DATA MINING - 1DL105, 1DL111

Fall 2007

An introductory class in data mining

http://user.it.uu.se/~udbl/dut-ht2007/
alt. http://www.it.uu.se/edu/course/homepage/infoutv/ht07

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Data in Data Mining

(Tan, Steinbach, Kumar ch. 2)

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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, or feature
- A collection of attributes describe an object
  - Object is also known as record, point, case, sample, entity, or instance

Attributes

Objects

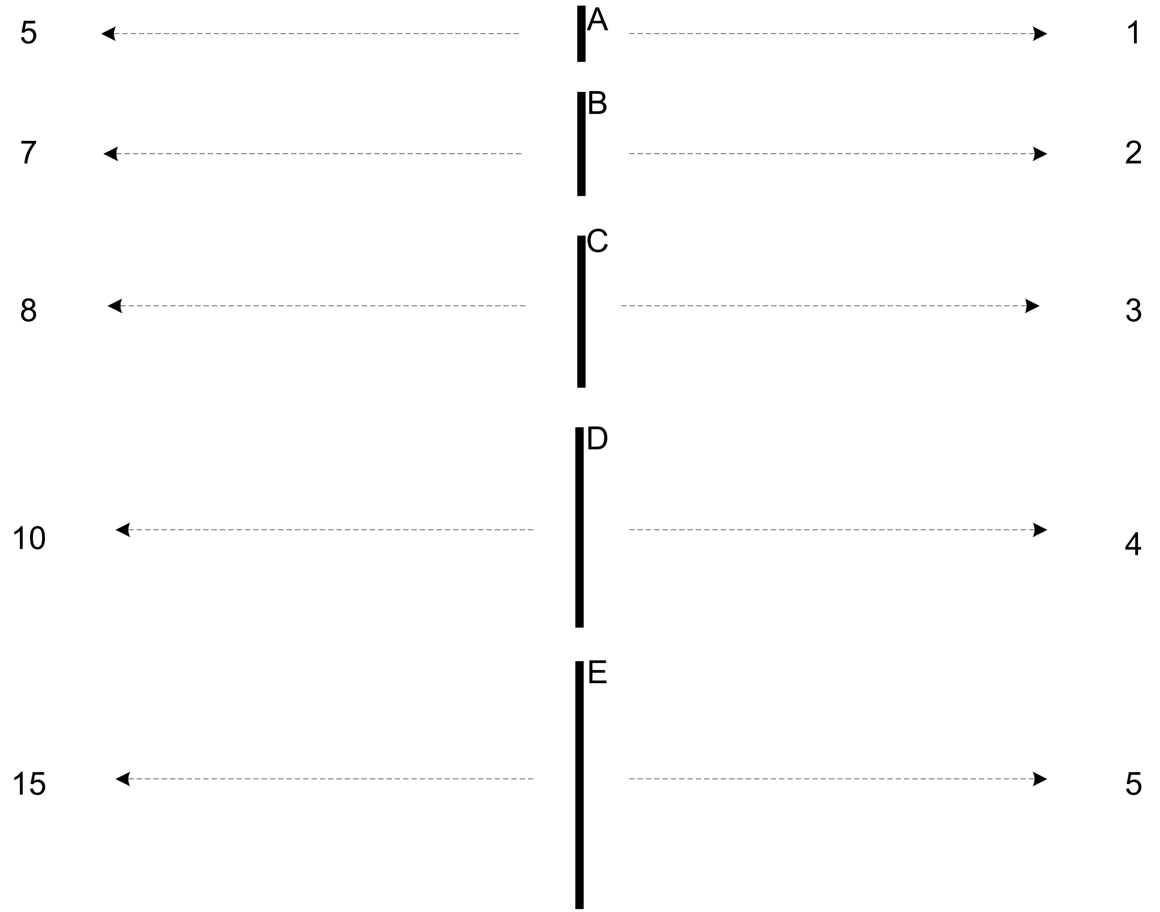
Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

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

Measurement of length

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



Types of attributes

- 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

Properties of attribute values

- The type of an attribute depends on which of the following properties it possesses:
  - Distinctness: $= \neq$
  - Order: $< >$
  - Addition: $+ -$
  - Multiplication: $* /$

  - Nominal attribute: distinctness
  - Ordinal attribute: distinctness & order
  - Interval attribute: distinctness, order & addition
  - Ratio attribute: all 4 properties

Attribute types continued …

Attribute Type	Description	Examples	Operations
Nominal	The values of a nominal attribute are just different names, i.e., nominal attributes provide only enough information to distinguish one object from another. (=, ≠)	zip codes, employee ID numbers, eye color, sex: {*male, female*}	mode, entropy, contingency correlation, χ^2 test
Ordinal	The values of an ordinal attribute provide enough information to order objects. (<, >)	hardness of minerals, {*good, better, best*}, grades, street numbers	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	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, electrical current	geometric mean, harmonic mean, percent variation

Attribute types continued …

Attribute Level	Transformation	Comments
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}.
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.

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.

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 Structured Data

- Dimensionality
  - Curse of Dimensionality
- Sparsity
  - Only presence counts
- Resolution
  - Patterns depend on the scale

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
5	No	Divorced	95K	Yes
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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

Projection of x Load	Projection of y load	Distance	Load	Thickness
10.23	5.27	15.22	2.7	1.2
12.65	6.25	16.22	2.2	1.1

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.

