CS 412 Intro. to Data Mining

Chapter 2. Data and Measurements

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Chapter 2. Getting to Know Your Data

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

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

- Transaction data

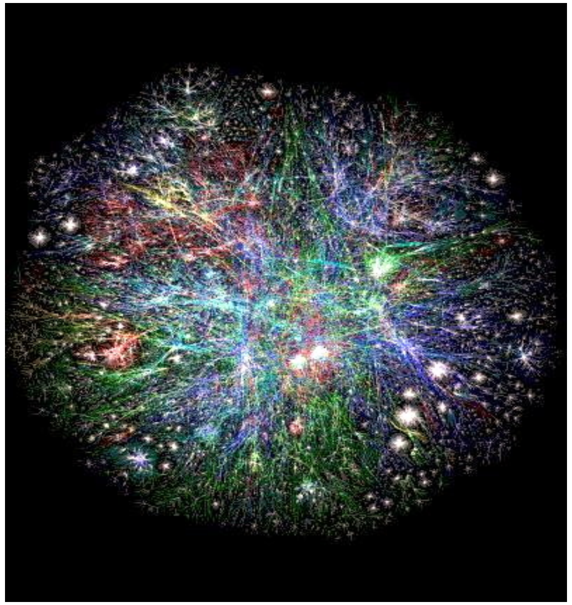
TID	*Items*
1	Bread, Coke, Milk
2	Beer, Bread
3	Beer, Coke, Diaper, Milk
4	Beer, Bread, Diaper, Milk
5	Coke, Diaper, Milk

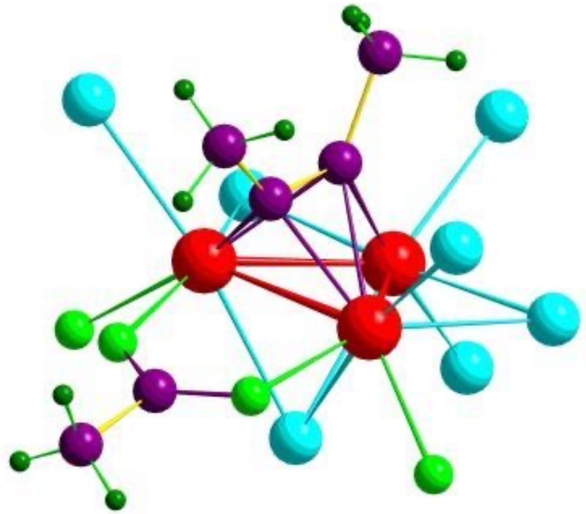
	team	coach	play	ball	score	game	win	lost	timeout	season
Document 1	3	0	5	0	2	6	0	2	0	2
Document 2	0	7	0	2	1	0	0	3	0	0
Document 3	0	1	0	0	1	2	2	0	3	0

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

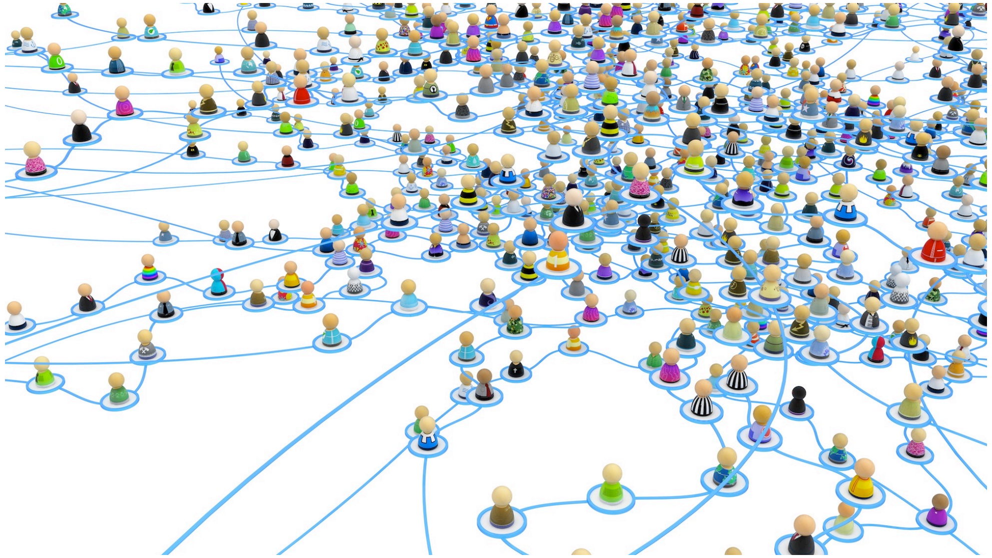
Types of Data Sets: (2) Graphs and Networks

