Università degli Studi di Milano

Master Degree in Computer Science

Information Management course

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Data Mining:

Concepts and Techniques

— Chapter 2 —

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Chapter 2: Getting to Know Your Data

- Data Objects and Attribute Types
- Basic Statistical Descriptions of Data
- Measuring Data Similarity and Dissimilarity
- Summary

Types of Data Sets

- Record
  - Relational records
  - Data matrix, e.g., numerical matrix, crosstabs
  - Document data: text documents: term-frequency vector
  - Transaction data
- Graph and network
  - World Wide Web
  - Social or information networks
  - Molecular Structures
- Ordered
  - Video data: sequence of images
  - Temporal data: time-series
  - Sequential Data: transaction sequences
  - Genetic sequence data
- Spatial, image and multimedia:
  - Spatial data: maps
  - Image data: .bmp
  - Video data: .avi

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

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

Important Characteristics of Structured Data

- Dimensionality
  - Curse of dimensionality

    (the volume of the space grows fast with the number of dimensions, and the available data becomes sparse)
- Sparsity
  - Only presence counts
- Resolution
  - Patterns depend on the scale
- Distribution
  - Centrality and dispersion

Data Objects

- Data sets are made up of data objects.
- A **data object** represents an entity (also called *samples , examples, instances, data points, objects, tuples …)*
- Examples:
    - sales database: customers, store items, sales
    - medical database: patients, treatments
    - university database: students, professors, courses
- Data objects are described by **attributes** (also called *variables, dimensions, features …*)

- In databases: rows -> data objects; columns ->attributes.

Attributes

- **Attribute (**or **dimensions, features, variables**): a data field, representing a characteristic or feature of a data object.
  - *E.g., customer _ID, name, address*
- Types:
  - Nominal
  - Binary
  - Ordinal
  - Numeric: quantitative
    - Interval-scaled
    - Ratio-scaled

Attribute Types

- **Nominal:** categories, states, or “names of things”
  - *Hair_color = {auburn, black, blond, brown, grey, red, white}*
  - marital status, occupation, ID numbers, zip codes
- **Binary**
  - Nominal attribute with only 2 states (0 and 1)
  - Symmetric binary: both outcomes equally important
    - e.g., gender
  - Asymmetric binary: outcomes not equally important.
    - e.g., medical test (positive vs. negative)
    - Convention: assign 1 to most important outcome (e.g., HIV positive)
- **Ordinal**
  - Values have a meaningful order (ranking) but magnitude between successive values is not known.
  - *Size = {small, medium, large}*, grades, army rankings

Numeric Attribute Types

- Quantity (integer or real-valued)
- **Interval**
  - Measured on a scale of **equal-sized units**
  - Values have order
    - E.g., *temperature in C˚or F˚, calendar dates*
  - No true zero-point
- **Ratio**
  - Inherent **zero-point**
  - We can speak of values as being an order of magnitude larger than the unit of measurement (10 K˚ is twice as high as 5 K˚).
    - e.g., *temperature in Kelvin, length, counts, monetary quantities*

Discrete vs. Continuous Attributes (ML view)

- **Discrete Attribute**
  - Has only a finite or countably infinite set of values
    - E.g., zip codes, profession, or the set of words in a collection of documents
  - Sometimes, represented as integer variables
  - Note: Binary attributes are a special case of discrete attributes
- **Continuous Attribute**
  - Has real numbers as attribute values
    - E.g., 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

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Basic Statistical Descriptions of Data

- Motivation
  - To better understand the data: central tendency, variation and spread
- Data dispersion characteristics
  - median, max, min, quantiles, outliers, variance...
- Numerical dimensions correspond to sorted intervals
  - Data dispersion: analyzed with multiple granularities of precision
  - Boxplot or quantile analysis on sorted intervals
- Dispersion analysis on computed measures
  - Folding measures into numerical dimensions
  - Boxplot or quantile analysis on the transformed cube

Measuring the Central Tendency

- Mean (algebraic measure) (sample vs. population):

  Note: *n* is sample size and *N* is population size.

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

  - Weighted arithmetic mean

$$\bar{x} = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i}$$

  - Sensitive to outliers: trimmed mean (chopping extreme values)

- Median:
  - Middle value if odd number of values, or average of the middle two values otherwise
  - Estimated by interpolation (for *grouped data*):

age	$frequency$
1–5	200
6–15	450
16–20	300
21–50	1500
51–80	700
81–110	44

$$median = L_1 + \left(\frac{\frac{n}{2} - \left(\sum freq\right)_l}{freq_{median}}\right) width$$

Lower boundary of the median interval

# values in the dataset

Freq. of the median interval

Sum of freq. of intervals preceding the median

Measuring the Central Tendency

- Mode
  - Value that occurs most frequently in the data
  - Unimodal, bimodal, trimodal
  - Empirical formula for moderately skewed:

$$mean - mode \simeq 3 \times (mean - median)$$

Mean: 58

Median: (52+56)/2 = 54

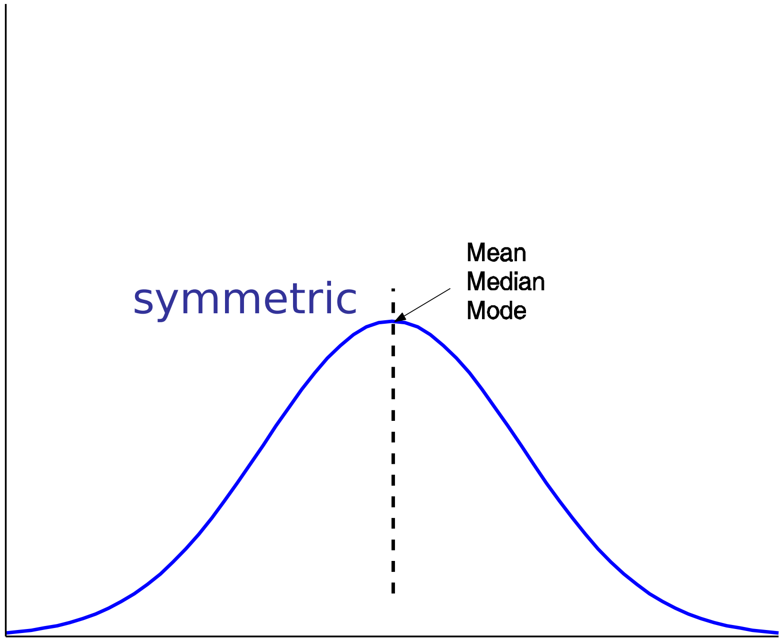
Mode: 52 and 70 (bimodal)

