.html#aaaa">
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```
Parallel Solution of Sparse Linear System of Equations </a>
```

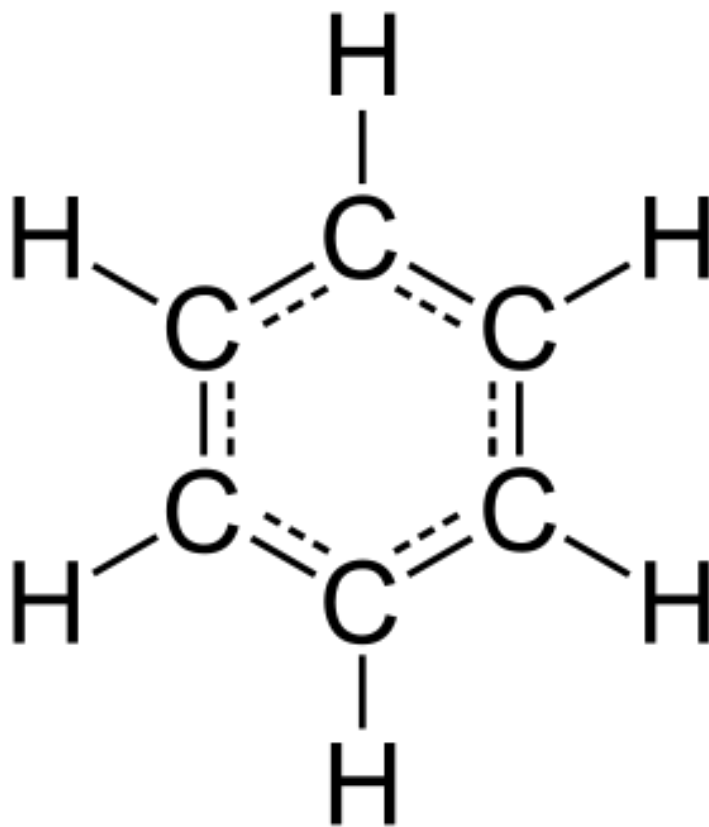
```
<li>
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<a href="papers/papers.html#ffff">
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```
N-Body Computation and Dense Linear System Solvers
```

# Chemical Data

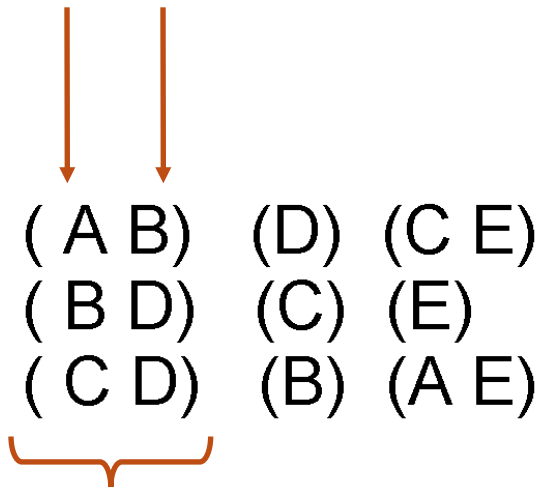
- Benzene Molecule: C<sub>6</sub>H<sub>6</sub>



# 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*

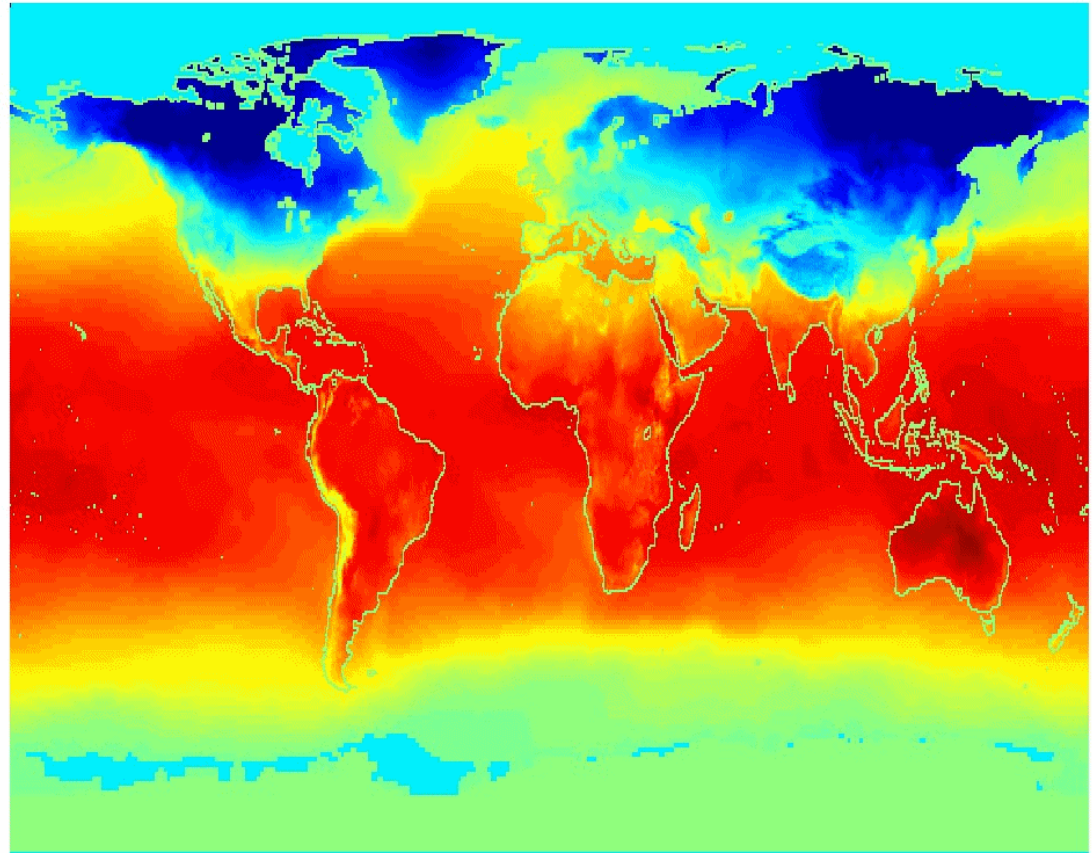


Source: FactSet

# Ordered Data: Spatio-Temporal

Jan, Feb, Mar, ...