- ❑ Transportation network
- ❑ World Wide Web



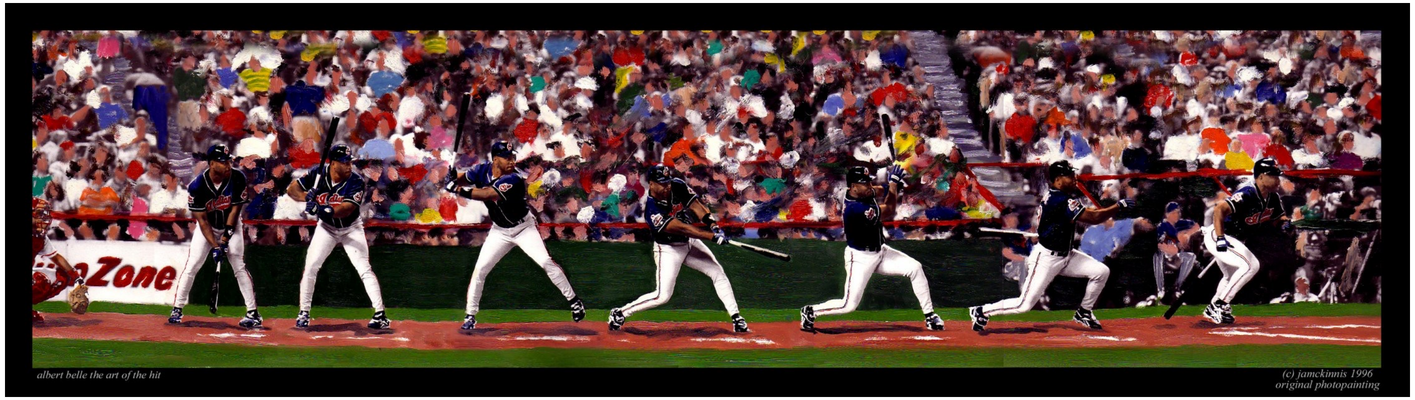


- ❑ Molecular Structures
- ❑ Social or information networks

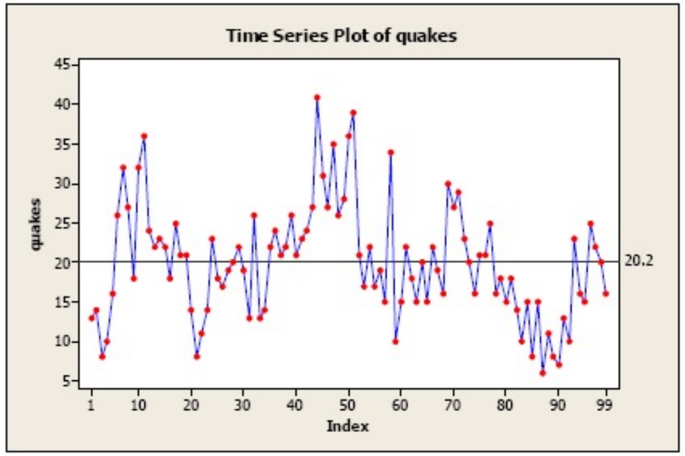


Types of Data Sets: (3) Ordered Data

- Video data: sequence of images



- Temporal data: time-series

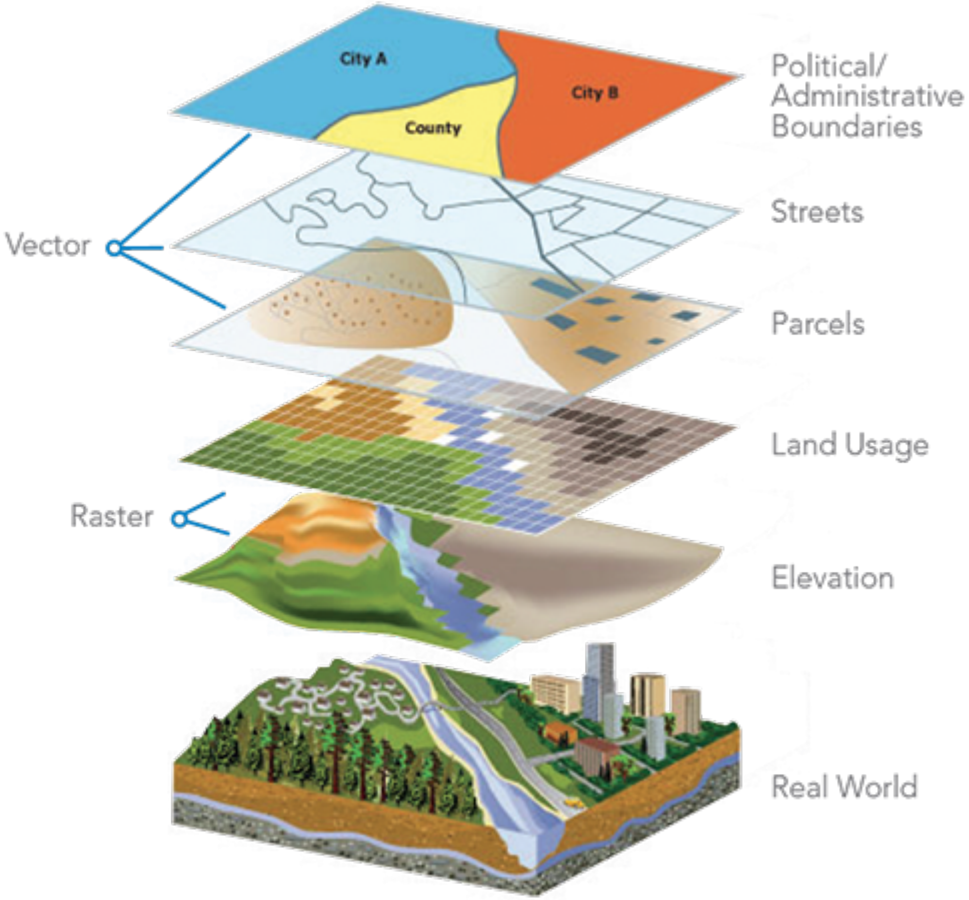


- Sequential Data: transaction sequences

- Genetic sequence data

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: No true zero, can compute differences, means, etc.
      - Examples: Temp in °C or °F, calendar year
    - Ratio-scaled: True zero, ratio scaled, e.g., 10 is twice as much as 5
      - Examples: Temp in °K, years of experience, number of words

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)
  - <u>Symmetric binary</u>: both outcomes equally important
    - e.g., gender