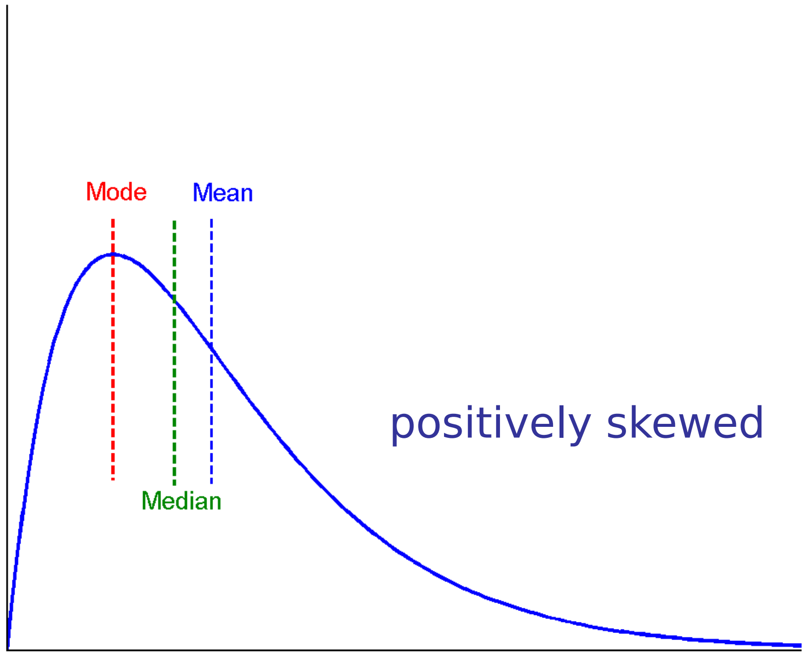
Midrange: (30+110) /2 = 70

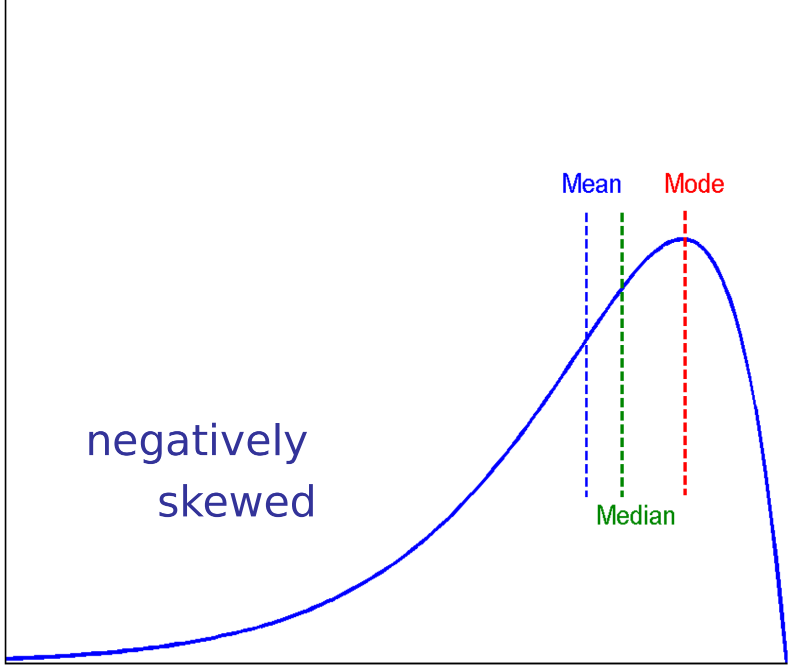
Employed	Salary
1	30
2	36
3	47
4	50
5	52
6	52
7	56
8	60
9	63
10	70
11	70
12	110

Symmetric vs. Skewed Data

- Median, mean and mode of symmetric, positively and negatively skewed data







Measuring the Dispersion of Data

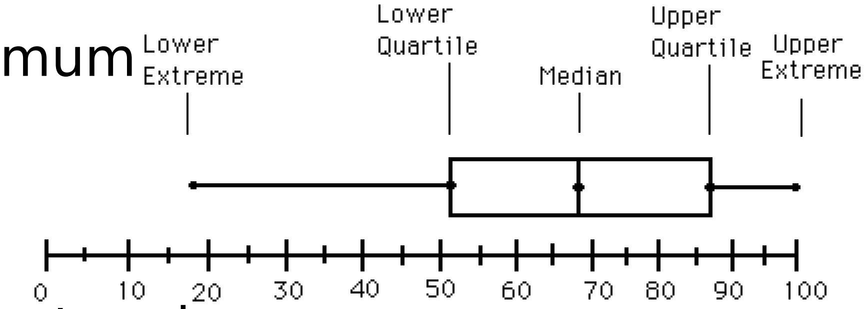
- Quartiles, outliers and boxplots
  - **Quartiles**: Q_1 (25th percentile), Q_3 (75th percentile)
  - **Inter-quartile range**: IQR = $Q_3 - Q_1$
  - **Five number summary**: min, Q_1, median, Q_3, max (nice for skewed distributions)
  - **Boxplot**: ends of the box are the quartiles; median is marked; add whiskers, and plot outliers individually
  - **Outlier**: usually, a value higher/lower than 1.5 x IQR
- Variance and standard deviation (*sample: s, population: σ)*
  - **Variance**: (algebraic, scalable computation)

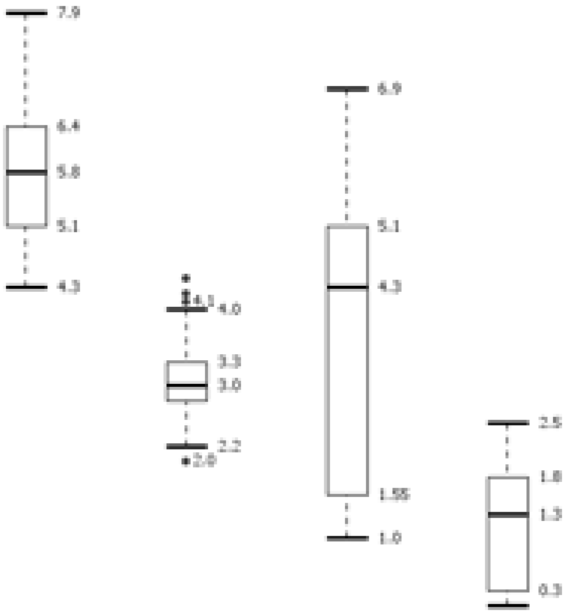
$$s^2=\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2=\frac{1}{n}[\sum_{i=1}^{n}x_i^2-\frac{1}{n}(\sum_{i=1}^{n}x_i)^2] \qquad \sigma^2=\frac{1}{N}\sum_{i=1}^{n}(x_i-\mu)^2=\frac{1}{N}\sum_{i=1}^{n}x_i^{\,2}-\mu^2$$

