



CS 412 Intro. to Data Mining

Chapter 2. Getting to Know Your Data

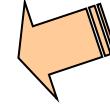
Jiawei Han, Computer Science, Univ. Illinois at Urbana-Champaign, 2017





Chapter 2. Getting to Know Your Data

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



Types of Data Sets: (1) Record Data

- Relational records
 - Relational tables, highly structured
- Data matrix, e.g., numerical matrix, crosstabs

| | China | England | France | Japan | USA | Total |
|-------------------------------|-------|---------|--------|-------|----------|----------|
| Active Outdoors Crochet Glove | | 12.00 | 4.00 | 1.00 | 240.00 | 257.00 |
| Active Outdoors Lycra Glove | | 10.00 | 6.00 | | 323.00 | 339.00 |
| InFlux Crochet Glove | 3.00 | 6.00 | 8.00 | | 132.00 | 149.00 |
| InFlux Lycra Glove | | 2.00 | | | 143.00 | 145.00 |
| Triumph Pro Helmet | 3.00 | 1.00 | 7.00 | | 333.00 | 344.00 |
| Triumph Vertigo Helmet | | 3.00 | 22.00 | | 474.00 | 499.00 |
| Xtreme Adult Helmet | 8.00 | 8.00 | 7.00 | 2.00 | 251.00 | 276.00 |
| Xtreme Youth Helmet | | 1.00 | | | 76.00 | 77.00 |
| Total | 14.00 | 43.00 | 54.00 | 3.00 | 1,972.00 | 2,086.00 |

- Transaction data

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

- Document data: Term-frequency vector (matrix) of text documents

Person:

| Pers_ID | Surname | First_Name | City |
|---------|-----------|------------|----------|
| 0 | Miller | Paul | London |
| 1 | Ortega | Alvaro | Valencia |
| 2 | Huber | Urs | Zurich |
| 3 | Blanc | Gaston | Paris |
| 4 | Bertolini | Fabrizio | Rom |

no relation

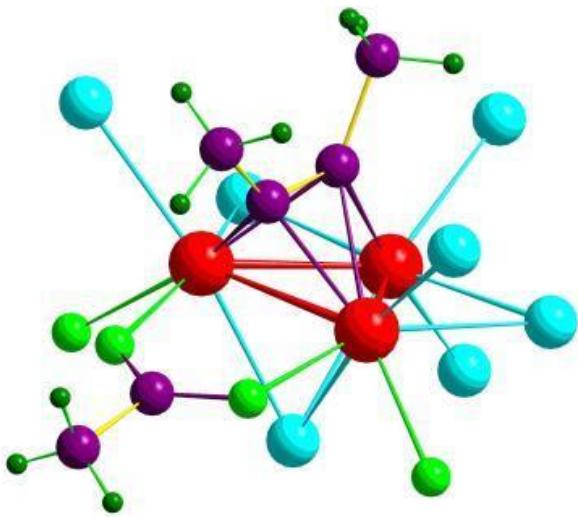
Car:

| Car_ID | Model | Year | Value | Pers_ID |
|--------|-------------|------|--------|---------|
| 101 | Bentley | 1973 | 100000 | 0 |
| 102 | Rolls Royce | 1965 | 330000 | 0 |
| 103 | Peugeot | 1993 | 500 | 3 |
| 104 | Ferrari | 2005 | 150000 | 4 |
| 105 | Renault | 1998 | 2000 | 3 |
| 106 | Renault | 2001 | 7000 | 3 |
| 107 | Smart | 1999 | 2000 | 2 |

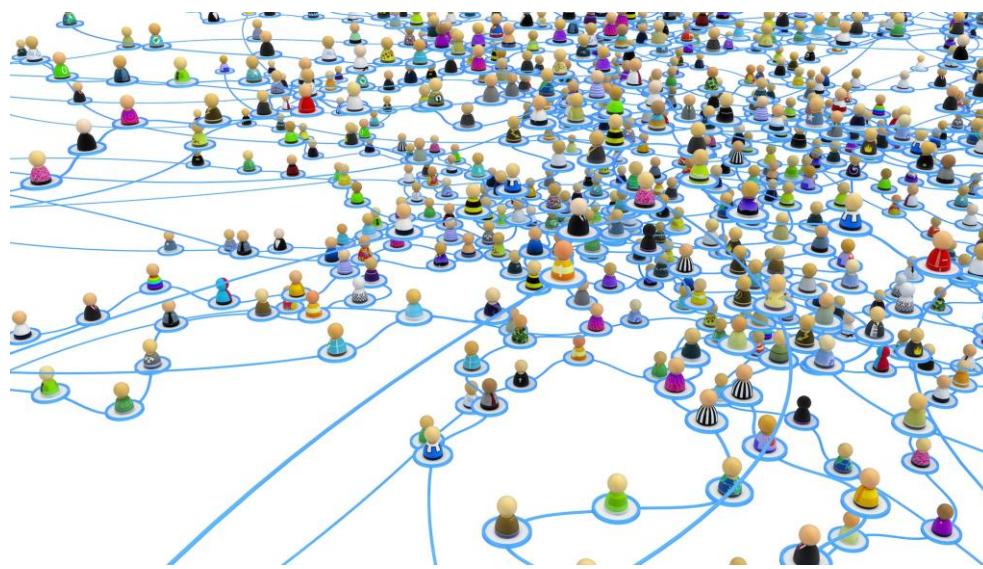
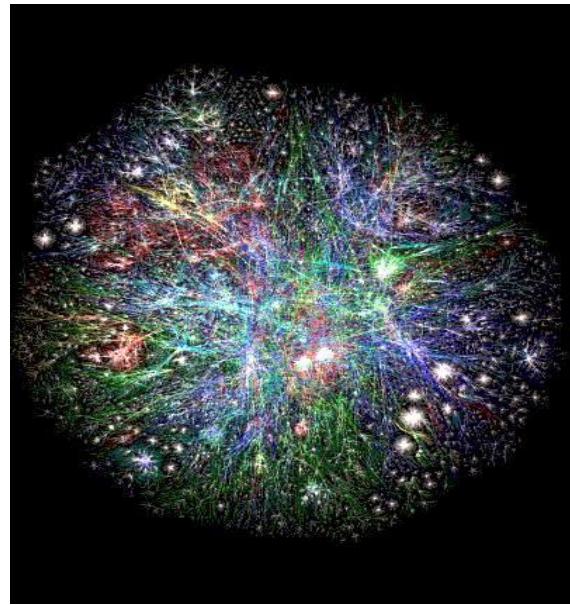
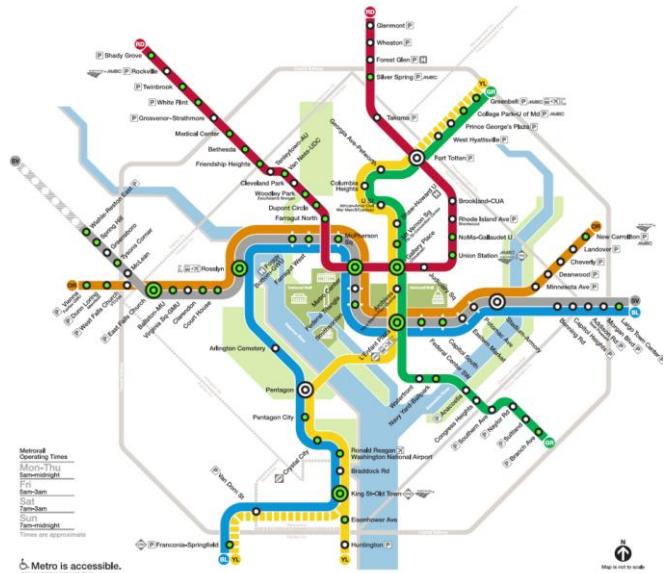
| team | coach | y | pla | ball | score | game | n | wi | lost | timeout | season |
|------------|-------|---|-----|------|-------|------|---|----|------|---------|--------|
| Document 1 | 3 | 0 | 5 | 0 | 2 | 6 | 0 | 2 | 0 | 2 | |
| Document 2 | 0 | 7 | 0 | 2 | 1 | 0 | 0 | 3 | 0 | 0 | |
| Document 3 | 0 | 1 | 0 | 0 | 1 | 2 | 2 | 0 | 3 | 0 | |

Types of Data Sets: (2) Graphs and Networks

- Transportation network
- World Wide Web

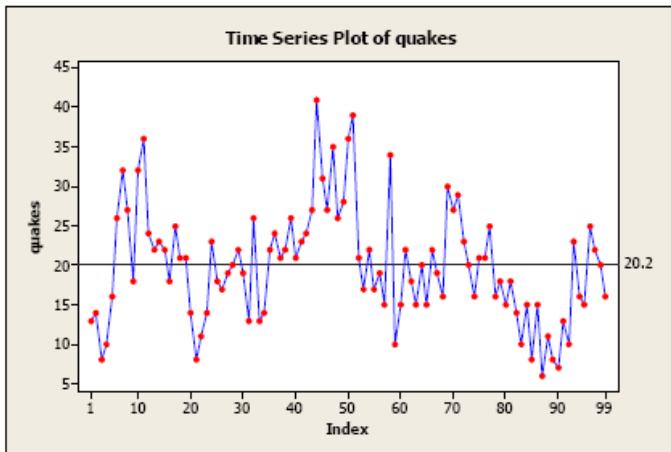


- Molecular Structures
- Social or information networks



Types of Data Sets: (3) Ordered Data

- Video data: sequence of images



- Temporal data: time-series



- Sequential Data: transaction sequences

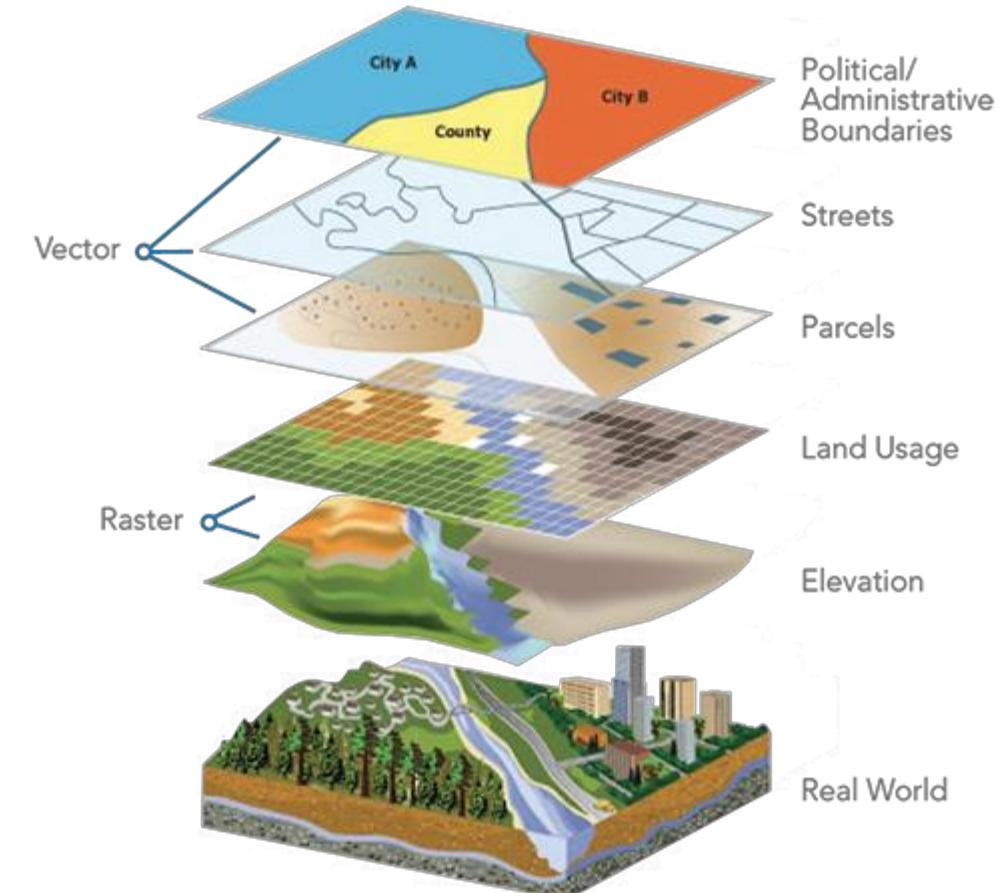
- Genetic sequence data

Start

| | | |
|------------|---|--|
| Human | GTTTGAGG | - - - ATGTTCAACAAATGCTCCTTCATTCCCTATTTACAGACCTGCCGCA |
| Chimpanzee | GTTTGAGG | - - - ATGTTCAATAATGCTGCTTCACTCCCTATTTACAGACCTGCCGCA |
| Macaque | GTTTGAGG | - - - ATGCTCAATAATGCTCCTTCATTCCCTCATTACAAACTTGCGCA |
| Human | GACAATTCTGCTAGCAGCCTTGTGCTATTATCTGTTTCTAAACCTTAGTAATTGAGTGT | |
| Chimpanzee | GACAATTCTGCTAGCAGCCTTGTGCTATTATCTGTTTCTAAACCTTAGTAATTGAGTGT | |
| Macaque | GACAATTCTGCTAGCAGCCTTGTGCTATTATCTGTTTCTAAACCTTAGTAATTGAGTGT | |
| Human | GATCTGGAGACTAACTCTGAAATAAAAGCTGATTATTTATTTATTTCTCAAAACAA | |
| Chimpanzee | GATCTGGAGACTAAACTCTGAAATAAAAGCTGATTATTTATTTATTTCTCAAAACAA | |
| Macaque | TATCTGGAGACTAAACTCTGAAATAAAAGCTGATTATTTATTTATTTCTCAAAACAA | |
| Human | CAGAACACGATTTAGCAAATTACTCTTAAGATAATTATTTACATTTCATATTCTCTA | |
| Chimpanzee | CAGAACACGATTTAGCAAATTACTCTTAAGATAACTATTTCATATTCTCTA | |
| Macaque | CAGAACATGATTTAGCAAATTACCTCTTAAGATAATTATTTGCACCTTCATATTCTCTA | |
| Human | CCCTGAGTTGATGTGAGCAATATGTCACCTTCATAAAGCCAGGTATACAC- - - TTATG | |
| Chimpanzee | CCCTGAGTTGATGTGAGCCGATGTCACCTTCATAAAGCCAGGTATACAC- - - TTATG | |
| Macaque | CCCTGAGTTGATGTGAGCAATATGTCACCTCCACAAAGCCAGGTATATACATTACG | |
| Human | GACAGGTAAGTAAAAACATATTATTTATCTACGTTTGTCCAAGAATTAAATTTC | |
| Chimpanzee | GACAGGTAAGTAAAAACATATTATTTATCTACGTTTGTCCAAGAATTAAATTTC | |
| Macaque | GACAGGTAAGTAAAAACATATTATTTATCTACGTTTGTCCAAGAATTAAATTTC | |
| Human | AACTGTTGCGCGTGTGGTAA- - - TGTAAAACAAACTCAGTACA | |
| Chimpanzee | AACTGTTGCGCGTGTGGTAA- - - TGTAAAACAAACTCAGTACA | |
| Macaque | AACTGTTGCGCGTGTGGTAA- - - CBAAAACAAACTCAGTACA | |

Types of Data Sets: (4) Spatial, image and multimedia Data

- Spatial data: maps



- Image data:

- Video data:

Important Characteristics of Structured Data

- ❑ Dimensionality
 - ❑ Curse of dimensionality
- ❑ 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
- ❑ Examples:
 - ❑ sales database: customers, store items, sales
 - ❑ medical database: patients, treatments
 - ❑ university database: students, professors, courses
- ❑ Also called *samples* , *examples*, *instances*, *data points*, *objects*, *tuples*
- ❑ Data objects are described by **attributes**
- ❑ Database 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 (e.g., red, blue)
 - Binary (e.g., {true, false})
 - Ordinal (e.g., {freshman, sophomore, junior, senior})
 - Numeric: quantitative
 - Interval-scaled: 100°C is interval scales
 - Ratio-scaled: 100°K is ratio scaled since it is twice as high as 50°K
- Q1: Is student ID a nominal, ordinal, or interval-scaled data?
- Q2: What about eye color? Or color in the color spectrum of physics?

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

□ Discrete Attribute

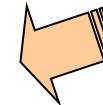
- Has only a finite or countably infinite set of values
 - E.g., zip codes, profession, or the set of words in a collection of documents
- Sometimes, represented as integer variables
- Note: Binary attributes are a special case of discrete attributes

□ 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

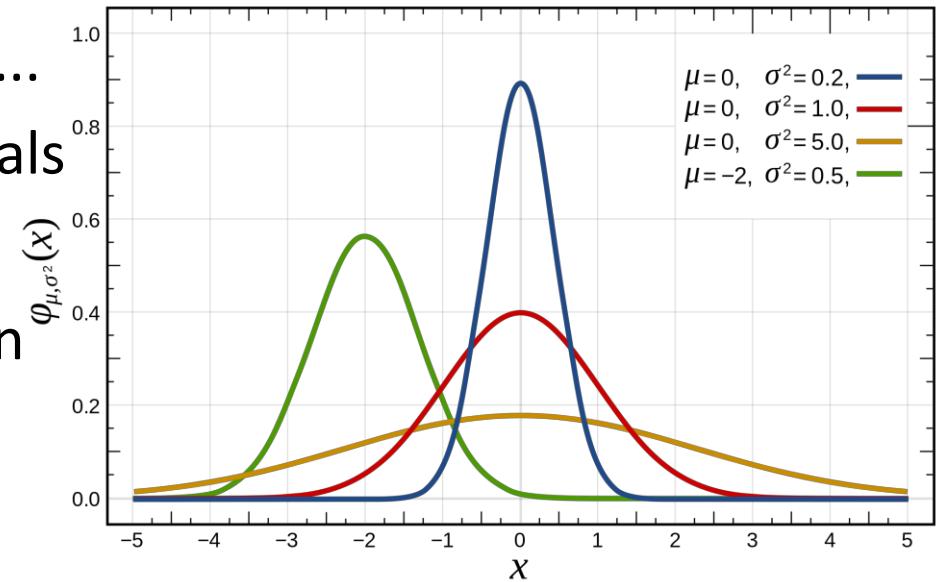
Chapter 2. Getting to Know Your Data

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



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: (1) Mean

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

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

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i \quad \mu = \frac{\sum x}{N}$$

- Weighted arithmetic mean:

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

- Trimmed mean:

- Chopping extreme values (e.g., Olympics gymnastics score computation)

Measuring the Central Tendency: (2) Median

- 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 |

Approximate
median



Sum before the median interval

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

Low interval limit



Interval width ($L_2 - L_1$)



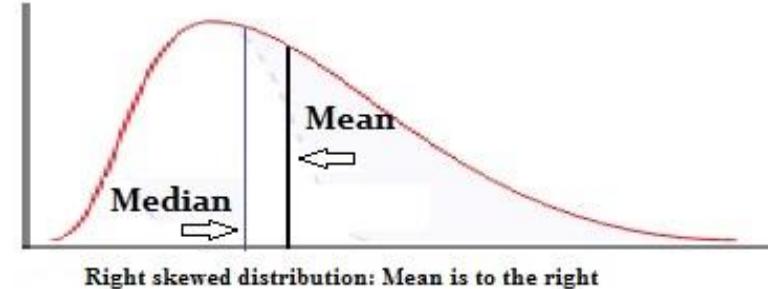
Measuring the Central Tendency: (3) Mode