  - <u>Asymmetric binary</u>: 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

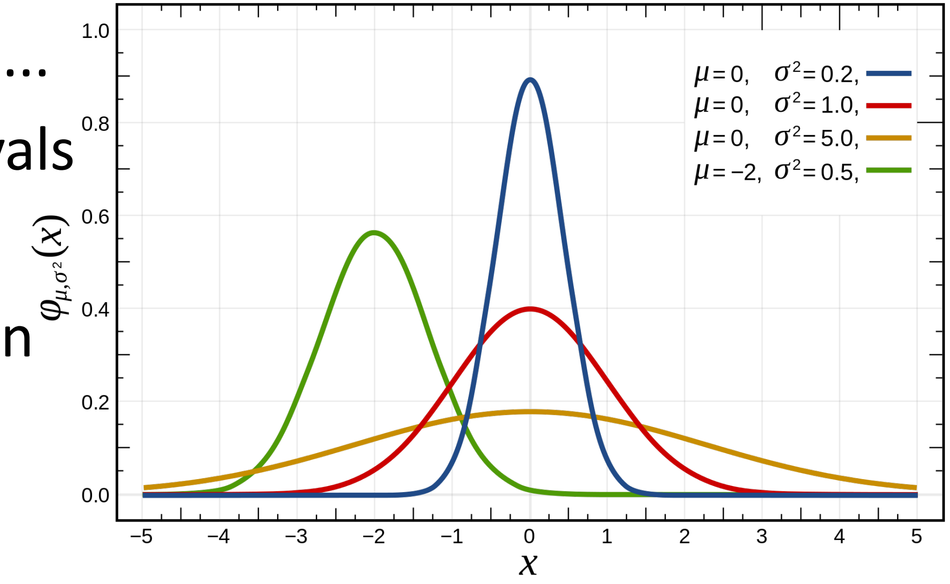
- **Discrete Attribute**
  - Has only a finite or countably infinite set of values
    - E.g., zip codes, profession, or the set of words in a collection of documents
  - Sometimes, represented as integer variables
  - Note: Binary attributes are a special case of discrete attributes
- **Continuous Attribute**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

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

sample mean

$$\mu = \frac{1}{N}\sum_{j=1}^{N} x_j$$

population mean

- Weighted arithmetic mean:

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

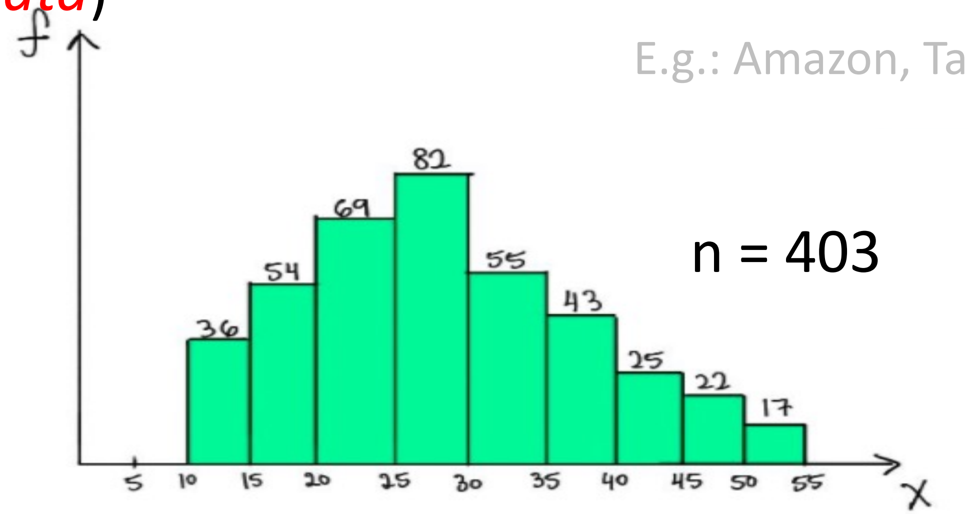
- Trimmed mean:
  - Chopping extreme values (e.g., Olympics gymnastics score computation)