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

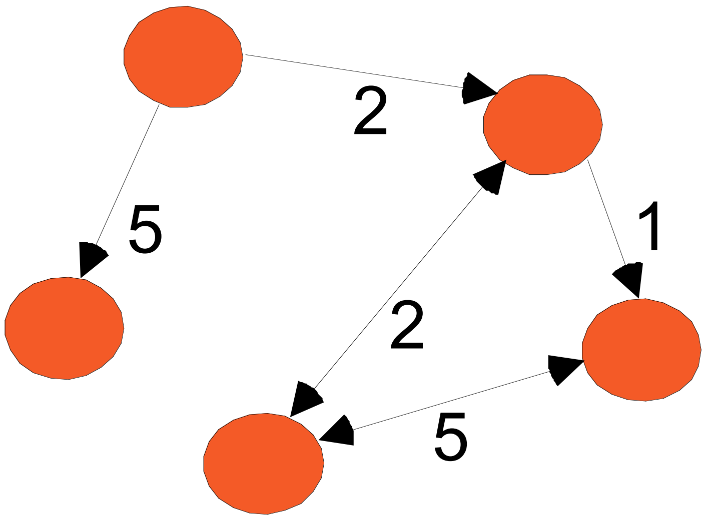
Transaction Data

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

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

Graph Data

- Examples: Generic graph and HTML Links



Data Mining

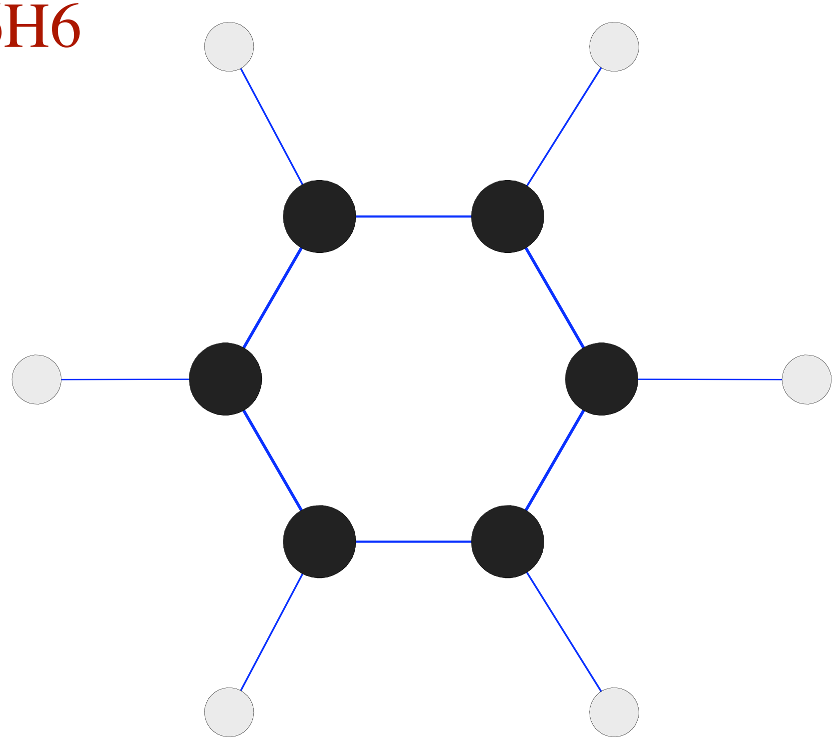
Graph Partitioning

Parallel Solution of Sparse Linear System of Equations

<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

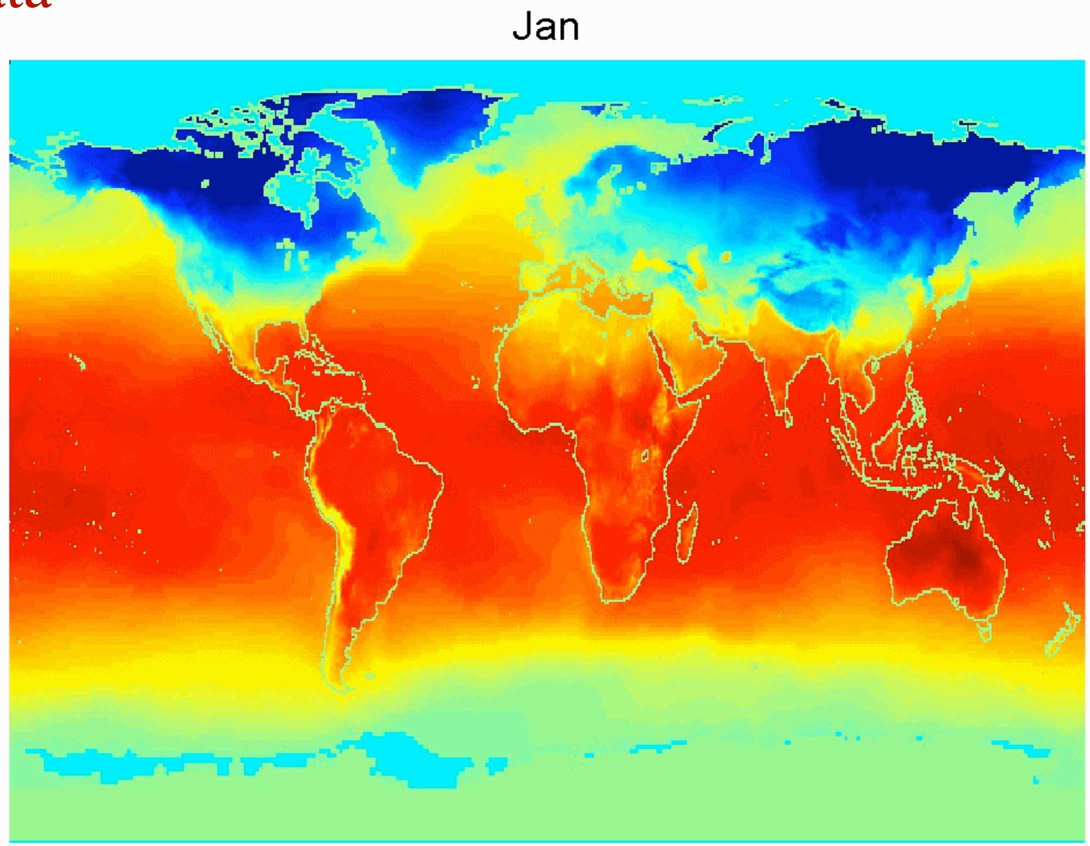
- Genomic sequence data

GGTTCCGCCTTCAGCCCCGCGCC
CGCAGGGCCCGCCCCGCGCCGTC
GAGAAGGGCCCGCCTGGCGGGCG
GGGGGAGGCGGGGCCGCCCGAGC
CCAACCGAGTCCGACCAGGTGCC
CCCTCTGCTCGGCCTAGACCTGA
GCTCATTAGGCGGCAGCGGACAG
GCCAAGTAGAACACGCGAAGCGC
TGGGCTGCCTGCTGCGACCAGGG

Ordered Data

- Spatio-Temporal Data

Average Monthly Temperature of land and ocean



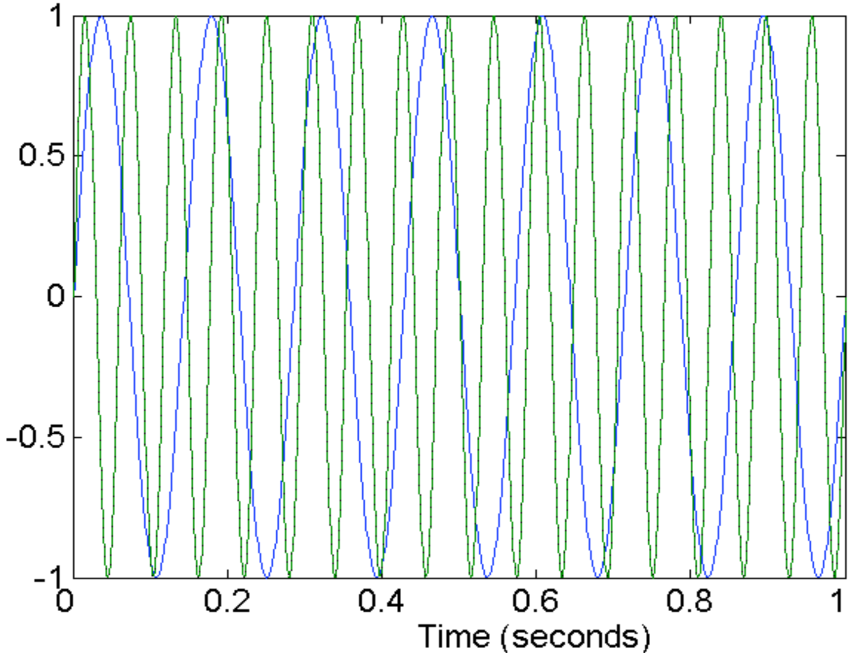
Data Quality

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

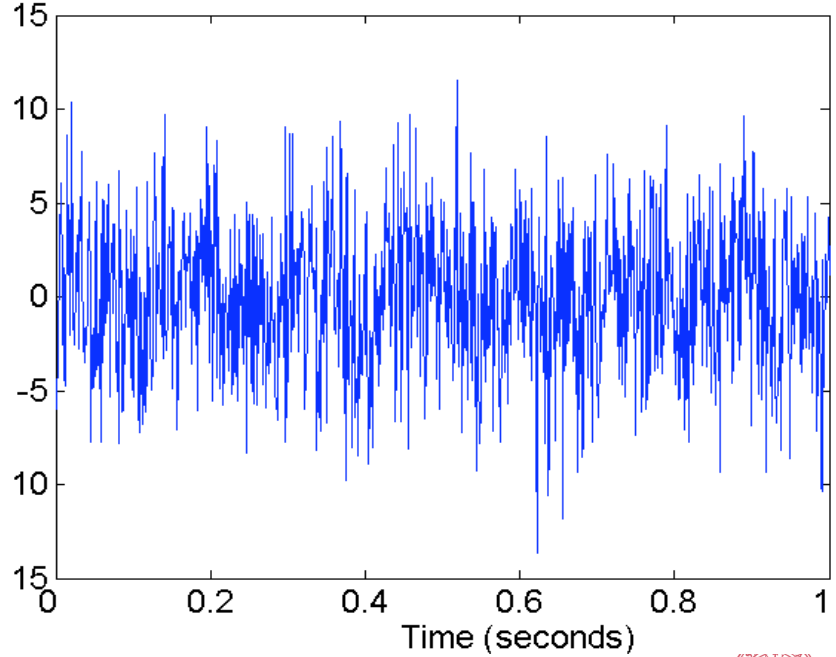
- Examples of data quality problems:
  - Noise and outliers
  - missing values
  - duplicate data

Noise

- Noise refers to modification of original values
  - Examples: distortion of a person's voice when talking on a poor phone and "snow" on television screen



