Data Mining: Data

Introduction to Data Mining

Lecture by

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Originally Produced by Tan, Steinbach, Karpatne, and Kumar for the book <<Introduction to Data Mining>>, Modified by S. Liang

Outline

- Attributes and Objects
- Types of Data
- Data Quality
- Similarity and Distance
- Data Preprocessing

What is Data?

- Collection of ***data objects*** and their ***attributes***
- An ***attribute*** is a property or characteristic of an object
  - Examples: eye color of a person, temperature, etc.
  - Attribute is also known as variable, field, characteristic, dimension, or feature
- 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

A More Complete View of Data

- Data may have parts
- The different parts of the data may have relationships
- More generally, data may have structure
- Data can be incomplete
- We will discuss this in more details later

Attribute Values

- ***Attribute values*** are numbers or symbols assigned to an attribute for a particular object

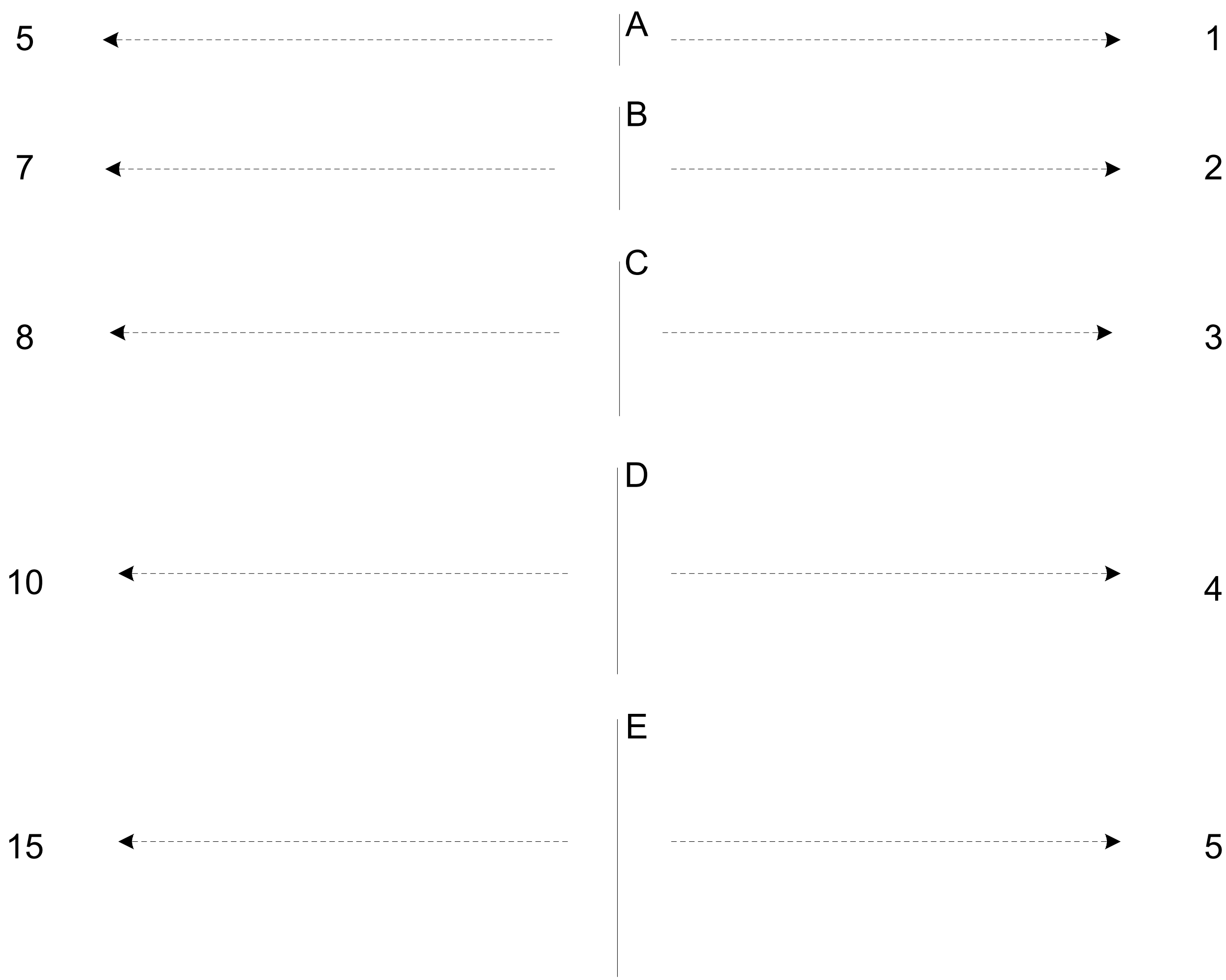
- Distinction between attributes and attribute values
  - Same attribute can be mapped to different attribute values
    - Example: height can be measured in feet or meters

  - 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

Measurement of Length

- The way you measure an attribute may not match the attributes properties.

This scale preserves the ordering and additvity properties of length.



This scale preserves only the ordering property of length.

Types of Attributes

- There are different types of attributes
  - Nominal (标称 / 名词词组)
    - Examples: ID numbers, eye color, zip codes
  - Ordinal
    - Examples: rankings (e.g., taste of potato chips on a scale from 1-10), grades, height {tall, medium, short}
  - Interval
    - Examples: calendar dates, temperatures in Celsius or Fahrenheit.
  - Ratio
    - Examples: temperature in Kelvin, length, time, counts

Properties/operations of Attribute Values

- The type of an attribute depends on which of the following properties/operations it possesses:
  - Distinctness: $= \; \neq$
  - Order: $< \; >$
  - Differences are meaningful : $+ \; -$
  - Ratios are meaningful $* \; /$

  - Nominal attribute: distinctness
  - Ordinal attribute: distinctness & order
  - Interval attribute: distinctness, order & meaningful differences
  - Ratio attribute: all 4 properties/operations

	Attribute Type	Description	Examples	Operations
Categorical Qualitative	Nominal	Nominal attribute values only distinguish. (=, ≠)	zip codes, employee ID numbers, eye color, sex: {*male, female*}	mode, entropy, contingency correlation, $\chi 2$ test
	Ordinal	Ordinal attribute values also order objects. (<, >)	hardness of minerals, {*good, better, best*}, grades, street numbers	median, percentiles, rank correlation, run tests, sign tests
Numeric Quantitative	Interval	For interval attributes, differences between values are meaningful. (+, -)	calendar dates, temperature in Celsius or Fahrenheit	mean, standard deviation, Pearson's correlation, *t* and *F* tests
	Ratio	For ratio variables, both differences and ratios are meaningful. (*, /)	temperature in Kelvin, monetary quantities, counts, age, mass, length, current	geometric mean, harmonic mean, percent variation

This categorization of attributes is due to S. S. Stevens

	Attribute Type	Transformation	Comments
Categorical Qualitative	Nominal	Any permutation of values	If all employee ID numbers were reassigned, would it make any difference?
	Ordinal	An order preserving change of values, i.e., *new_value = f(old_value)* where *f* is a monotonic function	An attribute encompassing the notion of good, better best can be represented equally well by the values {1, 2, 3} or by { 0.5, 1, 10}.
Numeric Quantitative	Interval	*new_value = a * old_value + b* where a and b are constants	Thus, the Fahrenheit and Celsius temperature scales differ in terms of where their zero value is and the size of a unit (degree).
	Ratio	*new_value = a * old_value*	Length can be measured in meters or feet.

This categorization of attributes is due to S. S. Stevens

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.

Asymmetric Attributes/ 不对称属性

- Only presence (a non-zero attribute value) is regarded as important
    - Words present in documents
    - Items present in customer transactions

- If we met a friend in the grocery store would we ever say the following?

  "I see our purchases are very similar since we didn't buy most of the same things."

- We need two asymmetric binary attributes to represent one ordinary binary attribute
    - Association analysis uses asymmetric attributes

- Asymmetric attributes typically arise from objects that are sets

Critiques

- Incomplete
  - Asymmetric binary
  - Cyclical
  - Multivariate
  - Partially ordered
  - Partial membership
  - Relationships between the data

- Real data is approximate and noisy
  - This can complicate recognition of the proper attribute type
  - Treating one attribute type as another may be approximately correct

Critiques ...

- Not a good guide for statistical analysis
  - May unnecessarily restrict operations and results
    - Statistical analysis is often approximate
    - Thus, for example, using interval analysis for ordinal values may be justified
  - Transformations are common but don't preserve scales
    - Can transform data to a new scale with better statistical properties
    - Many statistical analyses depend only on the distribution

More Complicated Examples

- ID numbers
  - Nominal, ordinal, or interval?

- Number of cylinders in an automobile engine
  - Nominal, ordinal, or ratio?

- Biased Scale
  - Interval or Ratio

Key Messages for Attribute Types

- The types of operations you choose should be "meaningful" for the type of data you have
  - Distinctness, order, meaningful intervals, and meaningful ratios are only four properties of data
  - The data type you see – often numbers or strings – may not capture all the properties or may suggest properties that are not there
  - Analysis may depend on these other properties of the data
    - Many statistical analyses depend only on the distribution
  - Many times what is meaningful is measured by statistical significance
  - But in the end, what is meaningful is measured by the domain

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

Important Characteristics of Data

- Dimensionality (number of attributes)
  - High dimensional data brings a number of challenges
- Sparsity
  - Only presence counts
- Resolution (分辨率)
  - Patterns depend on the scale
- Size
  - Type of analysis may depend on size of data

Record Data

- Data that consists of a collection of records, each of which consists of a fixed set of 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**
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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

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.

	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

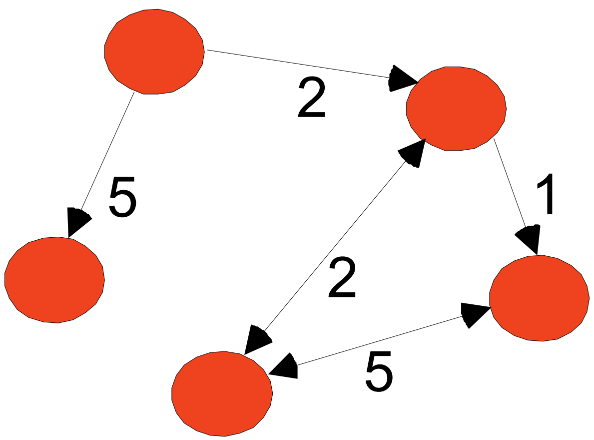
Transaction Data

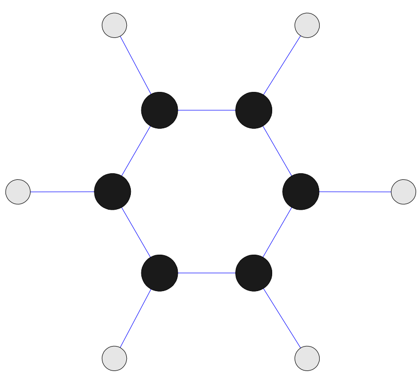
- A special type of record data, where
  - Each record (transaction) involves a set of items.
  - For example, consider a grocery store. The set of products purchased by a customer during one shopping trip constitute a transaction, while the individual products that were purchased are the items.