**Average Monthly  
Temperature of  
land and ocean**





## Topics

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



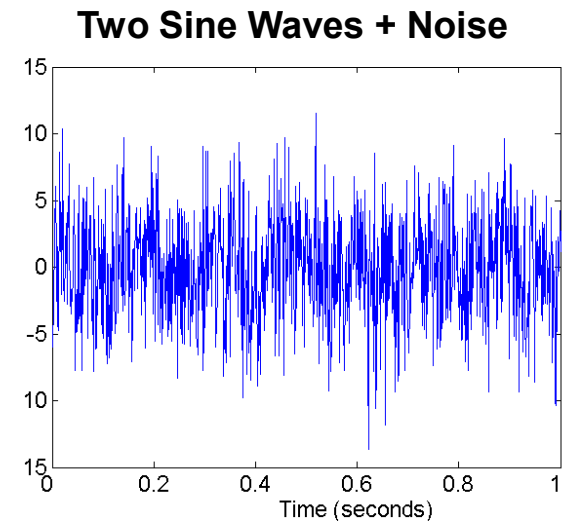
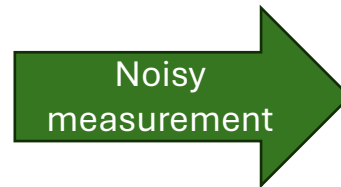
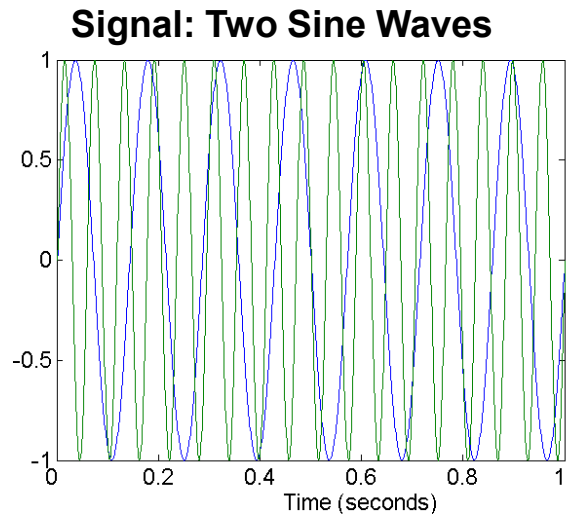
# Data Quality

- 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

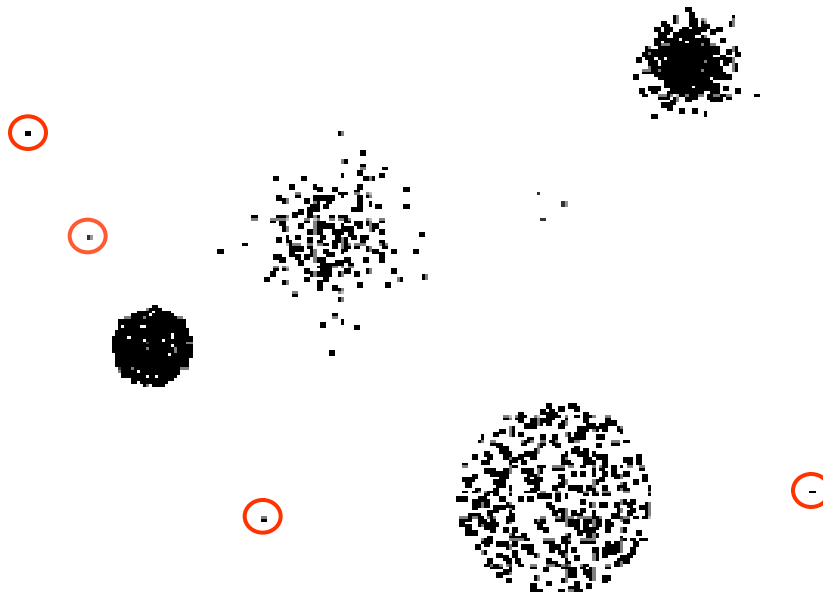
- Noise refers to modification of original values
  - Examples: distortion of a person's voice when talking on a poor phone, “snow” on television screen, measurement errors.



- 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

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- Attributes/Features
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- Data Quality
- **Data Preprocessing**
- Similarity and Dissimilarity
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# Data Preprocessing

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