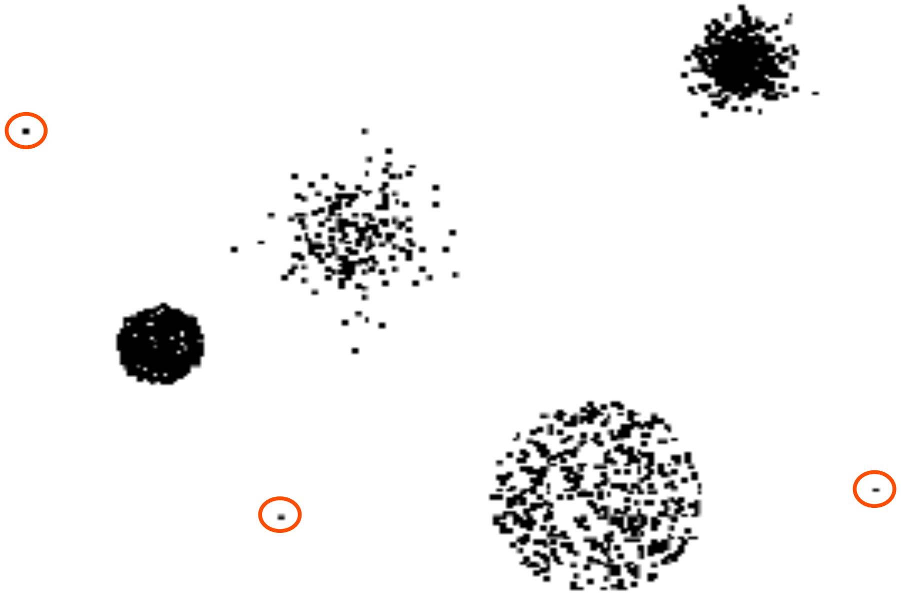
Two Sine Waves



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



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
  - Estimate Missing Values
  - Ignore the Missing Value During Analysis
  - Replace with all possible values (weighted by their probabilities)

Duplicate Data

- Data set may include data objects that are duplicates, or almost duplicates of one another
  - Major issue when merging data from heterogeous sources

- Examples:
  - Same person with multiple email addresses

- Data cleaning
  - Process of dealing with duplicate data issues

Data Preprocessing

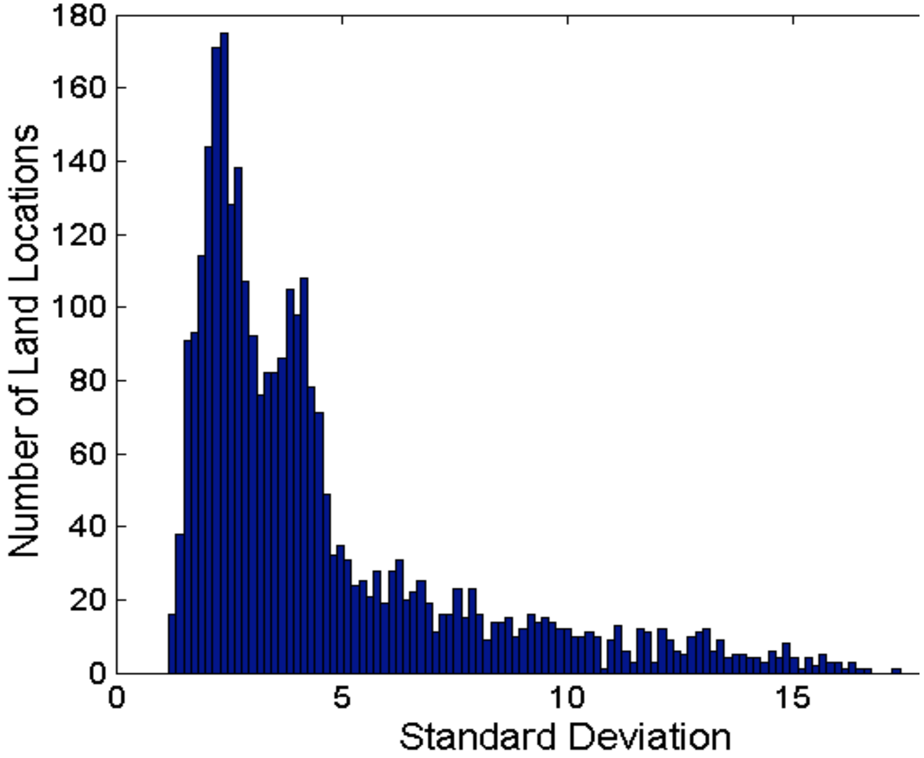
- Aggregation
- Sampling
- Dimensionality Reduction
- Feature subset selection
- Feature creation
- Discretization and Binarization
- Attribute Transformation

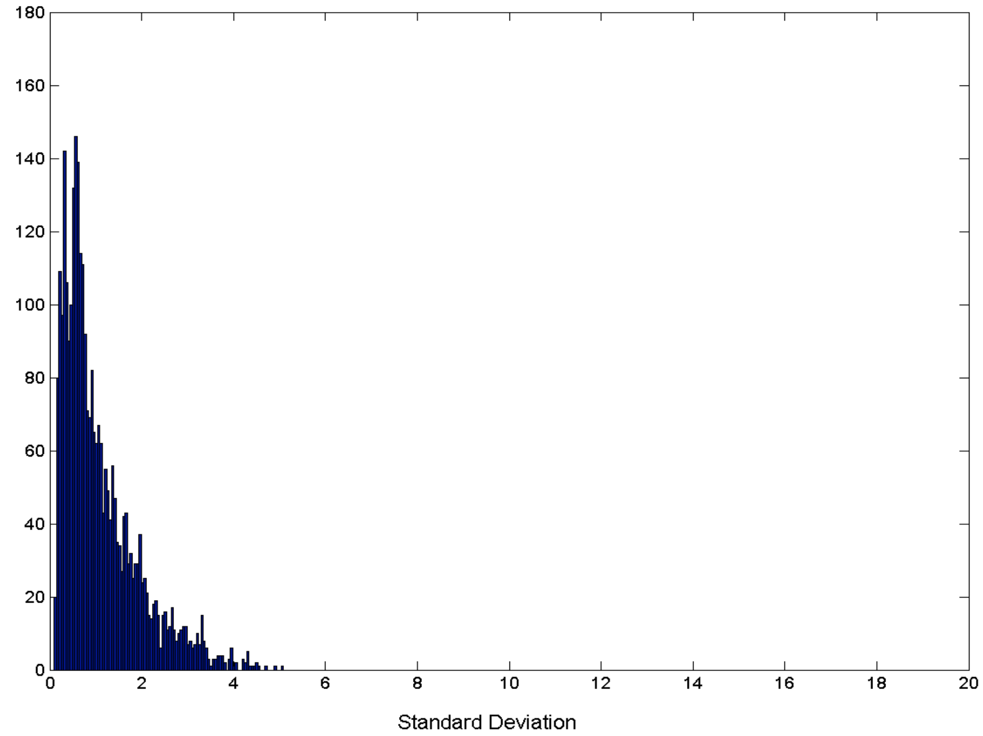
Aggregation

- 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

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 or time consuming.

Sampling …

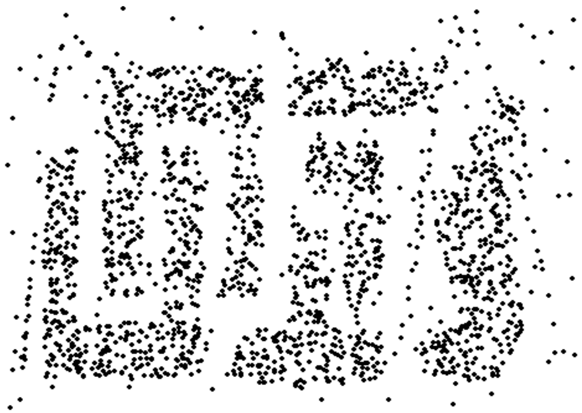
- The key principle for effective sampling is the following:
  - using a sample will work almost as well as using the entire data sets, if the sample is representative
  - A sample is representative if it has approximately the same property (of interest) as the original set of data