- Mode: Value that occurs most frequently in the data

- Unimodal

- Empirical formula:

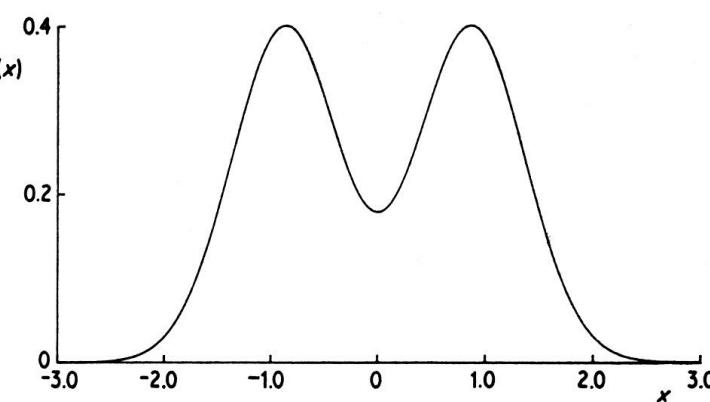
$$\text{mean} - \text{mode} = 3 \times (\text{mean} - \text{median})$$



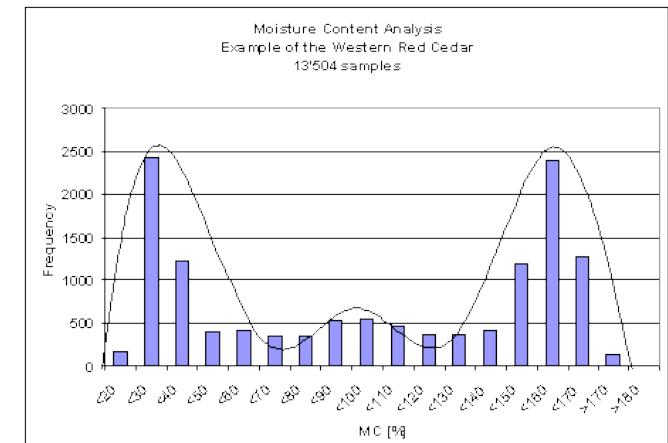
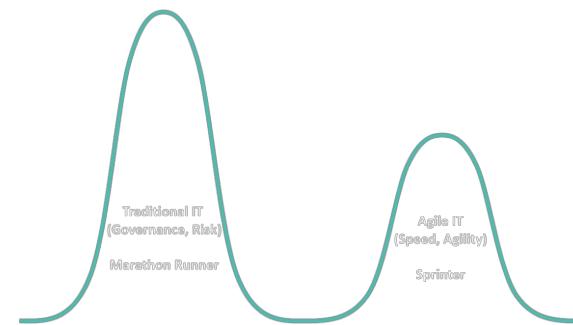
Right skewed distribution: Mean is to the right

- Multi-modal

- Bimodal



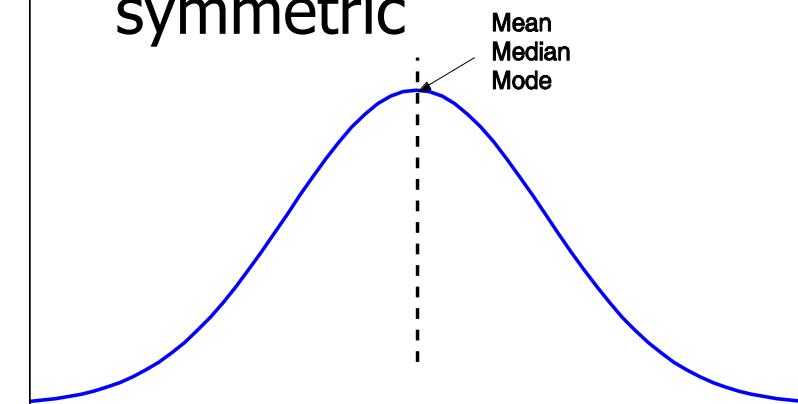
- Trimodal



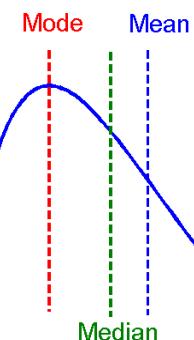
Symmetric vs. Skewed Data

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

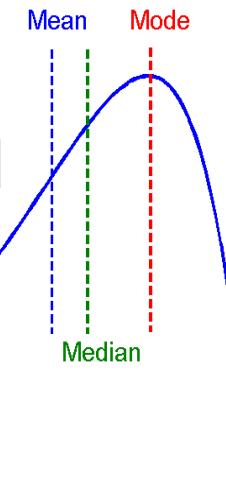
symmetric



positively skewed

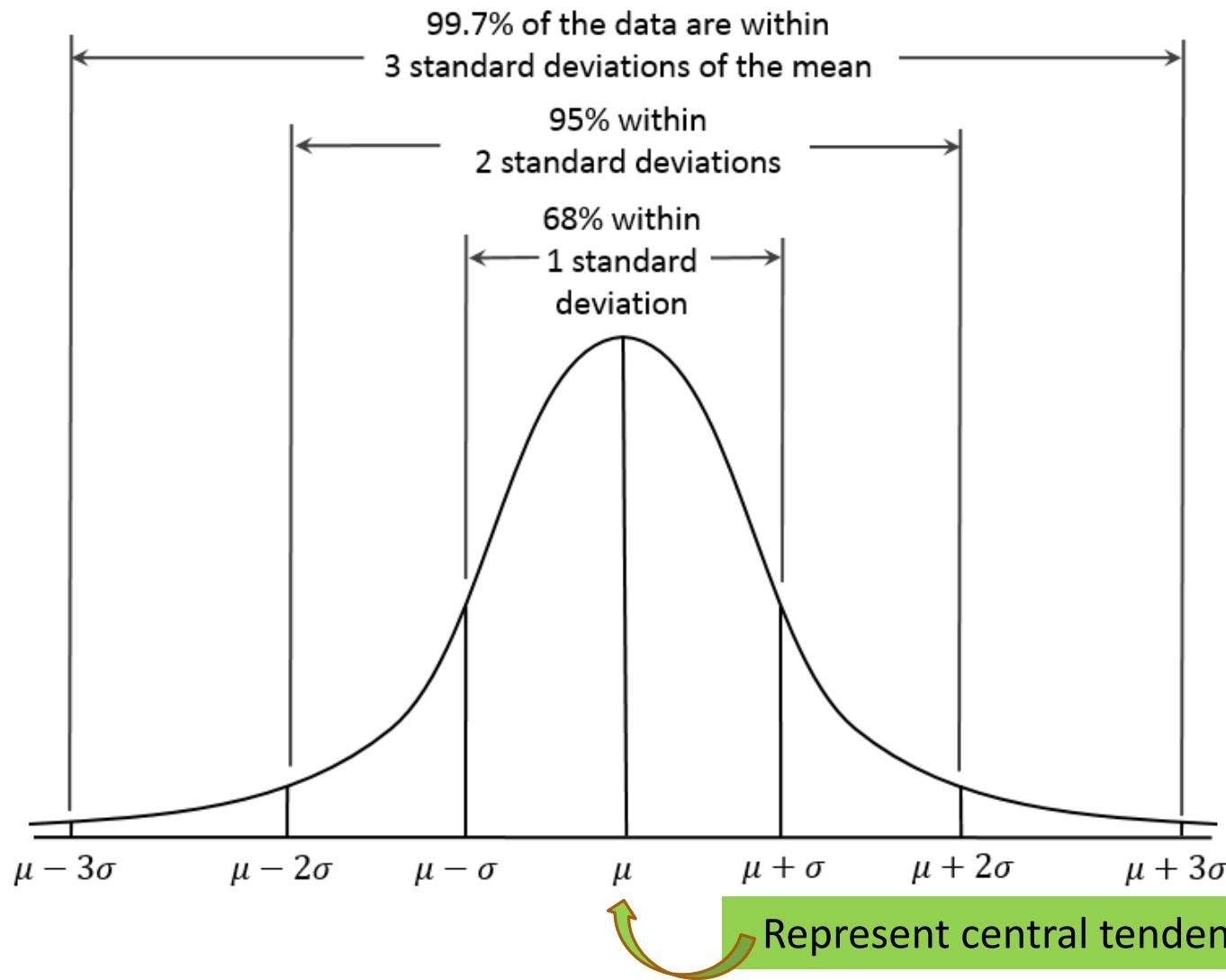


negatively skewed



Properties of Normal Distribution Curve

← —————— Represent data dispersion, spread —————— →



Measures Data Distribution: Variance and Standard Deviation

- ❑ Variance and standard deviation (*sample: s, population: σ*)

- ❑ **Variance:** (algebraic, scalable computation)

- ❑ Q: Can you compute it incrementally and efficiently?

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2 = \frac{1}{n-1} \left[\sum_{i=1}^n x_i^2 - \frac{1}{n} \left(\sum_{i=1}^n x_i \right)^2 \right]$$

$$\sigma^2 = \frac{1}{N} \sum_{i=1}^n (x_i - \mu)^2 = \frac{1}{N} \sum_{i=1}^n x_i^2 - \mu^2$$

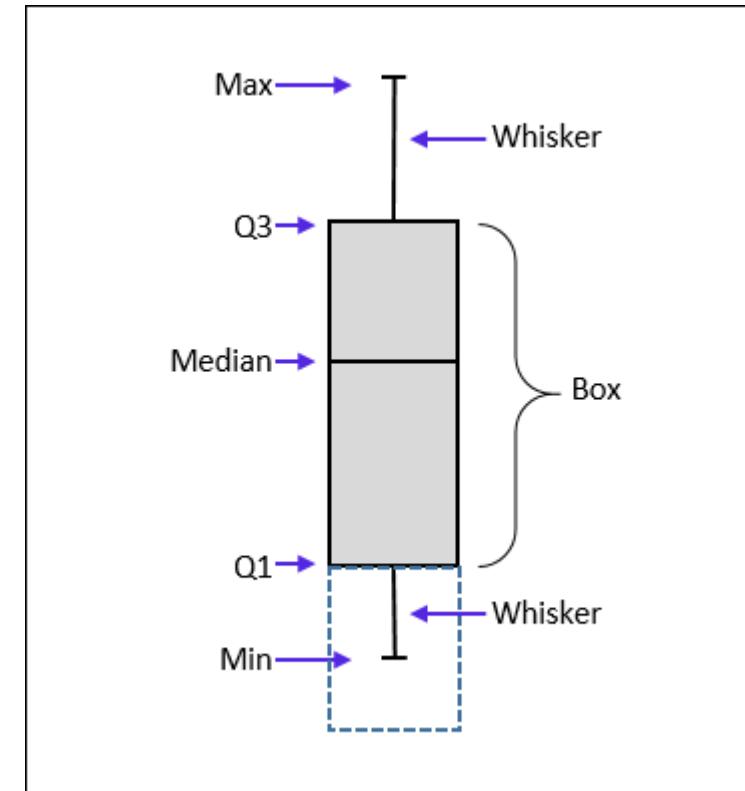
- ❑ **Standard deviation s (or σ)** is the square root of variance s^2 (or σ^2)

Graphic Displays of Basic Statistical Descriptions

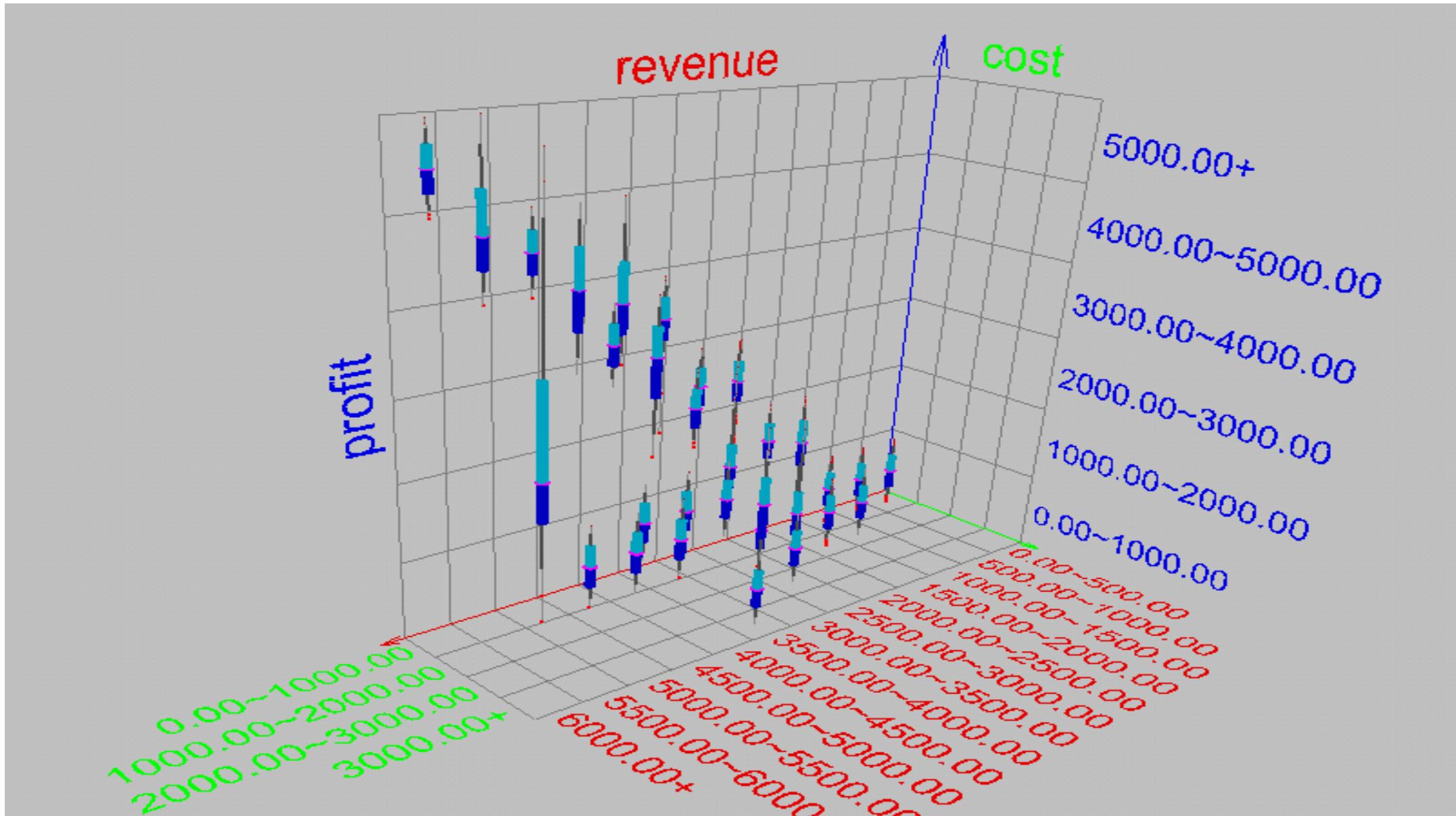
- **Boxplot:** graphic display of five-number summary
- **Histogram:** x-axis are values, y-axis repres. frequencies
- **Quantile plot:** each value x_i is paired with f_i , indicating that approximately $100 f_i \%$ of data are $\leq x_i$
- **Quantile-quantile (q-q) plot:** graphs the quantiles of one 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

Measuring the Dispersion of Data: Quartiles & Boxplots

- **Quartiles:** Q_1 (25^{th} percentile), Q_3 (75^{th} percentile)
- **Inter-quartile range:** $\text{IQR} = Q_3 - Q_1$
- **Five number summary:** min, Q_1 , median, Q_3 , max
- **Boxplot:** Data is represented with a box
 - Q_1 , Q_3 , IQR: The ends of the box are at the first and third quartiles, i.e., the height of the box is IQR
 - Median (Q_2) 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
 - **Outlier:** usually, a value higher/lower than $1.5 \times \text{IQR}$



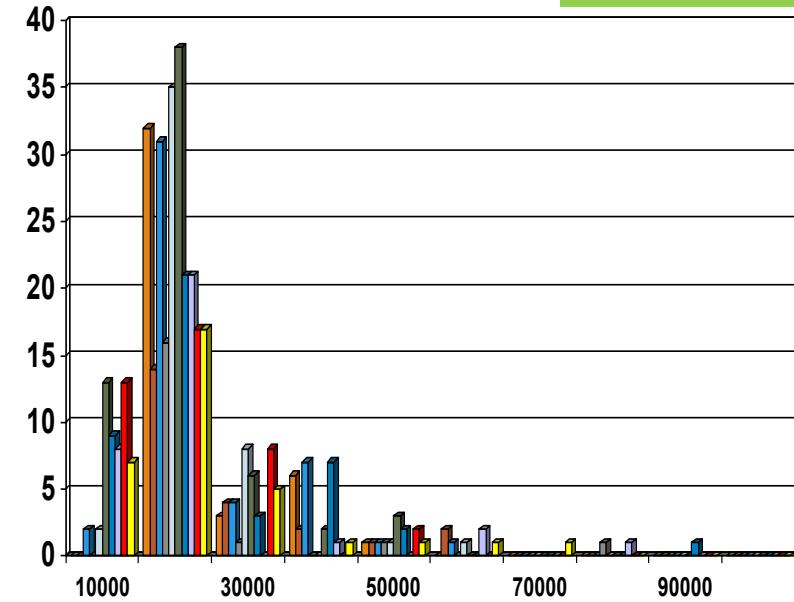
Visualization of Data Dispersion: 3-D Boxplots



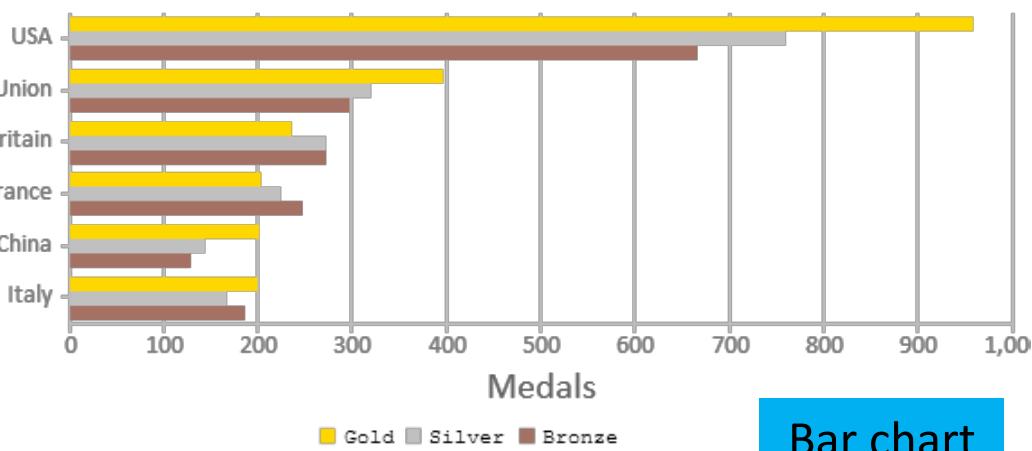
Histogram Analysis

- ❑ Histogram: Graph display of tabulated frequencies, shown as bars
- ❑ Differences between histograms and bar charts
 - ❑ Histograms are used to show distributions of variables while bar charts are used to compare variables
 - ❑ Histograms plot binned quantitative data while bar charts plot categorical data
 - ❑ Bars can be reordered in bar charts but not in histograms
 - ❑ 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