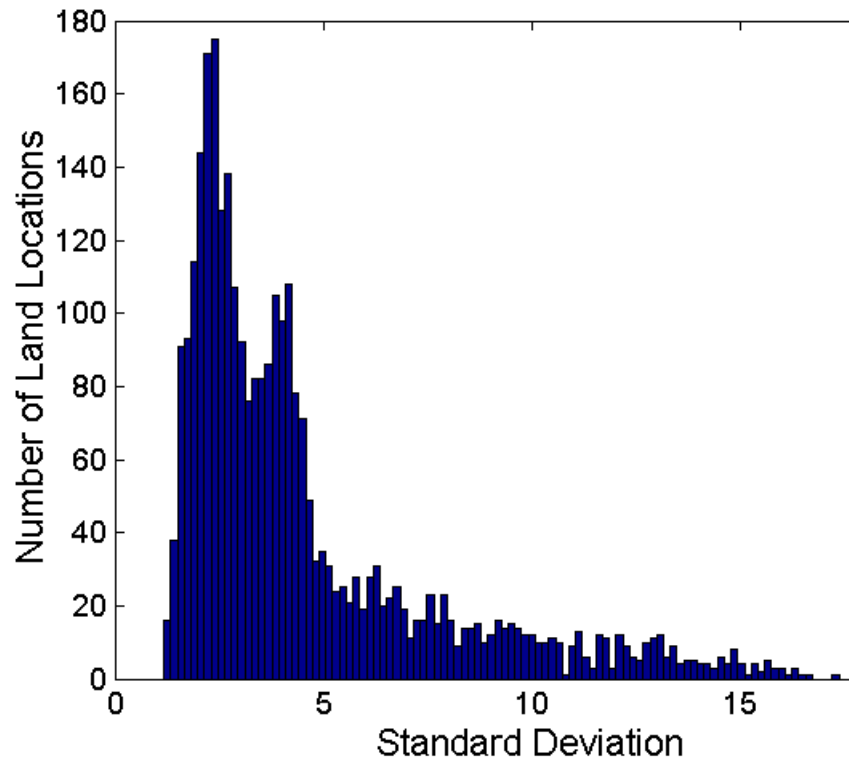
# Aggregation

- 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)

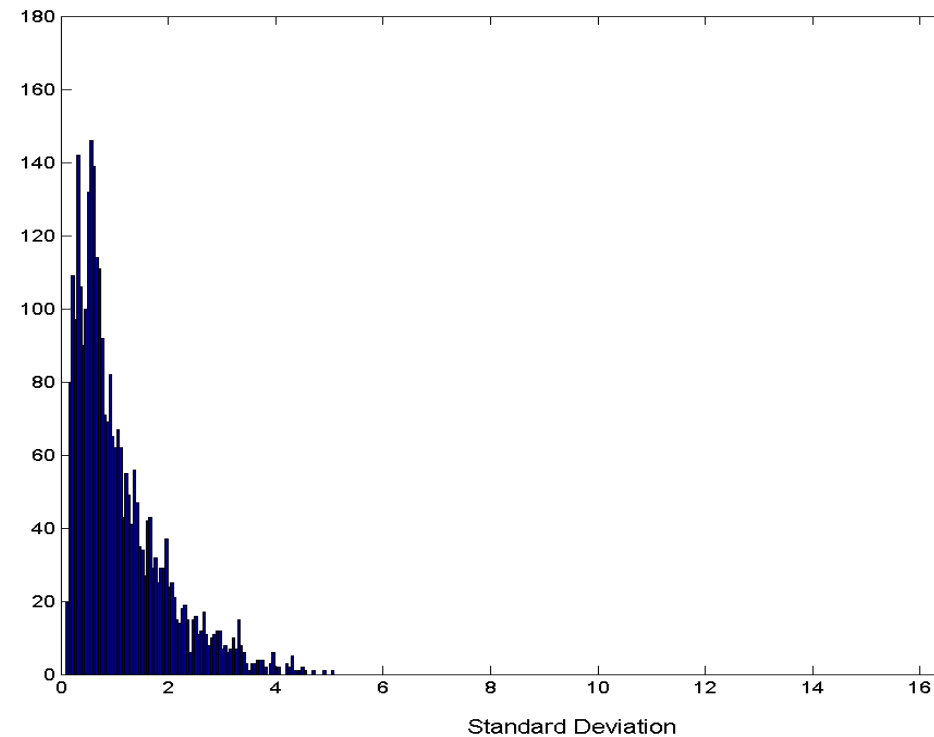


# Aggregation

## 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?

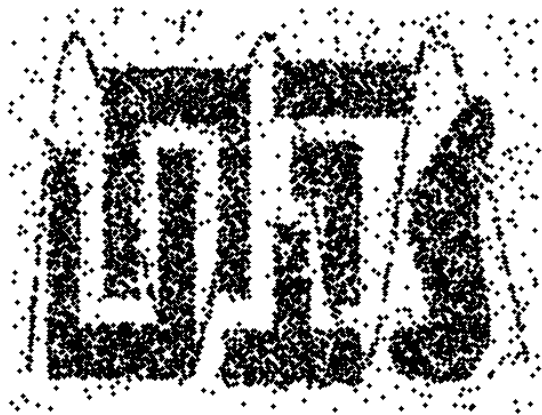
- **Simple random sampling**

There is an equal probability of selecting any particular item.

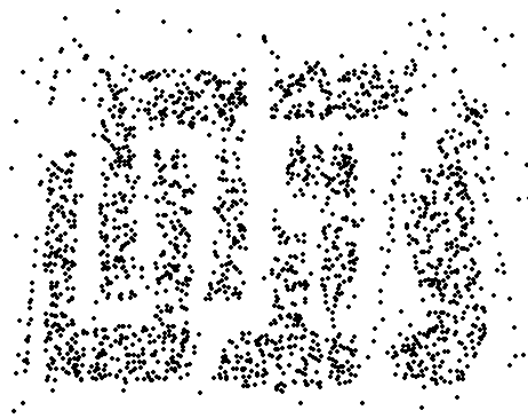
- **Stratified sampling**

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

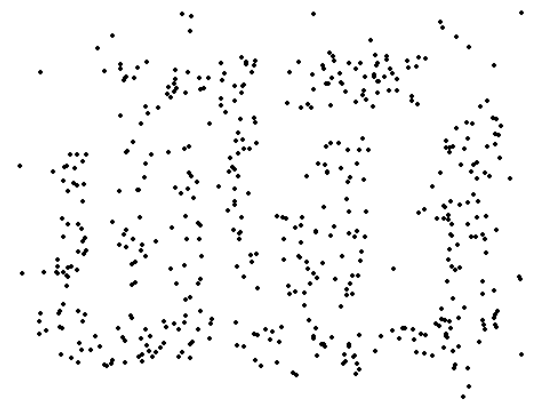
# Sample Size



**8000 points**



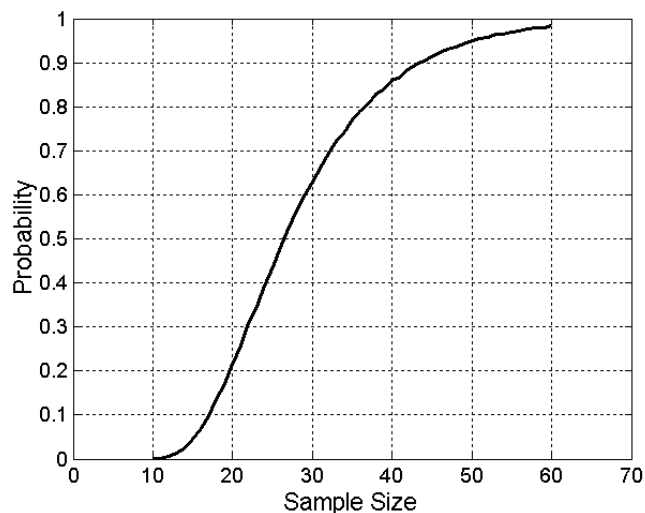
**2000 Points**



**500 Points**

# Sample Size

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

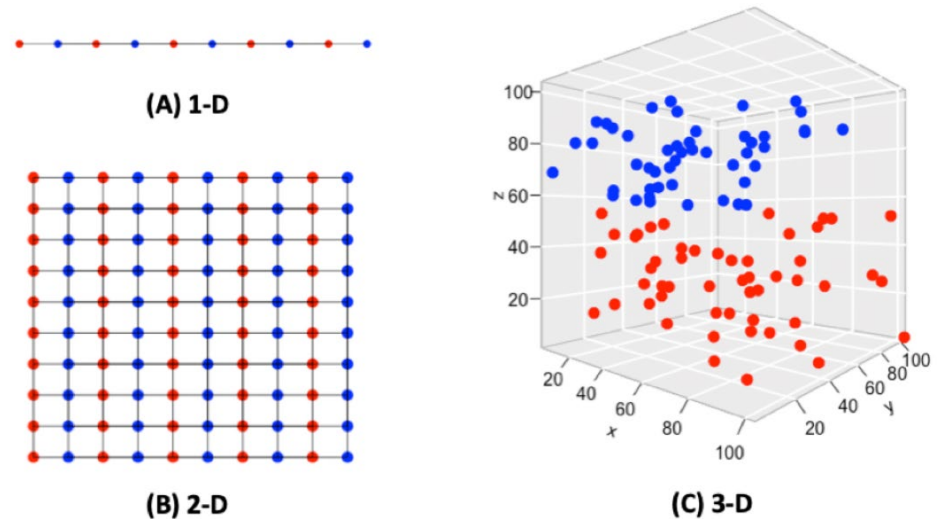


- Sample size determination:
  - Statistics: confidence interval for parameter estimate or desired statistical power of test.