Types of Sampling

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

Sample Size

8000 points

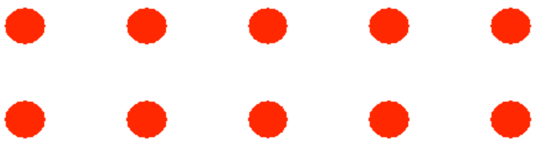


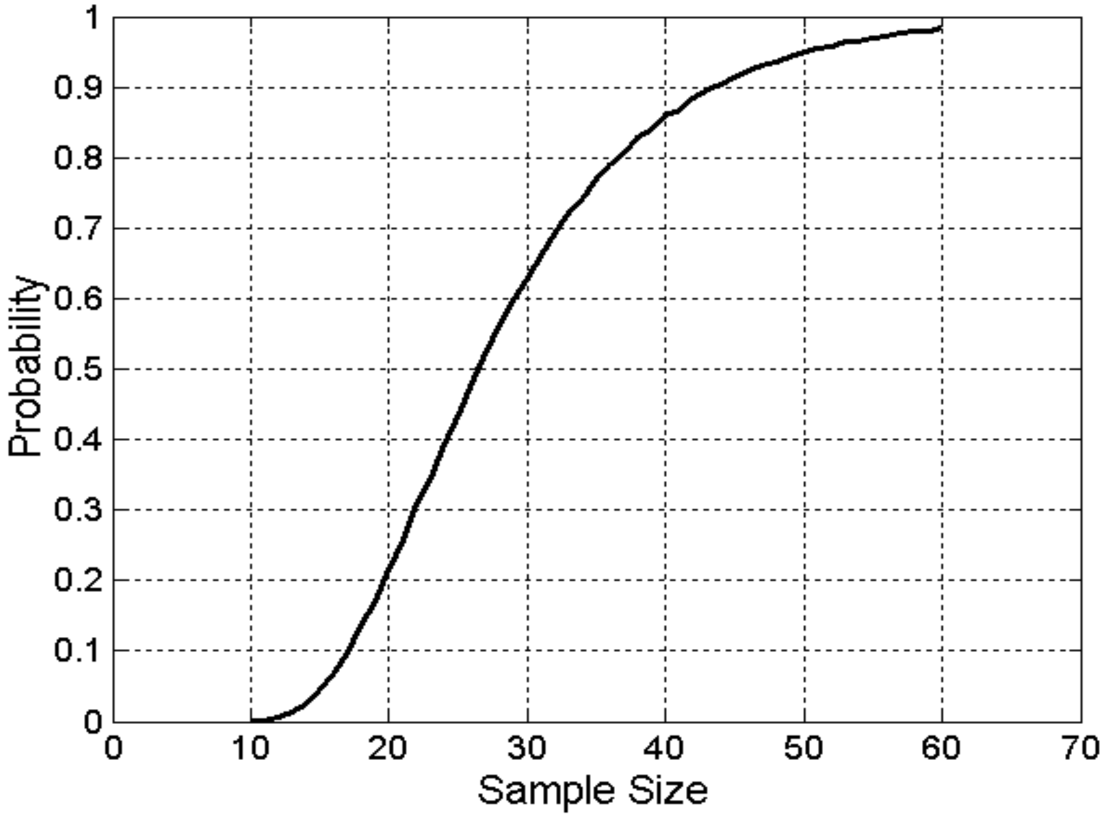
2000 Points

500 Points

Sample Size

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

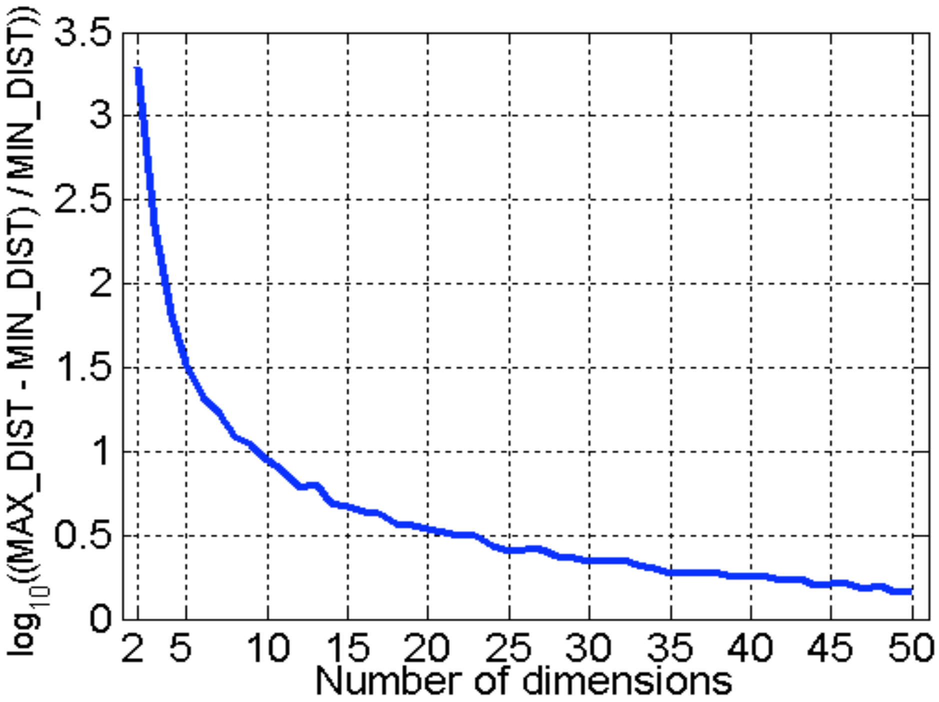




Curse of Dimensionality

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

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



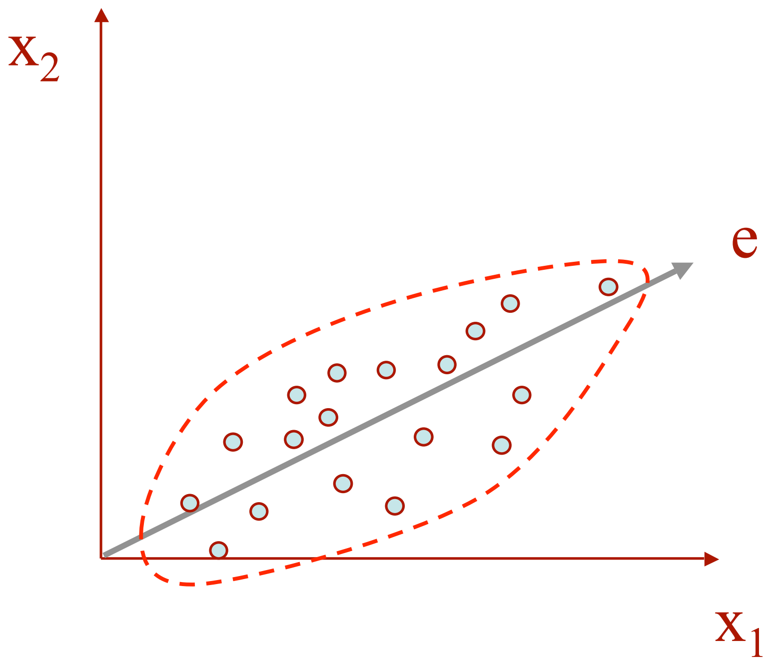
- **Randomly generate 500 points**
- **Compute difference between max and min distance between any pair of points**