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

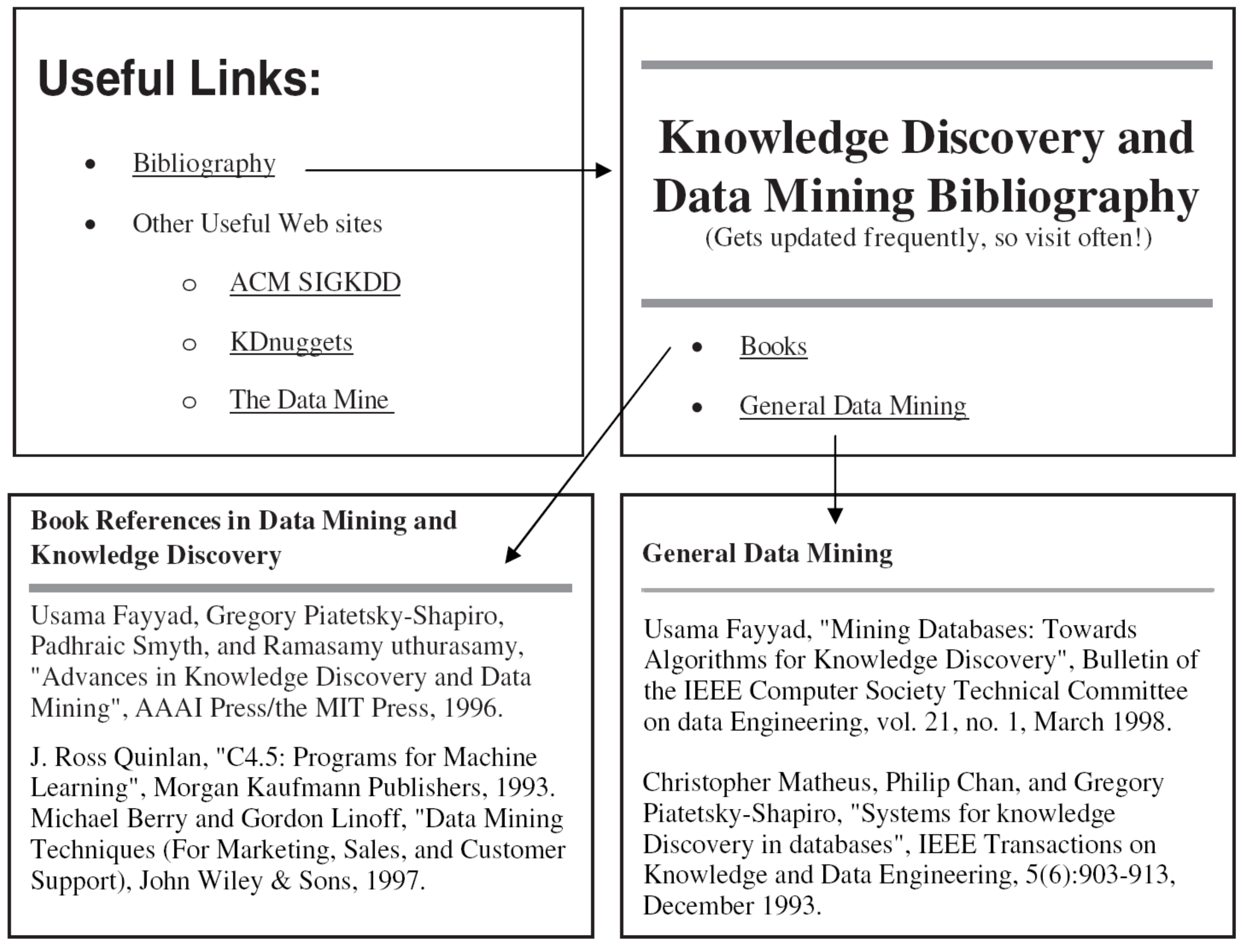
Graph Data

- Examples: Generic graph, a molecule, and webpages





Benzene Molecule: C_6H_6



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

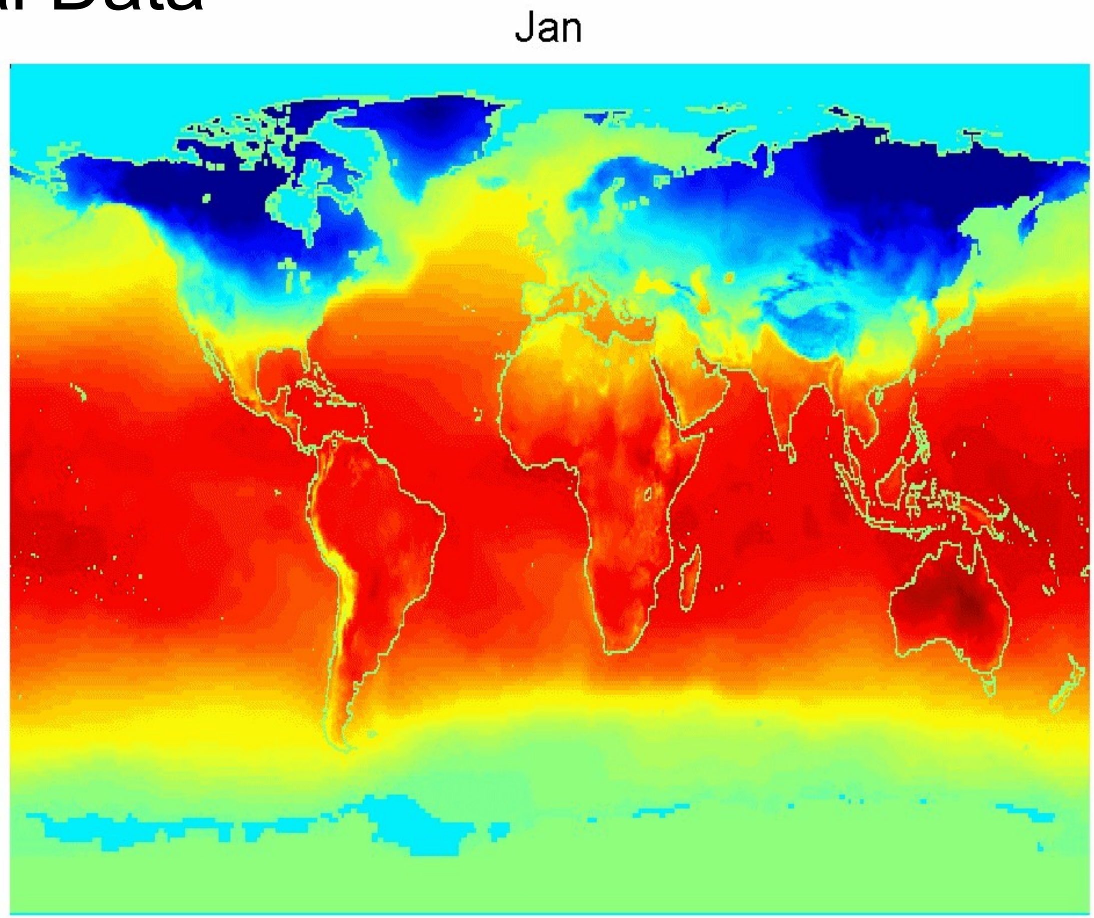
- Genomic sequence data

GGTTCCGCCTTCAGCCCCGCGCC
CGCAGGGCCCGCCCCGCGCCGTC
GAGAAGGGCCCGCCTGGCGGGCG
GGGGGAGGCGGGGCCGCCCGAGC
CCAACCGAGTCCGACCAGGTGCC
CCCTCTGCTCGGCCTAGACCTGA
GCTCATTAGGCGGCAGCGGACAG
GCCAAGTAGAACACGCGAAGCGC
TGGGCTGCCTGCTGCGACCAGGG

Ordered Data

- Spatio-Temporal Data

Average Monthly Temperature of land and ocean



Data Quality

- Poor data quality negatively affects many data processing efforts

"The most important point is that poor data quality is an unfolding disaster.

  – Poor data quality costs the typical company at least ten percent (10%) of revenue; twenty percent (20%) is probably a better estimate."

Thomas C. Redman, DM Review, August 2004

- Data mining example: a classification model for detecting people who are loan risks is built using poor data
  – Some credit-worthy candidates are denied loans
  – More loans are given to individuals that default

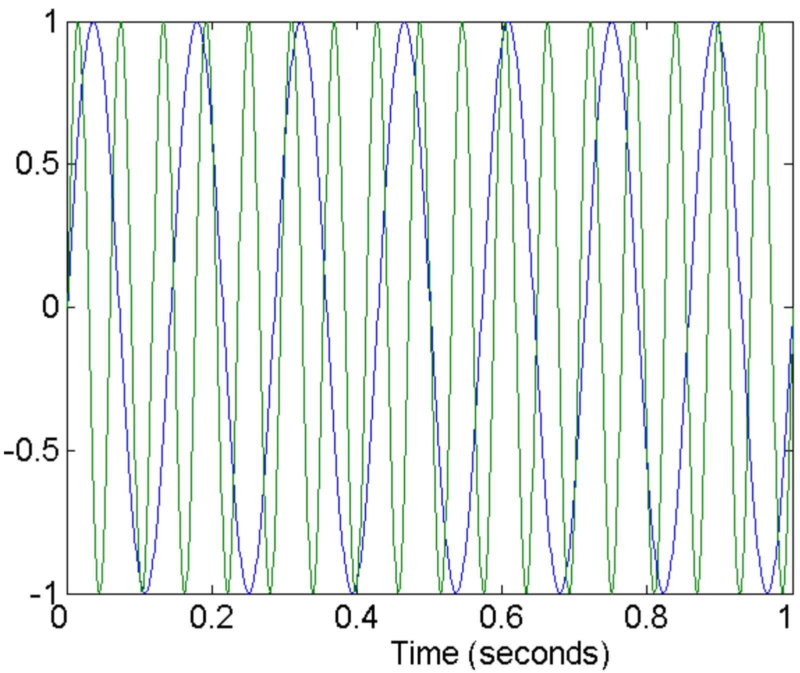
Data Quality …

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

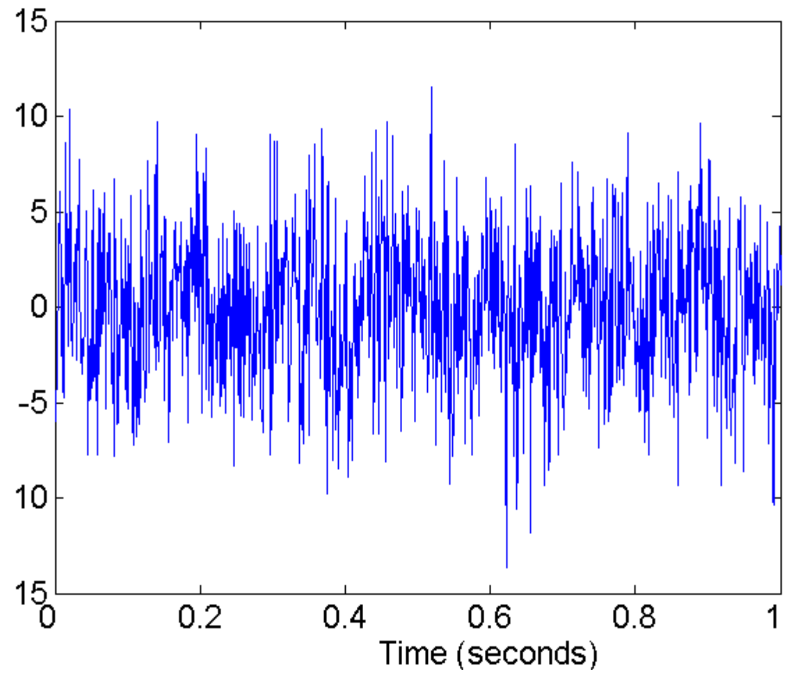
- Examples of data quality problems:
  - Noise and outliers
  - Missing values
  - Duplicate data
  - Wrong data

Noise

- For objects, noise is an extraneous (外来的) object
- For attributes, noise refers to modification of original values
  – Examples: distortion of a person's voice when talking on a poor phone and "snow" on television screen



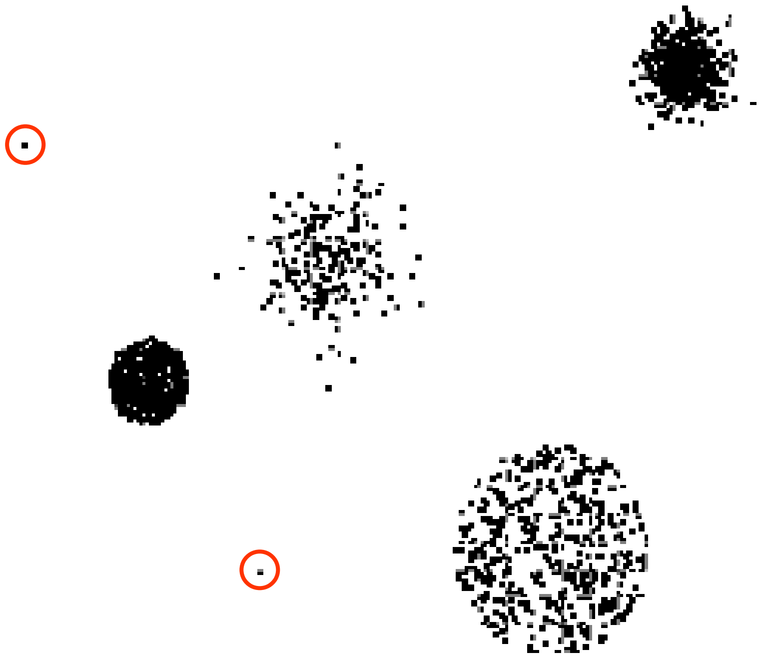
Two Sine Waves



Two Sine Waves + Noise

Outliers

- ***Outliers*** are data objects with characteristics that are considerably different than most of the other data objects in the data set
  - **Case 1:** Outliers are noise that interferes with data analysis
  - **Case 2:** Outliers are the goal of our analysis
    - Credit card fraud
    - Intrusion detection



- Causes?