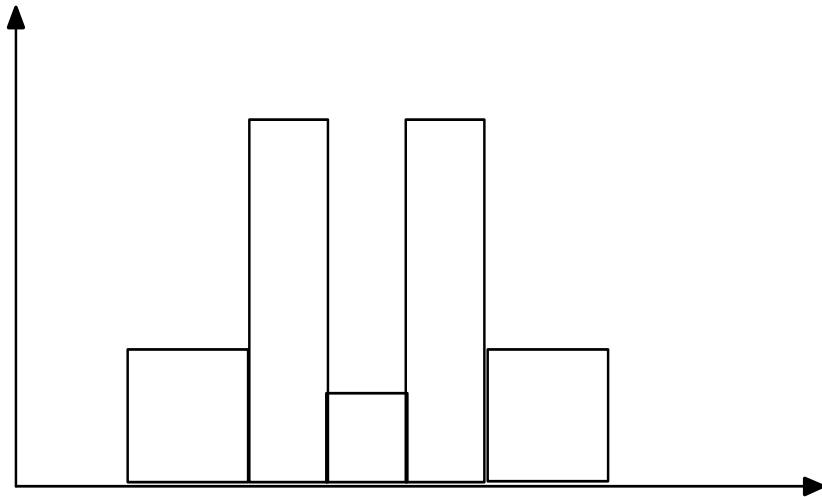
Histogram



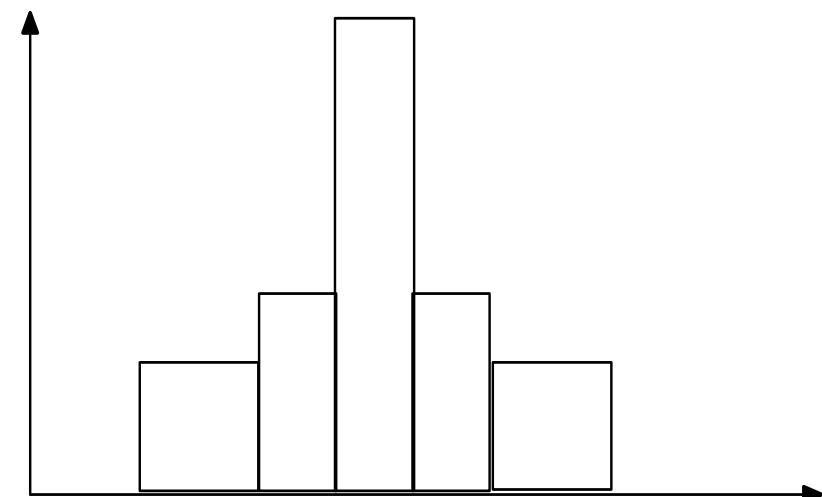
Olympic Medals of all Times (till 2012 Olympics)



Histograms Often Tell More than Boxplots

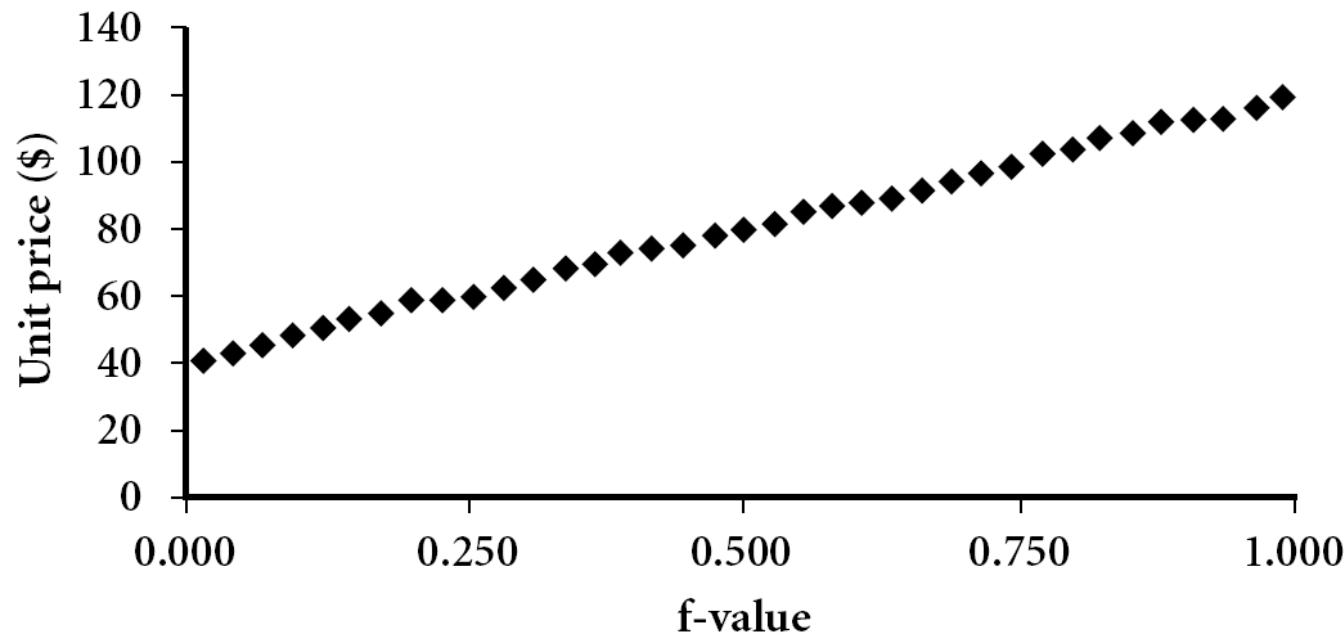


- ❑ The two histograms shown in the left may have the same boxplot representation
- ❑ The same values for: min, Q1, median, Q3, max
- ❑ But they have rather different data distributions



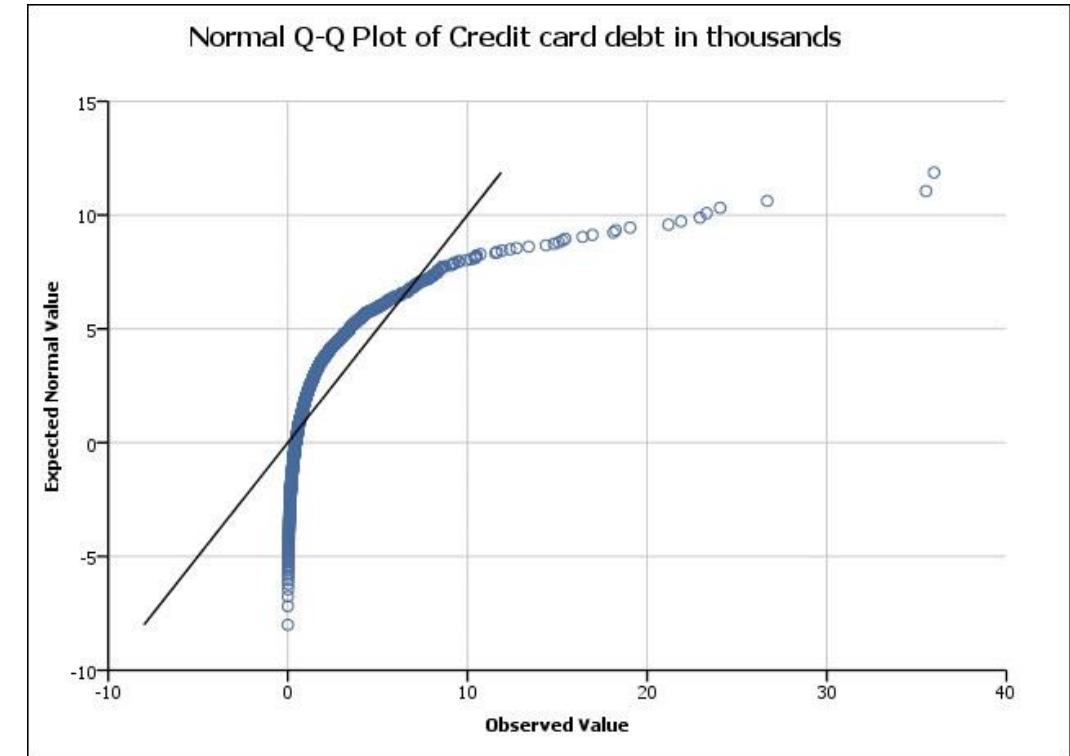
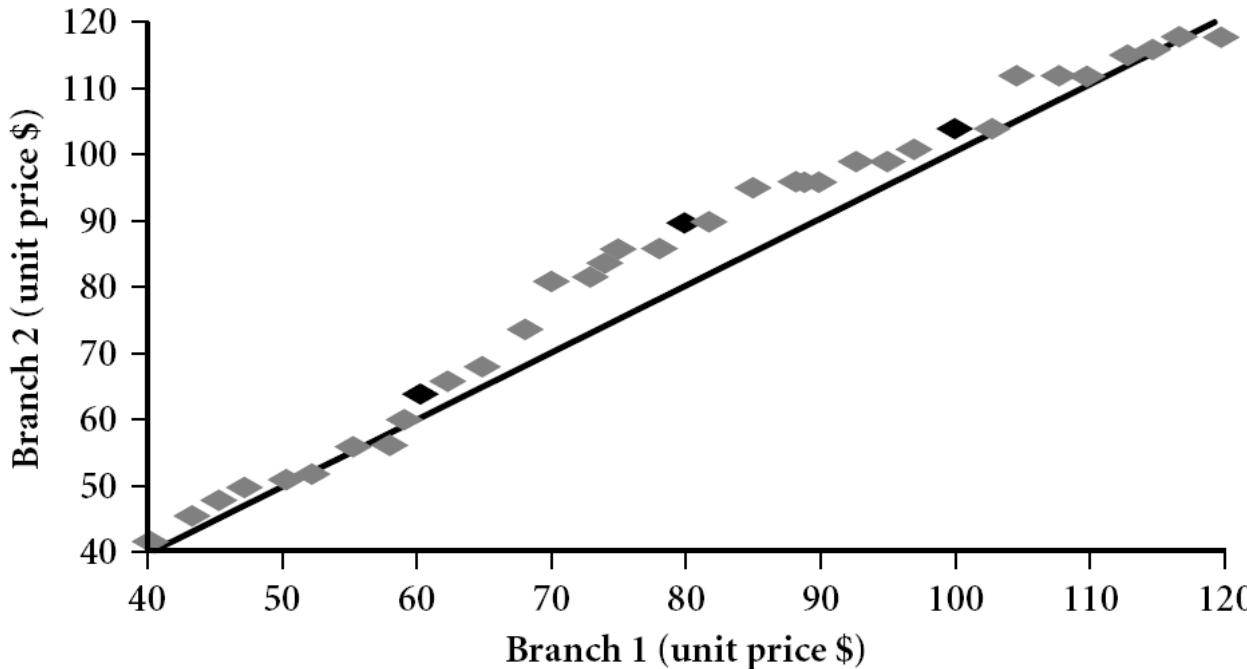
Quantile Plot

- Displays all of the data (allowing the user to assess both the overall behavior and unusual occurrences)
- Plots **quantile** information
 - For a data x_i , data sorted in increasing order, f_i indicates that approximately $100f_i\%$ of the data are below or equal to the value x_i



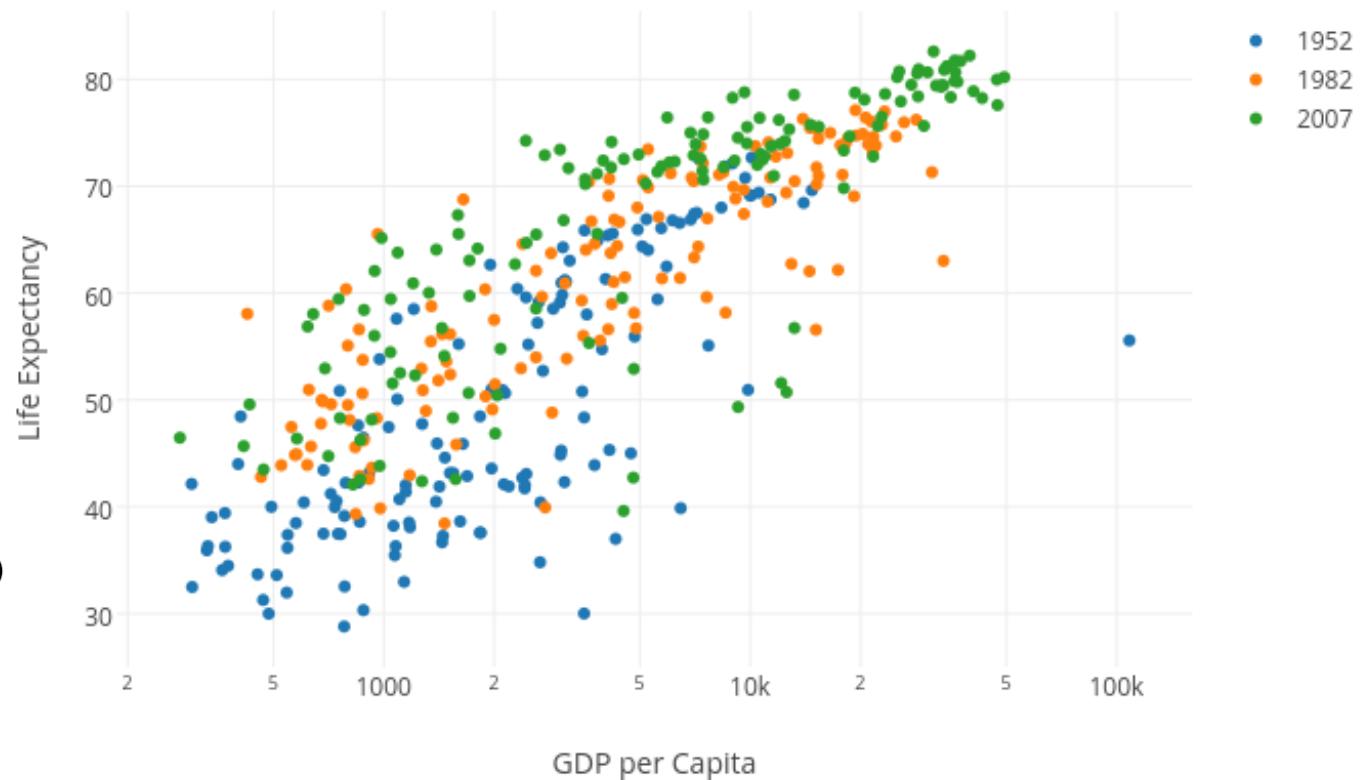
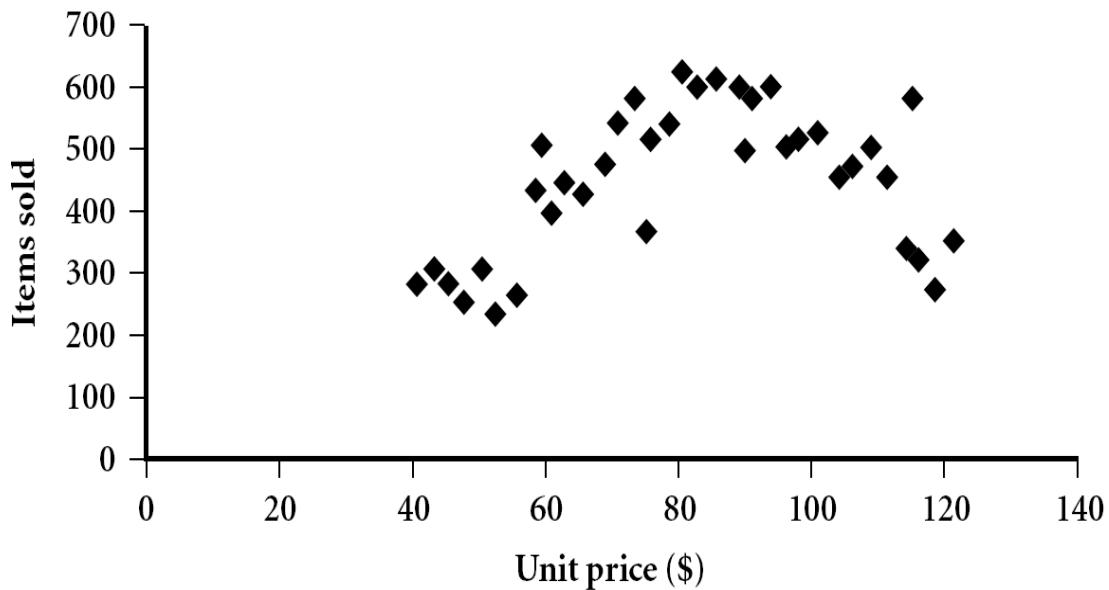
Quantile-Quantile (Q-Q) Plot

- 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

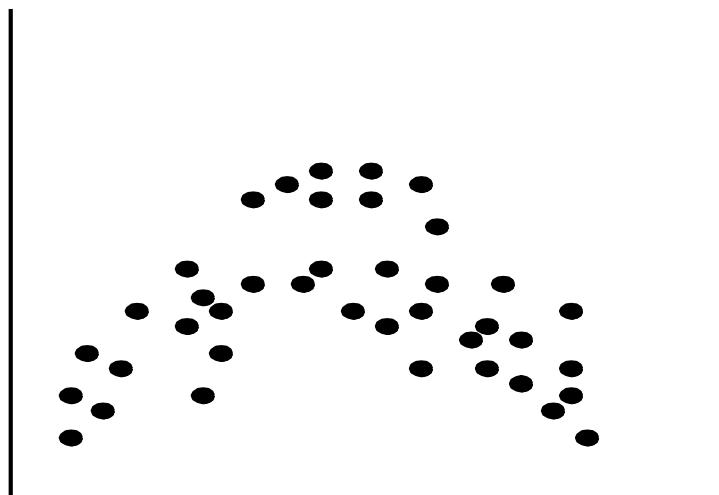
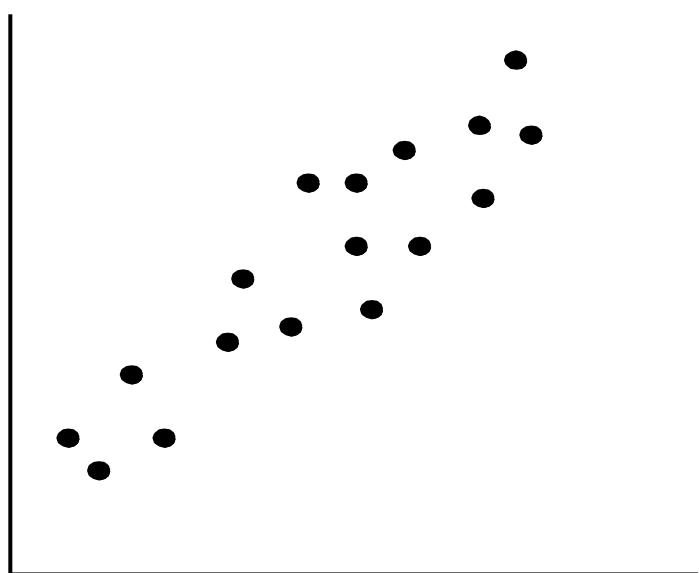