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

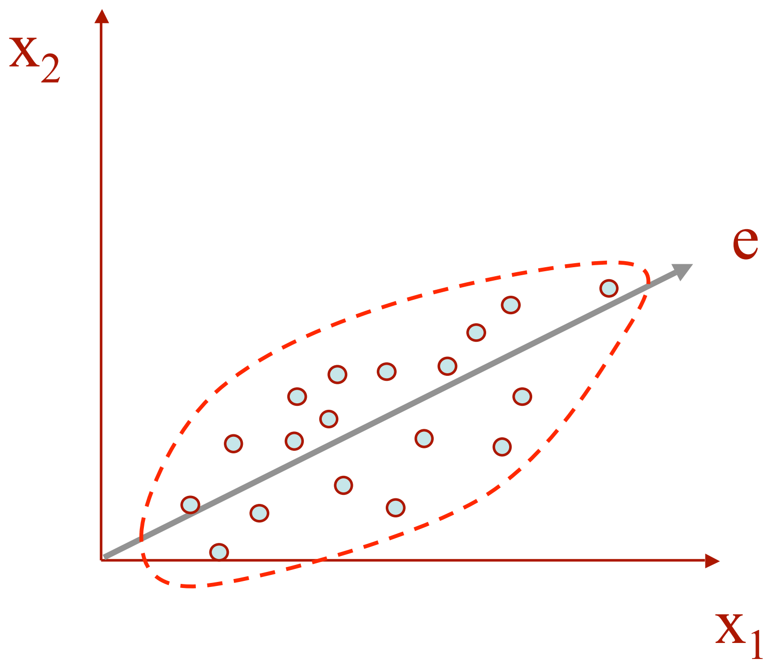
Dimensionality Reduction: PCA

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



Dimensionality Reduction: PCA

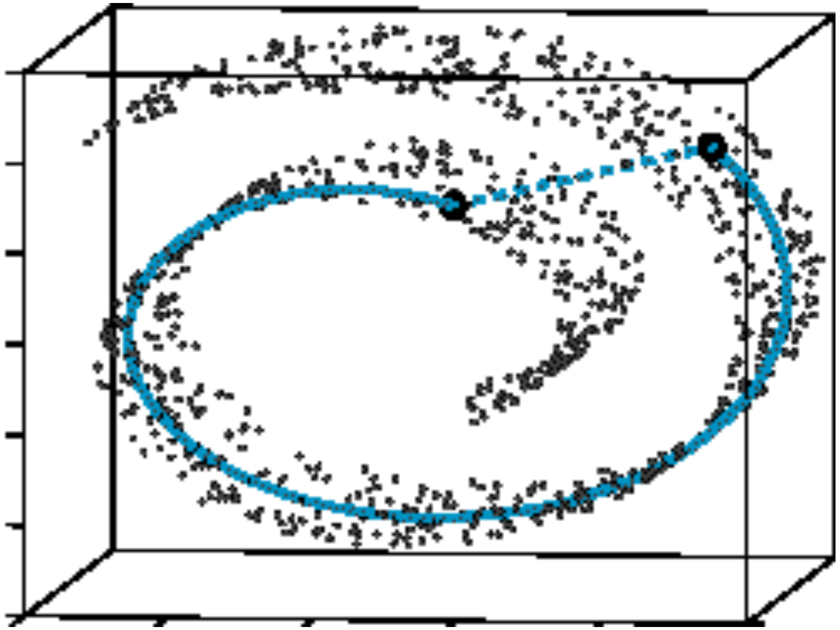
- Find the eigenvectors of the covariance matrix
- The eigenvectors define the new space



Dimensionality Reduction: ISOMAP

By: Tenenbaum, de Silva, Langford (2000)

- Construct a neighbourhood graph
- For each pair of points in the graph, compute the shortest path distances – geodesic distances



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

Feature Subset Selection

- Techniques:
  - Brute-force approch:
    - Try all possible feature subsets as input to data mining algorithm
  - Embedded approaches:
    - Feature selection occurs naturally as part of the data mining algorithm
  - Filter approaches:
    - Features are selected before data mining algorithm is run
  - Wrapper approaches:
    - Use the data mining algorithm as a black box to find best subset of attributes

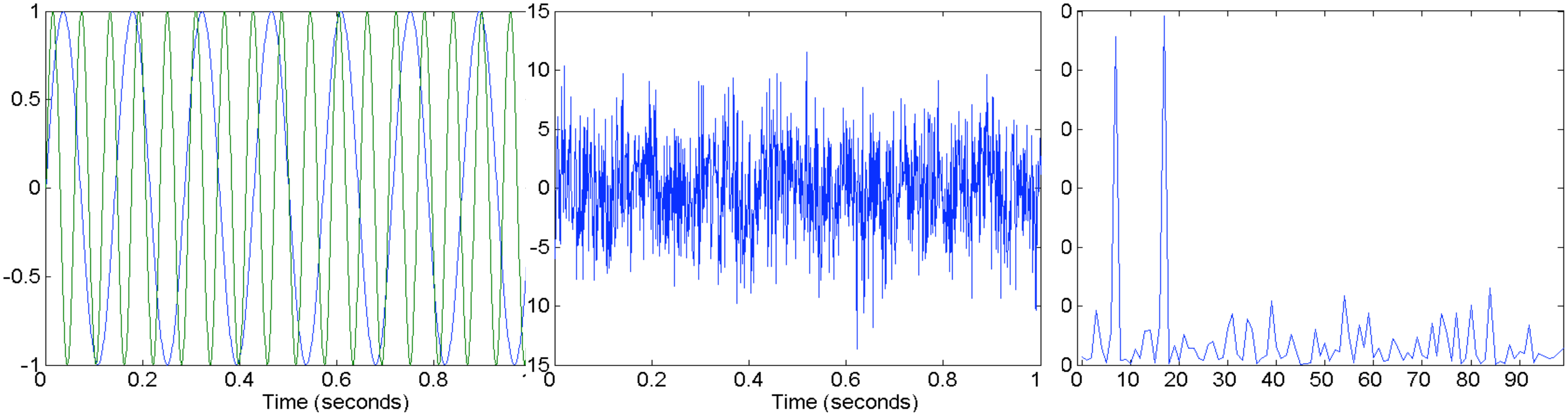
Feature Creation

- 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
  - Mapping Data to New Space
  - Feature Construction
    - combining features

Mapping Data to a New Space

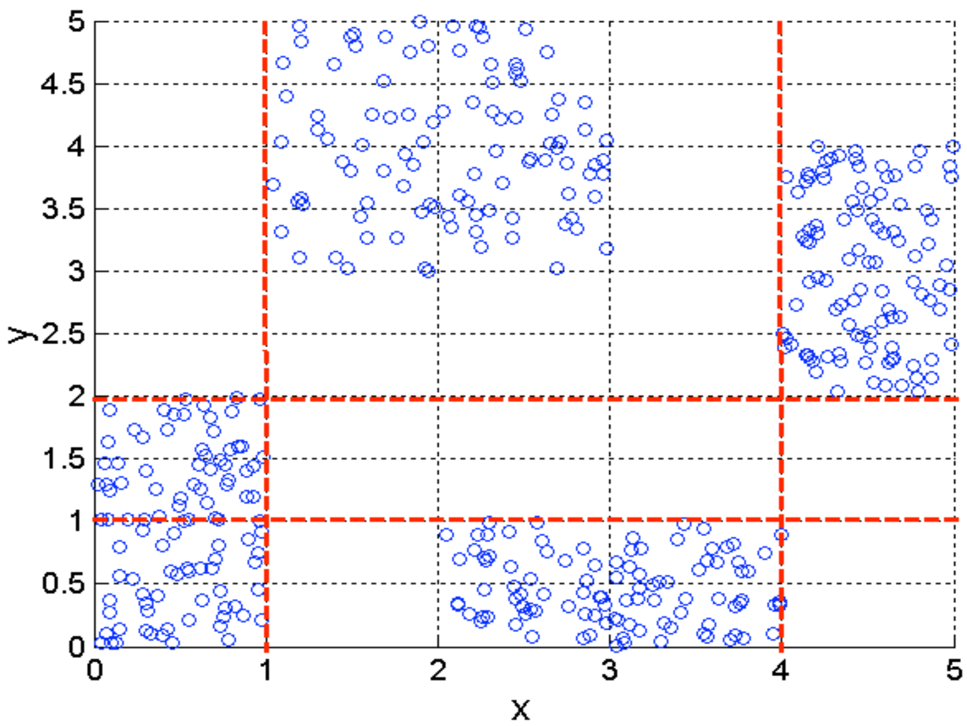
- **Fourier transform**
- **Wavelet transform**