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 or variables
  - Estimate missing values
    - Example: time series of temperature
    - Example: census results
  - Ignore the missing value during analysis

Missing Values …

- Missing completely at random (MCAR)
  – Missingness of a value is independent of attributes
  – Fill in values based on the attribute
  – Analysis may be unbiased overall
- Missing at Random (MAR)
  – Missingness is related to other variables
  – Fill in values based other values
  – Almost always produces a bias in the analysis
- Missing Not at Random (MNAR)
  – Missingness is related to unobserved measurements
  – Informative or non-ignorable missingness
- Not possible to know the situation from the data

Duplicate Data

- Data set may include data objects that are duplicates, or almost 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
- When should duplicate data not be removed?

Similarity and Dissimilarity Measures

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

The following table shows the similarity and dissimilarity between two objects, x and y, with respect to a single, simple attribute.

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

Euclidean Distance

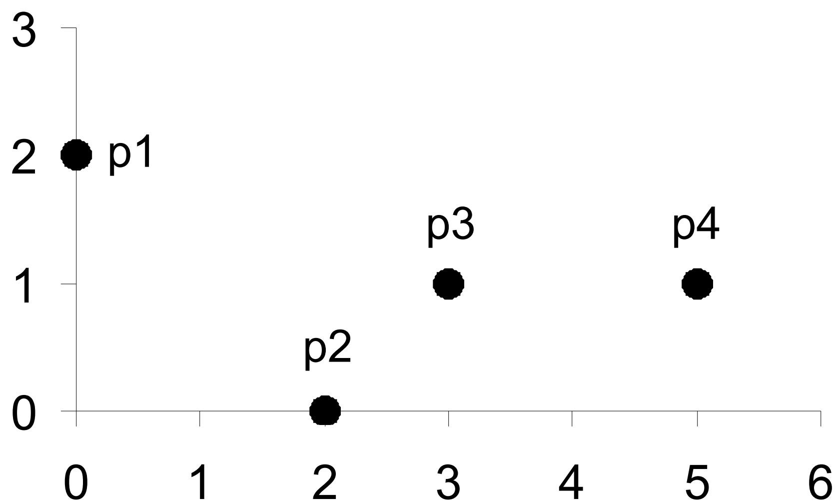
- Euclidean Distance

$$d(\mathbf{x},\mathbf{y}) = \sqrt{\sum_{k=1}^{n}(x_k - y_k)^2}$$

where *n* is the number of dimensions (attributes) and x_k and y_k are, respectively, the k^{th} attributes (components) or data objects $\mathbf{x}$ and $\mathbf{y}$.

- Standardization is necessary, if scales differ.

Euclidean Distance



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

	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Distance Matrix

Minkowski Distance(明式距离 / 明可夫斯基距离)

- Minkowski Distance is a generalization of Euclidean Distance

$$d(\mathbf{x}, \mathbf{y}) = \left(\sum_{k=1}^{n} |x_k - y_k|^r \right)^{1/r}$$

Where r is a parameter, n is the number of dimensions (attributes) and x_k and y_k are, respectively, the k^{th} attributes (components) or data objects $\boldsymbol{x}$ and $\boldsymbol{y}$.

Minkowski Distance: Examples

- $r = 1$. City block (Manhattan(曼哈顿), 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

- $r \rightarrow \infty$. "supremum" (Chebyshev(切比雪夫), L_{max} norm, L_∞ norm) distance.
  - This is the maximum difference between any component of the vectors

$$\lim_{r\to+\infty}\left(\sum_{k=1}^{n}|x_k-y_k|^r\right)^{1/r}=\max_{k=1}^{n}|x_k-y_k|$$

- Do not confuse r with n, i.e., all these distances are defined for all numbers of dimensions.

Minkowski Distance

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

L1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

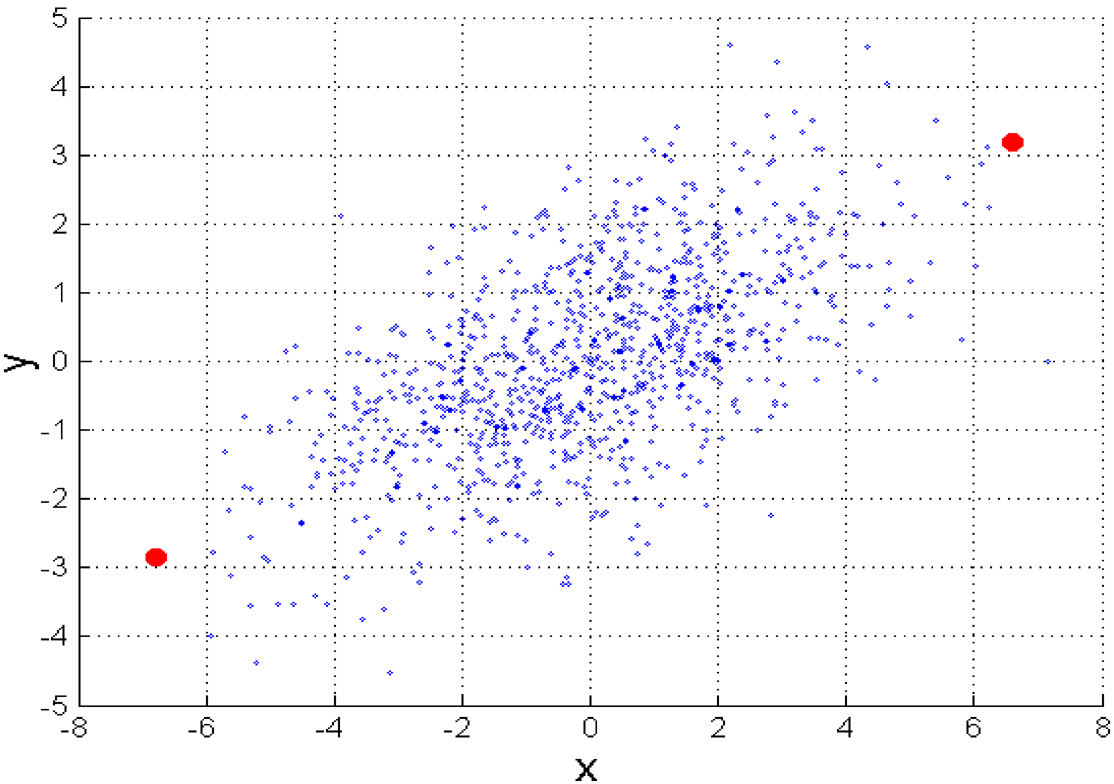
L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

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

Distance Matrix

Mahalanobis Distance(马哈拉诺比斯距离)

$$mahalanobis(x, y) = (x - y)^T \Sigma^{-1} (x - y)$$

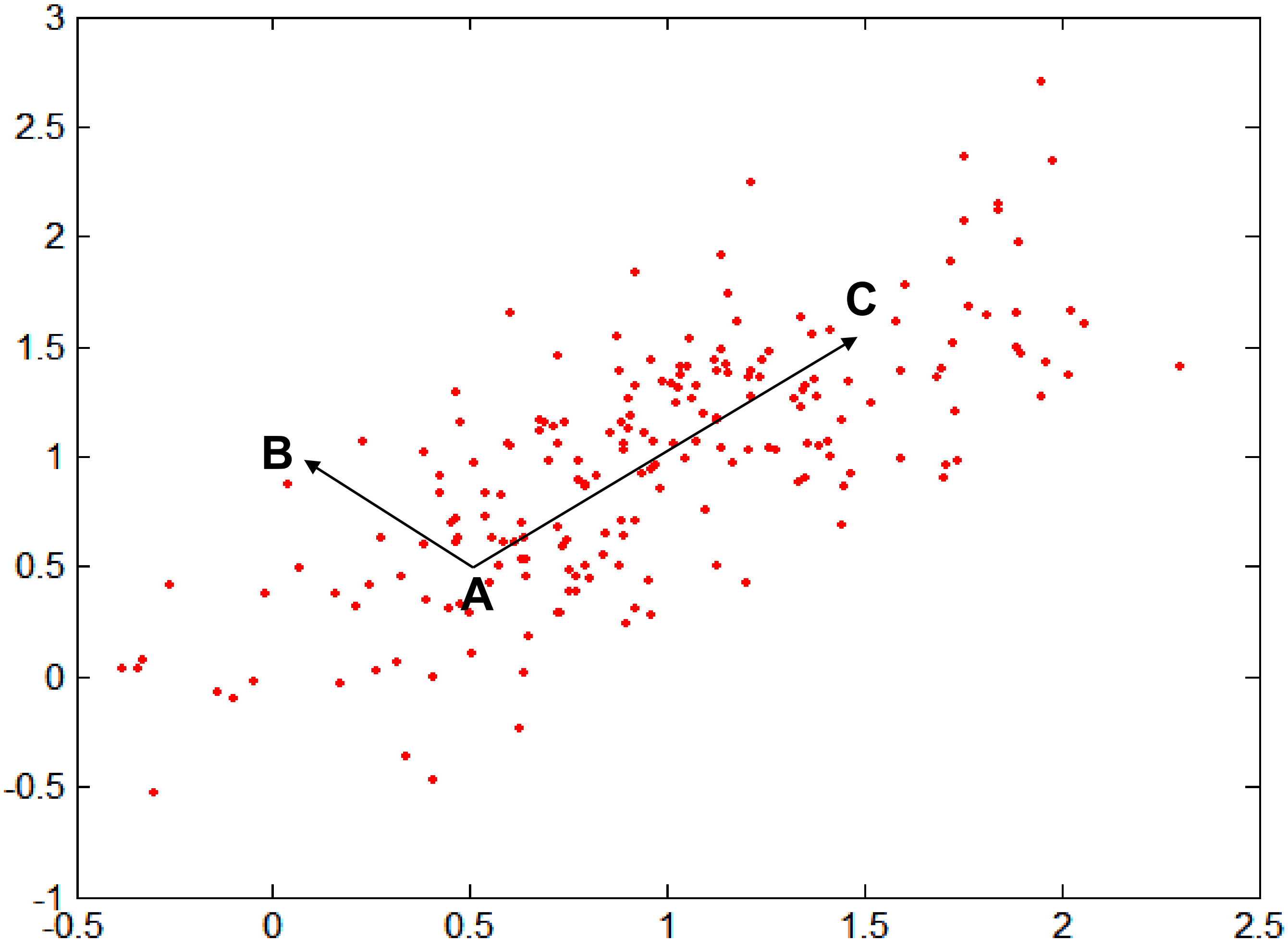


Σ is the covariance matrix

$$\begin{aligned} Cov(X,Y) &= E[(X - E[X])(Y - E[Y])] \\ &= E[XY] - 2E[Y]E[X] + E[X]E[Y] \\ &= E[XY] - E[X]E[Y] \end{aligned}$$

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

Mahalanobis Distance



Covariance Matrix:

$$\Sigma = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{bmatrix}$$

A: (0.5, 0.5)

B: (0, 1)

C: (1.5, 1.5)

Mahal(A,B) = 5

Mahal(A,C) = 4

Common Properties of a Distance

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

  1. $d(\mathbf{x}, \mathbf{y})\ \ 0$ for all *x* and *y* and $d(\mathbf{x}, \mathbf{y}) = 0$ only if $\mathbf{x} = \mathbf{y}$. (Positive definiteness)
  2. $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$ for all $\mathbf{x}$ and $\mathbf{y}$. (Symmetry)
  3. $d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z})$ for all points $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$. (Triangle Inequality)

  where $d(\mathbf{x}, \mathbf{y})$ is the distance (dissimilarity) between points (data objects), $\mathbf{x}$ and $\mathbf{y}$.

- A distance that satisfies these properties is a metric

$$D_{KL}(p||q) = \sum_{i=1}^{N} p(x_i) \cdot (\log p(x_i) - \log q(x_i))$$

Is Kullback–Leibler **divergence a metric? Why?**

Common Properties of a Similarity

- Similarities, also have some well known properties.

  1. $s(\mathbf{x}, \mathbf{y}) = 1$ (or maximum similarity) only if $\mathbf{x} = \mathbf{y}$.

  2. $s(\mathbf{x}, \mathbf{y}) = s(\mathbf{y}, \mathbf{x})$ for all $\mathbf{x}$ and $\mathbf{y}$. (Symmetry)

  where $s(\mathbf{x}, \mathbf{y})$ is the similarity between points (data objects), $\mathbf{x}$ and $\mathbf{y}$.