  - **Standard deviation** *s (or σ)* is the square root of variance

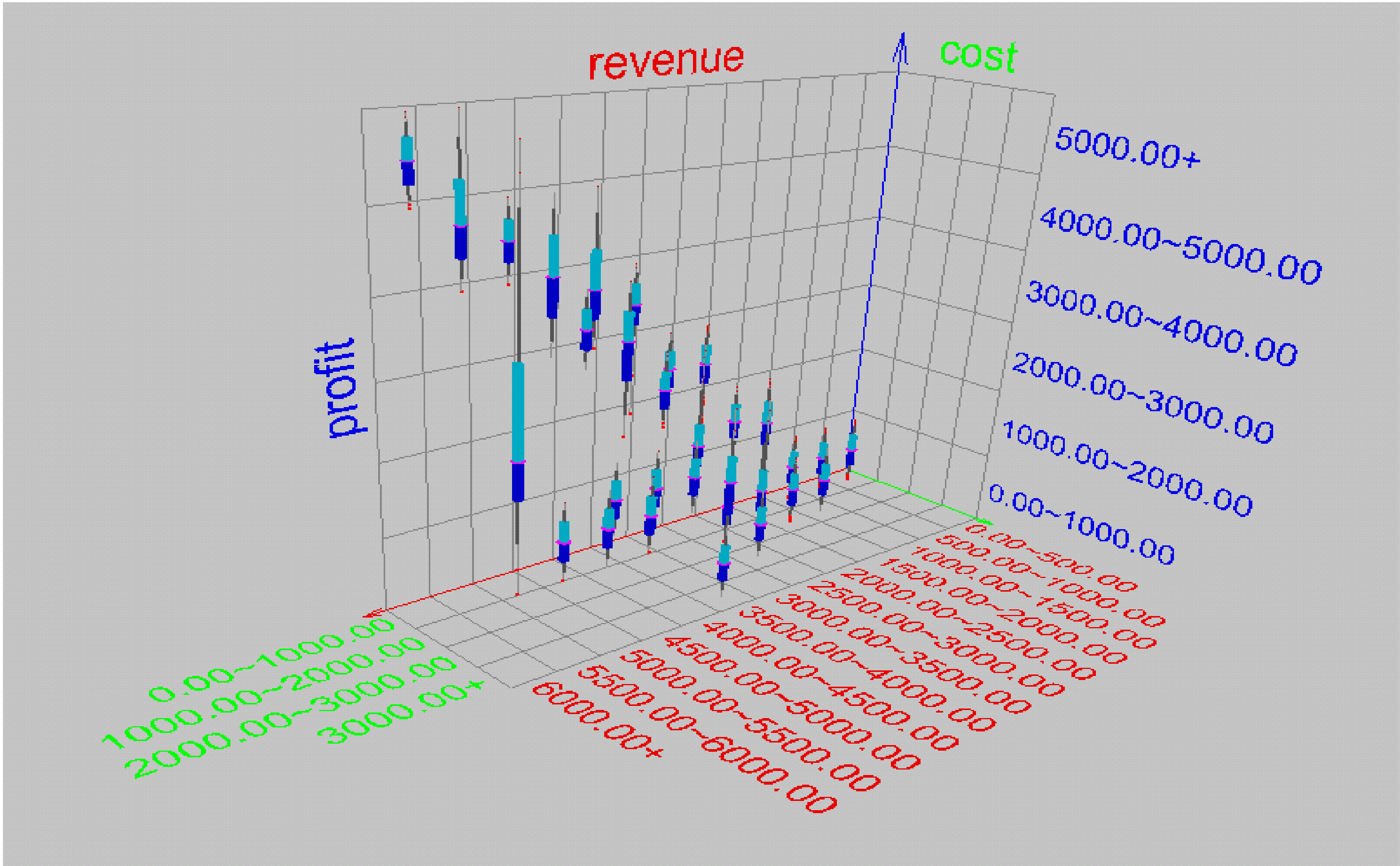
Boxplot Analysis

- **Five-number summary** of a distribution
  - Minimum, Q1, Median, Q3, Maximum
- **Boxplot**
  - Data is represented with a box
  - The ends of the box are at the first and third quartiles, i.e., the height of the box is IQR
  - The median is marked by a line within the box
  - Whiskers: two lines outside the box extended to Minimum and Maximum
  - Outliers: points beyond a specified outlier threshold, plotted individually





Visualization of Data Dispersion: 3-D Boxplots

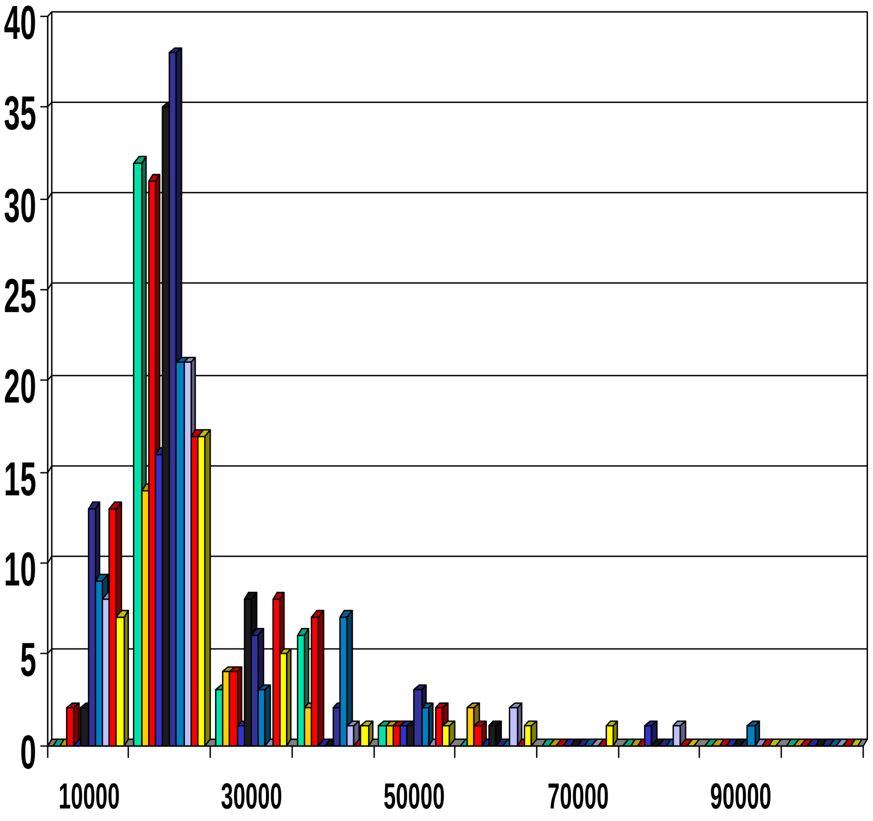


Graphic Displays of Basic Statistical Descriptions

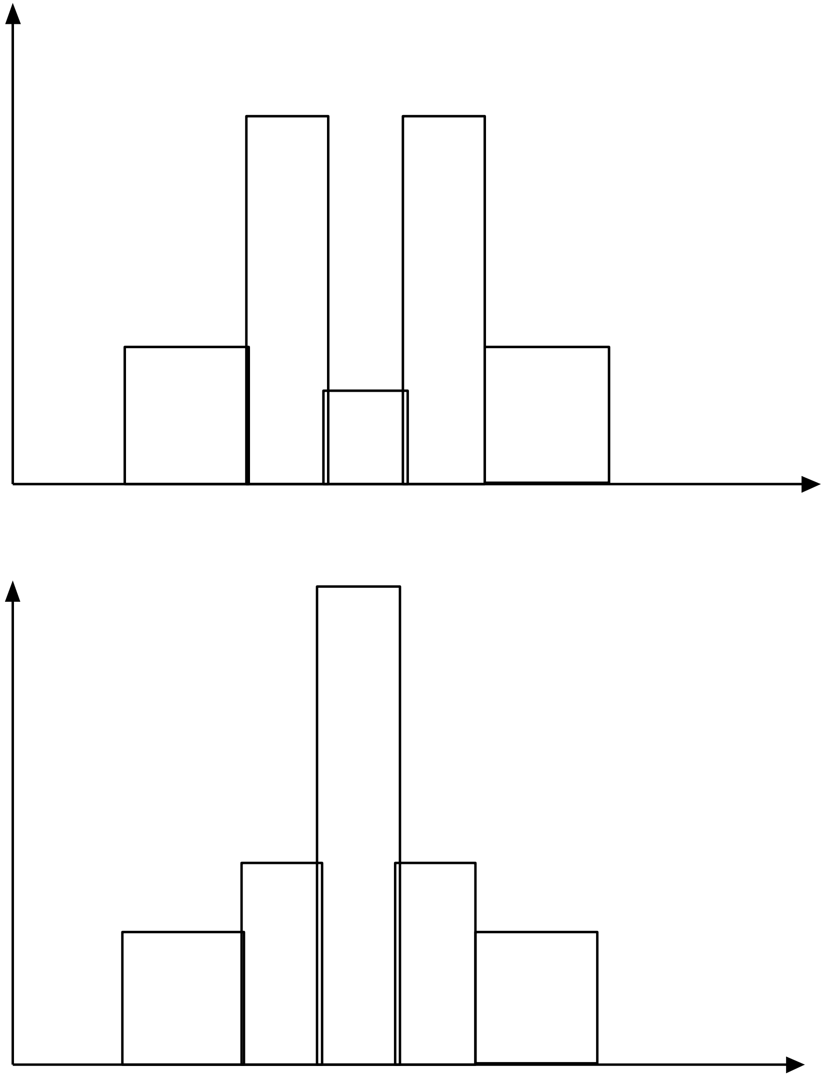
- **Boxplot**: graphic display of five-number summary
- **Histogram**: x-axis are values, y-axis repres. frequencies
- **Quantile plot**: each value x_i is paired with f_i indicating that approximately 100 f_i % of data are $\leq x_i$
- **Quantile-quantile (q-q) plot**: graphs the quantiles of one univariant distribution against the corresponding quantiles of another
- **Scatter plot**: each pair of values is a pair of coordinates and plotted as points in the plane

Histogram Analysis

- Histogram: Graph display of tabulated frequencies, shown as bars
- It shows what proportion of cases fall into each of several categories
- Differs from a bar chart in that it is the *area* of the bar that denotes the value, not the height as in bar charts, a crucial distinction when the categories are not of uniform width
- The categories are usually specified as non-overlapping intervals of some variable. The categories (bars) must be adjacent