Scatter plot

- ❑ 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

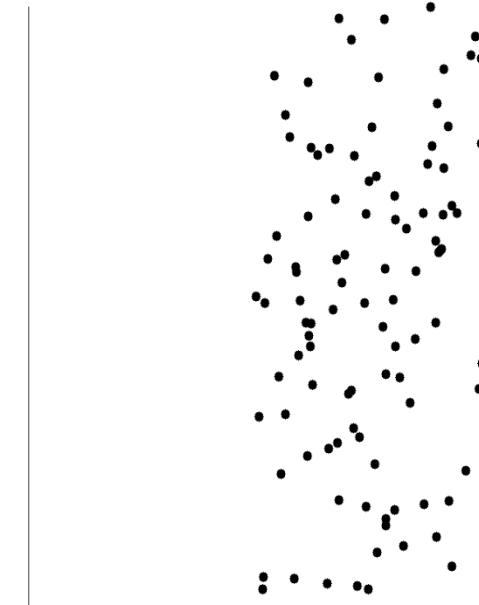
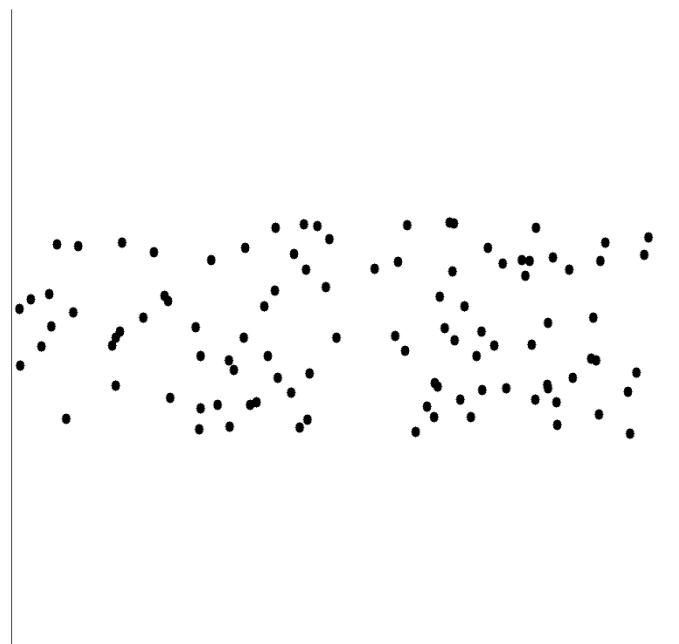
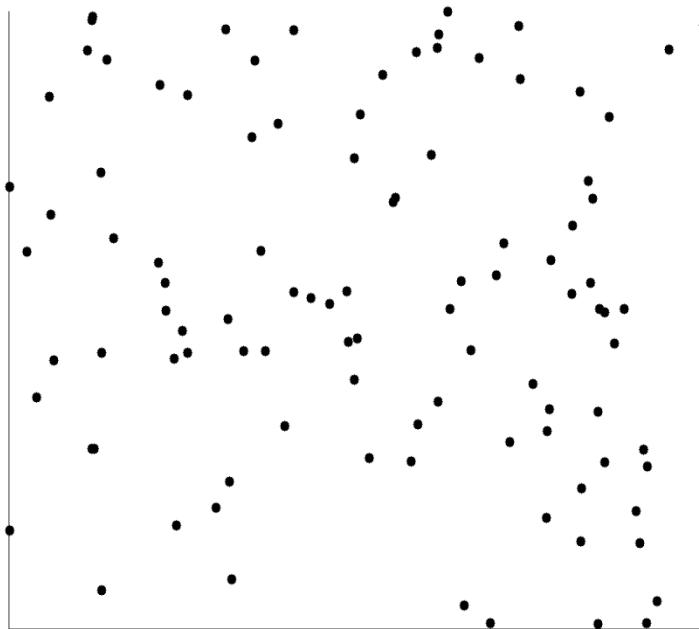


Positively and Negatively Correlated Data



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

Uncorrelated Data



Chapter 2. Getting to Know Your Data

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

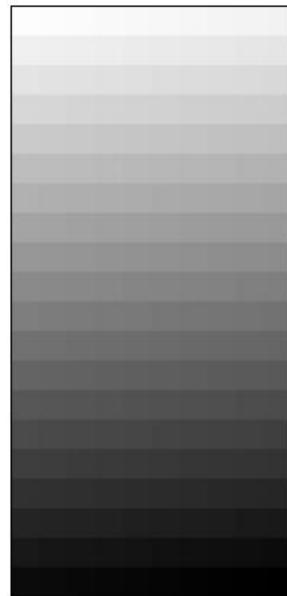


Data Visualization

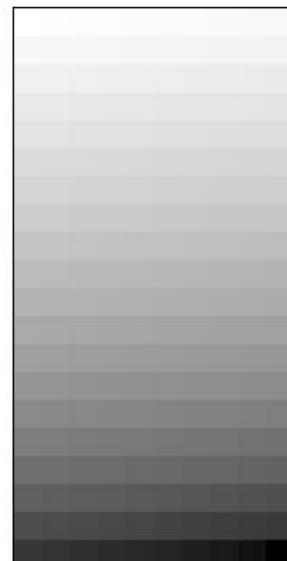
- Why data visualization?
 - Gain insight into an information space by mapping data onto graphical primitives
 - Provide qualitative overview of large data sets
 - Search for patterns, trends, structure, irregularities, relationships among data
 - Help find interesting regions and suitable parameters for further quantitative analysis
 - Provide a visual proof of computer representations derived
- Categorization of visualization methods:
 - Pixel-oriented visualization techniques
 - Geometric projection visualization techniques
 - Icon-based visualization techniques
 - Hierarchical visualization techniques
 - Visualizing complex data and relations

Pixel-Oriented Visualization Techniques

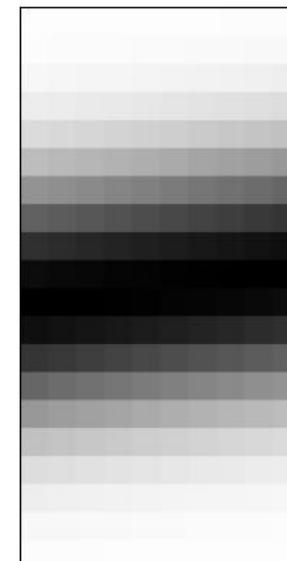
- ❑ For a data set of m dimensions, create m windows on the screen, one for each dimension
- ❑ The m dimension values of a record are mapped to m pixels at the corresponding positions in the windows
- ❑ The colors of the pixels reflect the corresponding values



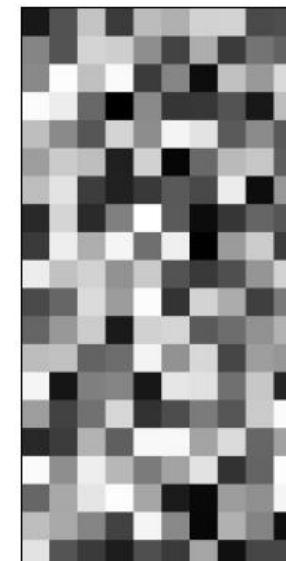
(a) Income



(b) Credit Limit



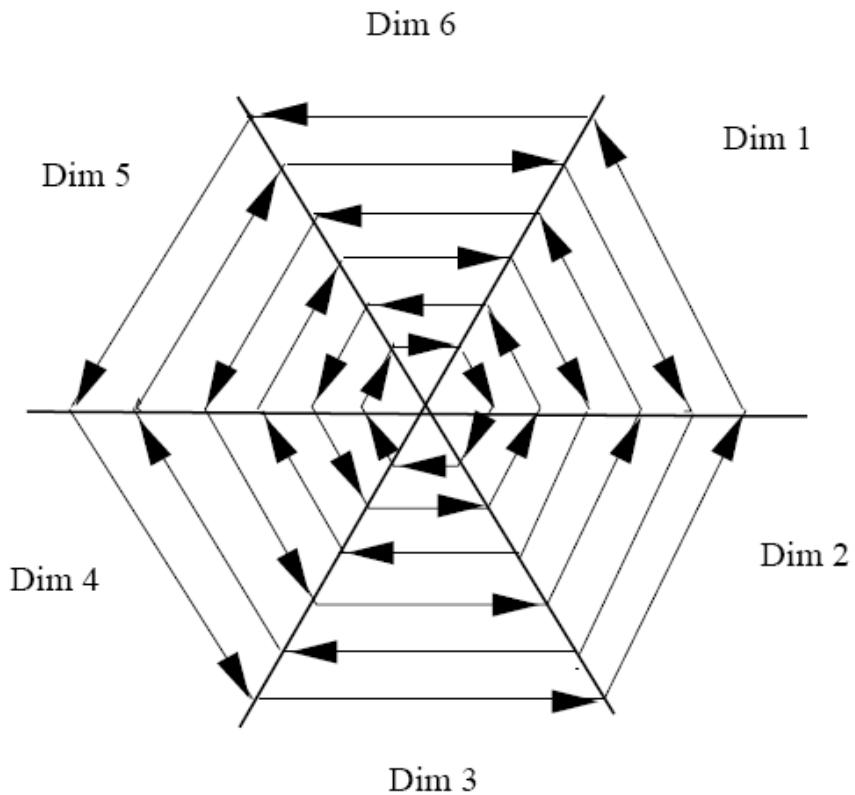
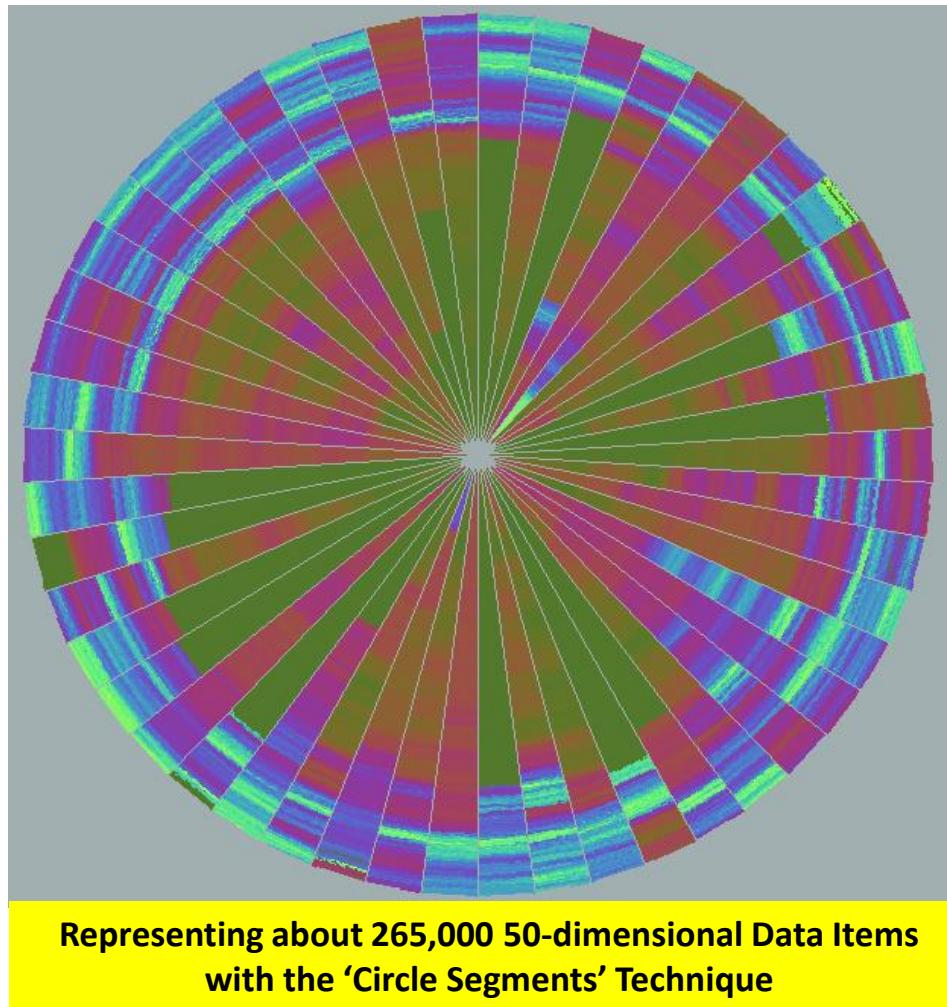
(c) transaction volume



(d) age

Laying Out Pixels in Circle Segments

- To save space and show the connections among multiple dimensions, space filling is often done in a circle segment



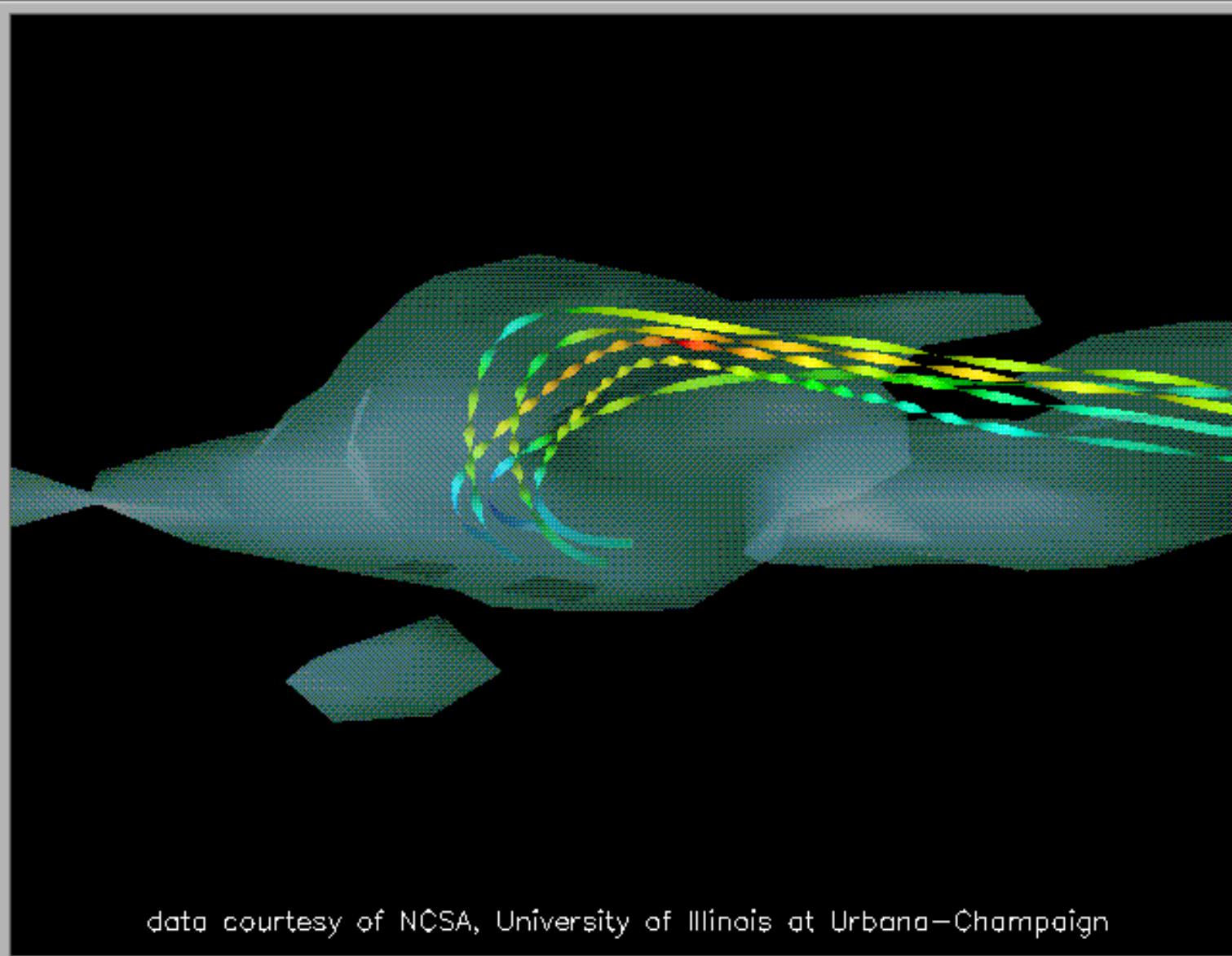
(b) Laying out pixels in circle segment

Geometric Projection Visualization Techniques

- Visualization of geometric transformations and projections of the data
- Methods
 - Direct visualization
 - Scatterplot and scatterplot matrices
 - Landscapes
 - Projection pursuit technique: Help users find meaningful projections of multidimensional data
 - Prosection views
 - Hyperslice
 - Parallel coordinates