Similarity Between Binary Vectors

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

- Compute similarities using the following quantities

  f_{01} = the number of attributes where *p* was 0 and *q* was 1

  f_{10} = the number of attributes where *p* was 1 and *q* was 0

  f_{00} = the number of attributes where *p* was 0 and *q* was 0

  f_{11} = the number of attributes where *p* was 1 and *q* was 1

- Simple Matching and Jaccard（雅卡尔）Coefficients

  SMC = number of matches / number of attributes

  $= (f_{11} + f_{00}) / (f_{01} + f_{10} + f_{11} + f_{00})$

  J = number of 11 matches / number of non-zero attributes

  $= (f_{11}) / (f_{01} + f_{10} + f_{11})$

SMC versus Jaccard: Example

$\mathbf{x} =$ 1 0 0 0 0 0 0 0 0 0

$\mathbf{y} =$ 0 0 0 0 0 0 1 0 0 1

$f_{01} = 2$ (the number of attributes where p was 0 and q was 1)

$f_{10} = 1$ (the number of attributes where p was 1 and q was 0)

$f_{00} = 7$ (the number of attributes where p was 0 and q was 0)

$f_{11} = 0$ (the number of attributes where p was 1 and q was 1)

$$\text{SMC} = (f_{11} + f_{00}) / (f_{01} + f_{10} + f_{11} + f_{00})$$
$$= (0+7) / (2+1+0+7) = 0.7$$

$$J = (f_{11}) / (f_{01} + f_{10} + f_{11}) = 0 / (2 + 1 + 0) = 0$$

Cosine Similarity

- If $\mathbf{d}_1$ and $\mathbf{d}_2$ are two document vectors, then

$$\cos(\mathbf{d}_1, \mathbf{d}_2) = \langle \mathbf{d}_1, \mathbf{d}_2 \rangle / \|\mathbf{d}_1\| \, \|\mathbf{d}_2\| ,$$

where $\langle \mathbf{d}_1, \mathbf{d}_2 \rangle$ indicates inner product or vector dot product of vectors, $\mathbf{d}_1$ and $\mathbf{d}_2$, and $\| \mathbf{d} \|$ is the length of vector $\mathbf{d}$.

- Example:

$$\mathbf{d}_1 = 3\ 2\ 0\ 5\ 0\ 0\ 0\ 2\ 0\ 0$$

$$\mathbf{d}_2 = 1\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 2$$

$\langle \mathbf{d}_1, \mathbf{d2} \rangle = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$

$\| \mathbf{d}_1 \| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5} = (42)^{0.5} = 6.481$

$\| \mathbf{d}_2 \| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5} = (6)^{0.5} = 2.449$

$\cos(\mathbf{d}_1, \mathbf{d}_2) = 0.3150$

Correlation measures the linear relationship between objects

$$\mathrm{corr}(\mathbf{x}, \mathbf{y}) = \frac{\mathrm{covariance}(\mathbf{x}, \mathbf{y})}{\mathrm{standard\_deviation}(\mathbf{x}) * \mathrm{standard\_deviation}(\mathbf{y})} = \frac{s_{xy}}{s_x\ s_y}, \quad (2.11$$

where we are using the following standard statistical notation and definitions

$$\mathrm{covariance}(\mathbf{x}, \mathbf{y}) = s_{xy} = \frac{1}{n-1}\sum_{k=1}^{n}(x_k - \overline{x})(y_k - \overline{y}) \quad (2.12$$

$$\begin{aligned}
\mathrm{standard_deviation}(\mathbf{x}) &= s_x = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(x_k - \overline{x})^2} \\
\mathrm{standard_deviation}(\mathbf{y}) &= s_y = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(y_k - \overline{y})^2}
\end{aligned}$$

$$\begin{aligned}
\overline{x} &= \frac{1}{n}\sum_{k=1}^{n} x_k \text{ is the mean of } \mathbf{x} \\
\overline{y} &= \frac{1}{n}\sum_{k=1}^{n} y_k \text{ is the mean of } \mathbf{y}
\end{aligned}$$

Visually Evaluating Correlation

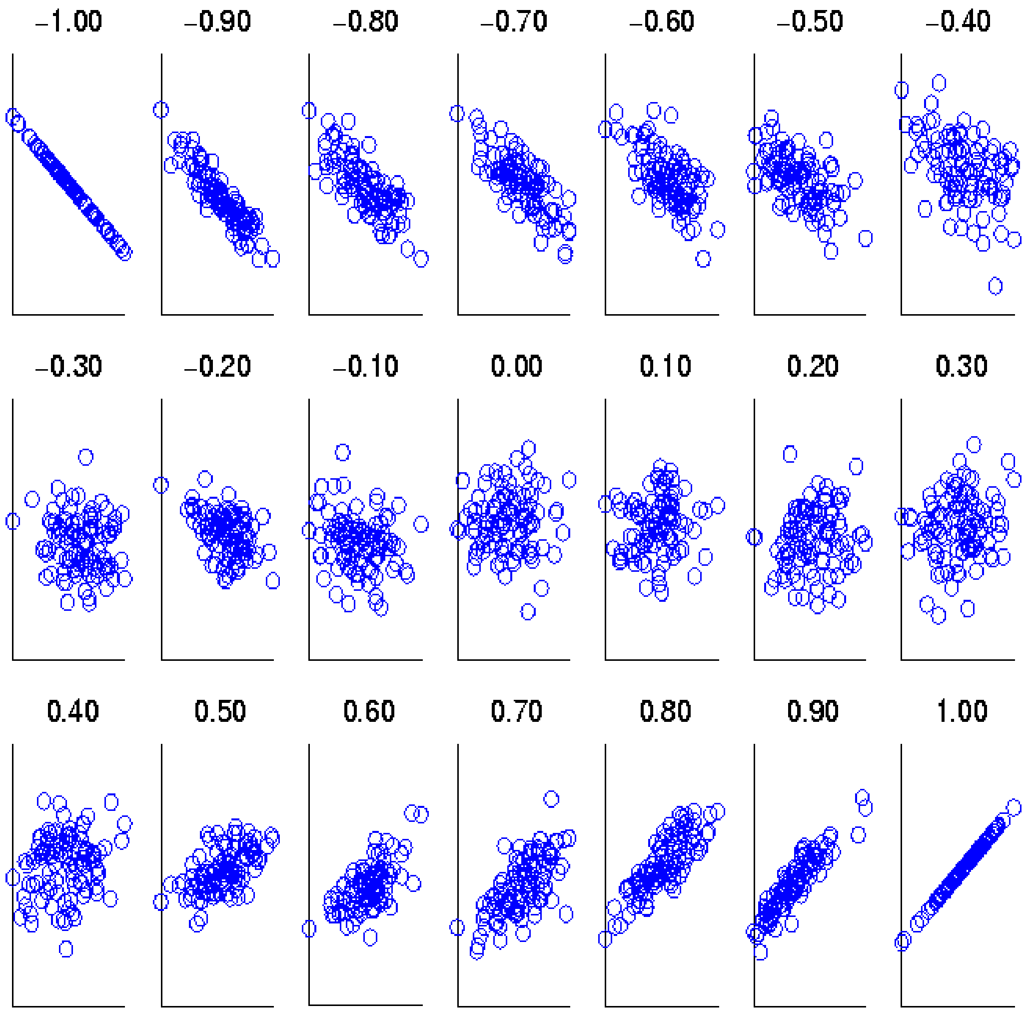


Figure 5.11. Scatter plots illustrating correlations from -1 to 1.

Scatter plots showing the similarity from –1 to 1.

Drawback of Correlation

- $\mathbf{x} = (-3, -2, -1, 0, 1, 2, 3)$
- $\mathbf{y} = (9, 4, 1, 0, 1, 4, 9)$

$$y_i = x_i^2$$

- $\text{mean}(\mathbf{x}) = 0$, $\text{mean}(\mathbf{y}) = 4$
- $\text{std}(\mathbf{x}) = 2.16$, $\text{std}(\mathbf{y}) = 3.74$

- corr = (-3)(5)+(-2)(0)+(-1)(-3)+(0)(-4)+(1)(-3)+(2)(0)+3(5) / (6 * 2.16 * 3.74)
  = 0

Comparison of Proximity Measures

- Domain of application
  - Similarity measures tend to be specific to the type of attribute and data
  - Record data, images, graphs, sequences, 3D-protein structure, etc. tend to have different measures
- However, one can talk about various properties that you would like a proximity measure to have
  - Symmetry is a common one
  - Tolerance to noise and outliers is another
  - Ability to find more types of patterns?
  - Many others possible
- The measure must be applicable to the data and produce results that agree with domain knowledge

Information Based Measures

- Information theory is a well-developed and fundamental disciple with broad applications

- Some similarity measures are based on information theory
  - Mutual information in various versions
  - General and can handle non-linear relationships
  - Can be complicated and time intensive to compute

Information and Probability

- Information relates to possible outcomes of an event
  - transmission of a message, flip of a coin, or measurement of a piece of d

- The more certain an outcome, the less information that it contains and vice-versa
  - For example, if a coin has two heads, then an outcome of heads provides no information
  - More quantitatively, the information is related the probability of an outcome
    - The smaller the probability of an outcome, the more information it provides and vice-versa
  - Entropy is the commonly used measure

Entropy

- For
  - a variable (event), X,
  - with n possible values (outcomes), $x_1, x_2 \ldots, x_n$
  - each outcome having probability, $p_1, p_2 \ldots, p_n$
  - the entropy of X , $H(X)$, is given by

- Entropy is between 0 and $\log_2 n$ and is measured in bits
  - Thus, entropy is a measure of how many bits it takes to represent an observation of X on average

Entropy Examples

- For a coin with probability p of heads and probability $q = 1 - p$ of tails

  - For $p = 0.5$, $q = 0.5$ (fair coin) $H = 1$
  - For $p = 1$ or $q = 1$, $H = 0$

- What is the entropy of a fair four-sided die?

Entropy for Sample Data: Example

Hair Color	Count	p	$-p\log_2 p$
Black	75	0.75	0.3113
Brown	15	0.15	0.4105
Blond	5	0.05	0.2161
Red	0	0.00	0
Other	5	0.05	0.2161
Total	100	1.0	1.1540

Maximum entropy is $\log_2 5 = 2.3219$

Entropy for Sample Data

- Suppose we have
  - a number of observations (m) of some attribute, X, e.g., the hair color of students in the class,
  - where there are n different possible values
  - And the number of observation in the i^{th} category is m_i
  - Then, for this sample

- For continuous data, the calculation is harder

Conditional Entropy

$$
\begin{aligned}
\mathrm{H}(Y|X) &\equiv \sum_{x\in\mathcal{X}} p(x)\,\mathrm{H}(Y|X=x) \\
&= -\sum_{x\in\mathcal{X}} p(x) \sum_{y\in\mathcal{Y}} p(y|x)\,\log p(y|x) \\
&= -\sum_{x\in\mathcal{X}} \sum_{y\in\mathcal{Y}} p(x,y)\,\log p(y|x) \\
&= -\sum_{x\in\mathcal{X},y\in\mathcal{Y}} p(x,y)\log p(y|x) \\
&= -\sum_{x\in\mathcal{X},y\in\mathcal{Y}} p(x,y)\log \frac{p(x,y)}{p(x)}. \\
&= \sum_{x\in\mathcal{X},y\in\mathcal{Y}} p(x,y)\log \frac{p(x)}{p(x,y)}.
\end{aligned}
$$

Mutual Information

- Information one variable provides about another

Formally, , where

H(X,Y) is the joint entropy of X and Y,

Where p_{ij} is the probability that the i^{th} value of X and the j^{th} value of Y occur together. It also can be computed as:

$$I(X;Y) = \sum_{y \in Y} \sum_{x \in X} p(x,y) \log \left(\frac{p(x,y)}{p(x)\,p(y)} \right)$$

- For discrete variables, this is easy to compute

- Maximum mutual information for discrete variables is $\log_2(\min(n_X, n_Y))$, where n_X (n_Y) is the number of values of X (Y)

Mutual Information Example

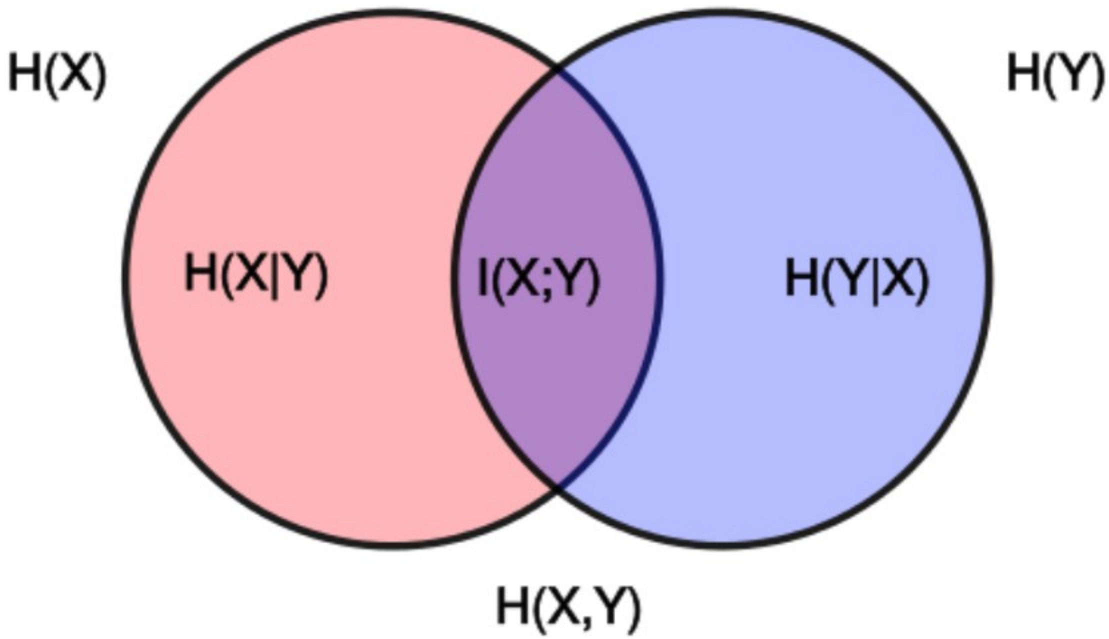
Student Status	Count	p	$-p\log_2 p$
Undergrad	45	0.45	0.5184
Grad	55	0.55	0.4744
Total	100	1.00	0.9928

Grade	Count	p	$-p\log_2 p$
A	35	0.35	0.5301
B	50	0.50	0.5000
C	15	0.15	0.4105
Total	100	1.00	1.4406

Student Status	Grade	Count	p	$-p\log_2 p$
Undergrad	A	5	0.05	0.2161
Undergrad	B	30	0.30	0.5211
Undergrad	C	10	0.10	0.3322
Grad	A	30	0.30	0.5211
Grad	B	20	0.20	0.4644
Grad	C	5	0.05	0.2161
Total		100	1.00	2.2710

Mutual information of Student Status and Grade = 0.9928 + 1.4406 - 2.2710 = 0.1624

Relationship



General Approach for Combining Similarities

- Sometimes attributes are of many different types, but an overall similarity is needed.