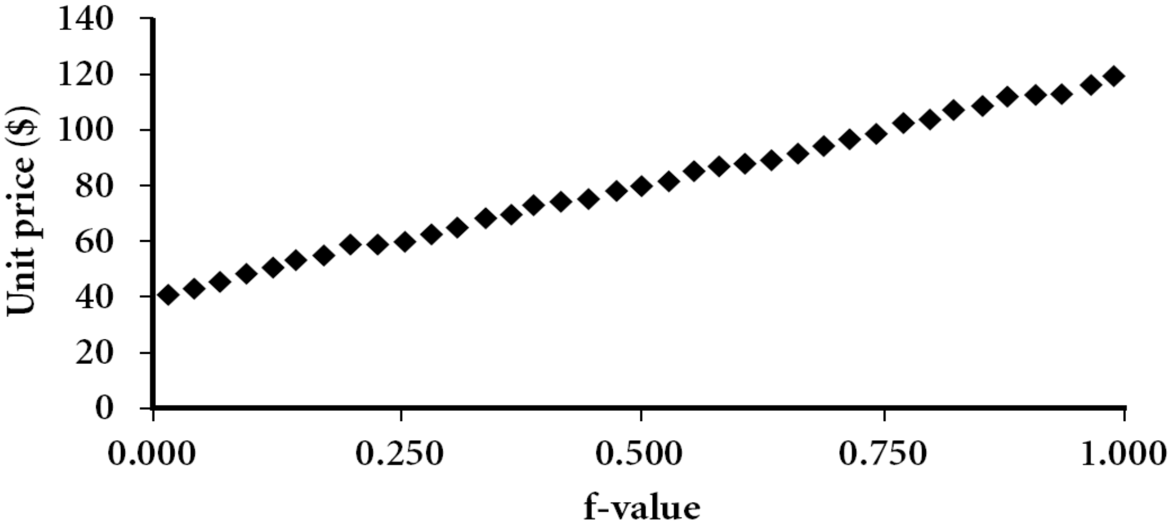
Histograms Often Tell More than Boxplots



- The two histograms shown in the left may have the same boxplot representation
  - The same values for: min, Q1, median, Q3, max
- But they have rather different data distributions

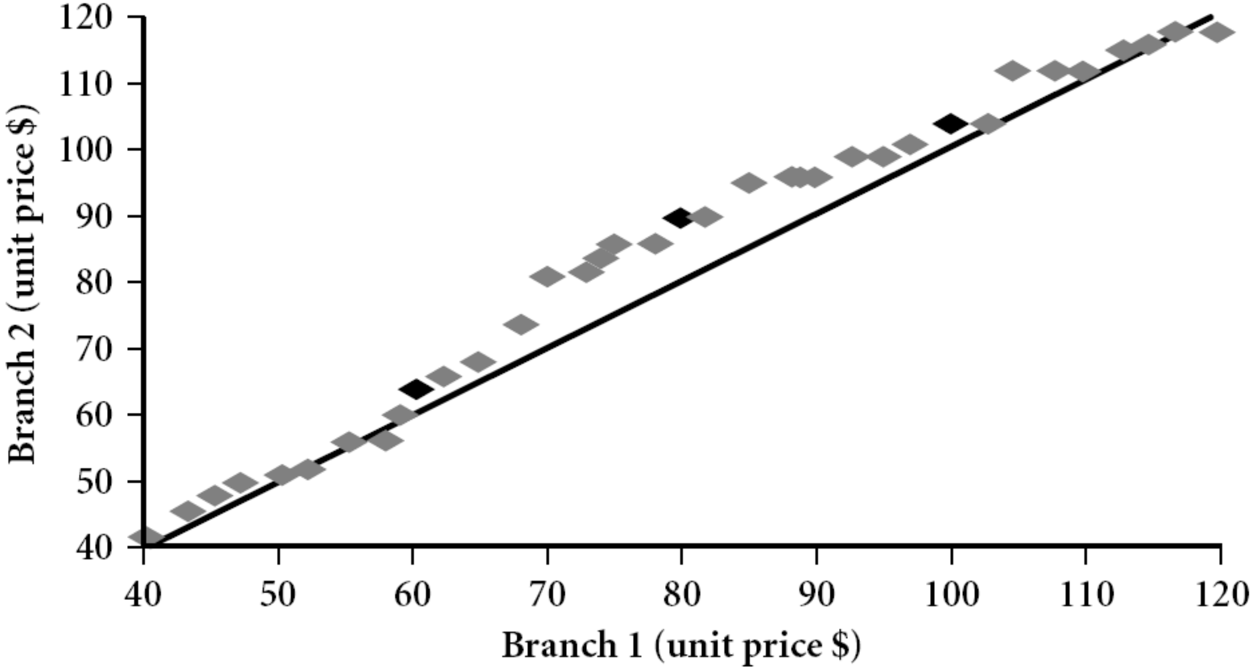
Quantile Plot

- Displays all of the data (assess both the overall behavior and unusual occurrences)
- Plots **quantile** information
  - Select an attribute x_i; *sort* data by non-decreasing x_i value; plot it equally spaced on the x axis
  - v(f) indicates the value s.t. a fraction f of data has value at most v(f)