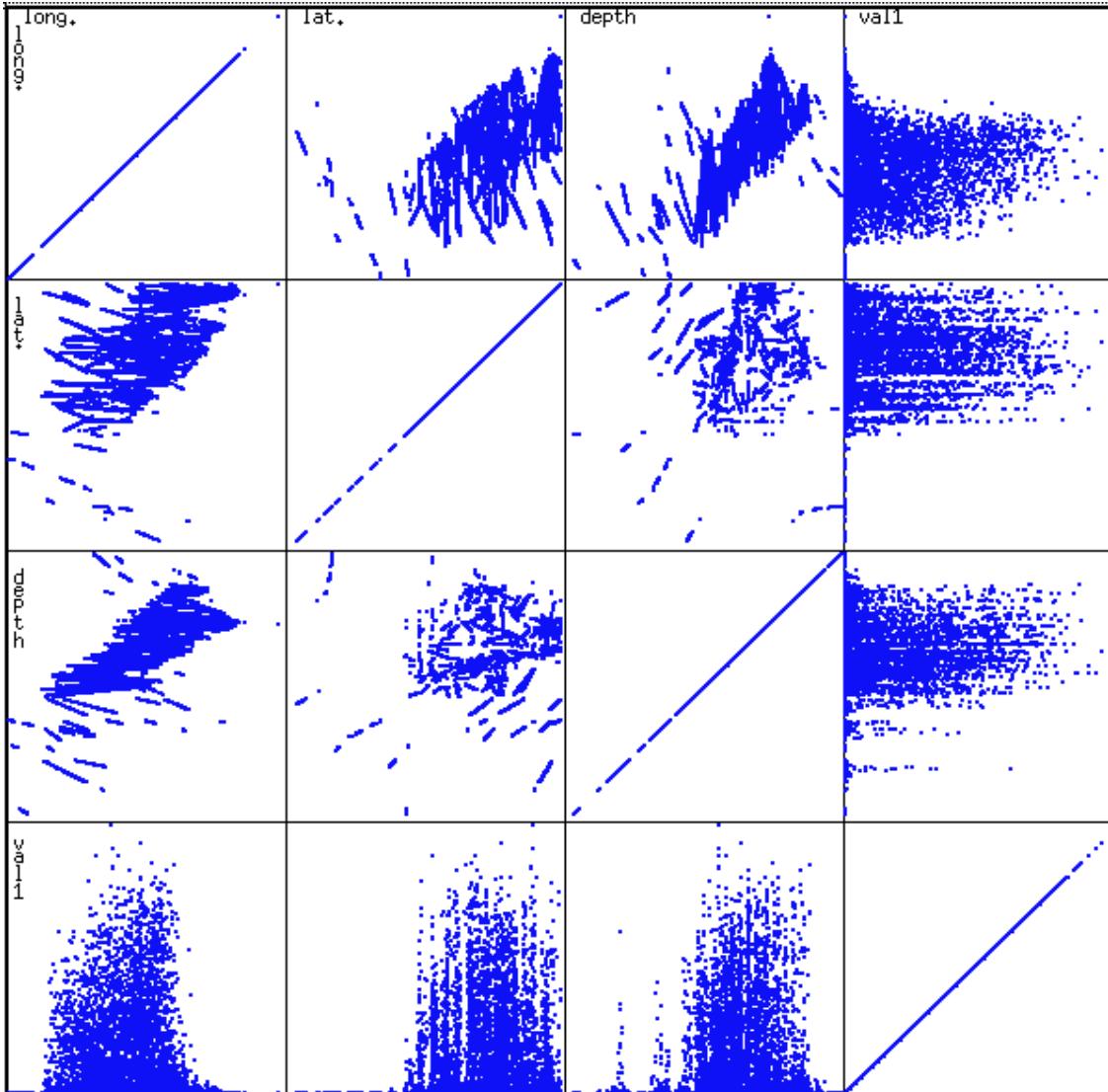
Direct Data Visualization

Ribbons with Twists Based on Vorticity



data courtesy of NCSA, University of Illinois at Urbana-Champaign

Scatterplot Matrices

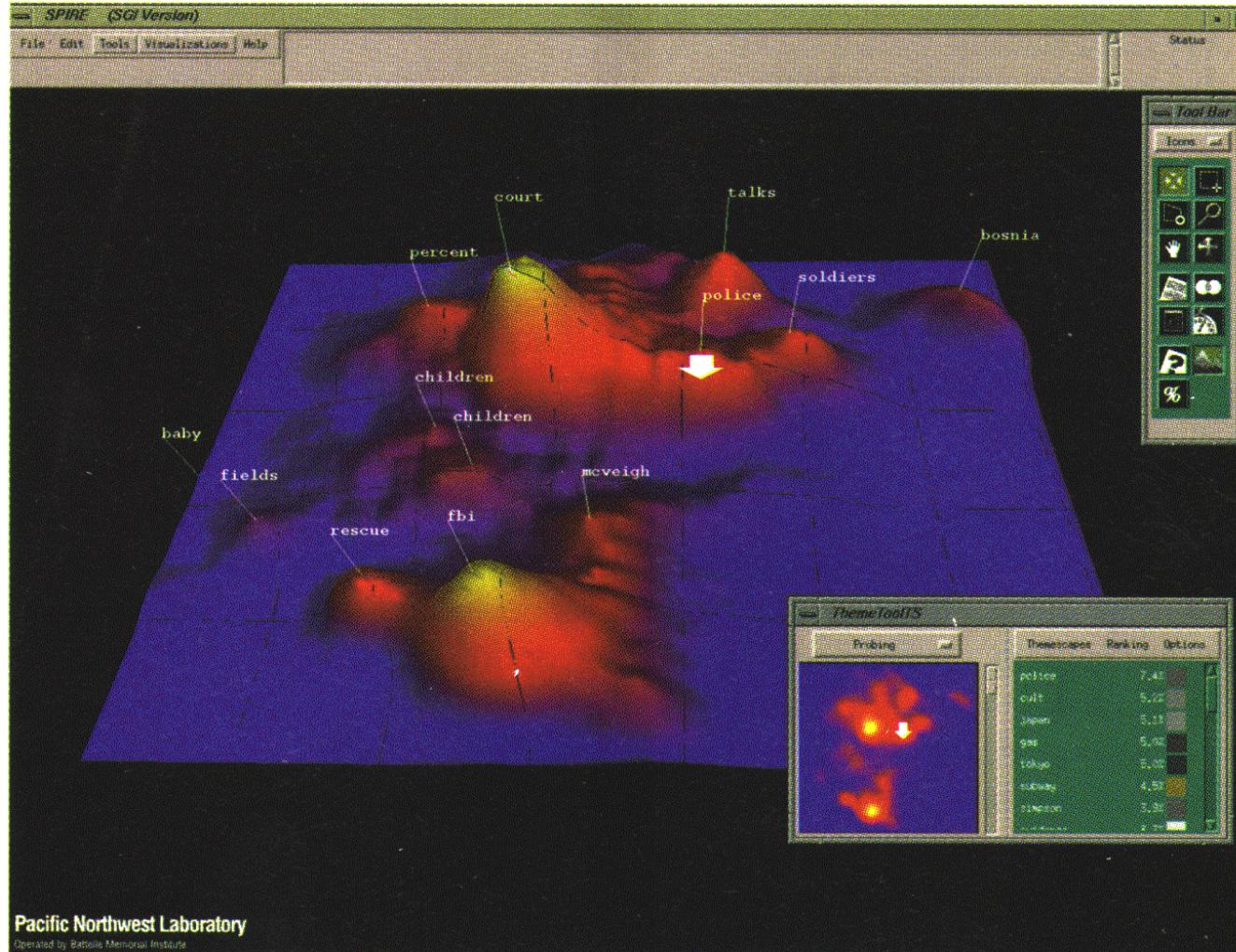


Used by permission of M. Ward, Worcester Polytechnic Institute

- Matrix of scatterplots (x-y-diagrams) of the k-dim. data
- A total of $k(k-1)/2$ distinct scatterplots

Landscapes

Used by permission of B. Wright, Visible Decisions Inc.

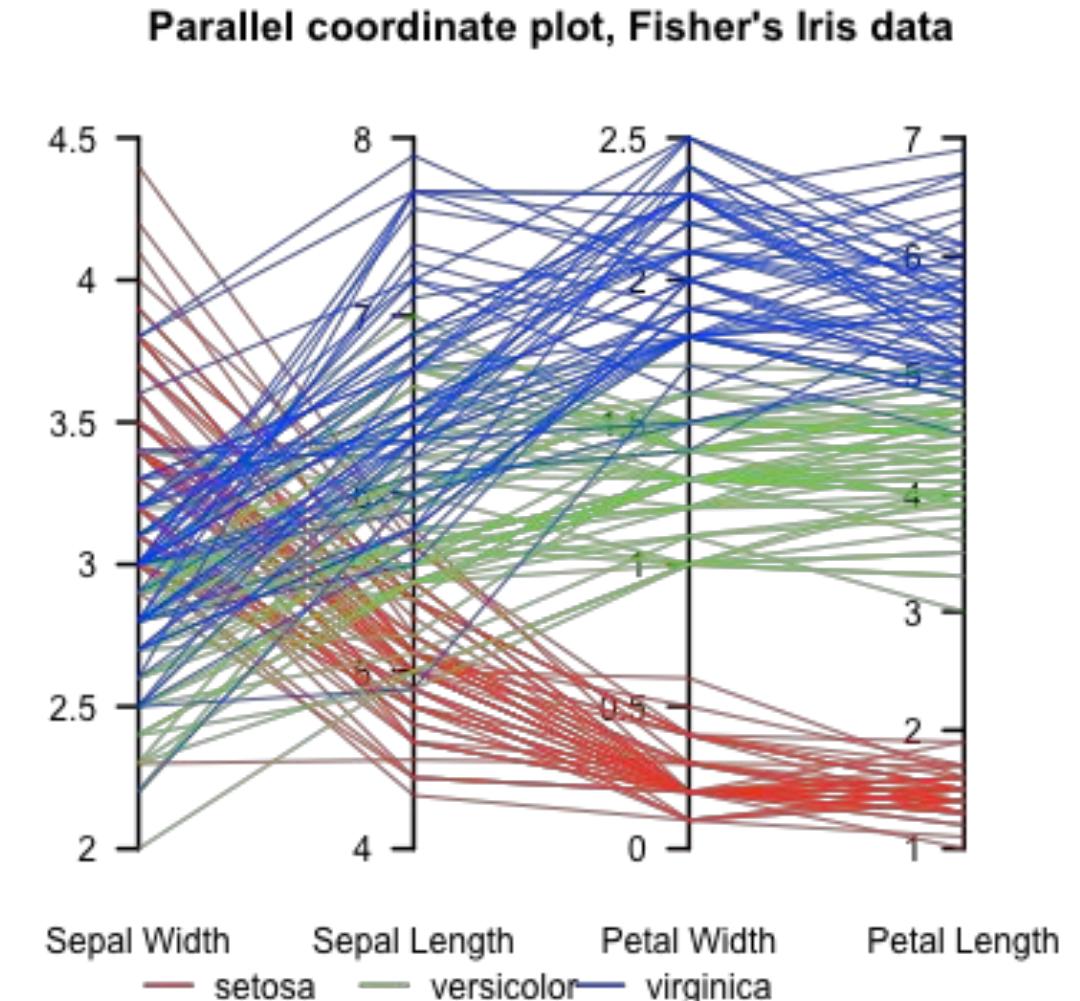


news articles visualized as a landscape

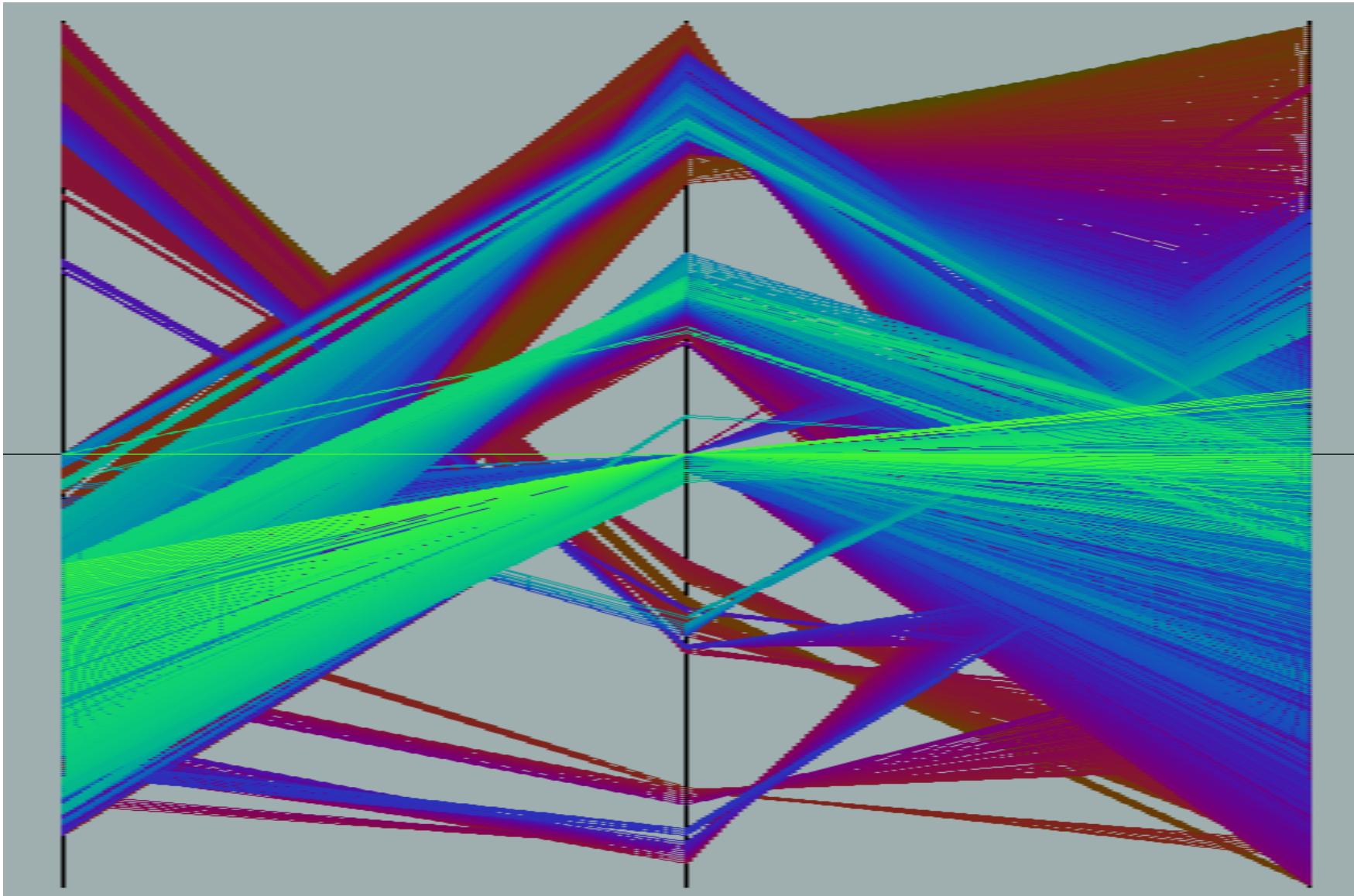
- Visualization of the data as perspective landscape
- The data needs to be transformed into a (possibly artificial) 2D spatial representation which preserves the characteristics of the data

Parallel Coordinates

- n equidistant axes which are parallel to one of the screen axes and correspond to the attributes
- The axes are scaled to the [minimum, maximum]: range of the corresponding attribute
- Every data item corresponds to a polygonal line which intersects each of the axes at the point which corresponds to the value for the attribute



Parallel Coordinates of a Data Set

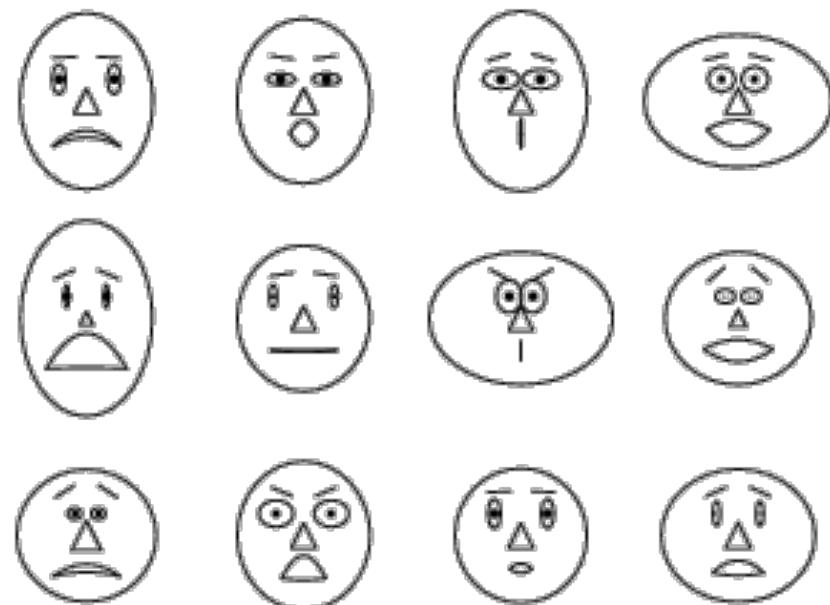


Icon-Based Visualization Techniques

- Visualization of the data values as features of icons
- Typical visualization methods
 - Chernoff Faces
 - Stick Figures
- General techniques
 - Shape coding: Use shape to represent certain information encoding
 - Color icons: Use color icons to encode more information
 - Tile bars: Use small icons to represent the relevant feature vectors in document retrieval

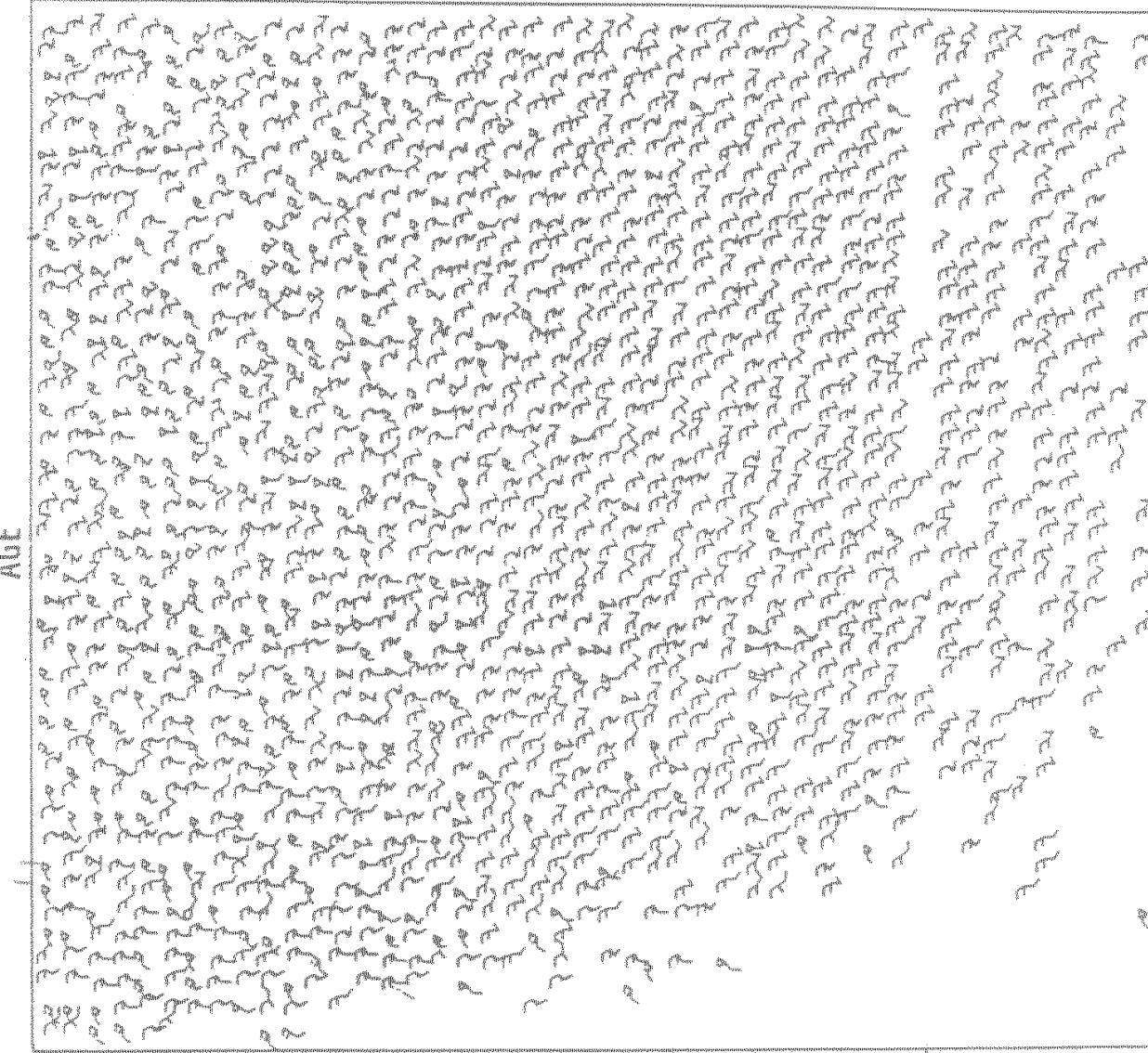
Chernoff Faces

- A way to display variables on a two-dimensional surface, e.g., let x be eyebrow slant, y be eye size, z be nose length, etc.
- The figure shows faces produced using 10 characteristics--head eccentricity, eye size, eye spacing, eye eccentricity, pupil size, eyebrow slant, nose size, mouth shape, mouth size, and mouth opening): Each assigned one of 10 possible values, generated using [*Mathematica*](#) (S. Dickson)
- REFERENCE: Gonick, L. and Smith, W. [*The Cartoon Guide to Statistics*](#). New York: Harper Perennial, p. 212, 1993
- Weisstein, Eric W. "Chernoff Face." From *MathWorld--A Wolfram Web Resource*.
mathworld.wolfram.com/ChernoffFace.html