1: For the k^{th} attribute, compute a similarity, $s_k(\mathbf{x}, \mathbf{y})$, in the range [0, 1].

2: Define an indicator variable, δ_k, for the k^{th} attribute as follows:

$\delta_k = 0$ if the k^{th} attribute is an asymmetric attribute and both objects have a value of 0, or if one of the objects has a missing value for the kth attribute

$\delta_k = 1$ otherwise

3. Compute

$$\text{similarity}(\mathbf{x}, \mathbf{y}) = \frac{\sum_{k=1}^{n} \delta_k s_k(\mathbf{x}, \mathbf{y})}{\sum_{k=1}^{n} \delta_k}$$

Using Weights to Combine Similarities

- May not want to treat all attributes the same.
  - Use non-negative weights

- Can also define a weighted form of distance

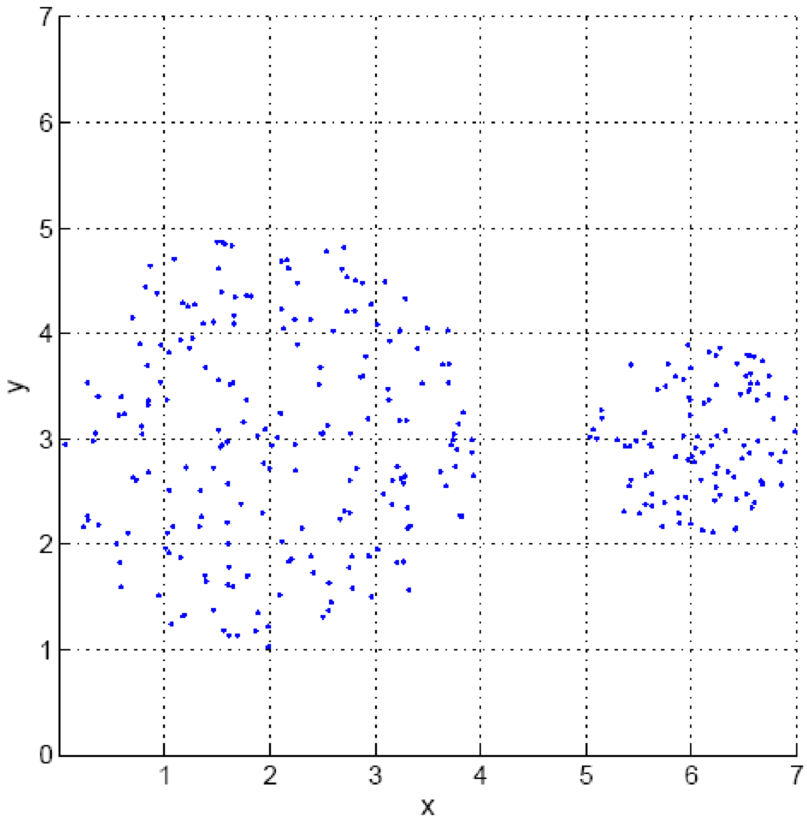
$$d(\mathbf{x}, \mathbf{y}) = \left(\sum_{k=1}^{n} w_k |x_k - y_k|^r \right)^{1/r}$$

Density

- Measures the degree to which data objects are close to each other in a specified area
- The notion of density is closely related to that of proximity
- Concept of density is typically used for clustering and anomaly detection
- Examples:
  - Euclidean density
    - Euclidean density = number of points per unit volume
  - Probability density
    - Estimate what the distribution of the data looks like
  - Graph-based density
    - Connectivity

Euclidean Density: Grid-based Approach

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



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

Euclidean Density: Center-Based

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

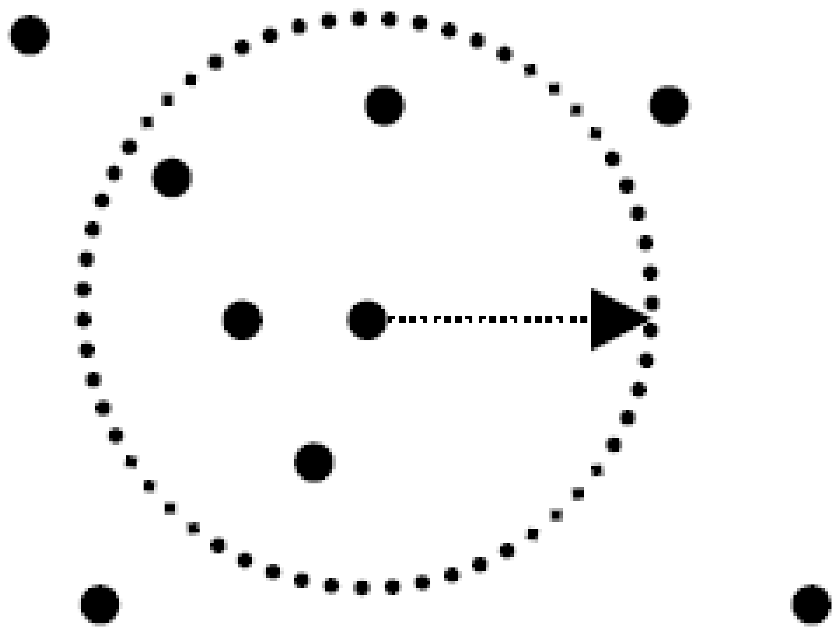


Illustration of center-based density.

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.
    - Days aggregated into weeks, months, or years
  - More "stable" data
    - Aggregated data tends to have less variability

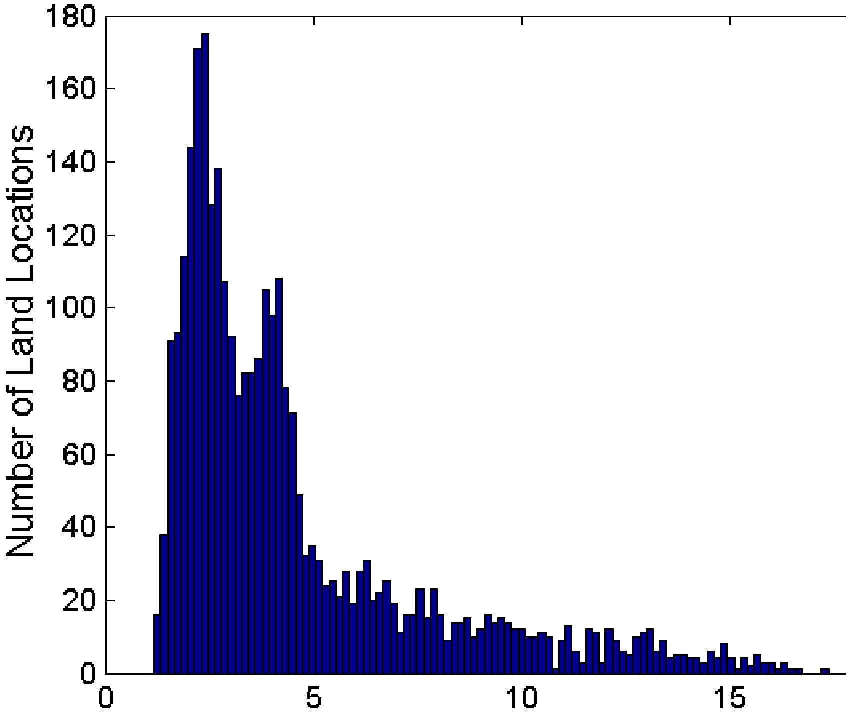
Example: Precipitation in Australia

- This example is based on precipitation（降雨量）in Australia from the period 1982 to 1993.

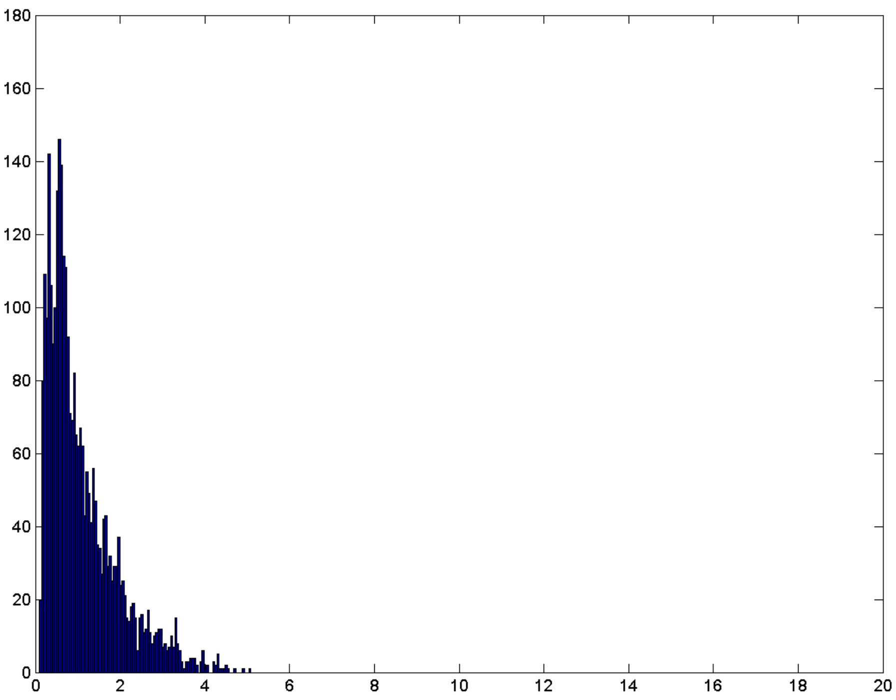
  The next slide shows
  - A histogram for the standard deviation of average monthly precipitation for 3,030 0.5◦ by 0.5◦ grid cells in Australia, and
  - A histogram for the standard deviation of the average yearly precipitation for the same locations.
- The average yearly precipitation has less variability than the average monthly precipitation.
- All precipitation measurements (and their standard deviations) are in centimeters.

Example: Precipitation in Australia …

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 reduction.
  - It is often used for both the preliminary investigation of the data and the final data analysis.

- Statisticians often sample because obtaining the entire set of data of interest is too expensive or time consuming.

- Sampling is typically used in data mining because processing the entire set of data of interest is too expensive or time consuming.