  - Machine learning: often more is better, cross-validated accuracy.



# Curse of Dimensionality

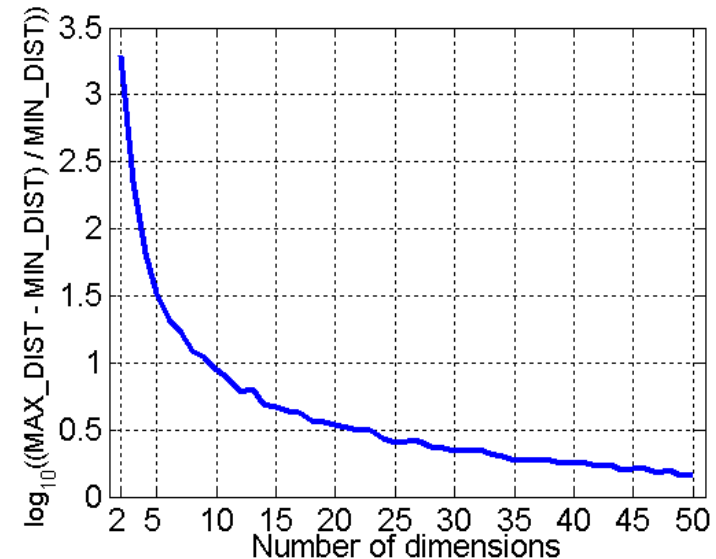
- When dimensionality increases, the size of the data space grows exponentially.



Points and space

- Definitions of density and distance between points, which is critical for clustering and outlier detection, become less meaningful
  - Density  $\rightarrow 0$
  - 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:

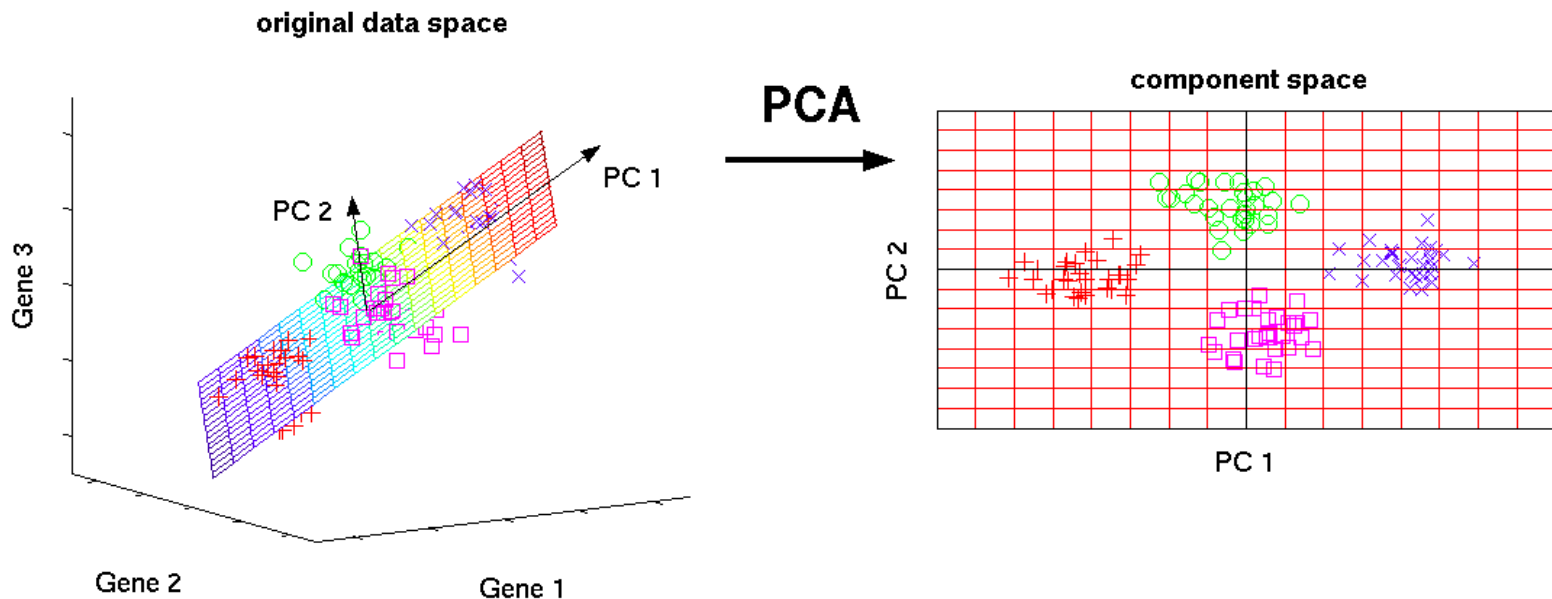
- Avoid curse of dimensionality
- Reduce amount of time and memory required by data mining algorithms
- Allow data to be more easily visualized
- May help to eliminate irrelevant features or reduce noise