Stick Figure

used by permission of G. Grinstein, University of Massachusetts at Lowell

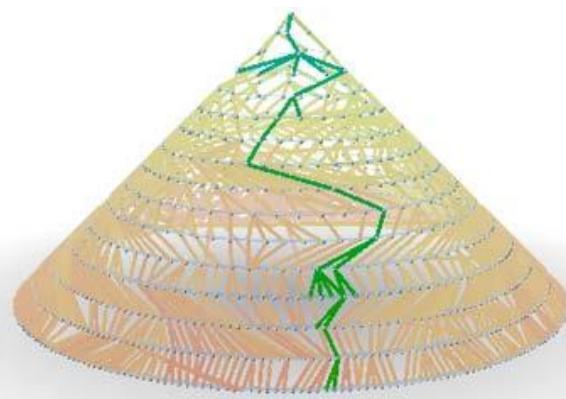
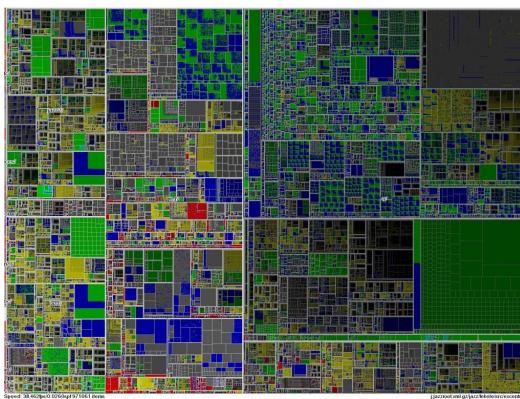
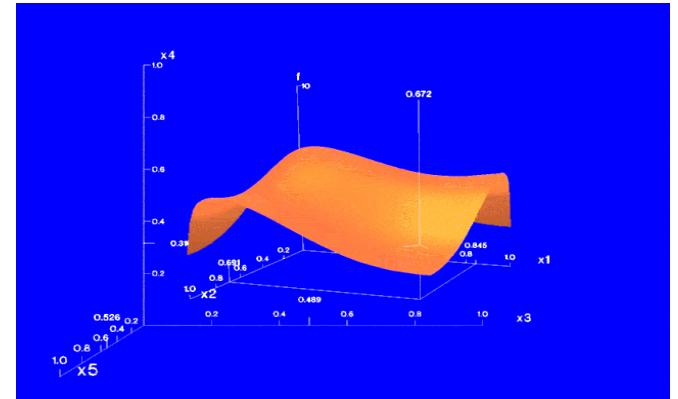
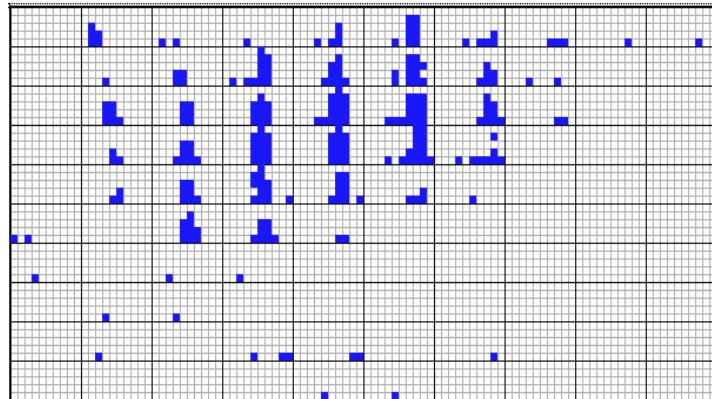


- A census data figure showing age, income, gender, education, etc.

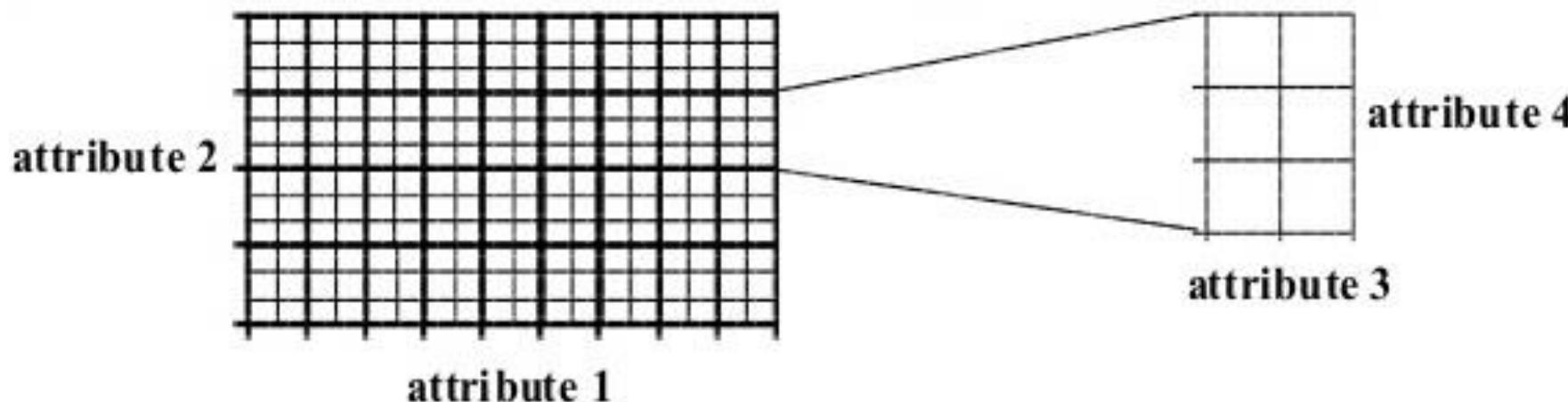
- A 5-piece stick figure (1 body and 4 limbs w. different angle/length)

Hierarchical Visualization Techniques

- ❑ Visualization of the data using a hierarchical partitioning into subspaces
- ❑ Methods
 - ❑ Dimensional Stacking
 - ❑ Worlds-within-Worlds
 - ❑ Tree-Map
 - ❑ Cone Trees
 - ❑ InfoCube



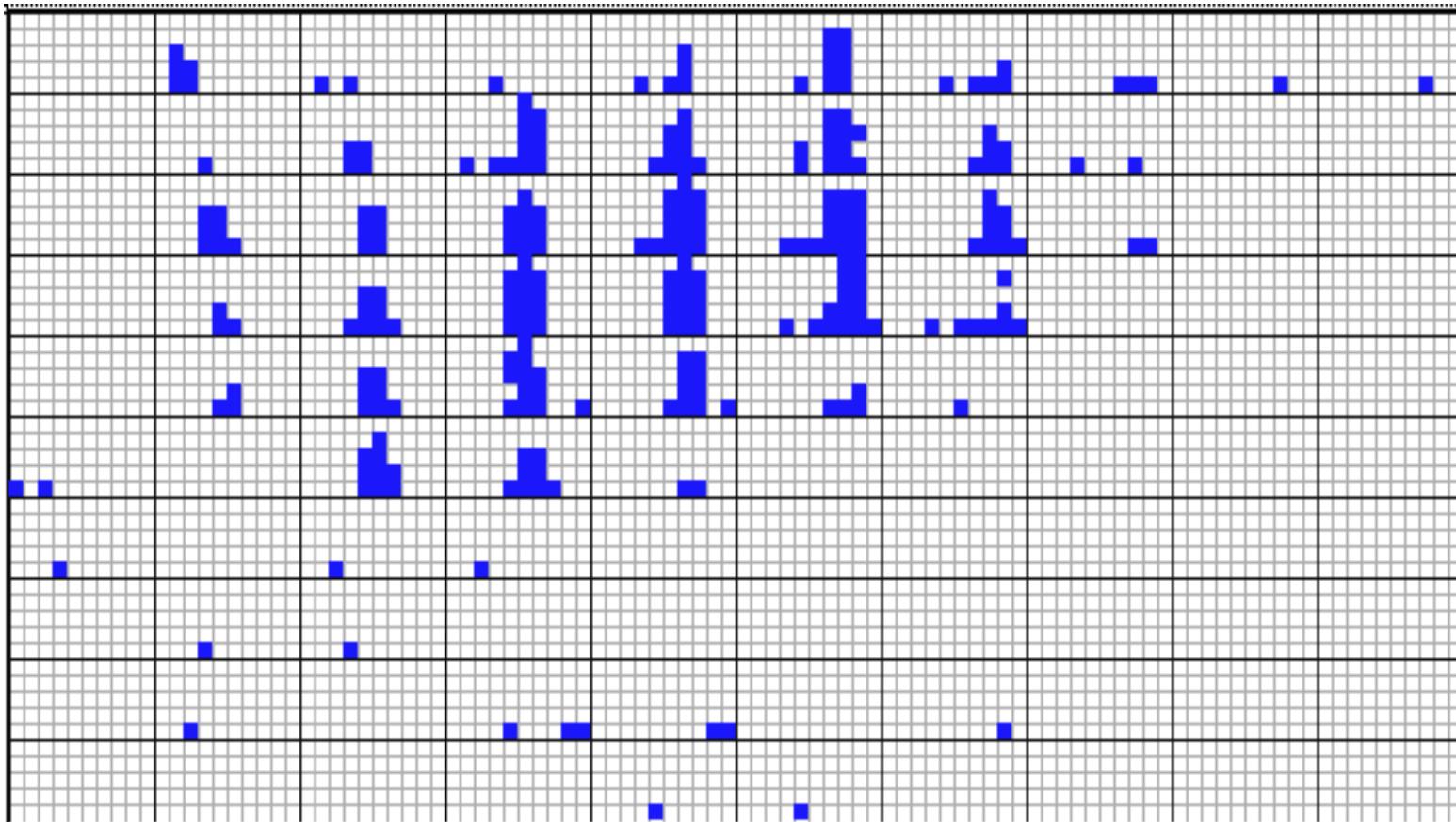
Dimensional Stacking



- Partitioning of the n-dimensional attribute space in 2-D subspaces, which are ‘stacked’ into each other
- Partitioning of the attribute value ranges into classes. The important attributes should be used on the outer levels.
- Adequate for data with ordinal attributes of low cardinality
- But, difficult to display more than nine dimensions
- Important to map dimensions appropriately

Dimensional Stacking

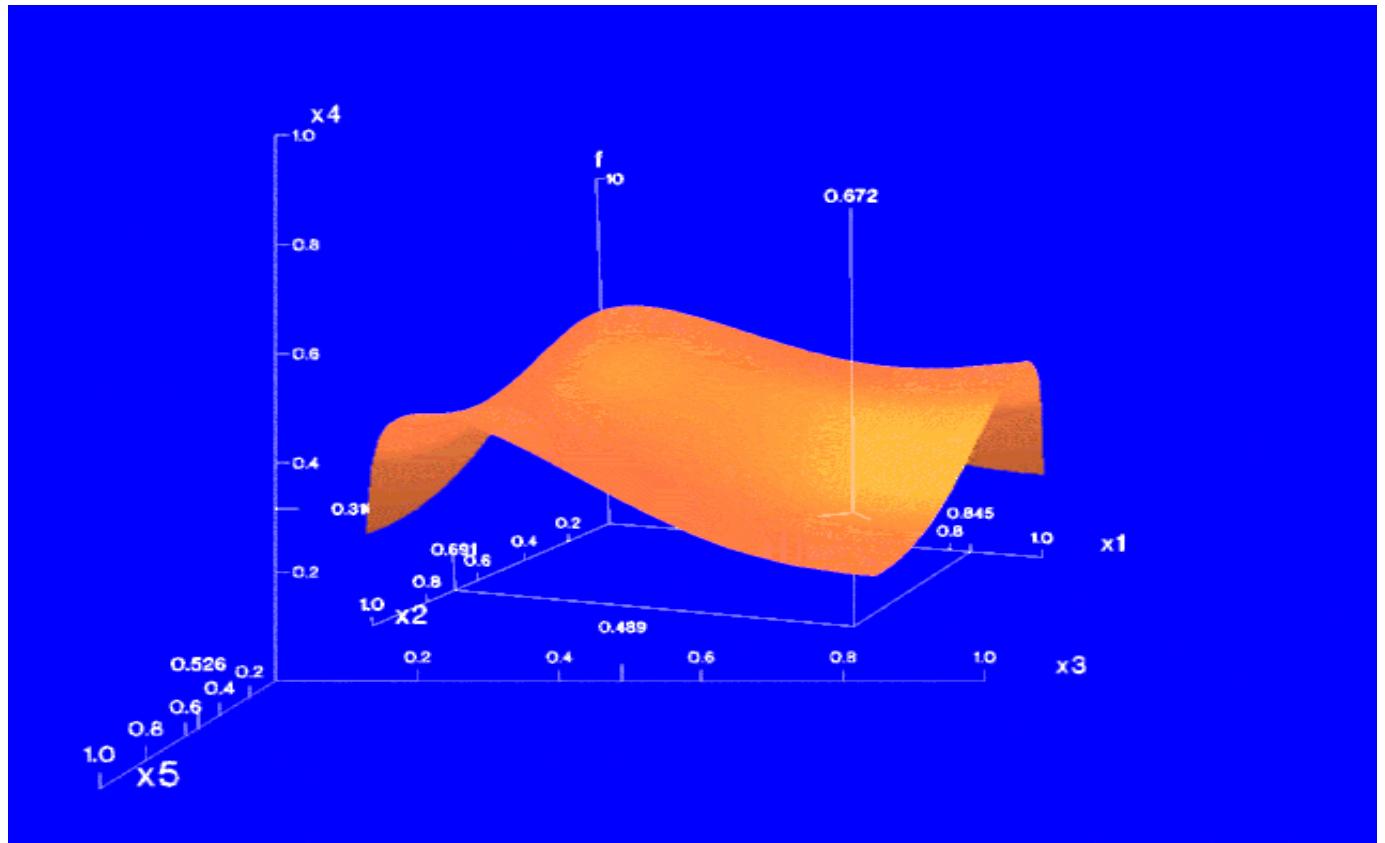
Used by permission of M. Ward, Worcester Polytechnic Institute



Visualization of oil mining data with longitude and latitude mapped to the outer x-, y-axes and ore grade and depth mapped to the inner x-, y-axes

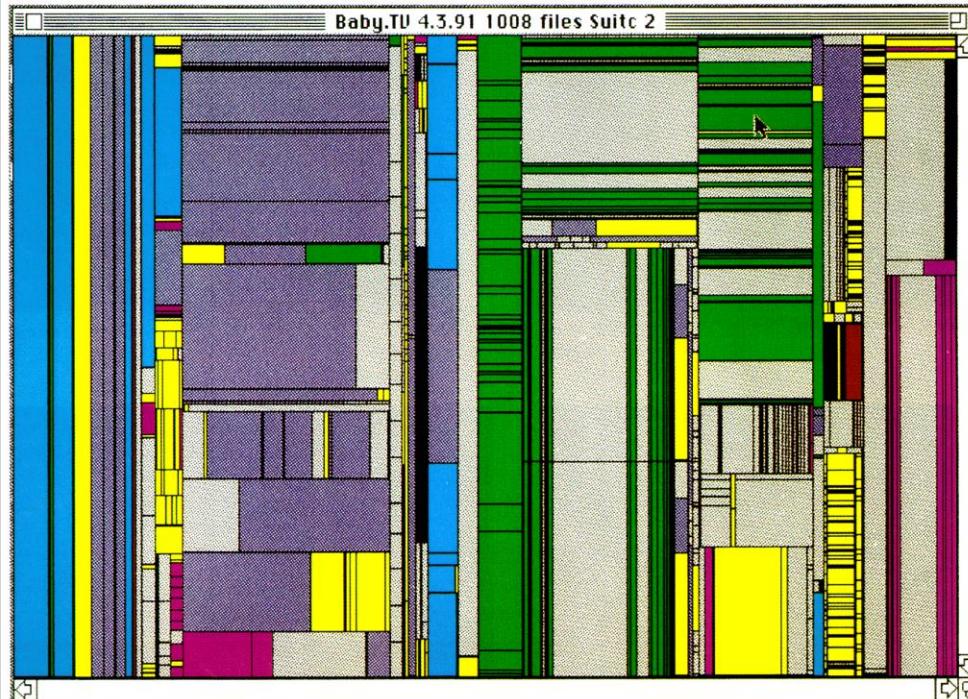
Worlds-within-Worlds

- ❑ Assign the function and two most important parameters to innermost world
- ❑ Fix all other parameters at constant values - draw other (1 or 2 or 3 dimensional worlds choosing these as the axes)
- ❑ Software that uses this paradigm
 - ❑ N-vision: Dynamic interaction through data glove and stereo displays, including rotation, scaling (inner) and translation (inner/outer)
 - ❑ Auto Visual: Static interaction by means of queries

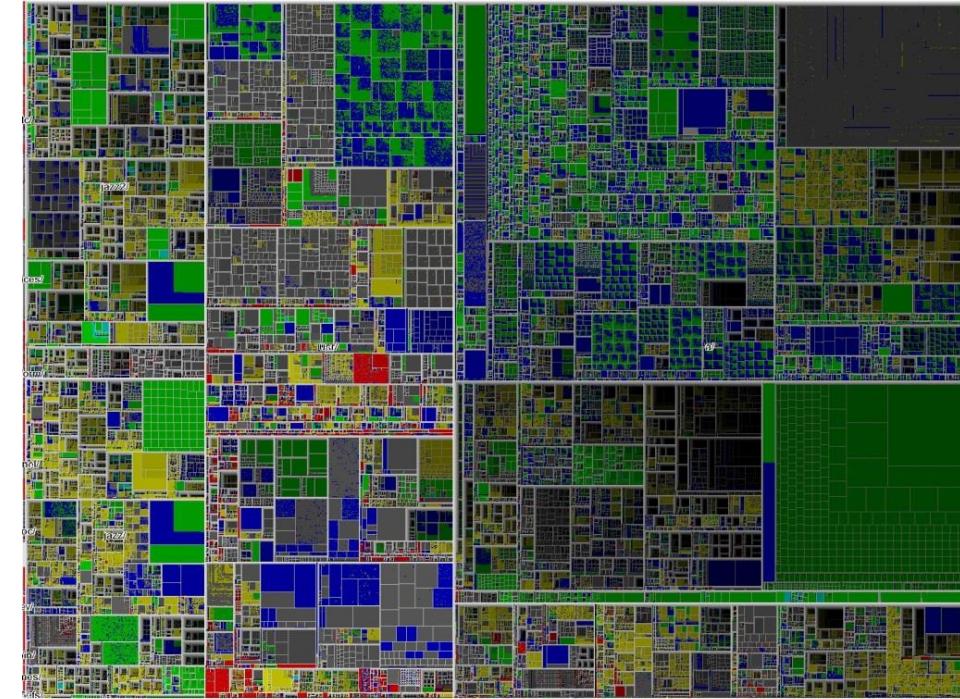


Tree-Map

- Screen-filling method which uses a hierarchical partitioning of the screen into regions depending on the attribute values
- The x- and y-dimension of the screen are partitioned alternately according to the attribute values (classes)