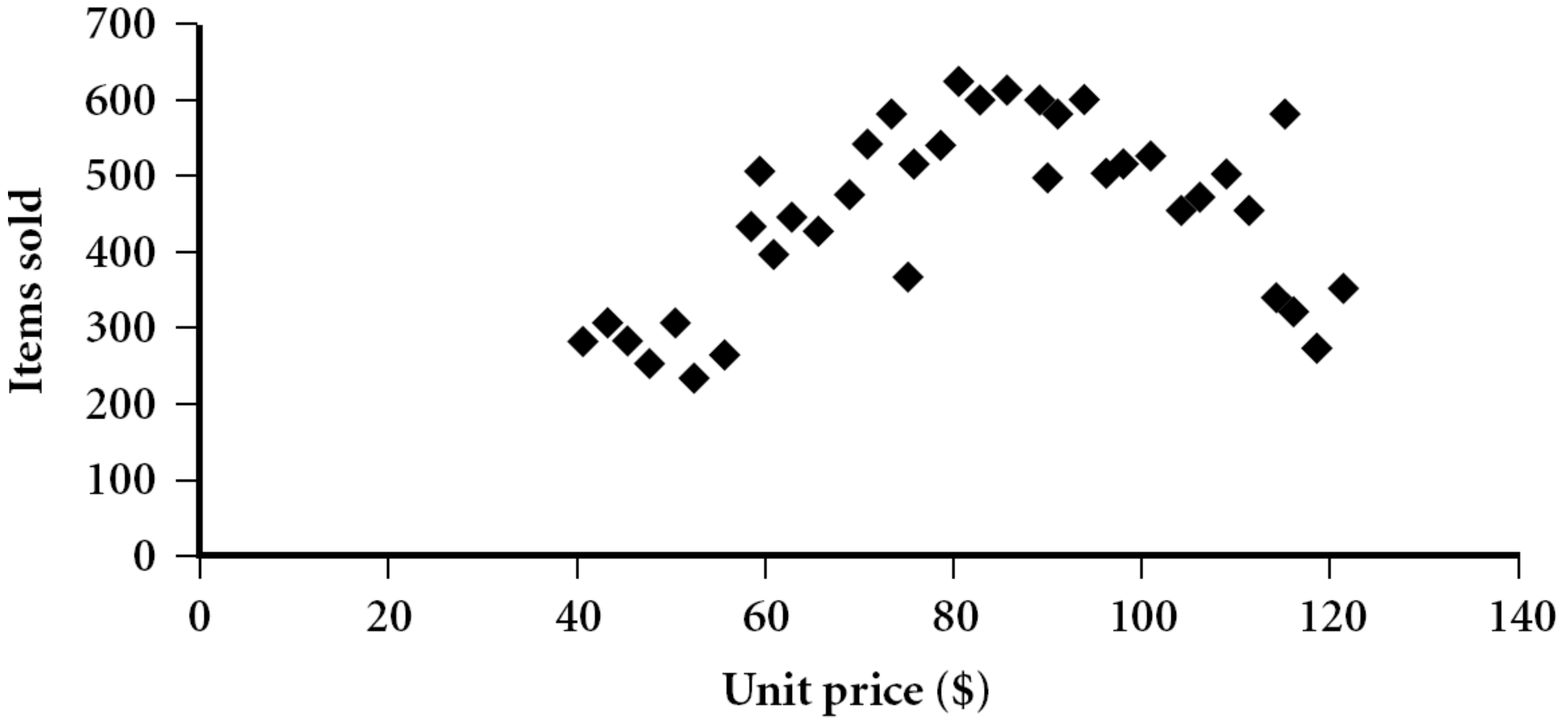
Quantile-Quantile (Q-Q) Plot

- Graphs the quantiles of one univariate distribution against the corresponding quantiles of another
- View: Is there is a shift in going from one distribution to another?
- Example shows unit price of items sold at Branch 1 vs. Branch 2 for each quantile. Unit prices of items sold at Branch 1 tend to be lower than those at Branch 2.

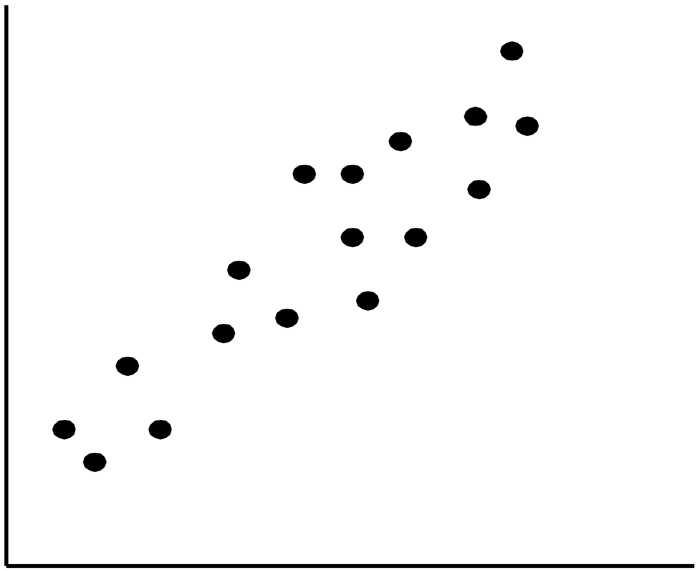


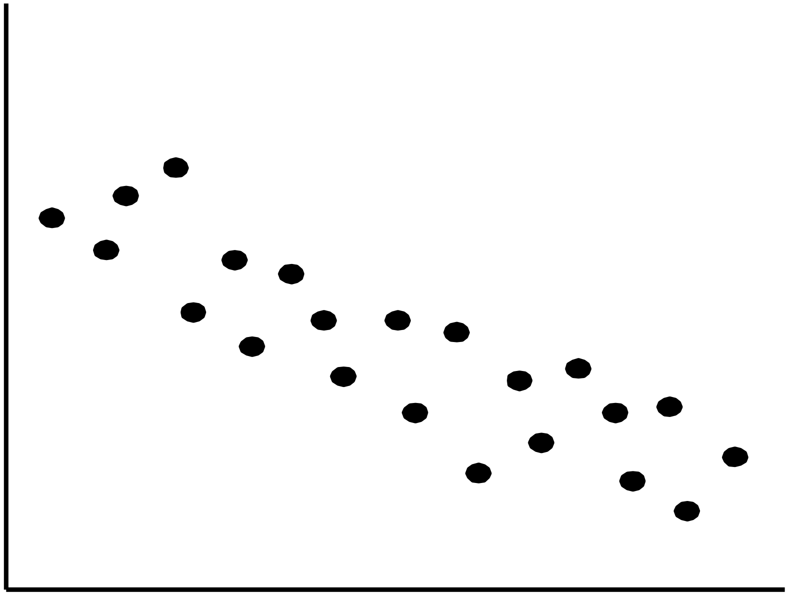
Scatter plot

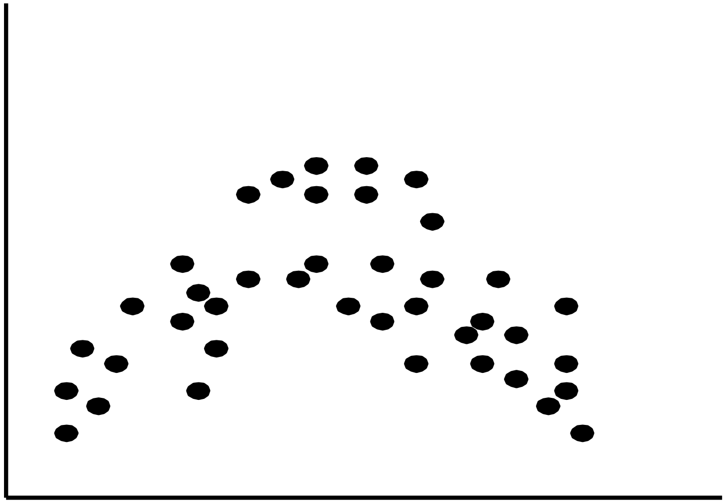
- Provides a first look at bivariate data to see clusters of points, outliers, etc
- Each pair of values is treated as a pair of coordinates and plotted as points in the plane