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*)

E.g.: Amazon, Taiga, Borneo

Bins: 1,2,…,M
Frequencies: $f_1, f_2, \ldots, f_M$
Cumulative frequencies $F_m = \sum_{l=1}^{m} f_l$



n = 403

Median falls in the m^th bin, $F_{m-1} \le n/2 \le F_m$
Interval [L_m, L_{m+1}], e.g., [25,30]

Approximate median

Sum before the median interval

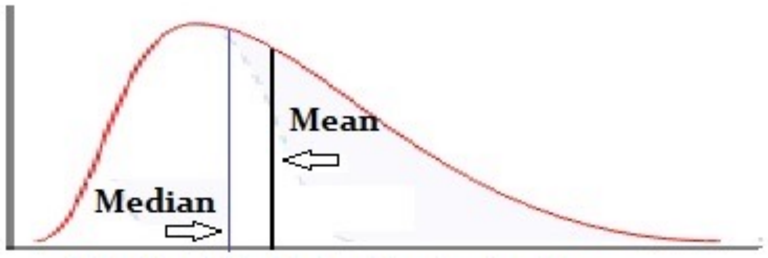
Interval width

$$median \approx L_m + \left(\frac{n/2 - F_{m-1}}{f_m}\right) \times (L_{m+1} - L_m)$$

Low interval limit

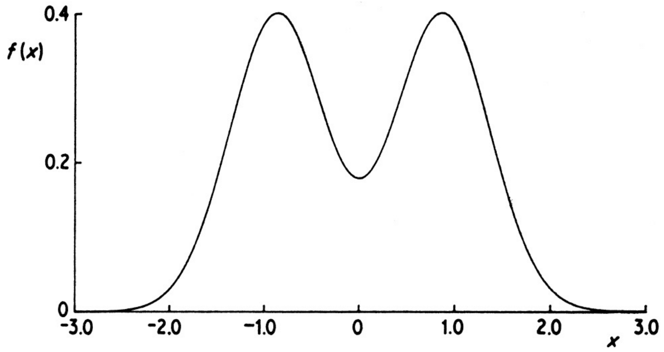
Measuring the Central Tendency: (3) Mode

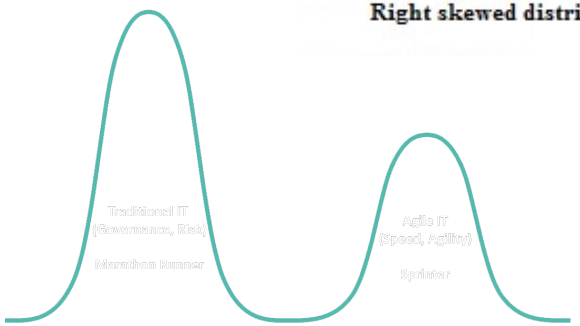
- Mode: Value that occurs most frequently in the data
- Unimodal
  - Empirical formula: $mean - mode = 3 \times (mean - median)$



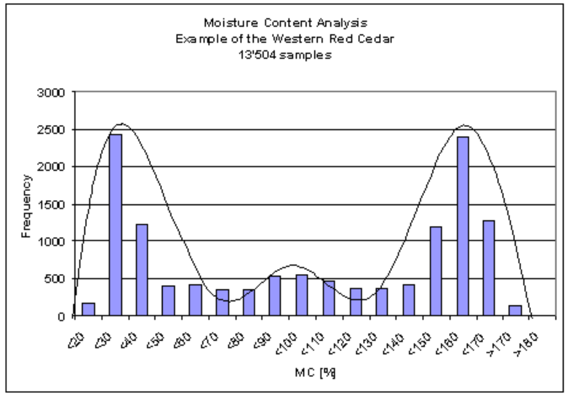
Right skewed distribution: Mean is to the right