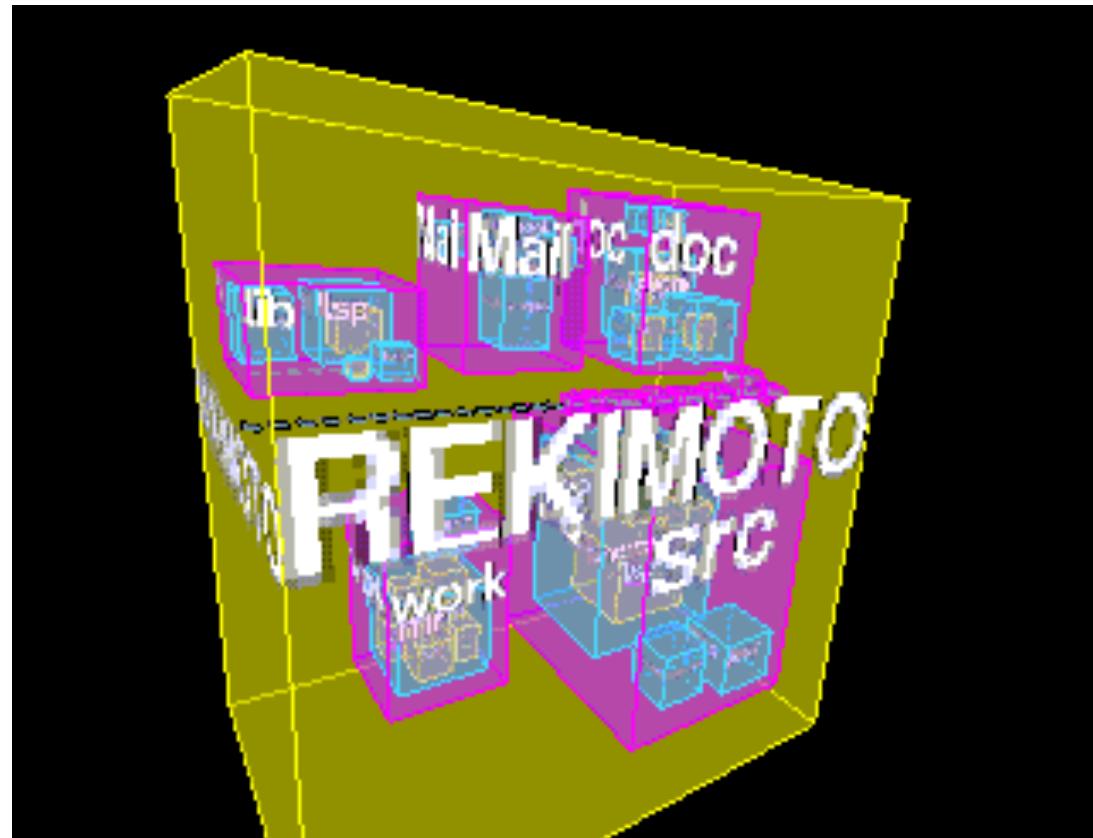
Schneiderman@UMD: Tree-Map of a File System



Schneiderman@UMD: Tree-Map to support
large data sets of a million items

InfoCube

- ❑ A 3-D visualization technique where hierarchical information is displayed as nested semi-transparent cubes
 - ❑ The outermost cubes correspond to the top level data, while the subnodes or the lower level data are represented as smaller cubes inside the outermost cubes, etc.



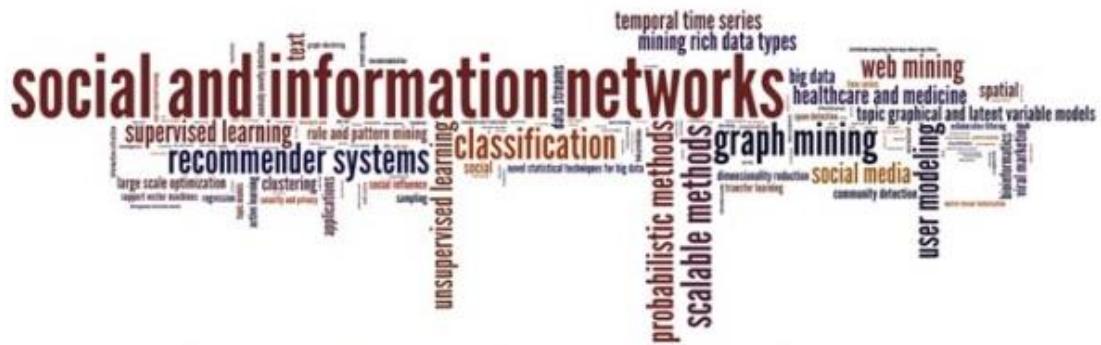
Three-D Cone Trees

- *3D cone tree* visualization technique works well for up to a thousand nodes or so
- First build a *2D circle tree* that arranges its nodes in concentric circles centered on the root node
- Cannot avoid overlaps when projected to 2D
- G. Robertson, J. Mackinlay, S. Card. “Cone Trees: Animated 3D Visualizations of Hierarchical Information”, *ACM SIGCHI'91*
- Graph from Nadeau Software Consulting website: Visualize a social network data set that models the way an infection spreads from one person to the next

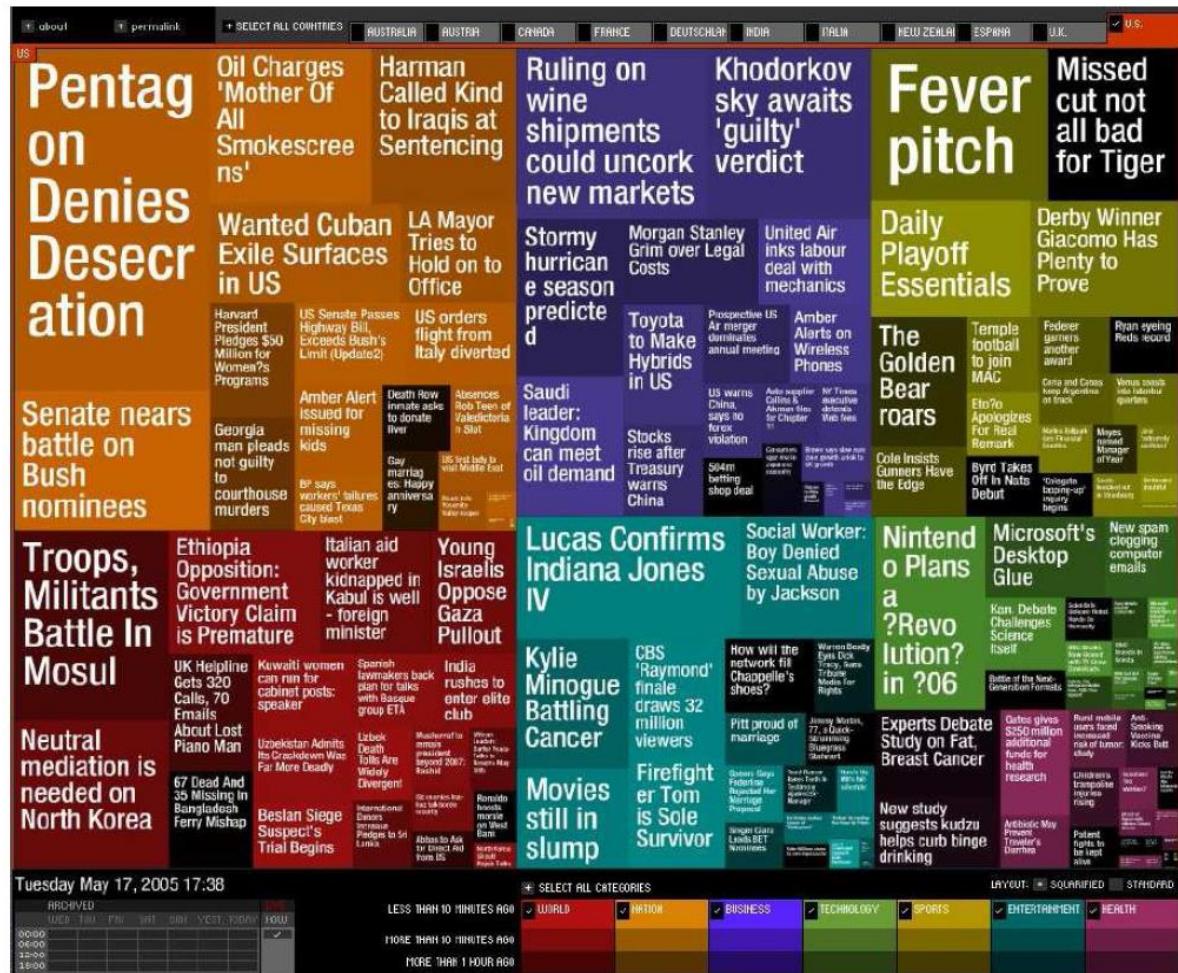


Visualizing Complex Data and Relations: Tag Cloud

- ❑ Tag cloud: Visualizing user-generated tags
 - ❑ The importance of tag is represented by font size/color
 - ❑ Popularly used to visualize word/phrase distributions



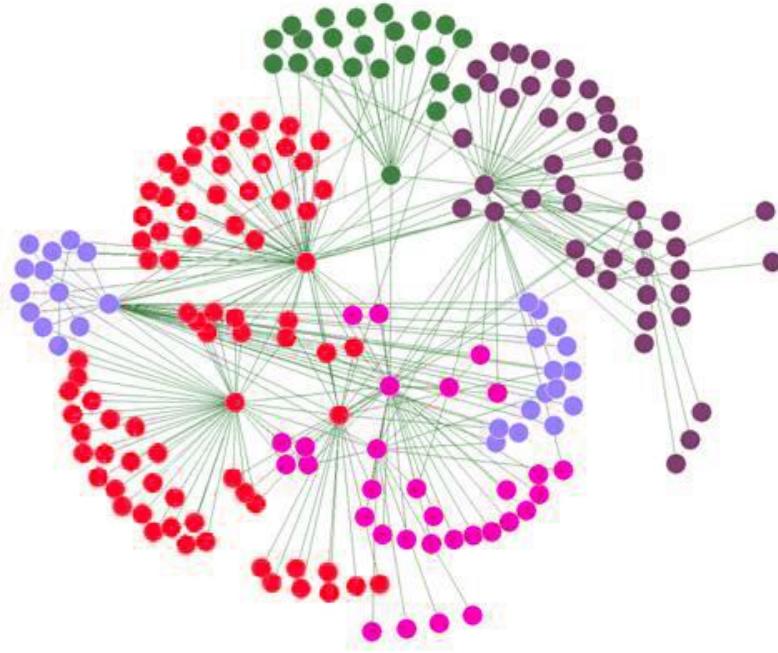
KDD 2013 Research Paper Title Tag Cloud



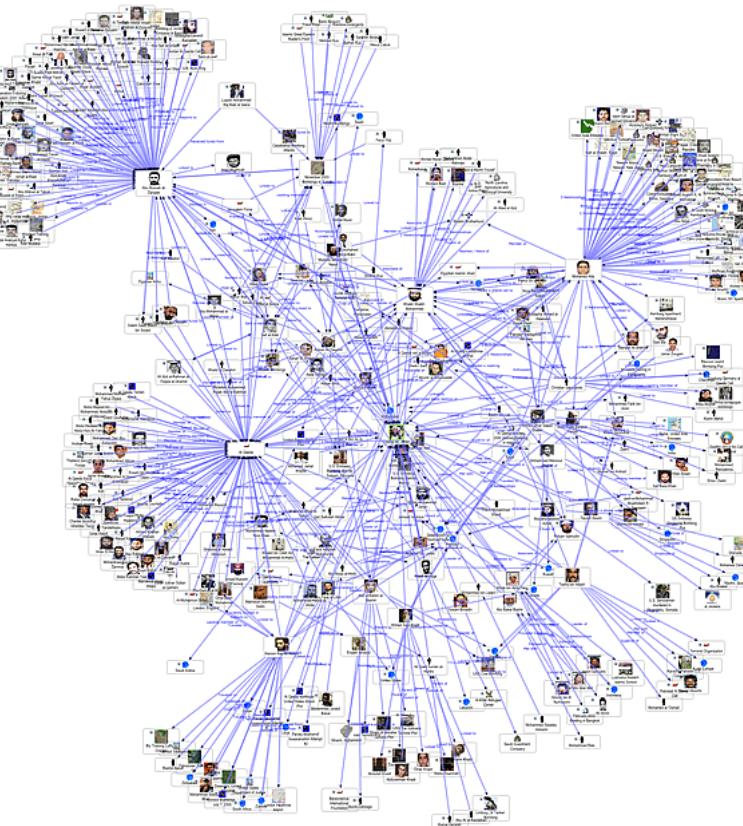
Newsmap: Google News Stories in 2005

Visualizing Complex Data and Relations: Social Networks

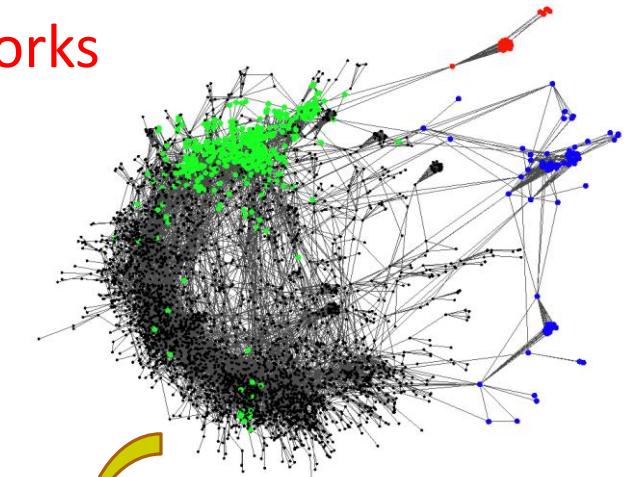
- Visualizing non-numerical data: social and information networks



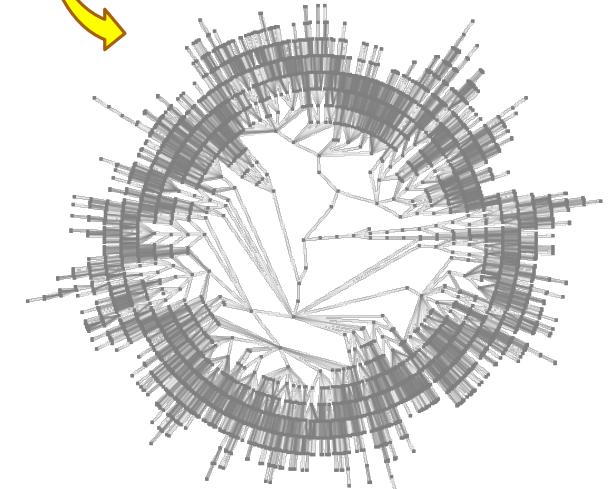
A typical network structure



A social network



organizing
information networks



Chapter 2. Getting to Know Your Data

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



Similarity, Dissimilarity, and Proximity

- **Similarity measure** or **similarity function**
 - A real-valued function that quantifies the similarity between two objects
 - Measure how two data objects are alike: The higher value, the more alike
 - Often falls in the range $[0,1]$: 0: no similarity; 1: completely similar
- **Dissimilarity** (or **distance**) **measure**
 - Numerical measure of how different two data objects are
 - In some sense, the inverse of similarity: The lower, the more alike
 - Minimum dissimilarity is often 0 (i.e., completely similar)
 - Range $[0, 1]$ or $[0, \infty)$, depending on the definition
- **Proximity** usually refers to either similarity or dissimilarity

Data Matrix and Dissimilarity Matrix

- Data matrix

- A data matrix of n data points with l dimensions

- Dissimilarity (distance) matrix

- n data points, but registers only the distance $d(i, j)$ (typically metric)

- Usually symmetric, thus a triangular matrix

- **Distance functions** are usually different for real, boolean, categorical, ordinal, ratio, and vector variables

- Weights can be associated with different variables based on applications and data semantics

$$D = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1l} \\ x_{21} & x_{22} & \dots & x_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nl} \end{pmatrix}$$

$$\begin{array}{ccccccc} & 0 & & & & & \\ & d(2,1) & & 0 & & & \\ & \vdots & & \vdots & & \ddots & \\ & d(n,1) & d(n,2) & \dots & 0 & & \end{array}$$

Standardizing Numeric Data

- Z-score:

$$z = \frac{x - \mu}{\sigma}$$

- X: raw score to be standardized, μ : mean of the population, σ : standard deviation
- the distance between the raw score and the population mean in units of the standard deviation
- negative when the raw score is below the mean, “+” when above
- An alternative way: Calculate the mean absolute deviation

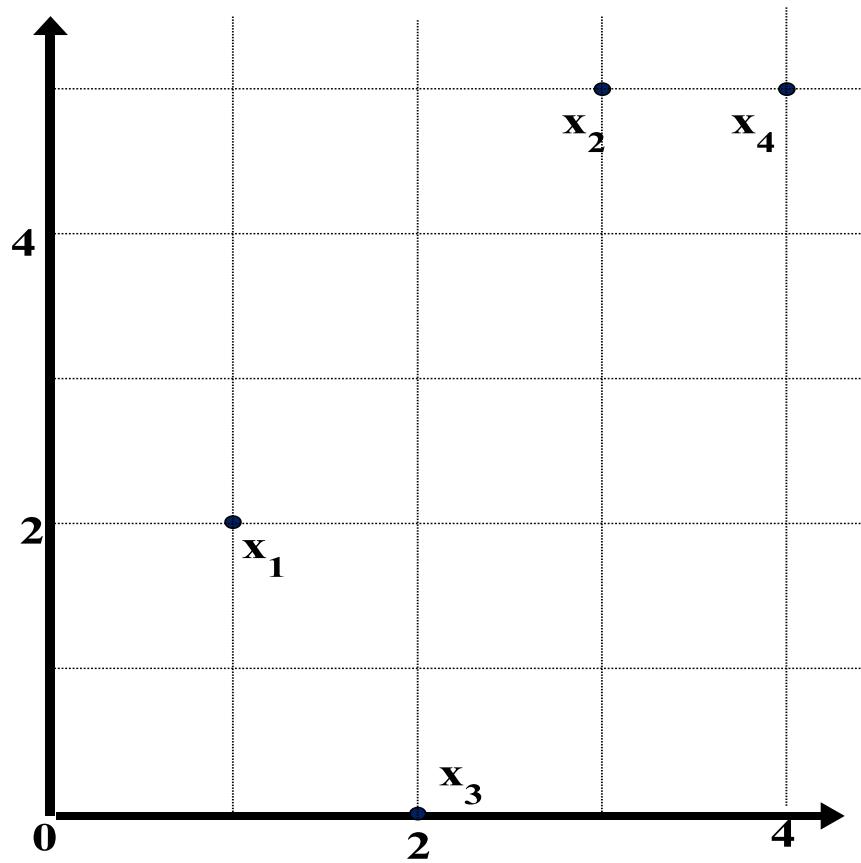
$$s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + \dots + |x_{nf} - m_f|)$$

where

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

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

Example: Data Matrix and Dissimilarity Matrix



Data Matrix

| point | attribute1 | attribute2 |
|-------|------------|------------|
| $x1$ | 1 | 2 |
| $x2$ | 3 | 5 |
| $x3$ | 2 | 0 |
| $x4$ | 4 | 5 |