- Techniques

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

# Dimensionality Reduction: Principal Components Analysis (PCA)

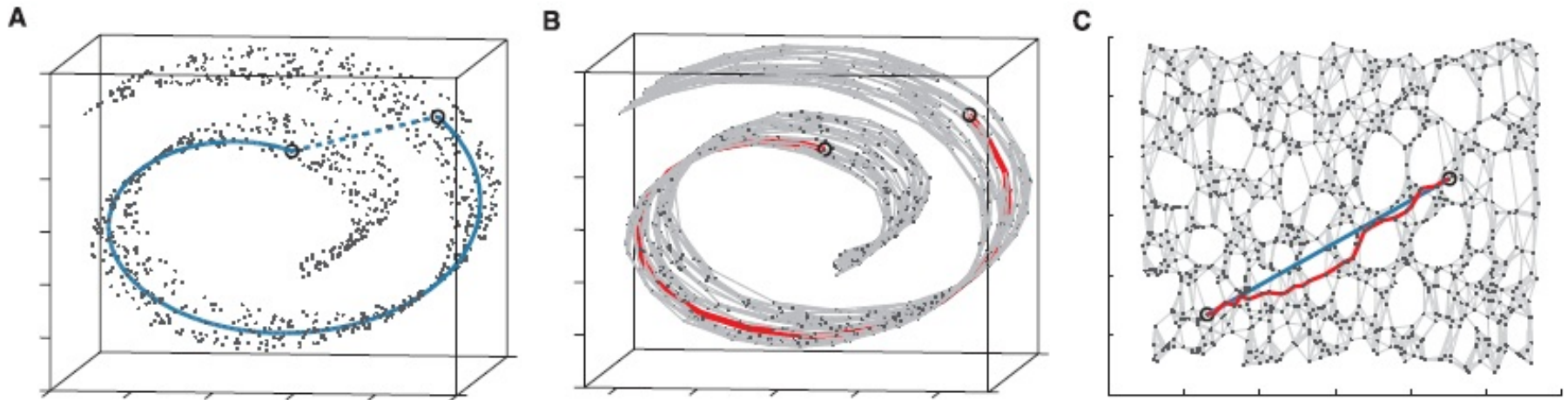
- **Goal:** Map points to a lower dimensional space while preserving distance information.



- **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).



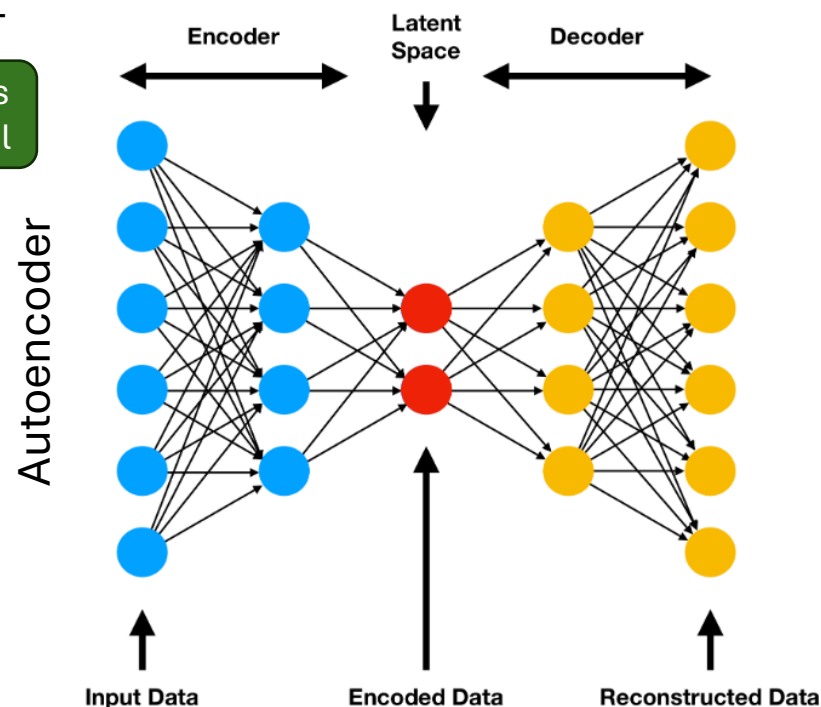
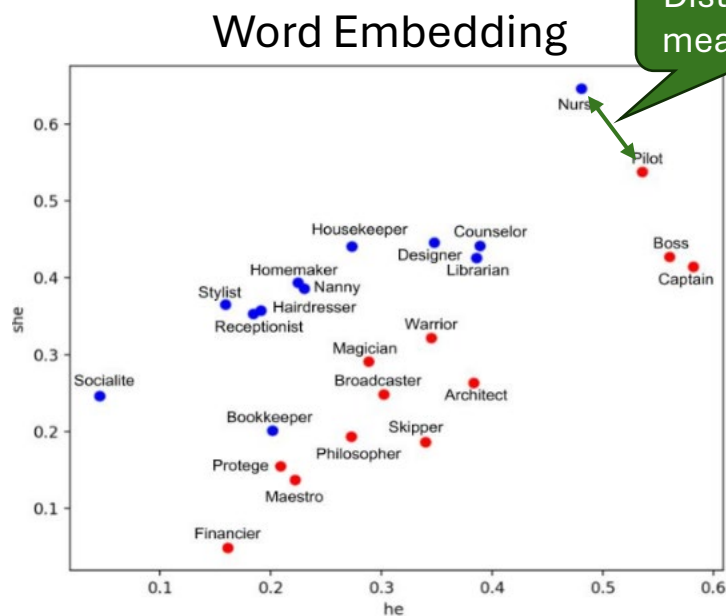
# Dimensionality Reduction: ISOMAP



- **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

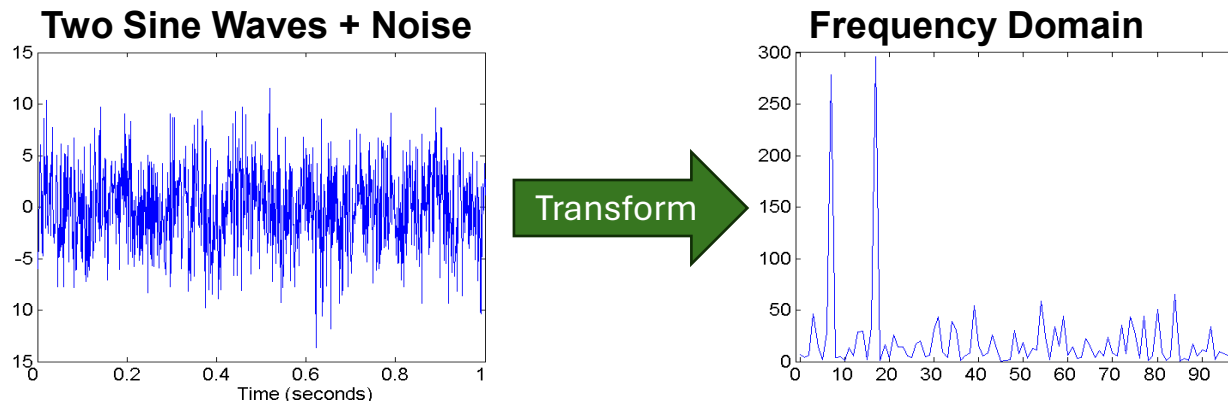
- Embedded approaches:
  - Feature selection occurs naturally as part of the data mining algorithm (e.g., regression, decision trees).