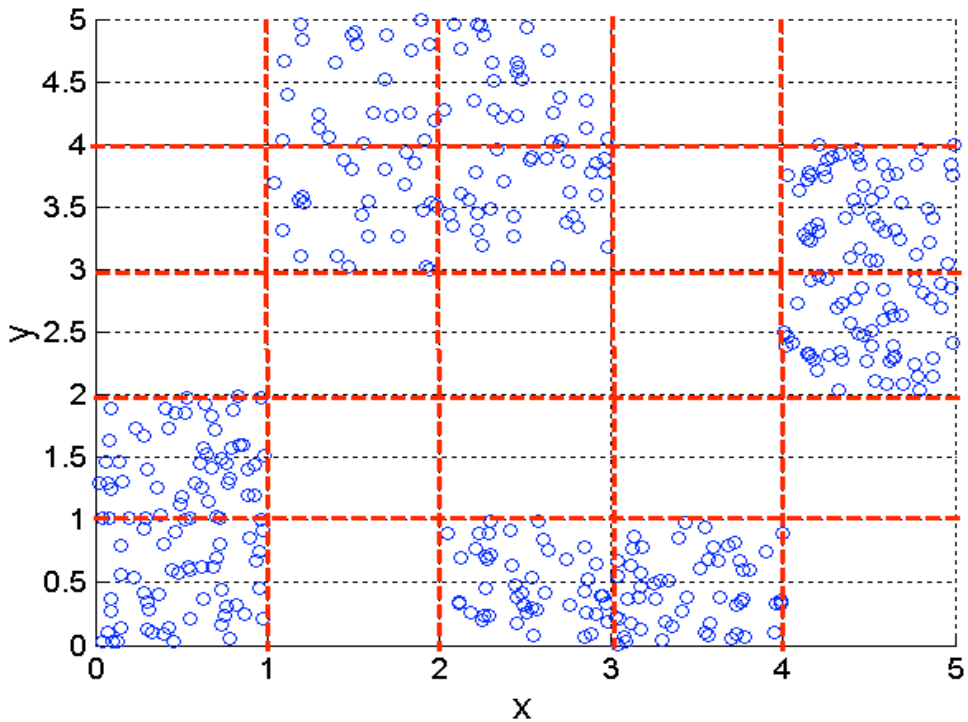
Two Sine Waves **Two Sine Waves + Noise** **Frequency**

Discretization Using Class Labels

entropy based approach

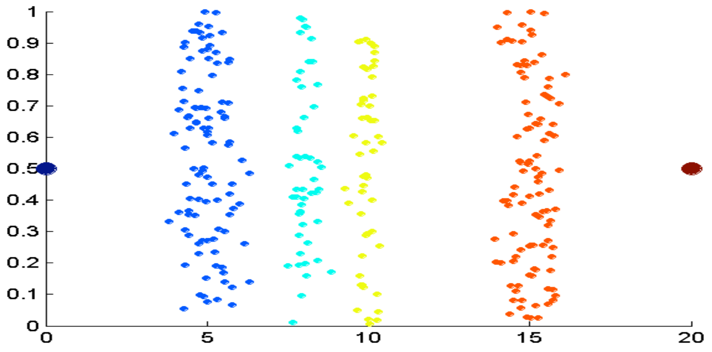


3 categories for both x and y

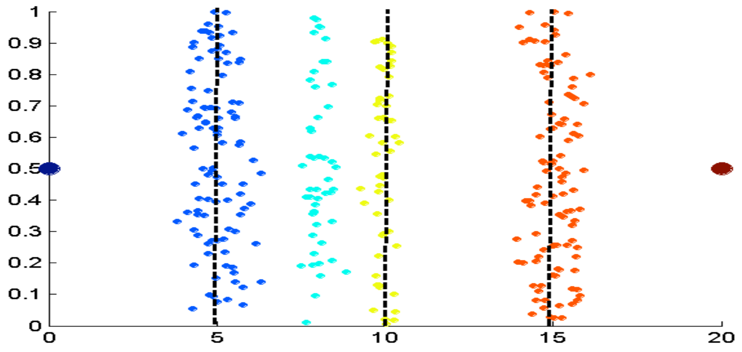


5 categories for both x and y

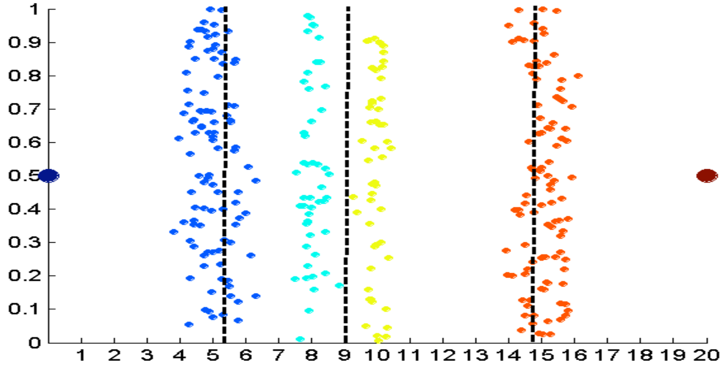
Discretization Without Using Class Labels



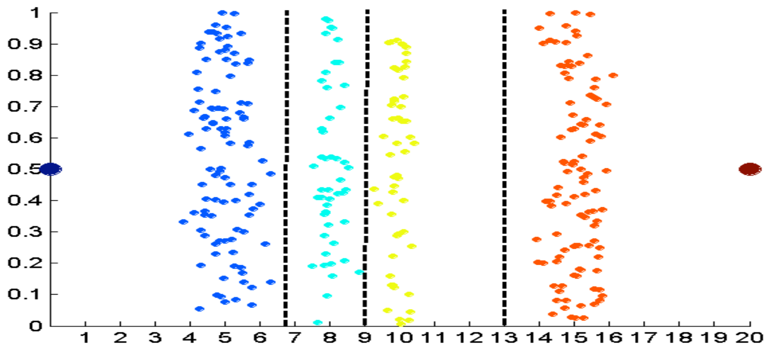
Data



Equal interval width



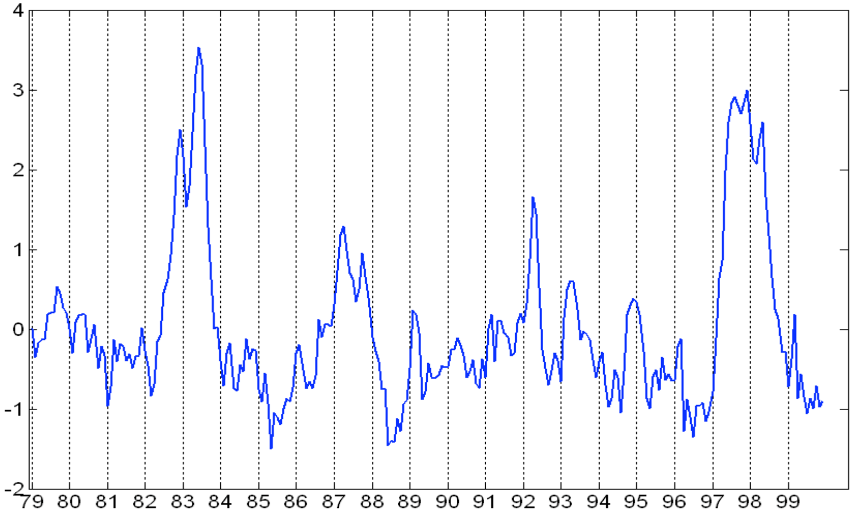
Equal frequency



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



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 $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Table 5.1. Similarity and dissimilarity for simple attributes

Euclidean Distance

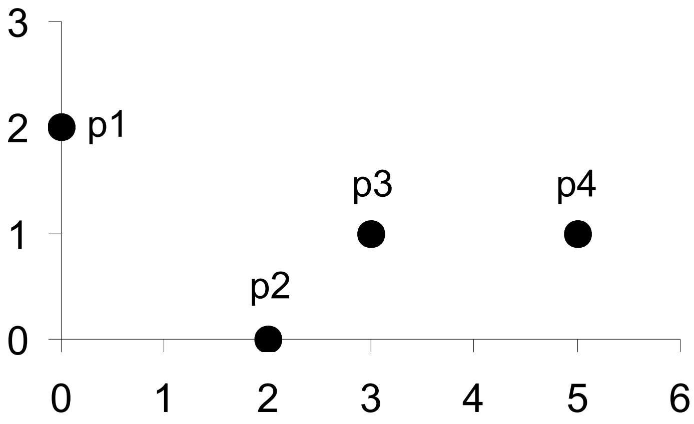
- Euclidean Distance

$$dist = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

  – Where n is the number of dimensions (attributes) and pk and qk are, respectively, the kth attributes (components) or data objects p and q.

- 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

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Minkowski Distance

- Minkowski Distance is a generalization of Euclidean Distance

$$dist = \left(\sum_{k=1}^{n} | p_k - q_k |^r \right)^{\frac{1}{r}}$$

  - Where r is a parameter, n is the number of dimensions (attributes) and pk and qk are, respectively, the kth attributes (components) or data objects p and q.