- Multi-modal
  - Bimodal





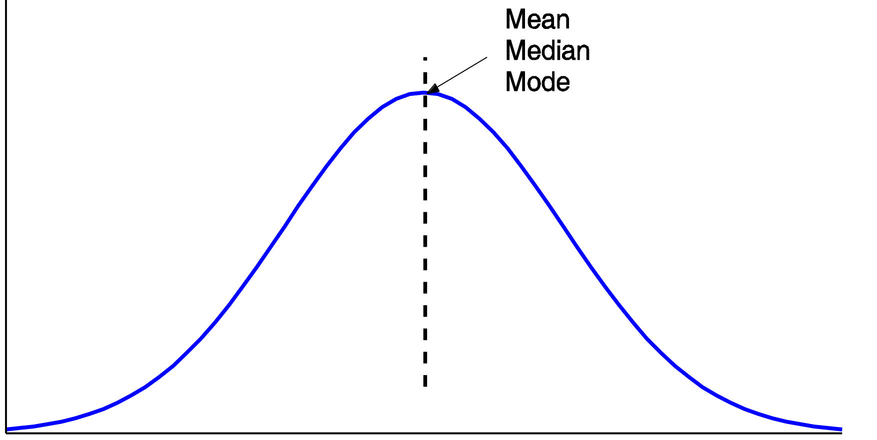
  - Trimodal

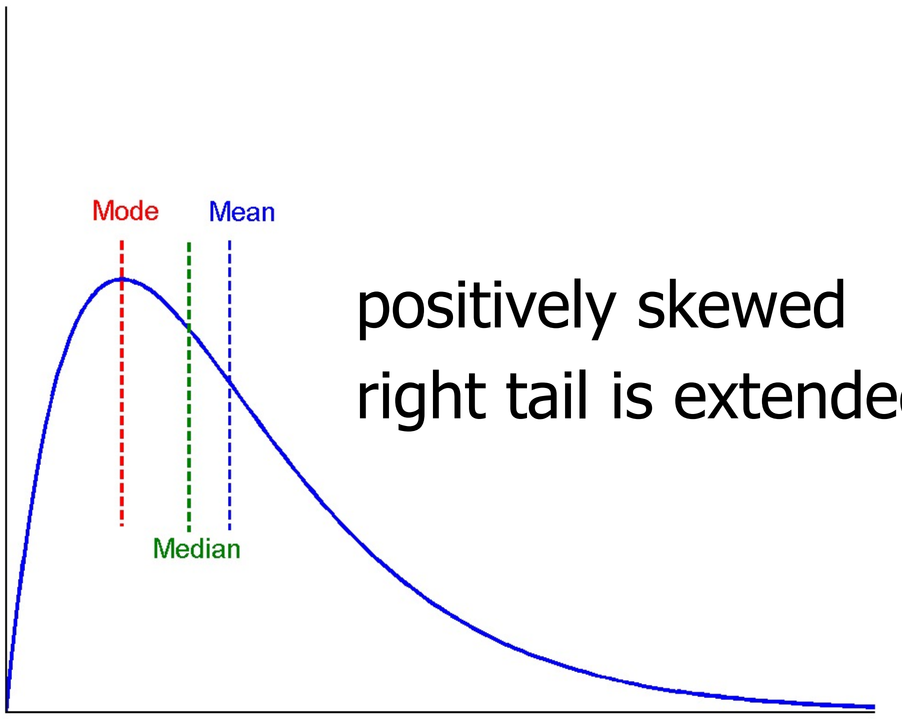


Symmetric vs. Skewed Data

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

symmetric



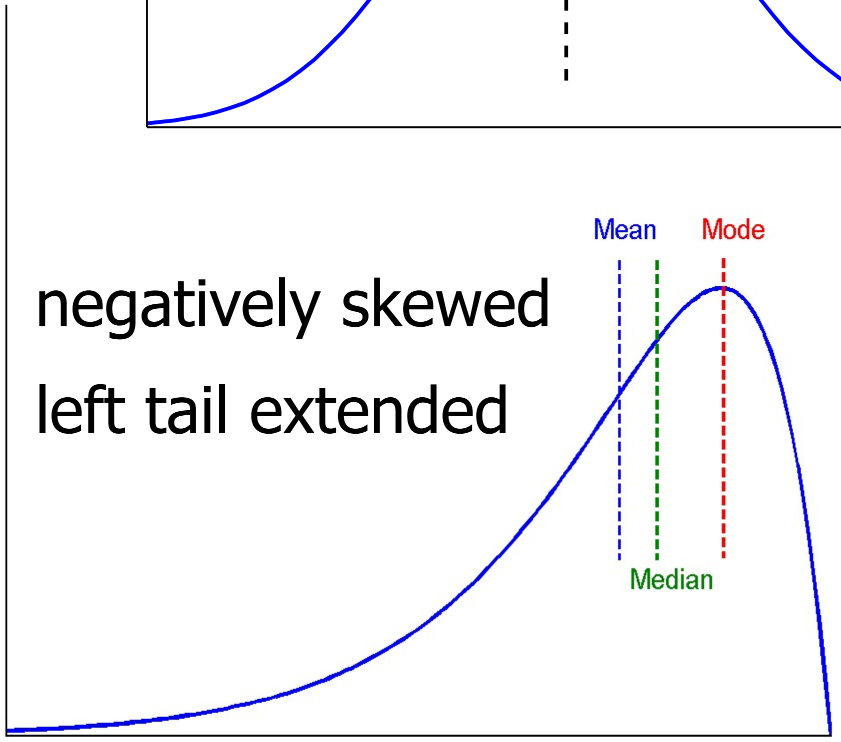


positively skewed

right tail is extended

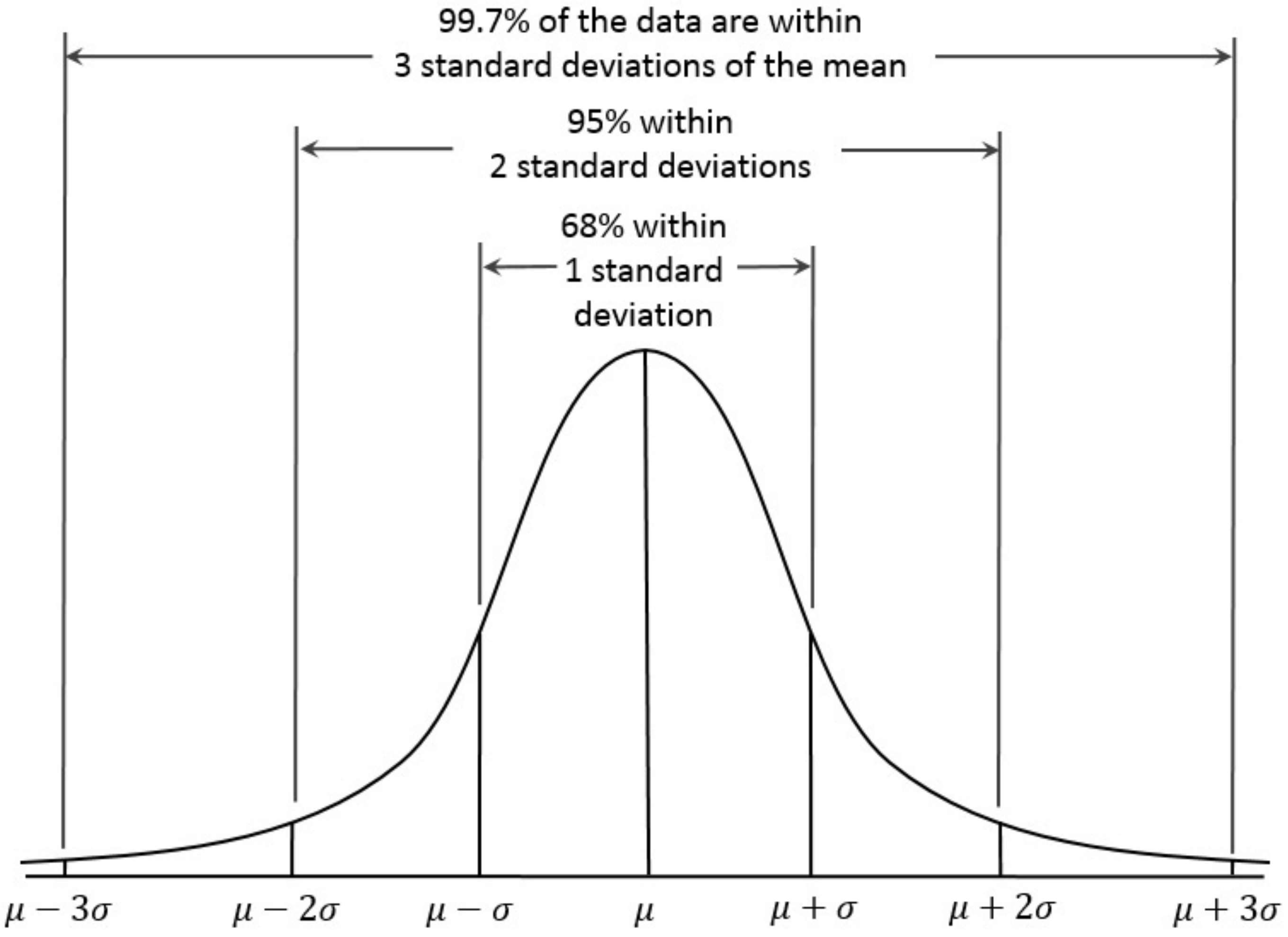
negatively skewed

left tail extended



Properties of Normal Distribution Curve

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



$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

$f(x)$ = probability density function

σ = standard deviation

μ = mean

Represent central tendency

Measures Data Distribution: Variance and Standard Deviation

- Variance and standard deviation (*sample, population)*
  - **Variance**: (algebraic, scalable computation)
    - Q: Can you compute it incrementally and efficiently?