- Filter approaches:
  - Features are selected before data mining algorithm is run
  - (e.g., highly correlated features)
- Brute-force approach:
  - Try all possible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

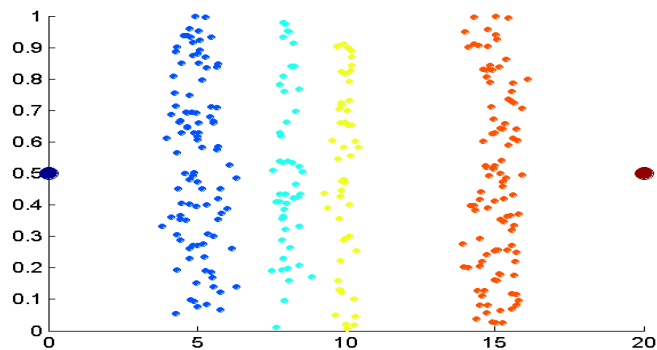
Create new attributes that can capture the important information in a data set much more efficiently than the original attributes

## Three general methodologies

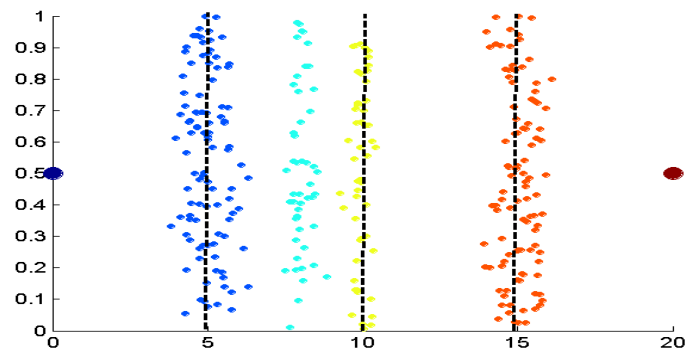
- Feature Extraction
  - Domain-specific (e.g., face recognition in image mining)
- Feature Construction / Feature Engineering
  - combining features (interactions: multiply features)
  - Example: Calculate the body mass index from height and weight
- Mapping Data to New Space
  - Example: Fourier transform/Wavelet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



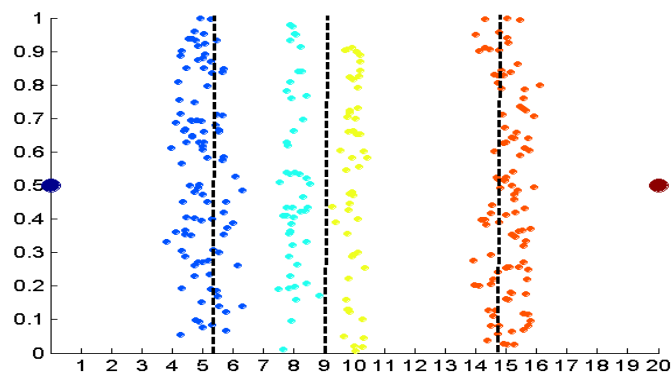
# Unsupervised Discretization



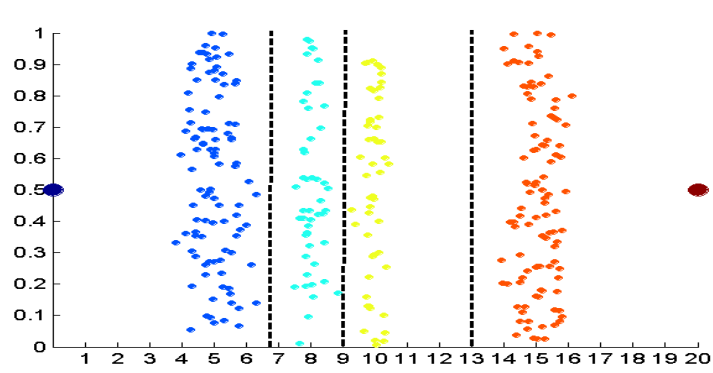
Data



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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- Attributes/Features