Positively and Negatively Correlated Data

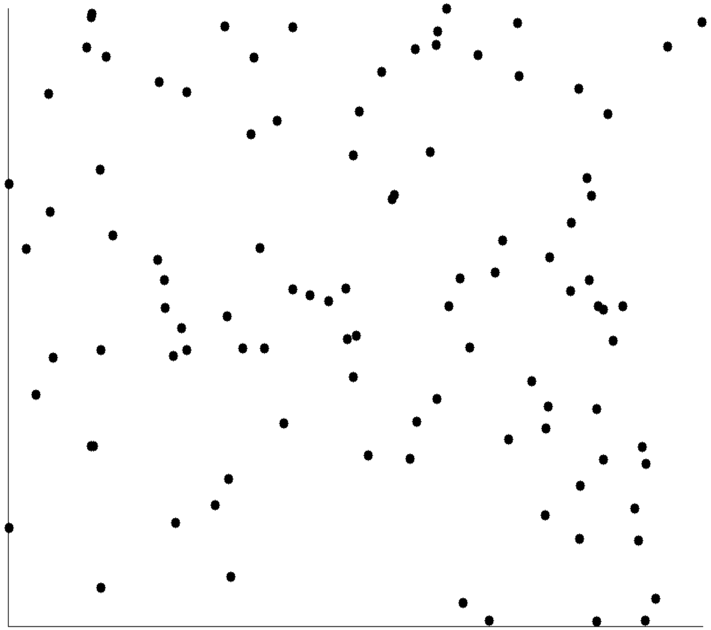


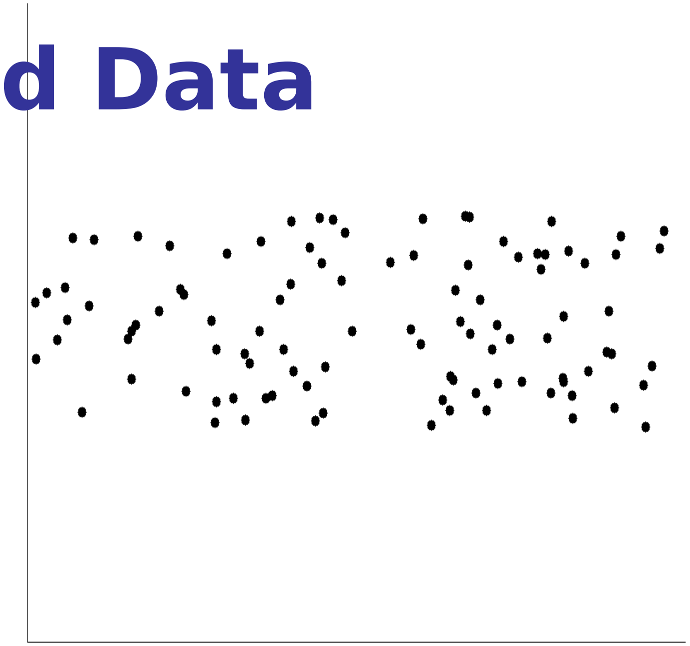


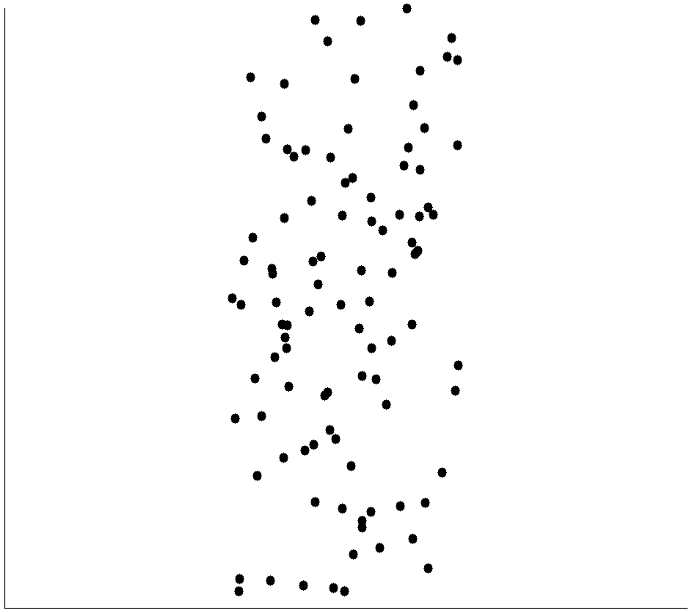


- The left half fragment is positively correlated
- The right half is negative correlated

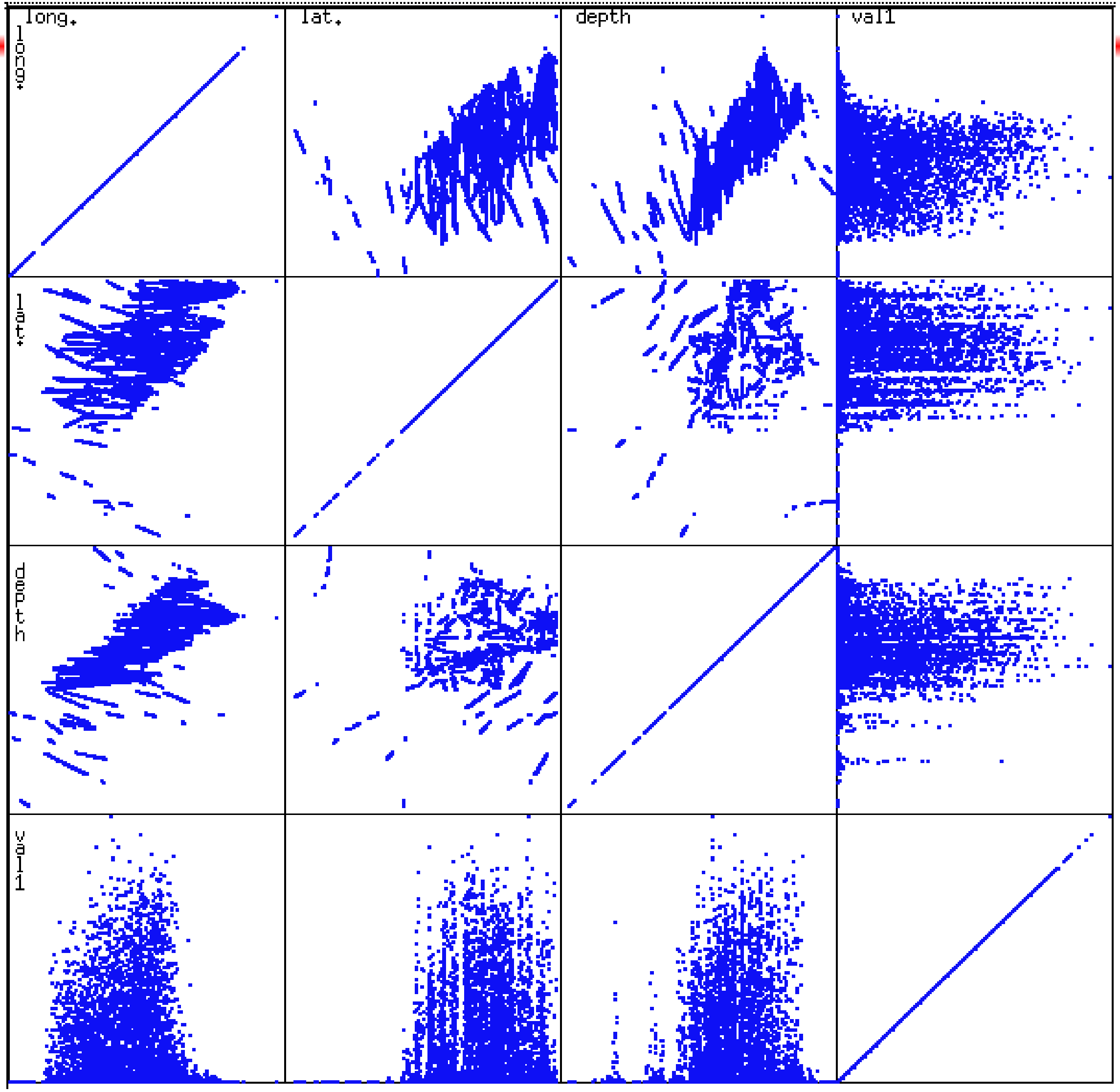
Uncorrelated Data







Scatterplot Matrices



Used by_ermission of M. Ward, Worcester Polytechnic Institute

Matrix of scatterplots (x-y-diagrams) of the k-dim. data [total of (k2/2-k) scatterplots]

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Similarity and Dissimilarity

- **Similarity**
  - Numerical measure of how alike two data objects are
  - Value is higher when objects are more alike
  - Often falls in the range [0,1]
- **Dissimilarity** (e.g., distance)
  - 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

Data Matrix and Dissimilarity Matrix

- Data matrix
  - n data points (objects) with p dimensions (features)

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

- Dissimilarity matrix
  - n data points, but registers only the distance
  - A triangular matrix

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}$$

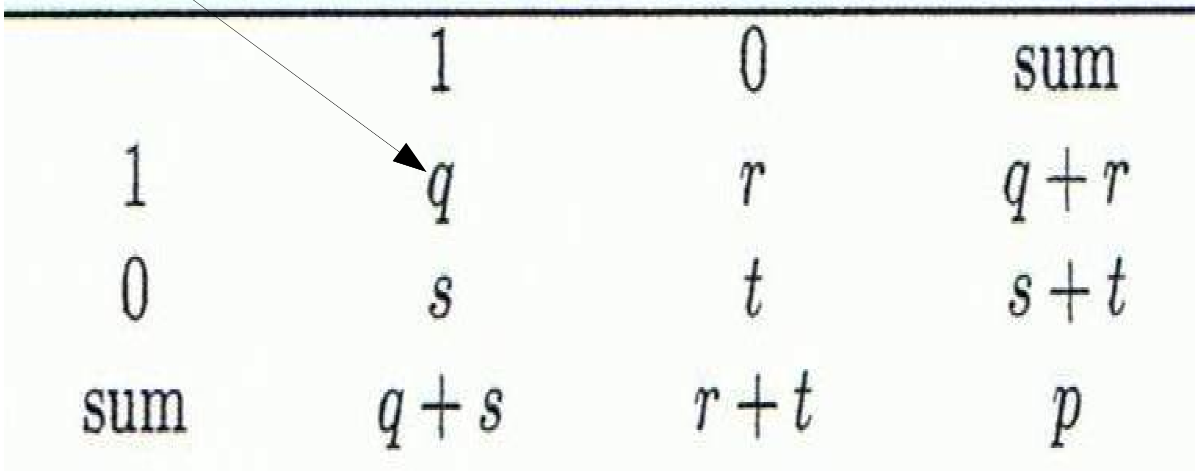
Proximity Measures for Binary Attributes