Dissimilarity Matrix (by Euclidean Distance)

| | $x1$ | $x2$ | $x3$ | $x4$ |
|------|------|------|------|------|
| $x1$ | 0 | | | |
| $x2$ | 3.61 | 0 | | |
| $x3$ | 2.24 | 5.1 | 0 | |
| $x4$ | 4.24 | 1 | 5.39 | 0 |

Distance on Numeric Data: Minkowski Distance

- **Minkowski distance:** A popular distance measure

$$d(i, j) = \sqrt[p]{|x_{i1} - x_{j1}|^p + |x_{i2} - x_{j2}|^p + \dots + |x_{il} - x_{jl}|^p}$$

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

- Properties
 - $d(i, j) > 0$ if $i \neq j$, and $d(i, i) = 0$ (Positivity)
 - $d(i, j) = d(j, i)$ (Symmetry)
 - $d(i, j) \leq d(i, k) + d(k, j)$ (Triangle Inequality)
- A distance that satisfies these properties is a **metric**
- Note: There are nonmetric dissimilarities, e.g., set differences

Special Cases of Minkowski Distance

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

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

- $p = 2$: (L_2 norm) Euclidean distance

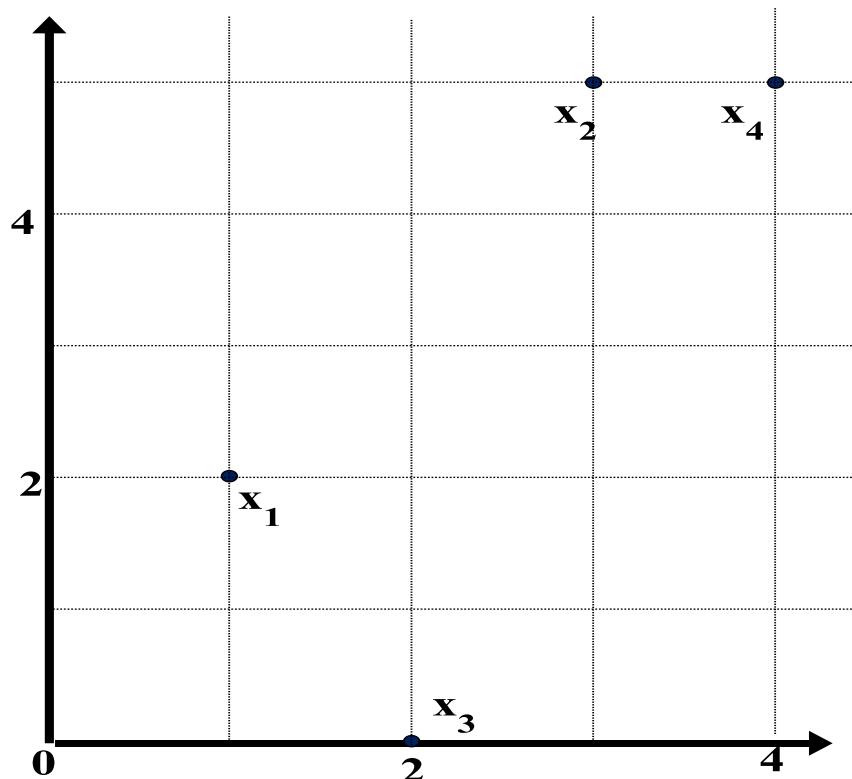
$$d(i, j) = \sqrt{|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \dots + |x_{il} - x_{jl}|^2}$$

- $p \rightarrow \infty$: (L_{\max} norm, L_∞ norm) “supremum” distance
 - The maximum difference between any component (attribute) of the vectors

$$d(i, j) = \lim_{p \rightarrow \infty} \sqrt[p]{|x_{i1} - x_{j1}|^p + |x_{i2} - x_{j2}|^p + \dots + |x_{il} - x_{jl}|^p} = \max_{f=1}^l |x_{if} - x_{jf}|$$

Example: Minkowski Distance at Special Cases

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



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_∞)

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

Proximity Measure for Binary Attributes

- A contingency table for binary data

| | | Object <i>j</i> | | |
|-----------------|---|-----------------|---------|---------|
| | | 1 | 0 | sum |
| Object <i>i</i> | 1 | q | r | $q + r$ |
| | 0 | s | t | $s + t$ |
| sum | | $q + s$ | $r + t$ | p |

- Distance measure for symmetric binary variables

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

- Distance measure for asymmetric binary variables:

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

- Jaccard coefficient (*similarity* measure for

asymmetric binary variables):

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

- Note: Jaccard coefficient is the same as

(a concept discussed in Pattern Discovery)

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

Example: Dissimilarity between Asymmetric Binary Variables

| Name | Gender | Fever | Cough | Test-1 | Test-2 | Test-3 | Test-4 |
|------|--------|-------|-------|--------|--------|--------|--------|
| Jack | M | Y | N | P | N | N | N |
| Mary | F | Y | N | P | N | P | N |
| Jim | M | Y | P | N | N | N | N |

- Gender is a symmetric attribute (not counted in)
- The remaining attributes are asymmetric binary
- Let the values Y and P be 1, and the value N be 0
- Distance: $d(i, j) = \frac{r + s}{q + r + s}$

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

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

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

| | | Mary | | |
|----------------|--|------|---|----------------|
| | | 1 | 0 | Σ_{row} |
| Jack | | 1 | 2 | 0 |
| | | 0 | 1 | 3 |
| Σ_{col} | | 3 | 3 | 6 |

| | | Jim | | |
|----------------|--|-----|---|----------------|
| | | 1 | 0 | Σ_{row} |
| Jack | | 1 | 1 | 2 |
| | | 0 | 1 | 3 |
| Σ_{col} | | 2 | 4 | 6 |

| | | Mary | | |
|----------------|--|------|---|----------------|
| | | 1 | 0 | Σ_{row} |
| Jim | | 1 | 1 | 2 |
| | | 0 | 2 | 4 |
| Σ_{col} | | 3 | 3 | 6 |

Proximity Measure for Categorical Attributes

- Categorical data, also called nominal attributes
 - Example: Color (red, yellow, blue, green), profession, etc.
- Method 1: Simple matching
 - m : # of matches, p : total # of variables

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

- Method 2: Use a large number of binary attributes
 - Creating a new binary attribute for each of the M nominal states

Ordinal Variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank (e.g., freshman, sophomore, junior, senior)
- Can be treated like interval-scaled
 - Replace *an ordinal variable value* by its rank: $r_{if} \in \{1, \dots, M_f\}$
 - Map the range of each variable onto $[0, 1]$ by replacing i -th object in the f -th variable by
$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$
- Example: freshman: 0; sophomore: 1/3; junior: 2/3; senior 1
 - Then distance: $d(\text{freshman}, \text{senior}) = 1$, $d(\text{junior}, \text{senior}) = 1/3$
- Compute the dissimilarity using methods for interval-scaled variables

Attributes of Mixed Type

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

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

- If f is numeric: Use the normalized distance
- If f is binary or nominal: $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$; or $d_{ij}^{(f)} = 1$ otherwise
- If f is ordinal
 - Compute ranks z_{if} (where $z_{if} = \frac{r_{if} - 1}{M_f - 1}$)
 - Treat z_{if} as interval-scaled

Cosine Similarity of Two Vectors

- A **document** can be represented by a bag of terms or a long vector, with each attribute recording the *frequency* of a particular term (such as word, keyword, 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, etc.
- Cosine measure: If d_1 and d_2 are two vectors (e.g., term-frequency vectors), then

$$\cos(d_1, d_2) = \frac{d_1 \bullet d_2}{\|d_1\| \times \|d_2\|}$$

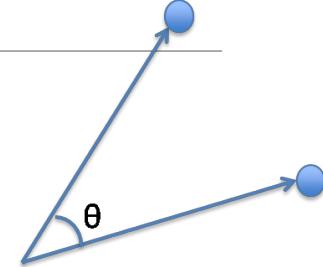
where \bullet indicates vector dot product, $\|d\|$: the length of vector d

Example: Calculating Cosine Similarity

- Calculating Cosine Similarity:

$$\cos(d_1, d_2) = \frac{d_1 \bullet d_2}{\|d_1\| \times \|d_2\|}$$

$$sim(A, B) = \cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|}$$



where • indicates vector dot product, ||d||: the length of vector d

- Ex: Find the **similarity** between documents 1 and 2.

$$d_1 = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0) \quad d_2 = (3, 0, 2, 0, 1, 1, 1, 0, 1, 0)$$

- First, calculate vector dot product

$$d_1 \bullet d_2 = 5 \times 3 + 0 \times 0 + 3 \times 2 + 0 \times 0 + 2 \times 1 + 0 \times 1 + 0 \times 1 + 2 \times 1 + 0 \times 0 + 0 \times 1 = 25$$

- Then, calculate ||d₁|| and ||d₂||

$$\|d_1\| = \sqrt{5 \times 5 + 0 \times 0 + 3 \times 3 + 0 \times 0 + 2 \times 2 + 0 \times 0 + 0 \times 0 + 2 \times 2 + 0 \times 0 + 0 \times 0} = 6.481$$

$$\|d_2\| = \sqrt{3 \times 3 + 0 \times 0 + 2 \times 2 + 0 \times 0 + 1 \times 1 + 1 \times 1 + 0 \times 0 + 1 \times 1 + 0 \times 0 + 1 \times 1} = 4.12$$

- Calculate cosine similarity: $\cos(d_1, d_2) = 25 / (6.481 \times 4.12) = 0.94$

Announcements: Meetine of the 4th Credit Project

- ❑ CS412: Assignment #1 was distributed last Tuesday!
 - ❑ The due date is Sept. 15. No late homework will be accepted!!
- ❑ Waitlist is cleared: We took 50 additional students into the video only session
 - ❑ Please find your status with Holly. You are either in or out (wait for Spring 2017)
- ❑ Meeting for Project for the 4th Credit
 - ❑ You can change from 4 to 3 credit or from 3 to 4 credits by sending me e-mails
 - ❑ Meeting time and location: **10-11am Friday (tomorrow!) at 0216 SC**
 - ❑ This project is part of WSDM 2017 Cup
 - ❑ Choice #1: **Triple Scoring**: Computing relevance scores for triples from type-like relations
 - ❑ Choice #2: **Vandalism Detection** for Wikipages
 - ❑ Tas/PhD student/postdoc will give you the details in the Friday meeting! **Must attend if you want to do the 4th credit project!!!**

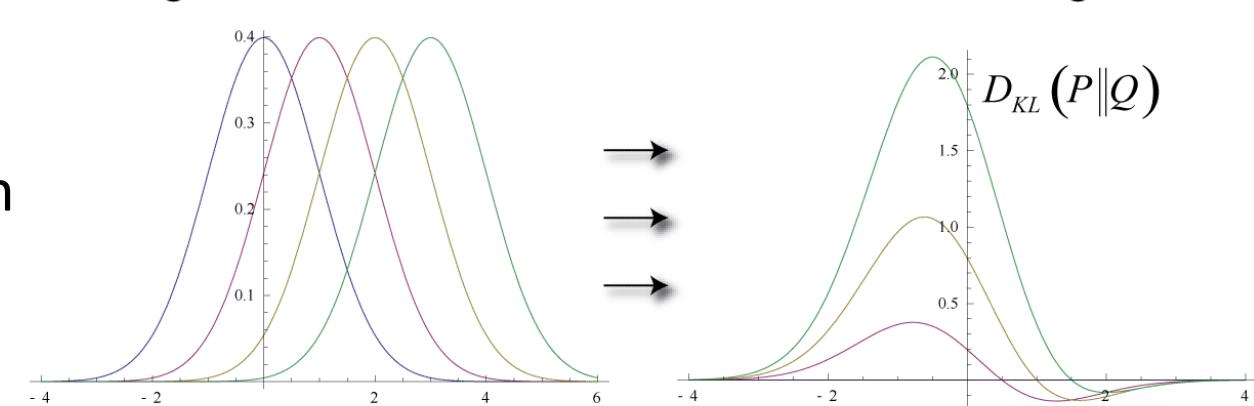
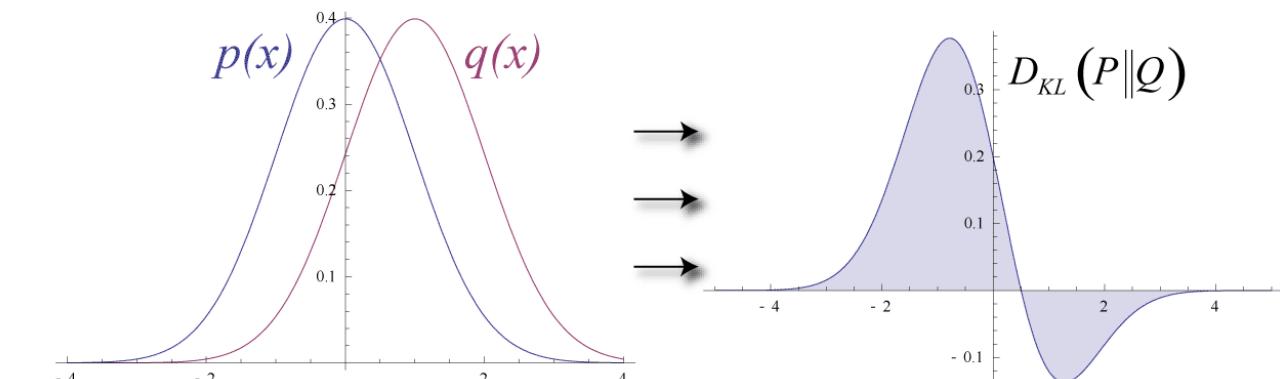
KL Divergence: Comparing Two Probability Distributions

- *The Kullback-Leibler (KL) divergence:*
Measure the difference between two probability distributions over the same variable x
 - From information theory, closely related to *relative entropy*, *information divergence*, and *information for discrimination*
- $D_{KL}(p(x) \parallel q(x))$: divergence of $q(x)$ from $p(x)$, measuring the information lost when $q(x)$ is used to approximate $p(x)$

$$D_{KL}(p(x) \parallel q(x)) = \sum_{x \in X} p(x) \ln \frac{p(x)}{q(x)}$$

Discrete form 

$$D_{KL}(p(x) \parallel q(x)) = \int_{-\infty}^{\infty} p(x) \ln \frac{p(x)}{q(x)} dx$$



Ack.: Wikipedia entry: *The Kullback-Leibler (KL) divergence*

Continuous form 

More on KL Divergence

$$D_{KL}(p(x)||q(x)) = \sum_{x \in X} p(x) \ln \frac{p(x)}{q(x)}$$

- The KL divergence measures the expected number of extra bits required to code samples from $p(x)$ ("true" distribution) when using a code based on $q(x)$, which represents a theory, model, description, or approximation of $p(x)$
- The KL divergence is not a distance measure, not a metric: asymmetric, not satisfy triangular inequality ($D_{KL}(P||Q)$ does not equal $D_{KL}(Q||P)$)
- In applications, P typically represents the "true" distribution of data, observations, or a precisely calculated theoretical distribution, while Q typically represents a theory, model, description, or approximation of P .
- The Kullback–Leibler divergence from Q to P , denoted $D_{KL}(P||Q)$, is a measure of the information gained when one revises one's beliefs from the prior probability distribution Q to the posterior probability distribution P . In other words, it is the amount of information lost when Q is used to approximate P .
- The KL divergence is sometimes also called the information gain achieved if P is used instead of Q . It is also called the relative entropy of P with respect to Q .

Subtlety at Computing the KL Divergence

- Base on the formula, $D_{KL}(P, Q) \geq 0$ and $D_{KL}(P || Q) = 0$ if and only if $P = Q$
- How about when $p = 0$ or $q = 0$?
 - $\lim_{p \rightarrow 0} p \log p = 0$
 - when $p \neq 0$ but $q = 0$, $D_{KL}(p || q)$ is defined as ∞ , i.e., if one event e is possible (i.e., $p(e) > 0$), and the other predicts it is absolutely impossible (i.e., $q(e) = 0$), then the two distributions are absolutely different
- However, in practice, P and Q are derived from frequency distributions, not counting the possibility of unseen events. Thus *smoothing* is needed
- Example: $P : (a : 3/5, b : 1/5, c : 1/5)$. $Q : (a : 5/9, b : 3/9, d : 1/9)$
 - need to introduce a small constant ϵ , e.g., $\epsilon = 10^{-3}$
 - The sample set observed in P , $SP = \{a, b, c\}$, $SQ = \{a, b, d\}$, $SU = \{a, b, c, d\}$
 - Smoothing, add missing symbols to each distribution, with probability ϵ
 - $P' : (a : 3/5 - \epsilon/3, b : 1/5 - \epsilon/3, c : 1/5 - \epsilon/3, d : \epsilon)$
 - $Q' : (a : 5/9 - \epsilon/3, b : 3/9 - \epsilon/3, c : \epsilon, d : 1/9 - \epsilon/3)$
 - $D_{KL}(P' || Q')$ can then be computed easily

$$D_{KL}(p(x) || q(x)) = \sum_{x \in X} p(x) \ln \frac{p(x)}{q(x)}$$

Chapter 2. Getting to Know Your Data

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



Summary

- Data attribute types: nominal, binary, ordinal, interval-scaled, ratio-scaled
- Many types of data sets, e.g., numerical, text, graph, Web, image.
- Gain insight into the data by:
 - Basic statistical data description: central tendency, dispersion, graphical displays
 - Data visualization: map data onto graphical primitives
 - Measure data similarity
- Above steps are the beginning of data preprocessing
- Many methods have been developed but still an active area of research

References

- W. Cleveland, Visualizing Data, Hobart Press, 1993
- T. Dasu and T. Johnson. Exploratory Data Mining and Data Cleaning. John Wiley, 2003
- U. Fayyad, G. Grinstein, and A. Wierse. Information Visualization in Data Mining and Knowledge Discovery, Morgan Kaufmann, 2001
- L. Kaufman and P. J. Rousseeuw. Finding Groups in Data: an Introduction to Cluster Analysis. John Wiley & Sons, 1990.
- H. V. Jagadish et al., Special Issue on Data Reduction Techniques. Bulletin of the Tech. Committee on Data Eng., 20(4), Dec. 1997
- D. A. Keim. Information visualization and visual data mining, IEEE trans. on Visualization and Computer Graphics, 8(1), 2002
- D. Pyle. Data Preparation for Data Mining. Morgan Kaufmann, 1999
- S. Santini and R. Jain," Similarity measures", IEEE Trans. on Pattern Analysis and Machine Intelligence, 21(9), 1999
- E. R. Tufte. The Visual Display of Quantitative Information, 2nd ed., Graphics Press, 2001
- C. Yu, et al., Visual data mining of multimedia data for social and behavioral studies, Information Visualization, 8(1), 2009