- 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

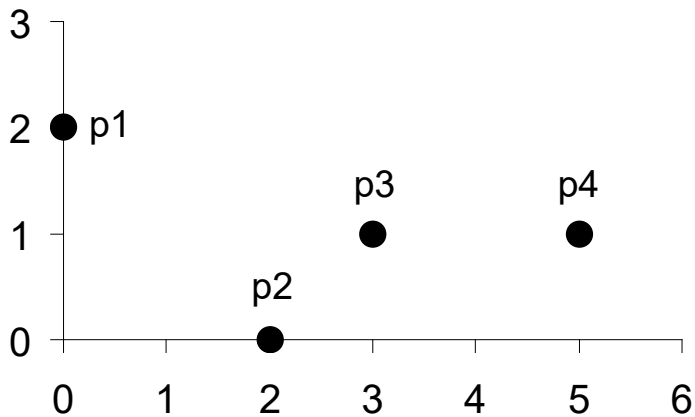
point	x	y
p	0	2
q	2	0

- 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,  $L^\infty$  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

## Distance Matrix

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

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

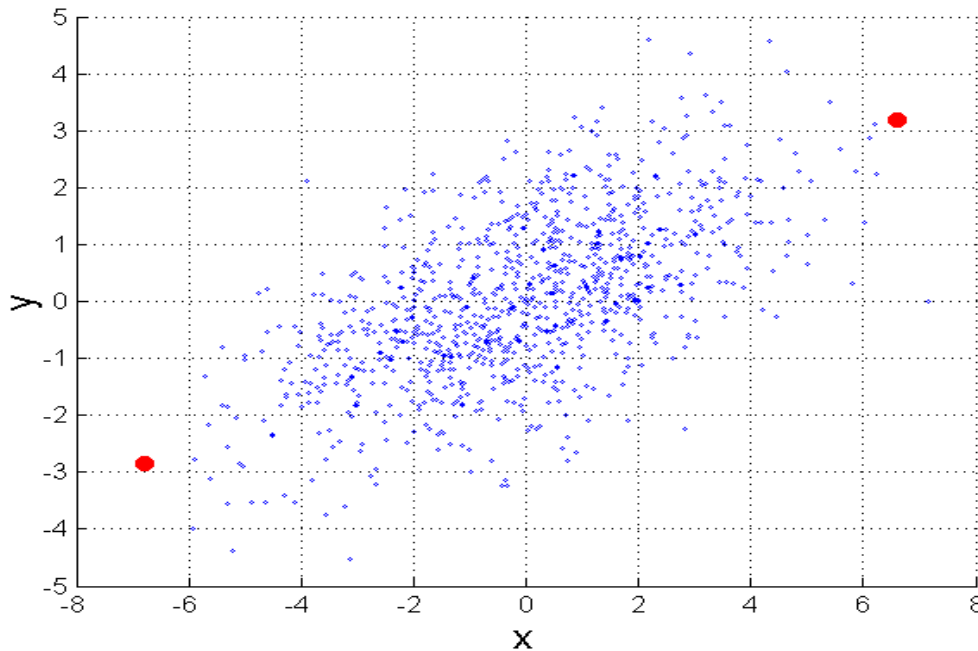
$L^2$	p1	p2	p3	p4
p1	0.00	2.83	3.16	5.10
p2	2.83	0.00	1.41	3.16
p3	3.16	1.41	0.00	2.00
p4	5.10	3.16	2.00	0.00

$L^\infty$	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

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

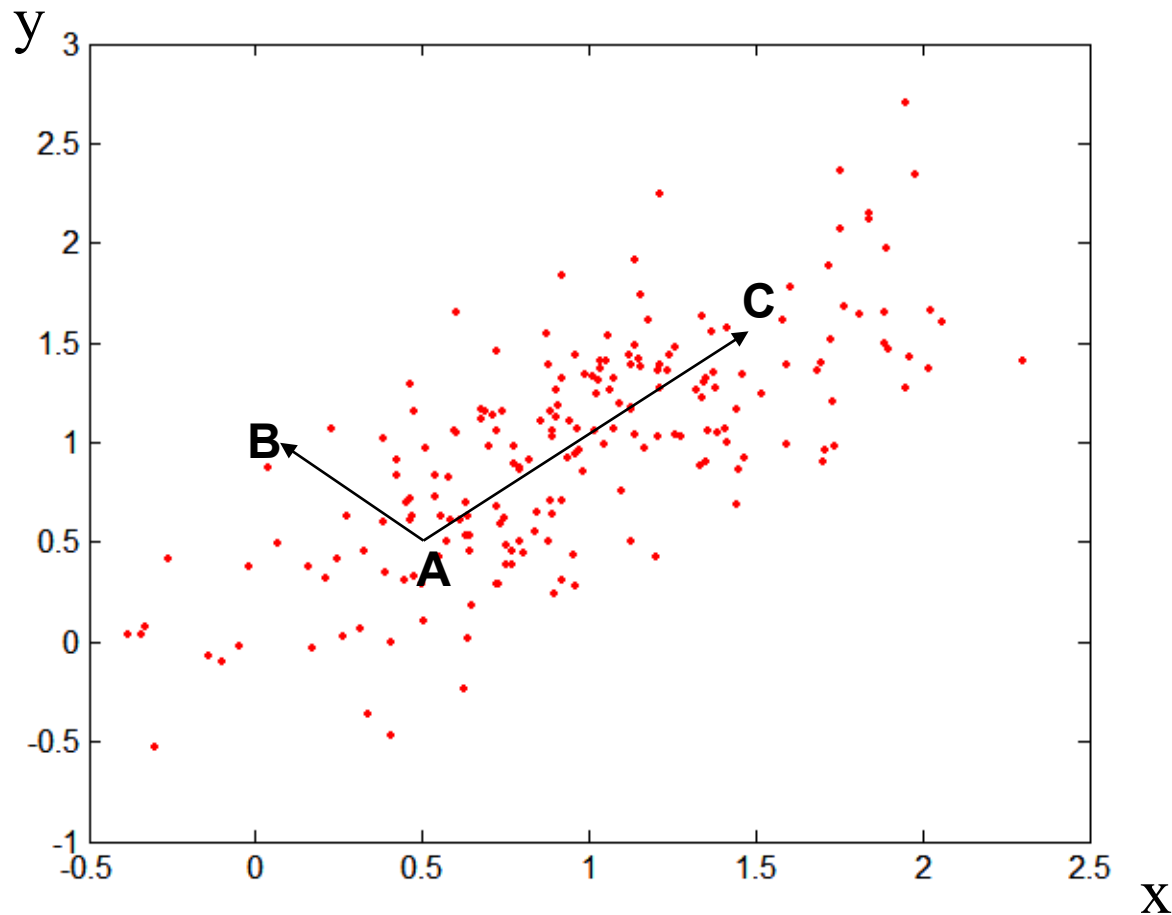


$\mathbf{S}^{-1}$  is the inverse of the covariance matrix of the input data

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

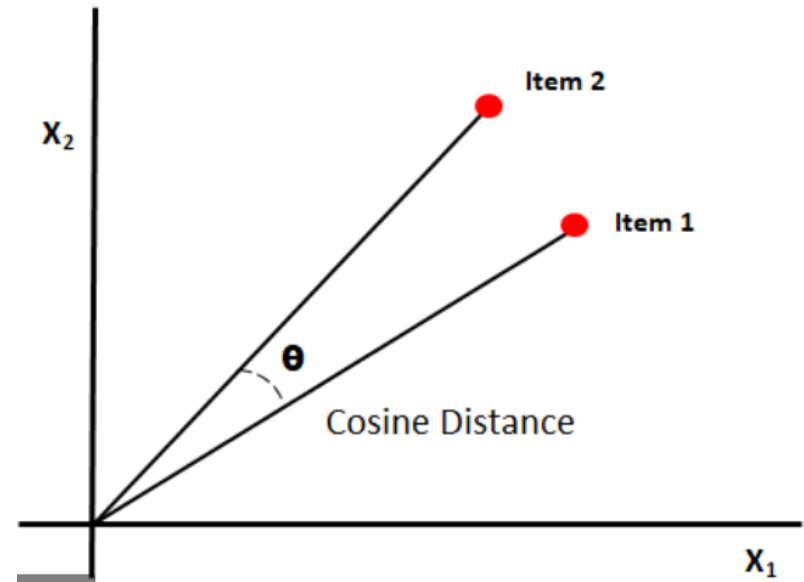
B = 1 0 0 0 0 0 0 1 0 2

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

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