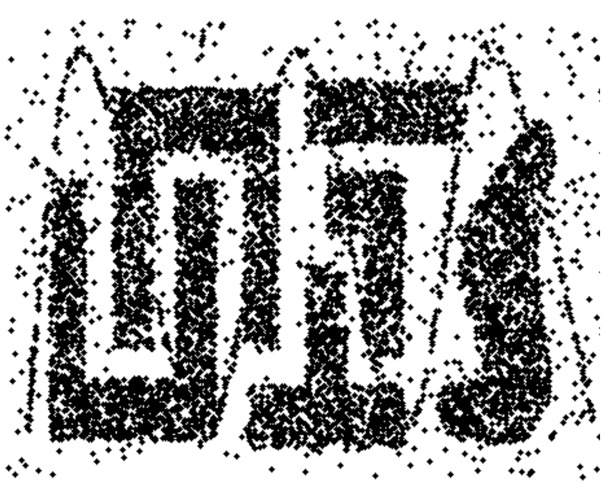
Sampling …

- The key principle for effective sampling is the following:

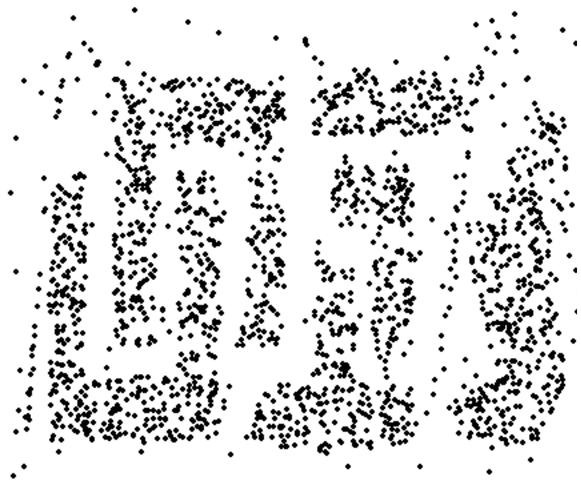
  – Using a sample will work almost as well as using the entire data set, if the sample is representative

  – A sample is representative if it has approximately the same properties (of interest) as the original set of data

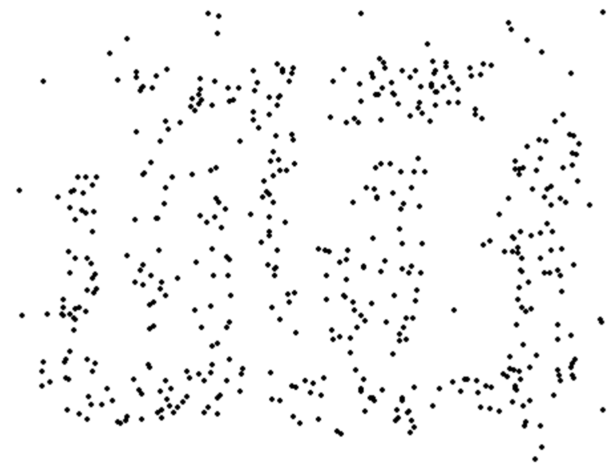
Sample Size



8000 points



2000 Points



500 Points

Types of Sampling

- Simple Random Sampling
  - There is an equal probability of selecting any particular item
  - 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.
    - In sampling with replacement, the same object can be picked up more than once
- Stratified (层级的) sampling
  - Split the data into several partitions; then draw random samples from each partition

Monte Carlo Methods

- Monte Carlo Estimator: Evaluating Integrals

$$E[f(X)] = \int f(X) P_X(X)\, dX.$$

$$\begin{aligned} Var(X) &= E[(X - E[X])^2], \\ &= E[X^2] - E[X]^2. \end{aligned}$$

Monte Carlo Methods

- Image that we want to integrate a one-dimensional function f(x) from a to b :

$$F = \int_a^b f(x)\, dx.$$

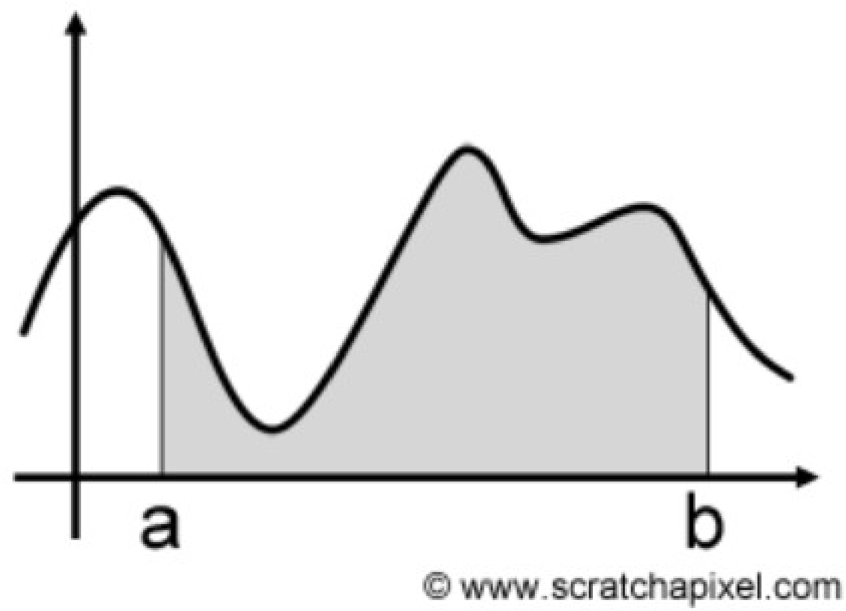


Figure 1: the integral over the domain [a,b] can be seen as the area under the curve.

Monte Carlo Methods

- Image that we want to integrate a one-dimensional function f(x) from a to b :

$$F = \int_a^b f(x)\,dx.$$

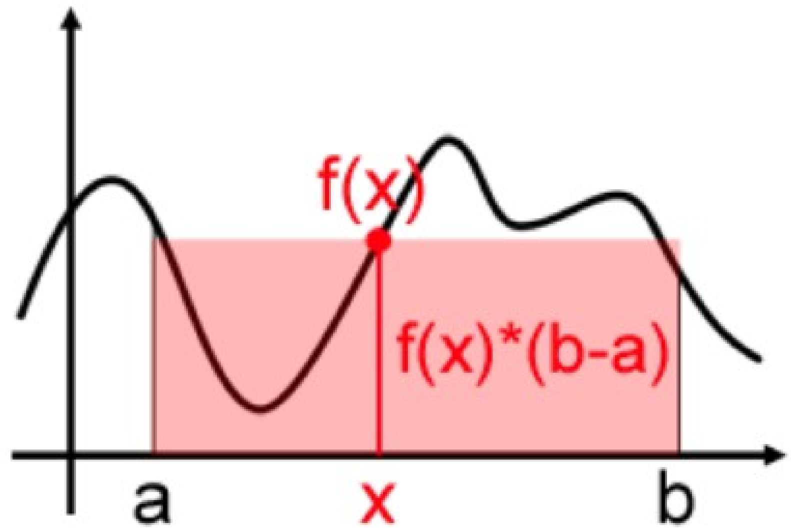
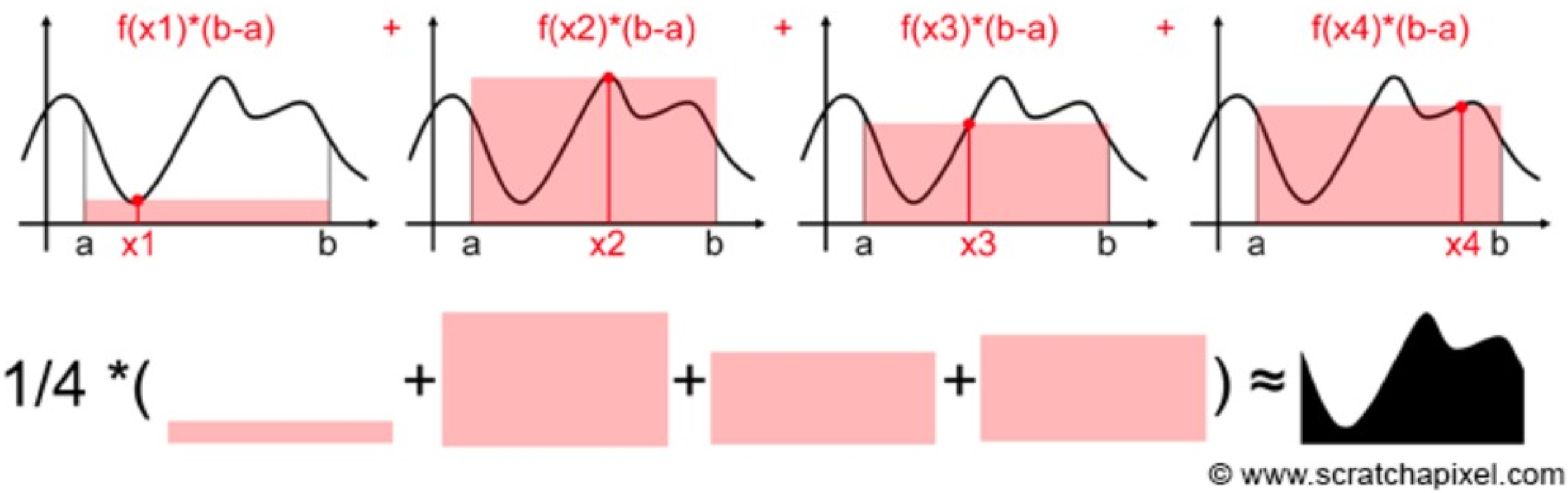


Figure 2: the curve can be evaluated at x and the result can be multiplied by (b - a). This defines a rectangle which can be seen as a very crude approximation of the integral.

Monte Carlo Methods

- Image that we want to integrate a one-dimensional function f(x) from a to b :

$$F = \int_a^b f(x)\, dx.$$



Monte Carlo Methods

- We can formalize this idea with the following formula:

$$\langle F^N \rangle = (b-a)\frac{1}{N}\sum_{i=0}^{N-1} f(X_i).$$

$X_i = a + \xi(b-a)$, where ξ is uniformly distributed between zero and one.

Basic Monte Carlo Estimator

Monte Carlo Methods

- Image that we want to integrate a one-dimensional function f(x) from a to b :

$$F = \int_a^b f(x)\, dx.$$

It is important here to note that:

$$Pr(\lim_{N\to\infty} \langle F^N \rangle = F) = 1.$$

Monte Carlo Methods

It is important here to note that:

$$Pr(\lim_{N\to\infty} \langle F^N \rangle = F) = 1.$$

Note also that $\langle F^N \rangle$ is a random variable, since it's actually made up of a sum of random numbers. We can now proof that the expected value of $\langle F^N \rangle$ is equal to F:

$$\begin{aligned}
E[< F^N >] &= E\left[(b-a)\frac{1}{N}\sum_{i=0}^{N-1} f(x_i)\right] \\
&= (b-a)\frac{1}{N}E\left[\sum_{i=0}^{N-1} f(x_i)\right] \\
&= (b-a)\frac{1}{N}\sum_{i=0}^{N-1}\int_a^b f(x)pdf(x)dx \\
&= \frac{1}{N}\sum_{i=0}^{N-1}\int_a^b f(x)dx \\
&= \int_a^b f(x)dx \\
&= F
\end{aligned}$$

Monte Carlo Methods

- Generalization to Arbitrary PDF
  - We can extend Monte Carlo integration to random variables with arbitrary PDFs. The more generic formula is then:

$$\langle F^N \rangle = \frac{1}{N} \sum_{i=0}^{N-1} \frac{f(X_i)}{pdf(X_i)}.$$

The pdf in the denominator is the same as the pdf of the random variable X

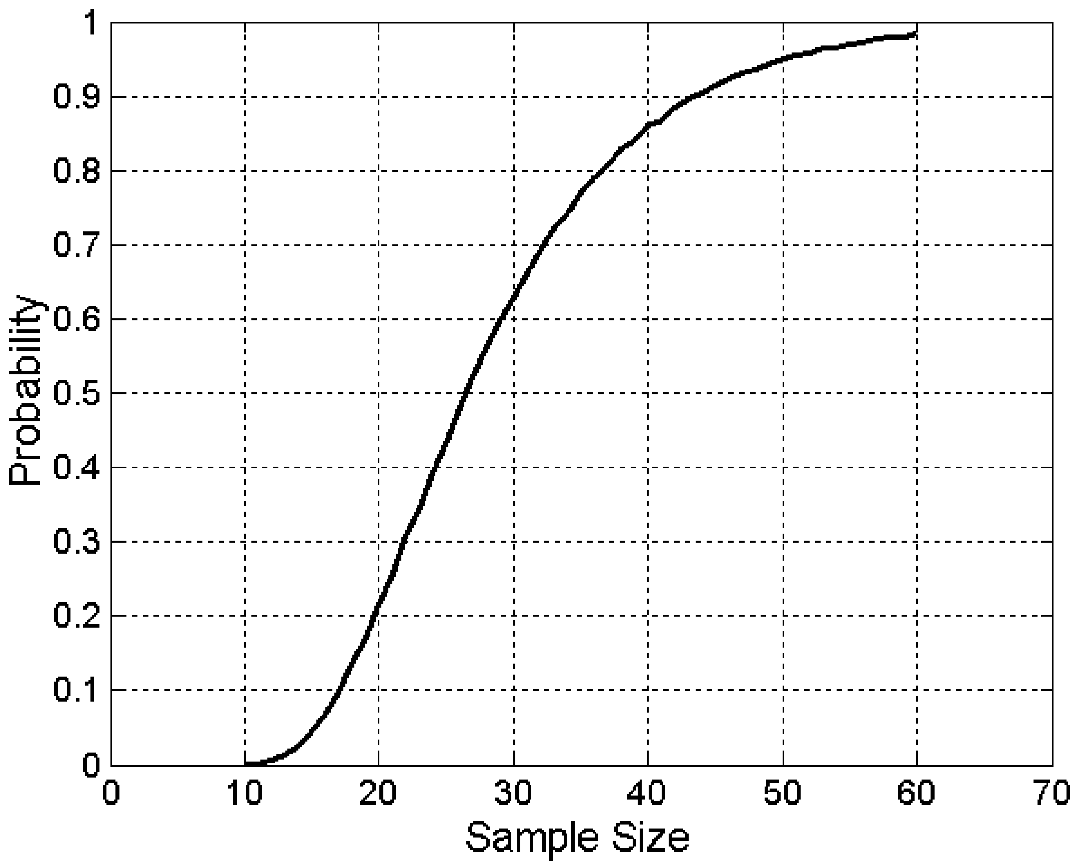
Monte Carlo Methods

- Generalization to Arbitrary PDF
  - We can extend Monte Carlo integration to random variables with arbitrary PDFs. The more generic formula is then:

$$
\begin{aligned}
E[\langle F^N \rangle] &= E\left[\frac{1}{N}\sum_{i=0}^{N-1}\frac{f(X_i)}{pdf X_i)}\right], \\
&= \frac{1}{N}\sum_{i=0}^{N-1} E\left[\frac{f(X_i)}{pdf(X_i)}\right], \\
&= \frac{1}{N}\sum_{i=0}^{N-1} \int_\Omega \frac{f(x)}{pdf(x)} pdf(x)\, dx, \\
&= \frac{1}{N}\sum_{i=0}^{N-1} \int_\omega f(x)\, dx, \\
&= F.
\end{aligned}
$$