Minkowski Distance: examples

- $r = 1$. City block (Manhattan, taxicab, L1 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
- $r \to \infty$. “supremum” (Lmax 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 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

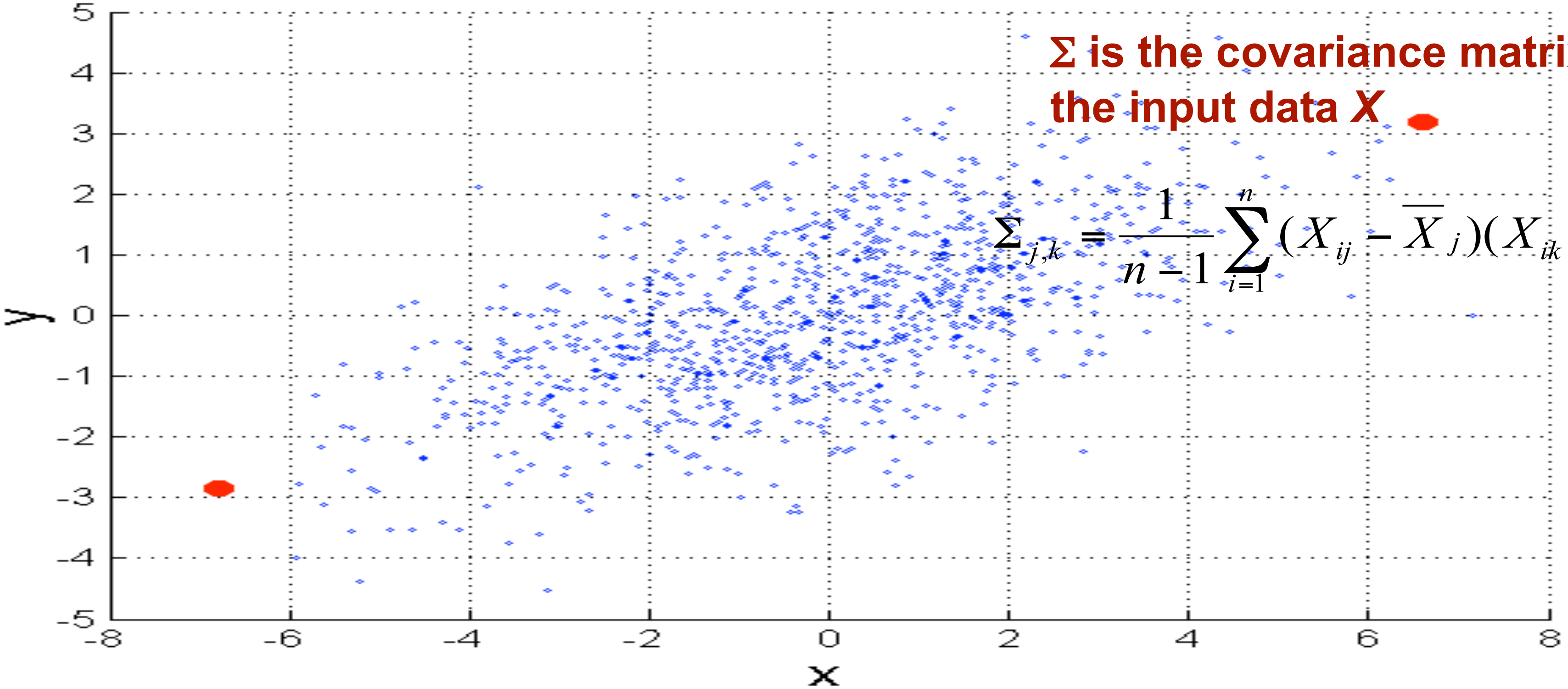
L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

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

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



Σ is the covariance matrix of the input data *X*

$$\Sigma_{j,k} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij} - \overline{X}_j)(X_{ik} - \overline{X}_k)$$

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

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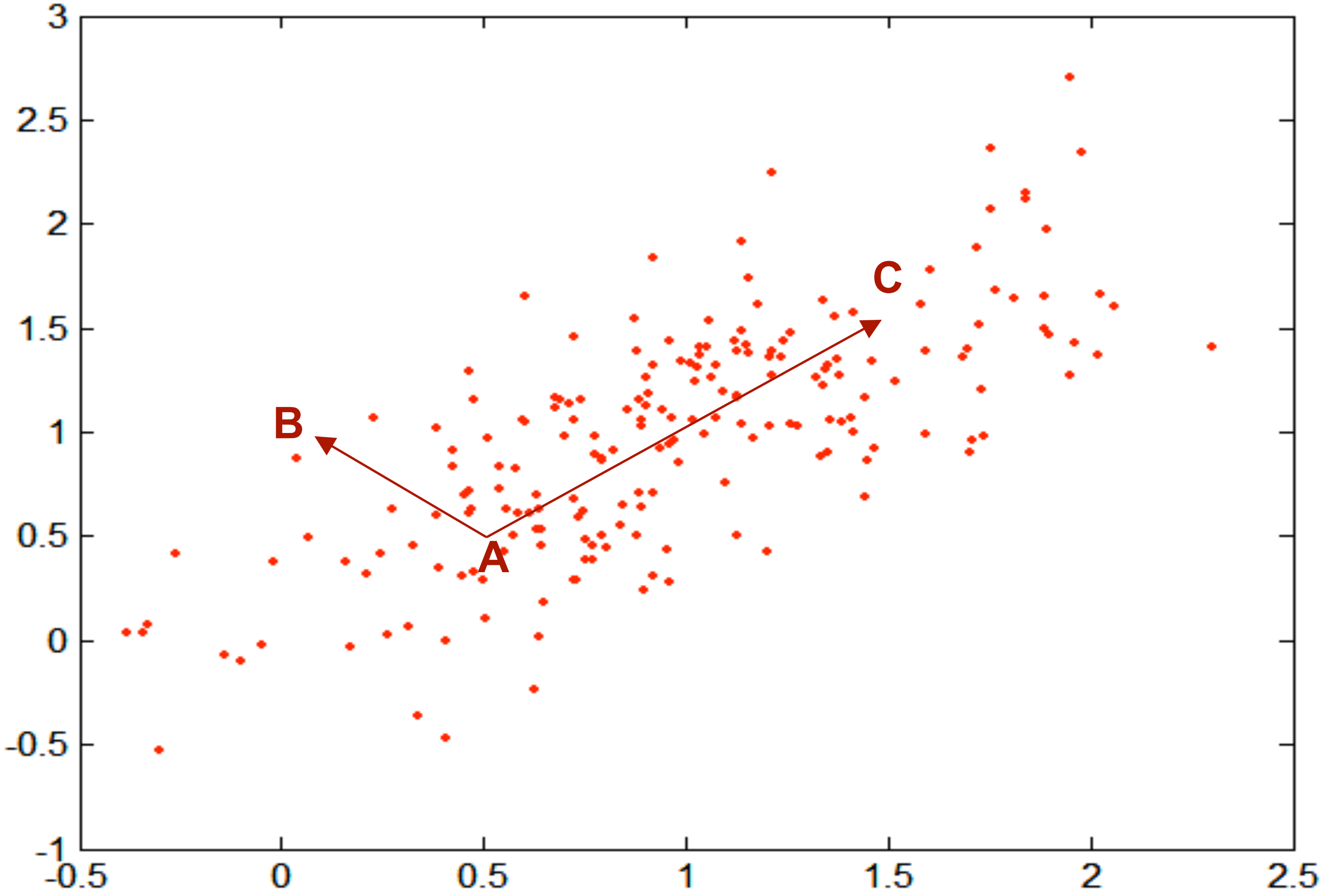
Mahalanobis Distance



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

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Common properties of a distance

- Distances, such as the Euclidean distance, have some well known properties.
  - $d(p, q) \geq 0$ for all p and q and $d(p, q) = 0$ only if $p = q$. (Positive definiteness)
  - $d(p, q) = d(q, p)$ for all p and q. (Symmetry)
  - $d(p, r) \leq d(p, q) + d(q, r)$ 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**

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.