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

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

Note: The subtle difference of formulae for sample vs. population
- n : the size of the sample
- N : the size of the population

- **Standard deviation** is the square root of variance

Covariance of Numeric Data

- Two numeric attributes A, B, and n observations: $\{(a_1,b_1),\ldots,(a_n,b_n)\}$
- Expected values:

$$E(A) = \bar{A} = \frac{\sum_{i=1}^{n} a_i}{n} \qquad E(B) = \bar{B} = \frac{\sum_{i=1}^{n} b_i}{n}$$

- Covariance

$$Cov(A,B) = E((A-\bar{A})(B-\bar{B})) = \frac{\sum_{i=1}^{n}(a_i-\bar{A})(b_i-\bar{B})}{n}$$

$$= E(A\cdot B) - \bar{A}\bar{B}$$

- Correlation coefficient

$$r_{A,B} = \frac{Cov(A,B)}{\sigma_A \sigma_B}$$

Correlation Coefficient of Numeric Data

- Correlation Coefficient

$$r_{A,B} = \frac{\sum_{i=1}^{n}(a_i - \bar{A})(b_i - \bar{B})}{n\sigma_A\sigma_B} = \frac{\sum_{i=1}^{n}(a_i b_i) - n\bar{A}\bar{B}}{n\sigma_A\sigma_B}$$

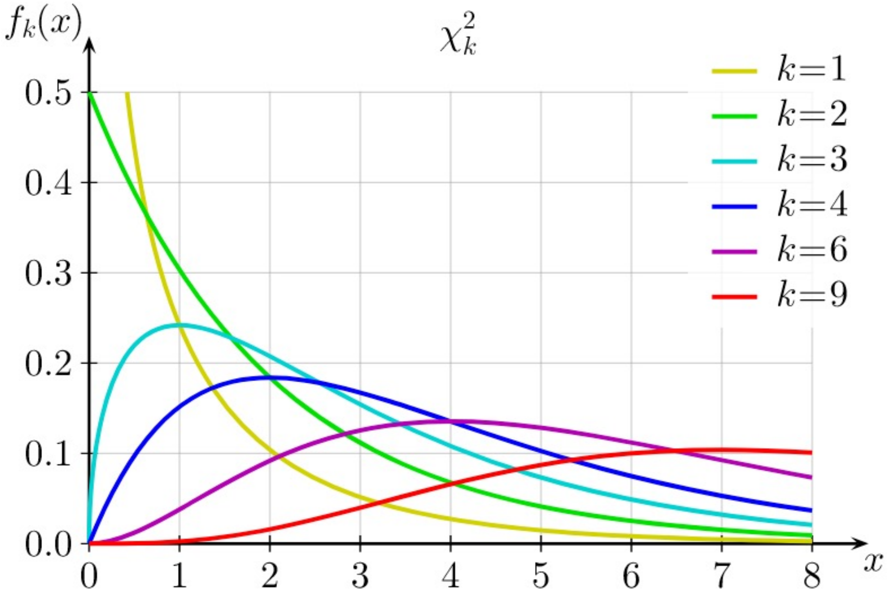
- $r_{A,B}$ lies in [-1,+1]
- Positive correlation: $r_{A,B} > 0$, typically increase/decrease together
- Negative correlation: $r_{A,B} < 0$, typically one increases when the other decreases
- Uncorrelated: $r_{A,B} = 0$, no correlation
- Correlation does not mean causation

Hypothesis Tests for Nominal Data

- Hypothesis testing, using a sample of *n* observations
  - Consider a `null hypothesis' and `alternative hypothesis'
  - Consider a test statistic, and set a significance level
  - Calculate the test statistic from observations
  - Calculate the p-value, accept or reject the null hypothesis

- Nominal data: χ^2 test
  - χ^2-distribution with k degrees of freedom

$$Q \sim \chi_k^2 \quad \equiv \quad Q = \sum_{i=1}^{k} g_i^2 \;, g_i \sim N(0,1)$$

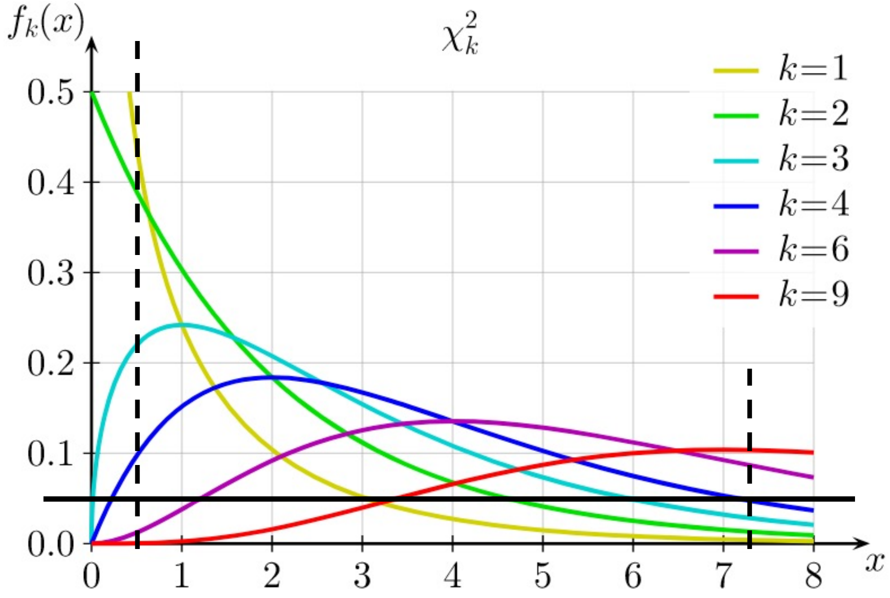


Example: Is My Coin Biased?