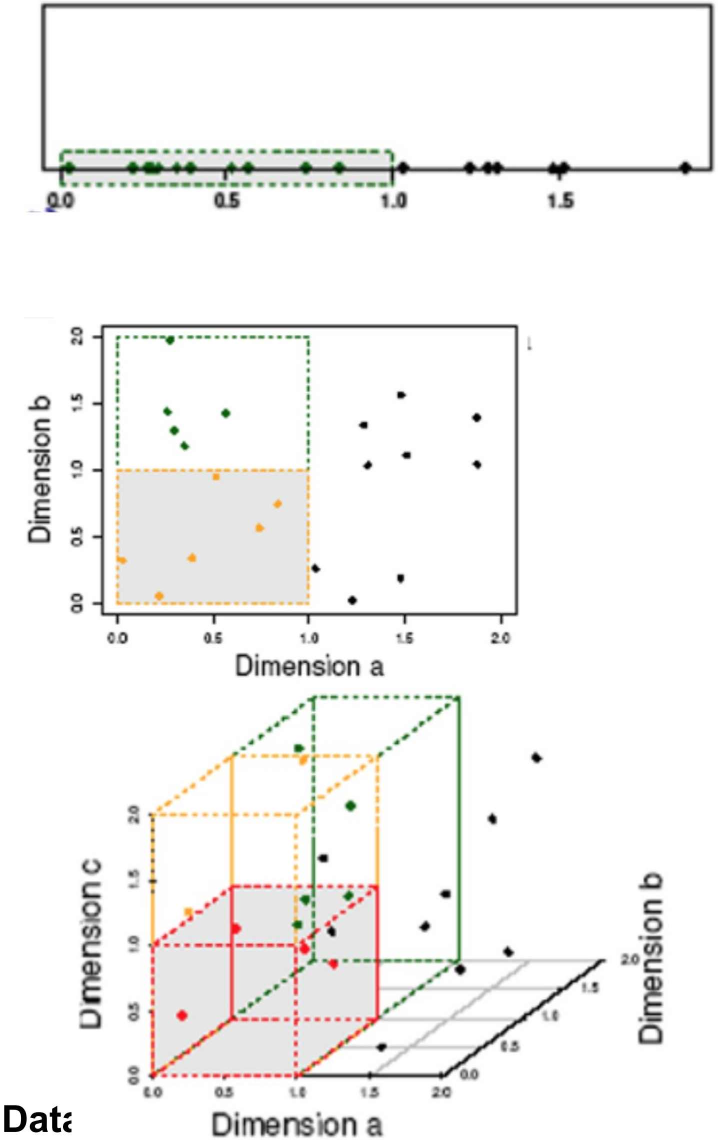
Sample Size

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



Curse of Dimensionality

- Data in only one dimension is relatively packed
- Adding a dimension “stretch” the points across the dimension, making them further apart
- Adding more dimensions will make the points further apart—high dimensional data is extremely sparse
- Distance measure become meaningless—due to equi-distance



(a) Many objects in one unit bin

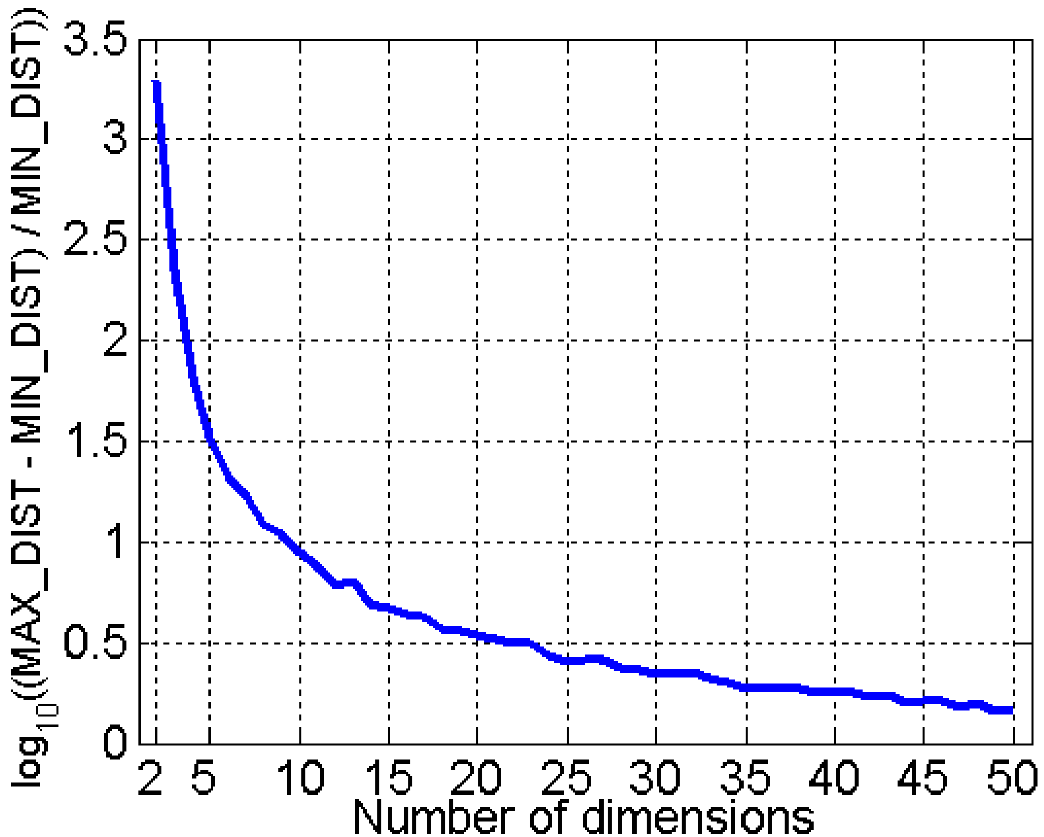
(b) 6 objects in one unit bin

(c) 4 objects in one unit bin

Curse of Dimensionality

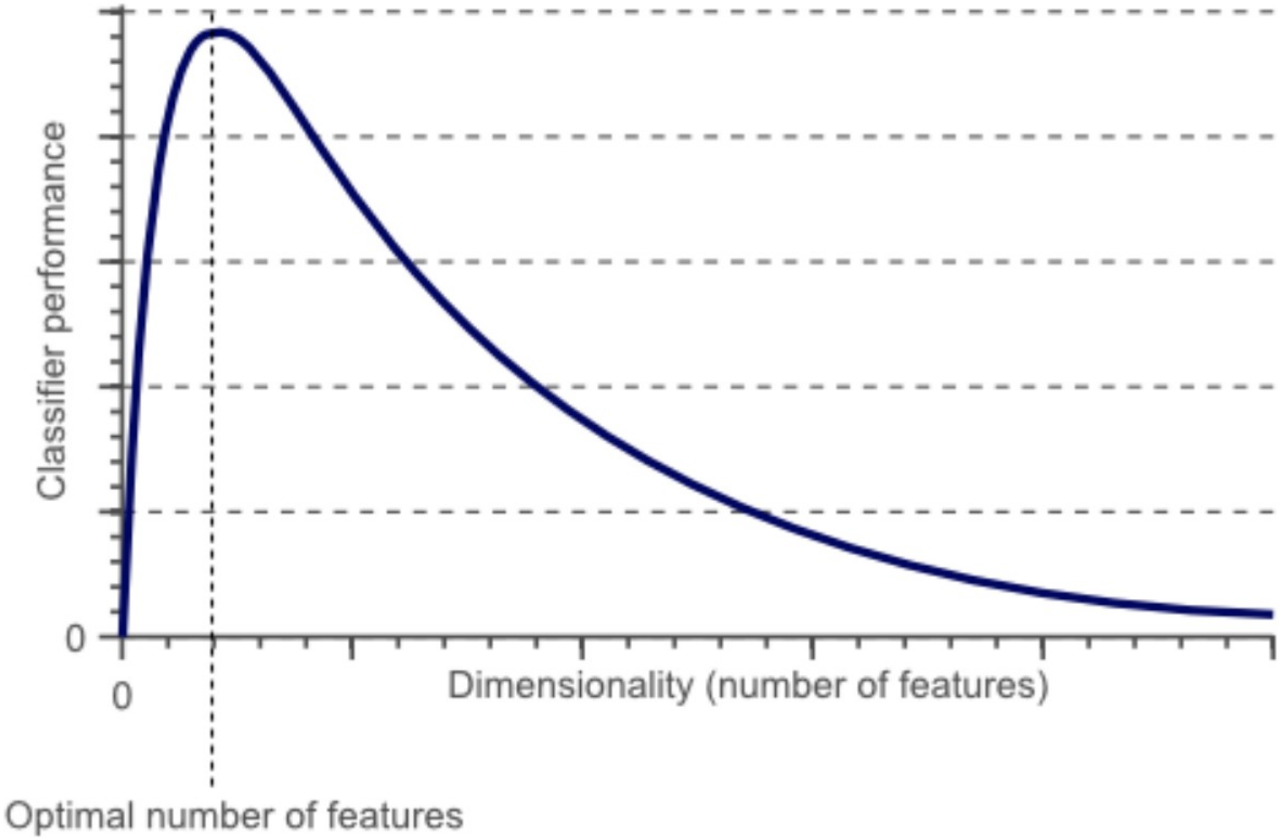
- When dimensionality increases, data becomes increasingly sparse in the space that it occupies

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



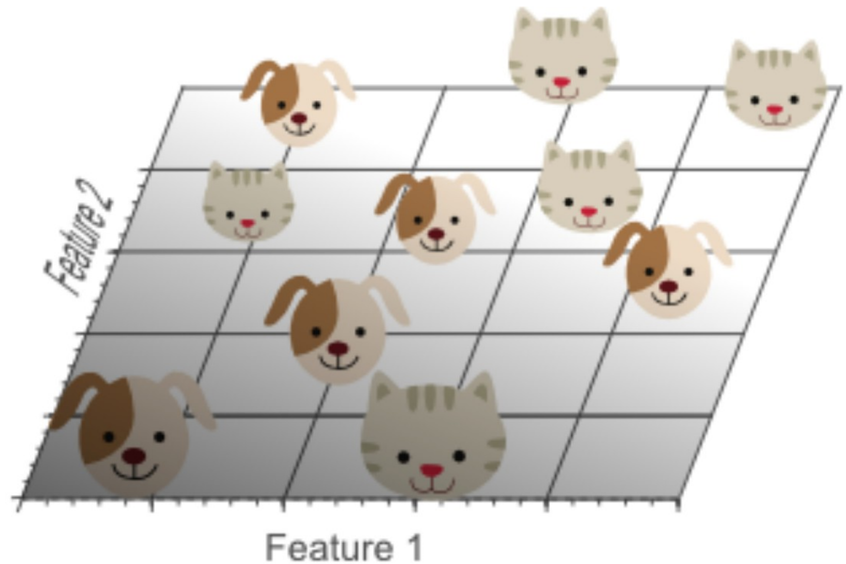
- **Randomly generate 500 points**
- **Compute difference between max and min distance between any pair of points**

Curse of Dimensionality



Curse of Dimensionality

Figure 2. A single feature does not result in a perfect separation of our training data.