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
  SMC = number of matches / number of attributes
  = (M11 + M00) / (M01 + M10 + M11 + M00)

  J = number of 11 matches / number of not-both-zero attributes values
  = (M11) / (M01 + M10 + M11)

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)

- SMC = (M11 + M00)/(M01 + M10 + M11 + M00) = (0+7) / (2+1+0+7) = 0.7

- J = (M11) / (M01 + M10 + M11) = 0 / (2 + 1 + 0) = 0

Cosine Similarity

- If d1 and d2 are two document vectors, then

  $$\cos(d1, d2) = (d1 \bullet d2) / ||d1||\,||d2|| ,$$

  where • indicates vector dot product and || d || is the length of vector d.

- Example:

  d1 = 3 2 0 5 0 0 0 2 0 0
  d2 = 1 0 0 0 0 0 0 1 0 2

  $$d1 \bullet d2 = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$$
  $$||d1|| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5} = (42)^{0.5} = 6.481$$
  $$||d2|| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5} = (6)^{0.5} = 2.245$$

  $$\cos(d1, d2) = .3150$$

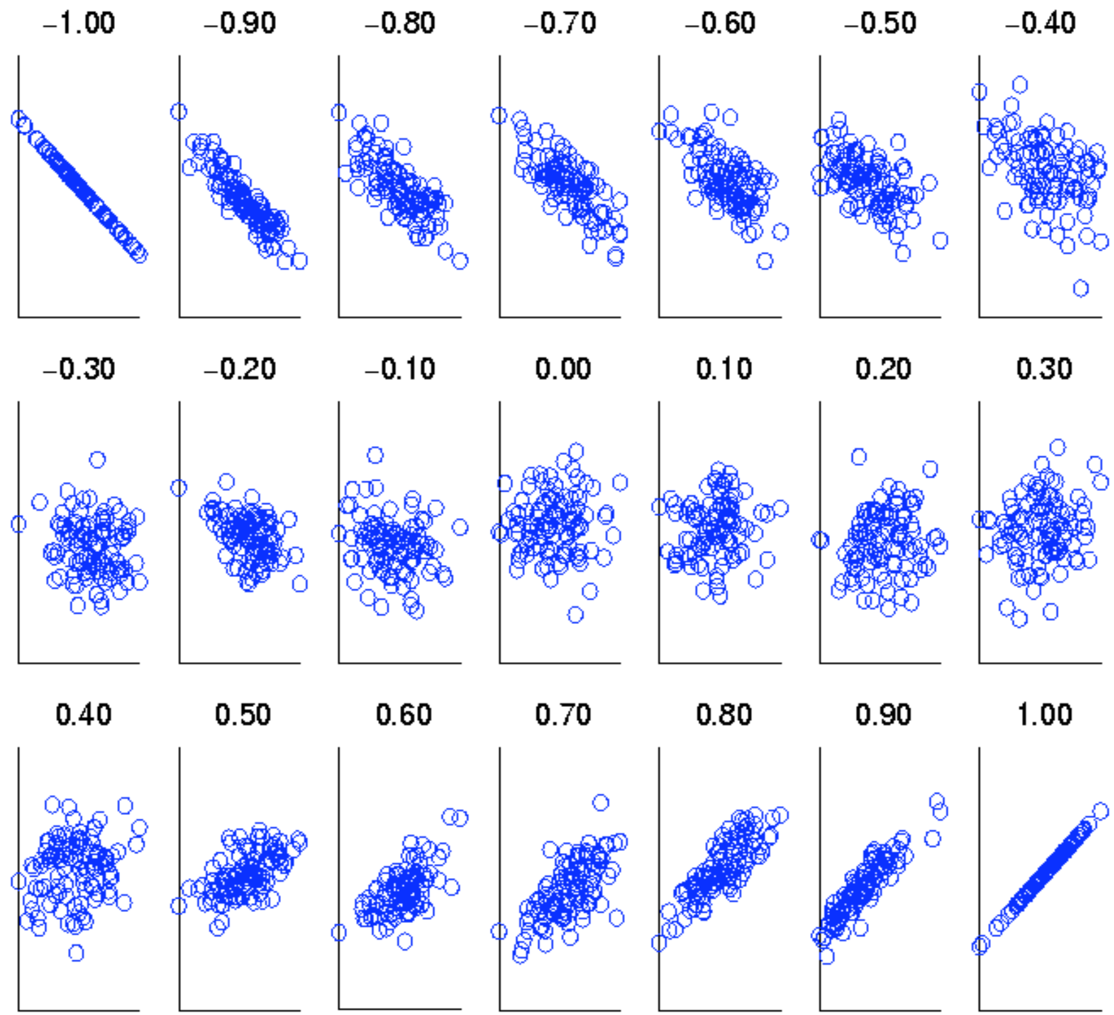
Correlation

- Correlation examines the degree to which the values for two variables behave similarly by measuring the linear relationship between objects.

$$c(x,y) = \frac{\sum(x_i - \bar{X})(y_i - \bar{Y})}{\sqrt{\sum(x_i - \bar{X})^2 \sum(y_i - \bar{Y})^2}}$$

- Correlation coefficient:
  - 1 = perfect positive correlation
  - -1 = perfect negative correlation
  - 0 = no correlation
- Correlation = -1: X = (-3, 6, 0, 3,-6)
  Y = (1,-2, 0,-1, 2)
- Correlation = +1: X = (3, 6, 0, 3, 6)
  Y = (1, 2, 0, 1, 2)

Visually Evaluating Correlation



Scatter plots showing the similarity from –1 to 1.

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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, 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:

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

Using weights to combine similarities

- May not want to treat all attributes the same.
  - Use weights w_k which are between 0 and 1 and sum to 1.

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

$$distance(p,q) = \left(\sum_{k=1}^{n} w_k |p_k - q_k|^r \right)^{1/r}$$

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Density

- Density-based clustering require a notion of density
- Examples:
  - Euclidean density
    - Euclidean density = number of points per unit volume
  - Probability density
  - Graph-based density

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

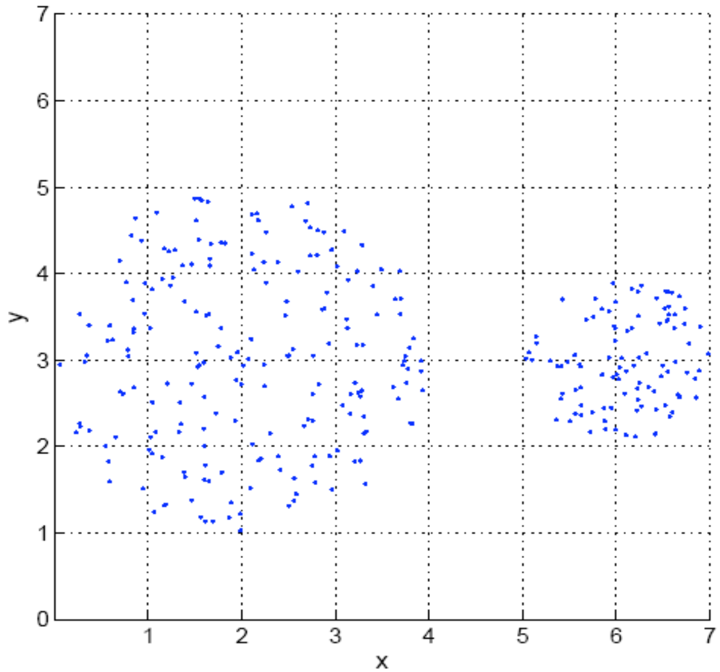

Figure 7.13. Cell-based density.

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

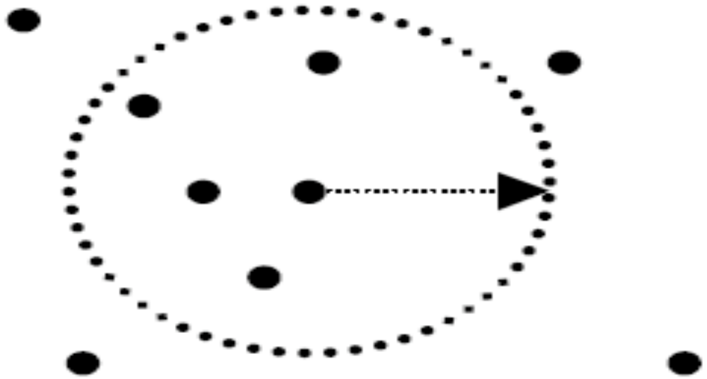

Figure 7.14. Illustration of center-based density.