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

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



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,  $\delta_k$ , 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

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- 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.~~

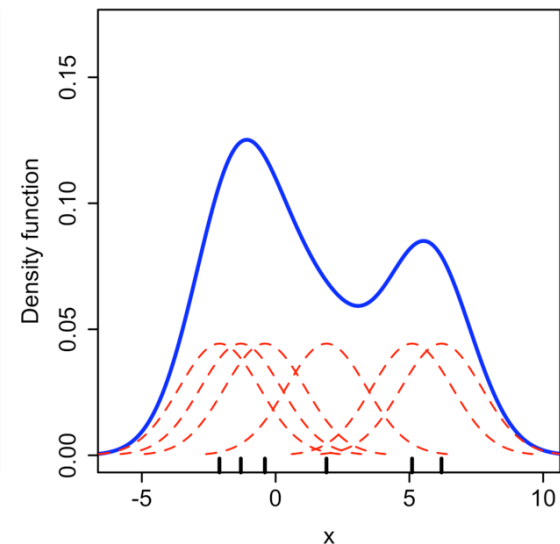
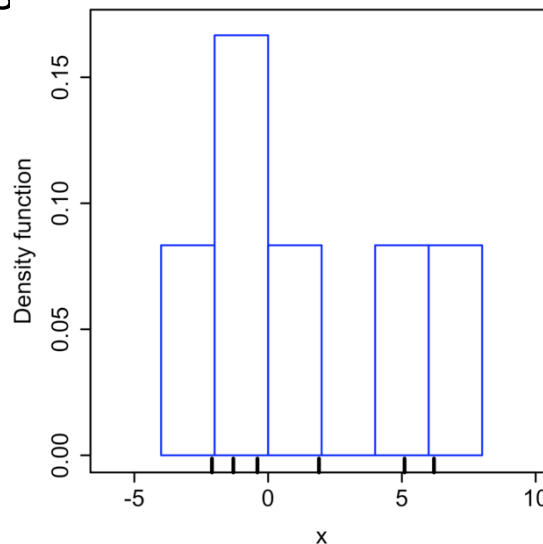
# Kernel Density Estimation (KDE)

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

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

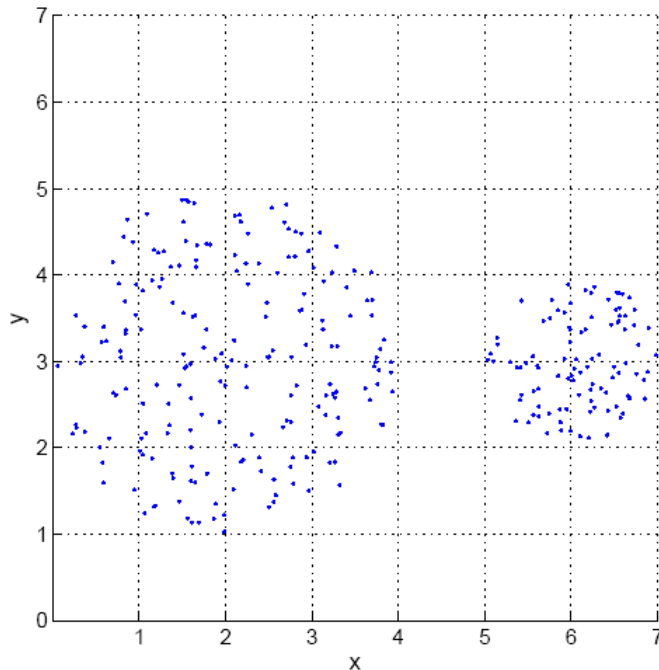
- K is the kernel (a non-negative function that integrates to one) and  $h > 0$  is a smoothing parameter called the bandwidth. Often a Gaussian kernel is used

- 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

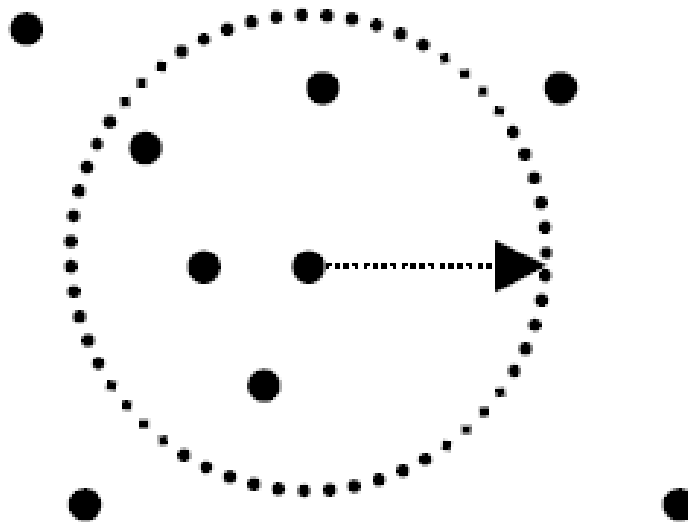


Figure 7.14. Illustration of center-based density.



## You should know now about...

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