Curse of Dimensionality

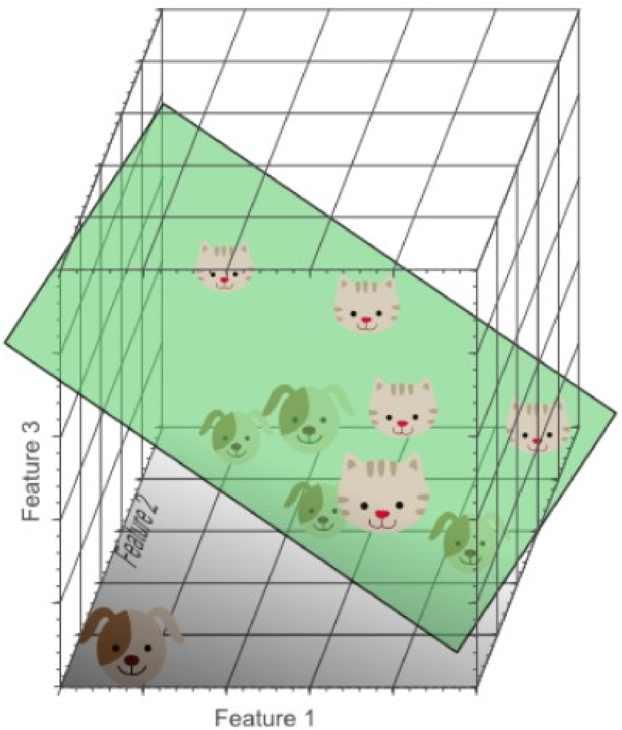
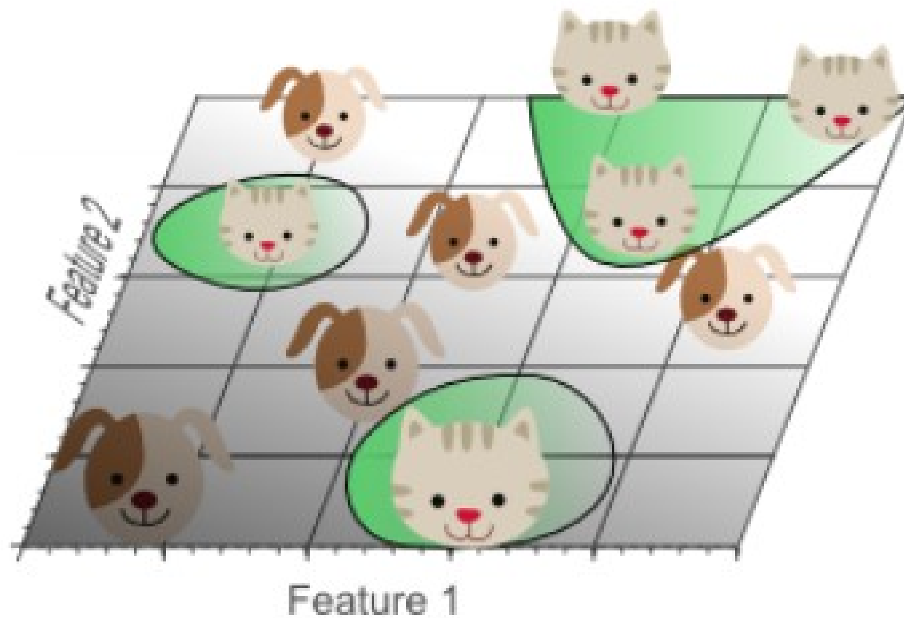


Figure 5. The more features we use, the higher the likelihood that we can successfully separate the classes perfectly.



https://www.visiondummy.com/2014/04/curse-dimensionality-affect-classification/

https://zhuanlan.zhihu.com/p/27488363

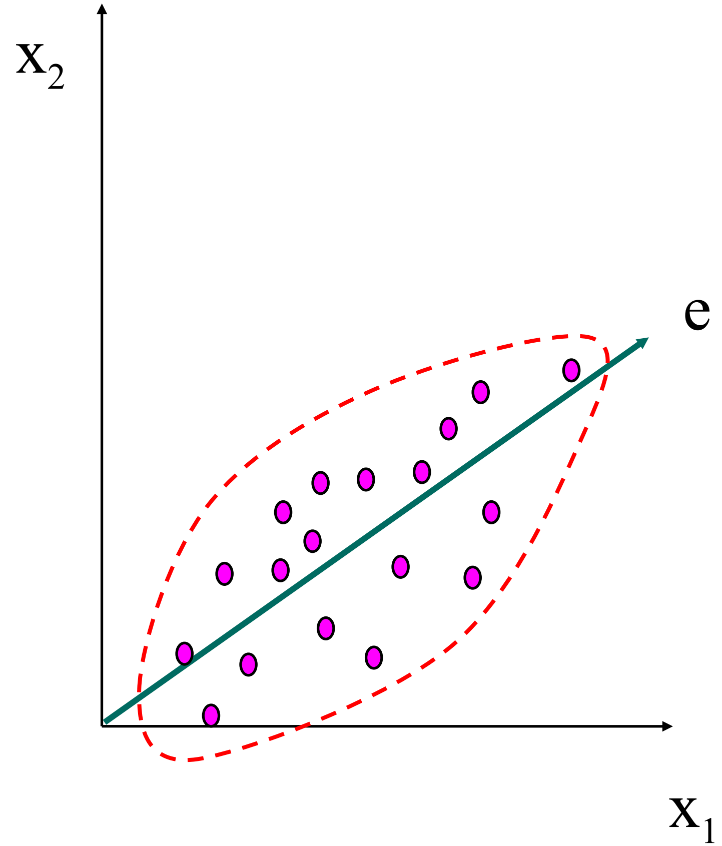
Dimensionality Reduction

- 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
  - Principal Components Analysis (PCA)
  - Singular Value Decomposition
  - Others: supervised and non-linear techniques

Dimensionality Reduction: PCA

- Goal is to find a projection that captures the largest amount of variation in data



Dimensionality Reduction: PCA

Feature Subset Selection

- Another way to reduce dimensionality of data
- Redundant features
  - Duplicate much or all of the information contained in one or more other attributes
  - 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 at hand
  - Example: students' ID is often irrelevant to the task of predicting students' GPA
- Many techniques developed, especially for classification

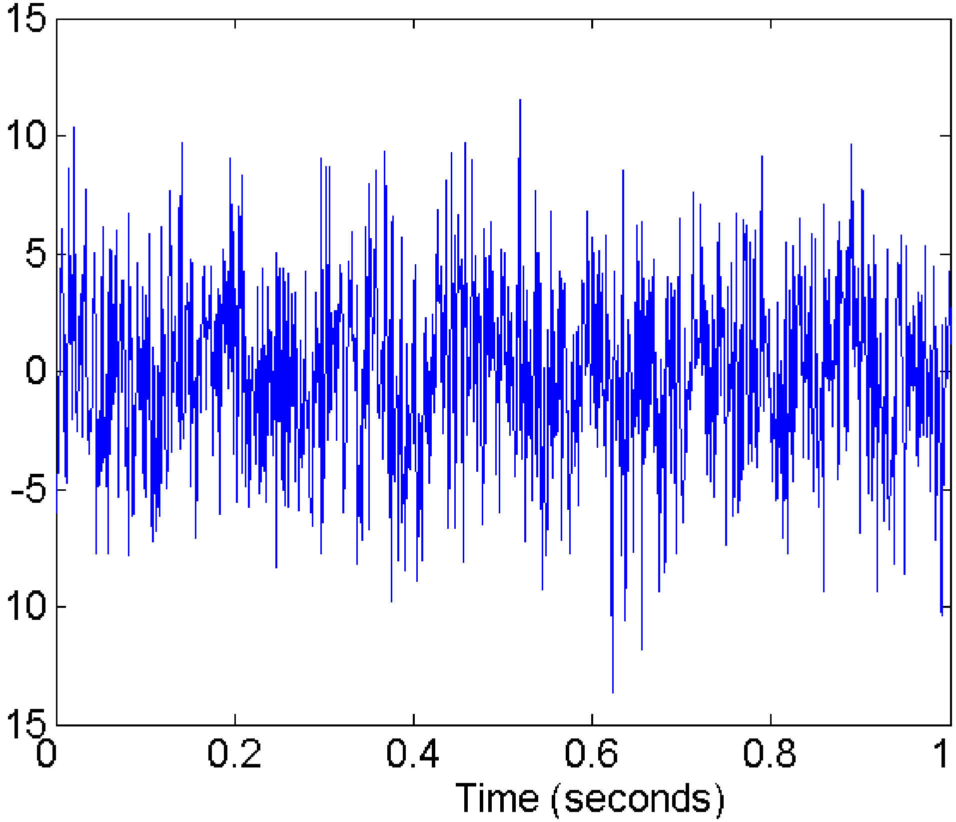
Feature Creation

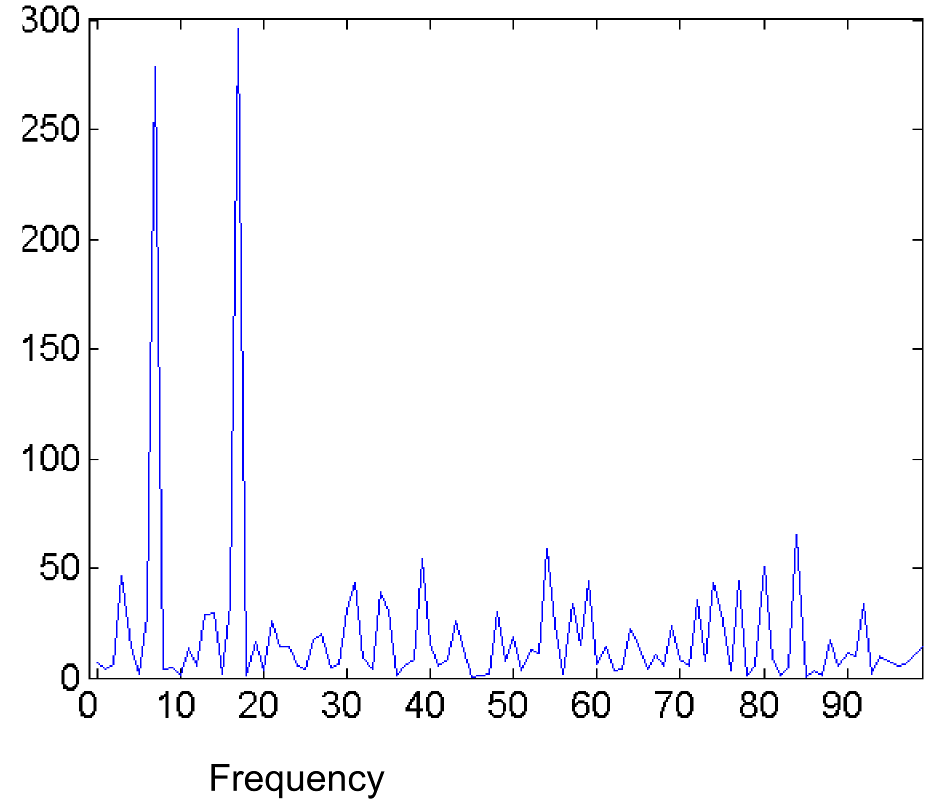
- Create new attributes that can capture the important information in a data set much more efficiently than the original attributes

- Three general methodologies:
  - Feature extraction
    - Example: extracting edges from images
  - Feature construction
    - Example: dividing mass by volume to get density
  - Mapping data to new space
    - Example: Fourier and wavelet analysis

Mapping Data to a New Space

- Fourier and wavelet transform





Two Sine Waves + Noise **Frequency**

Discretization

- Discretization is the process of converting a continuous attribute into an ordinal attribute
  - A potentially infinite number of values are mapped into a small number of categories
  - Discretization is commonly used in classification
  - Many classification algorithms work best if both the independent and dependent variables have only a few values
  - We give an illustration of the usefulness of discretization using the Iris data set

Binarization

- Binarization maps a continuous or categorical attribute into one or more binary variables
- Typically used for association analysis
- Often convert a continuous attribute to a categorical attribute and then convert a categorical attribute to a set of binary attributes
  – Association analysis needs asymmetric binary attributes
  – Examples: eye color and height measured as {low, medium, high}

Attribute Transformation

- An attribute transform is 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, $|x|$
  - Normalization
    - Refers to various techniques to adjust to differences among attributes in terms of frequency of occurrence, mean, variance, range
    - Take out unwanted, common signal, e.g., seasonality
  - In statistics, standardization refers to subtracting off the means and dividing by the standard deviation

Thank You!