- A contingency table for binary data

Number of attributes for which both data objects have value 1

Data object *j*

Data object *i*



	1	0	sum
1	q	r	$q+r$
0	s	t	$s+t$
sum	$q+s$	$r+t$	p

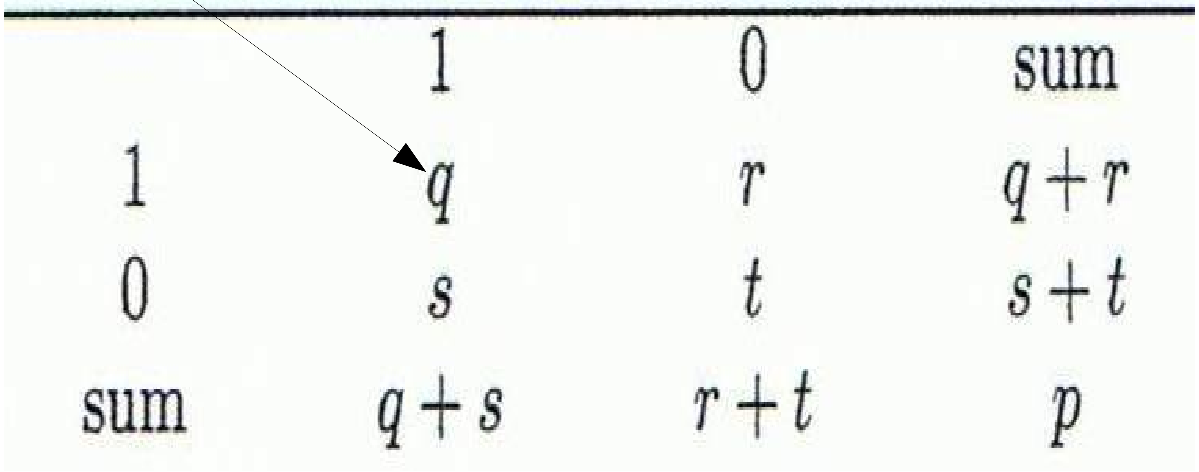
Proximity Measures for Binary Attributes

- … but we can do the same for attributes (transpose)

Number of data objects for which both attributes have value 1

Attribute *j*

Attribute *i*



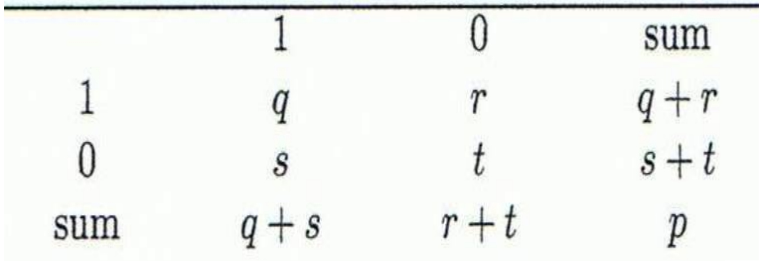
	1	0	sum
1	q	r	$q+r$
0	s	t	$s+t$
sum	$q+s$	$r+t$	p

Proximity Measures for Binary Attributes

- A contingency table for binary data

Data object *j*

Data object *i*



	1	0	sum
1	q	r	$q+r$
0	s	t	$s+t$
sum	$q+s$	$r+t$	p

- Distance measure for symmetric bin. vars (0 and 1 equally important):

$$d(i, j) = \frac{r + s}{q + r + s + t}$$

- Distance measure for asymm. bin. vars (1 more important – e.g. diseases):

$$d(i, j) = \frac{r + s}{q + r + s}$$

- Jaccard coefficient (*similarity* measure for *asymmetric* binary variables):

$$sim_{Jaccard}(i, j) = \frac{q}{q + r + s}$$

- Note: Jaccard coefficient is the same as “coherence”:

$$coherence(i, j) = \frac{sup(i, j)}{sup(i) + sup(j) - sup(i, j)} = \frac{q}{(q + r) + (q + s) - q}$$

Dissimilarity between Binary Attributes

- Example

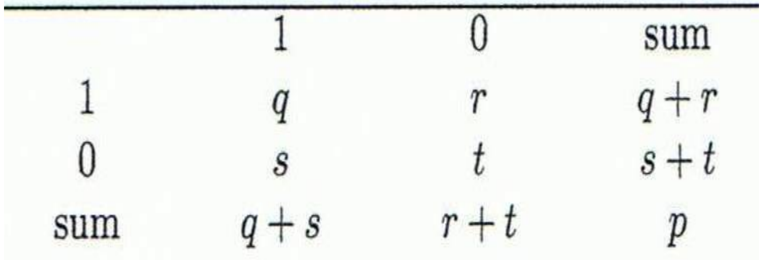
Name	Gender	Fever	Cough	Test-1	Test-2	Test-3
Jack	M	Y	N	P	N	N
Mary	F	Y	N	P	N	P
Jim	M	Y	P	N	N	N

  - Gender is a symmetric attribute (let's discard it!)
  - The remaining attributes are asymmetric binary
  - Let the values Y and P be 1, and the value N 0

$$d(jack, mary) = \frac{0+1}{2+0+1} = 0.33$$

$$d(jack, jim) = \frac{1+1}{1+1+1} = 0.67$$

$$d(jim, mary) = \frac{1+2}{1+1+2} = 0.75$$



	1	0	sum
1	q	r	$q+r$
0	s	t	$s+t$
sum	$q+s$	$r+t$	p

$$d(i, j) = \frac{r+s}{q+r+s}$$

Proximity Measures for Categorical (or “nominal”) Attributes

- Can take 2 or more states, e.g., red, yellow, blue, green (generalization of a binary attribute)
- Method 1: Simple matching
  - *m*: # of matches, *p*: total # of attributes

$$d(i,j)=\frac{p-m}{p}$$

- Method 2: Use a large number of binary attributes
  - creating a new binary attribute for each of the *M* categories

Proximity on Numeric Data: Minkowski Distance

- *Minkowski distance*: A popular distance measure

$$d(i, j) = \sqrt[h]{|x_{i1} - x_{j1}|^h + |x_{i2} - x_{j2}|^h + \cdots + |x_{ip} - x_{jp}|^h}$$

where $i = (x_{i1}, x_{i2}, \ldots, x_{ip})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jp})$ are two p-dimensional data objects, and h is the order (the distance so defined is also called L-h norm)

- Properties
  - d(i, j) > 0 if i ≠ j, and d(i, i) = 0 (Positive definiteness)
  - d(i, j) = d(j, i) (Symmetry)
  - d(i, j) ≤ d(i, k) + d(k, j) (Triangle Inequality)
- A distance that satisfies these properties is a metric

Special Cases of Minkowski Distance

- *h* = 1: Manhattan (city block, L_1 norm) distance
  - E.g., the Hamming distance: the number of bits that are different between two binary vectors

$$d(i,j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ip} - x_{jp}|$$

- *h* = 2: (L_2 norm) Euclidean distance

$$d(i,j) = \sqrt{(|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \dots + |x_{ip} - x_{jp}|^2)}$$

- $h \to \infty$. "supremum" (L_{max} norm, L_∞ norm) distance.
  - This is the maximum difference between any component (attribute) of the vectors

$$d(i,j) = \lim_{h \to \infty} \left(\sum_{f=1}^{p} |x_{if} - x_{jf}|^h \right)^{\frac{1}{h}} = \max_{f}^{p} |x_{if} - x_{jf}|$$

Example: Minkowski Distance

point	attribute 1	attribute 2
x1	1	2
x2	3	5
x3	2	0
x4	4	5

Dissimilarity Matrices

Manhattan (L_1)

L	x1	x2	x3	x4
x1	0			
x2	5	0		
x3	3	6	0	
x4	6	1	7	0

Euclidean (L_2)

L2	x1	x2	x3	x4
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

Supremum (L_{inf})

L_∞	x1	x2	x3	x4
x1	0			
x2	3	0		
x3	2	5	0	
x4	3	1	5	0

Standardizing Numeric Data

- Z-score: $z = \frac{x - \mu}{\sigma}$
  - X: raw data, μ: mean of the population, σ: standard deviation
  - the distance between the raw score and the population mean in units of the standard deviation
  - <0 when the raw score is below the mean, >0 when above
- An alternative way: Calculate the mean absolute deviation

$$s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + ... + |x_{nf} - m_f|)$$

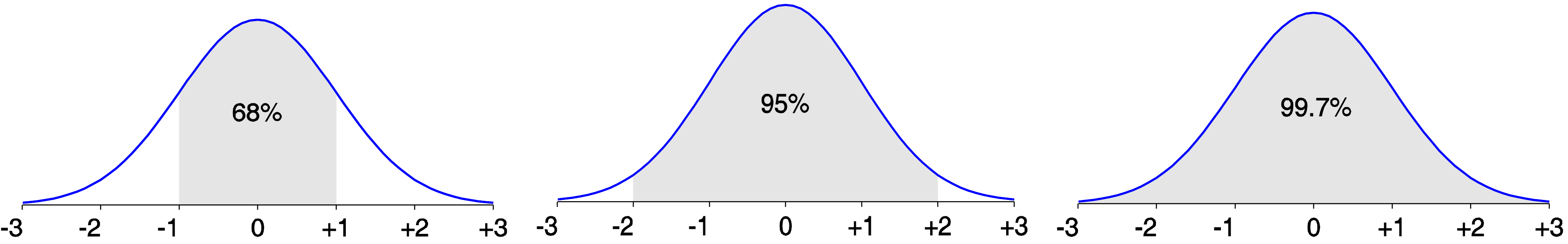
where

$$m_f = \frac{1}{n}(x_{1f} + x_{2f} + ... + x_{nf}).$$

  - standardized measure (*z-score*): $z_{if} = \frac{x_{if} - m_f}{s_f}$
- mean absolute deviation is more robust than std dev

Properties of Normal Distribution Curve

- The normal (distribution) curve
  - From μ–σ to μ+σ: contains about 68% of the measurements (μ: mean, σ: standard deviation)
  - From μ–2σ to μ+2σ: contains about 95% of it
  - From μ–3σ to μ+3σ: contains about 99.7% of it



Ordinal Variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank
- Can be treated like interval-scaled
  - replace x_{if} by their rank $r_{if} \in \{1, \ldots, M_f\}$
  - map (normalize) the range of each variable onto [0, 1] by replacing x_{if} by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

  - compute the dissimilarity using distance measures for numeric attributes

Attributes of Mixed Type

- A database may contain all attribute types
  - Nominal, symmetric binary, asymmetric binary, numeric, ordinal
- One may use a weighted formula to combine their effects

$$d(i,j)=\frac{\Sigma_{f=1}^{p}\delta_{ij}^{(f)}d_{ij}^{(f)}}{\Sigma_{f=1}^{p}\delta_{ij}^{(f)}}$$

- Choice of $\delta_{ij}^{(f)}$
  - Set $\delta_{ij}^{(f)}=0$ if
    - x_{if} or x_{jf} is missing
    - $x_{if} = x_{jf} = 0$ and f is asymmetric binary
  - Set $\delta_{ij}^{(f)}=1$ otherwise

Attributes of Mixed Type

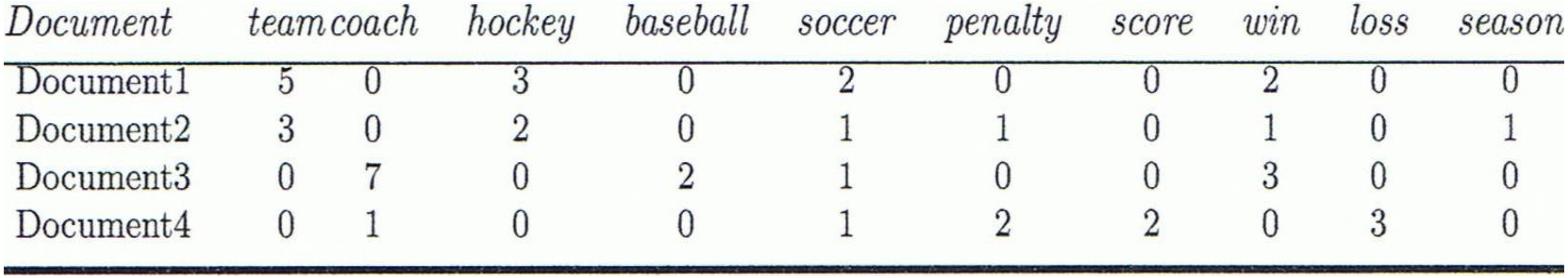
$$d(i,j) = \frac{\sum_{f=1}^{p} \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^{p} \delta_{ij}^{(f)}}$$

- *Choice of $d_{ij}^{(f)}$*
  - *when f* is binary or nominal:

    $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$, $d_{ij}^{(f)} = 1$ otherwise
  - *when f* is numeric: use the normalized distance
  - *when f* is ordinal
    - Compute ranks r_{if} and $z_{if} = \frac{r_{if} - 1}{M_f - 1}$
    - Treat z_{if} as interval-scaled

Cosine Similarity

- A **document** can be represented by thousands of attributes, each recording the *frequency* of a particular word (such as keywords) or phrase in the document.



Document	*team*	*coach*	*hockey*	*baseball*	*soccer*	*penalty*	*score*	*win*	*loss*	*season*
Document1	5	0	3	0	2	0	0	2	0	0
Document2	3	0	2	0	1	1	0	1	0	1
Document3	0	7	0	2	1	0	0	3	0	0
Document4	0	1	0	0	1	2	2	0	3	0

- Other vector objects: gene features in micro-arrays, …
- Applications: information retrieval, biologic taxonomy, gene feature mapping, ...
- Issue: very long and **sparse**

- Treat documents as vectors, and compute a **cosine similarity**

Cosine Similarity

- Cosine measure: If x and y are two vectors (e.g., term-frequency vectors), then

  cos(x, *y*) = (*x* • *y*) /||*x*|| ||*y*||

  where
  - • indicates vector dot product, $x \cdot y = \sum_{i=1}^{p} x_i y_i$
  - ||*x*||: the L2 norm (length) of vector x $\|x\| = \sqrt{x_1^2 + x_2^2 + \ldots + x_p^2}$

- Remark: when attributes are binary valued:
  - • indicates the number of shared features
  - ||*x*|| ||y|| is the geometric mean between the number of features of x and the number of features of y:

    sqrt(a) * sqrt(b) = sqrt(a * b)
  - cos (x, y) measures relative possession of common features

Example: Cosine Similarity

- cos(x, *y*) = (*x* • *y*) /||*x*|| ||*y*||
- Ex: Find the **similarity** between documents x and y.

x = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0)
***y* =** (3, 0, 2, 0, 1, 1, 0, 1, 0, 1)

x • y = 5*3+0*0+3*2+0*0+2*1+0*1+0*1+2*1+0*0+0*1=
= 25

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

$||y||= (3*3+0*0+2*2+0*0+1*1+1*1+0*0+1*1+0*0+1*1)^{\mathbf{0.5}}=$
= 4.12

cos(x, *y*) = 25 / (6.481 * 4.12) = 0.94

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