- Tossed a coin 100 times: 54 Heads, 46 Tails
  - Is my coin biased
- Hypothesis testing, using a sample of *n* observations
  - Null hypothesis: Coin is unbiased, *expected behavior* 50 Heads, 50 Tails
  - Test statistic: measures deviation from *expected behavior*

$$\frac{(54-50)^2}{50} + \frac{(46-50)^2}{50} = 0.64$$

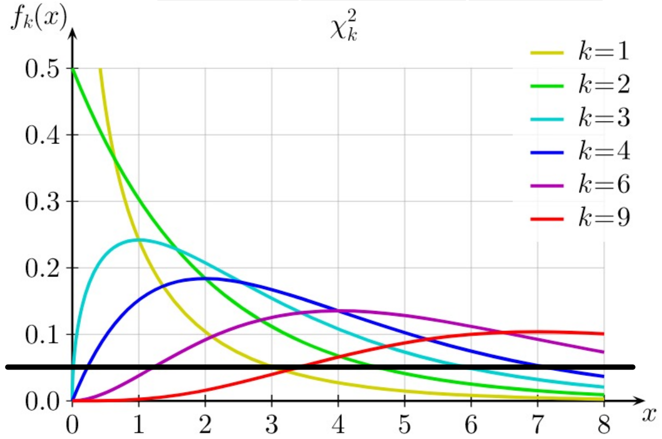
  - Test statistic follows the chi-square distribution
    - Degrees of freedom k = 1
  - Significance level: probability that the deviation is by random chance
    - α=0.05 or α=0.01 are typical


$f_k(x)$
χ^2_k
$k=1$
$k=2$
$k=3$
$k=4$
$k=6$
$k=9$
0.5
0.4
0.3
0.2
0.1
0.0
0
1
2
3
4
5
6
7
8
x

Chi-Squared Test for Nominal Data

- Hypothesis: Answers to multiple choice questions are uniformly distributed
  - Options: A, B, C, D; Null hypothesis says probability is ¼
  - Alternative hypothesis: Distribution is not uniform
- Set significance level α=0.05
  - Tail probability (distribution) threshold
  - 3 degrees of freedom, χ^2 value to reject null = 7.815
- Sample n=100 questions for the analysis
- χ^2 statistic: $\sum_{i=1}^{4} \frac{(o_i - e_i)^2}{e_i} = 6$
  - Probability is ≥ 0.1 > α, cannot reject null hypothesis

Correct Choice	Expected	Actual
A	25	20
B	25	20
C	25	25
D	25	35



Correlation Analysis for Nominal Data

- Two nominal attributes A and B
  - A has values $\{a_1, a_2, \ldots, a_c\}$
  - B has values $\{b_1, b_2, \ldots, b_r\}$
- Create a contingency table from data
  - Counts of joint events ($A=a_i$, $B=b_j$)
- Null hypothesis: A and B are independent
- The expected frequency in each entry: $$e_{ij} = \frac{count(A = a_i) \times count(B = b_j)}{n}$$
- The χ^2 statistic, (r-1)(c-1) degrees of freedom

$$\chi^2 = \sum_{i=1}^{c} \sum_{j=1}^{r} \frac{(o_{ij} - e_{ij})^2}{e_{ij}}$$

Table 2.2: Example 2.1's 2×2 Contingency Table Data

	male	*female*	*Total*
fiction	250 (90)	200 (360)	450
non_fiction	50 (210)	1000 (840)	1050
Total	300	1200	1500

Note: Are *gender* and *preferred_reading* correlated?

Example: Correlation Analysis for Nominal Data

- Compute expected frequency

$$e_{11} = \frac{count(male) \times count(fiction)}{n} = \frac{300 \times 450}{1500} = 90$$

Table 2.2: Example 2.1's 2×2 Contingency Table Data

	male	*female*	*Total*
fiction	250 (90)	200 (360)	450
non_fiction	50 (210)	1000 (840)	1050
Total	300	1200	1500

Note: Are *gender* and *preferred_reading* corre-

- The χ^2 statistic

$$\chi^2 = \frac{(250-90)^2}{90} + \frac{(50-210)^2}{210} + \frac{(200-360)^2}{360} + \frac{(1000-840)^2}{840}$$
$$= 284.44 + 121.90 + 71.11 + 30.48 = 507.93.$$

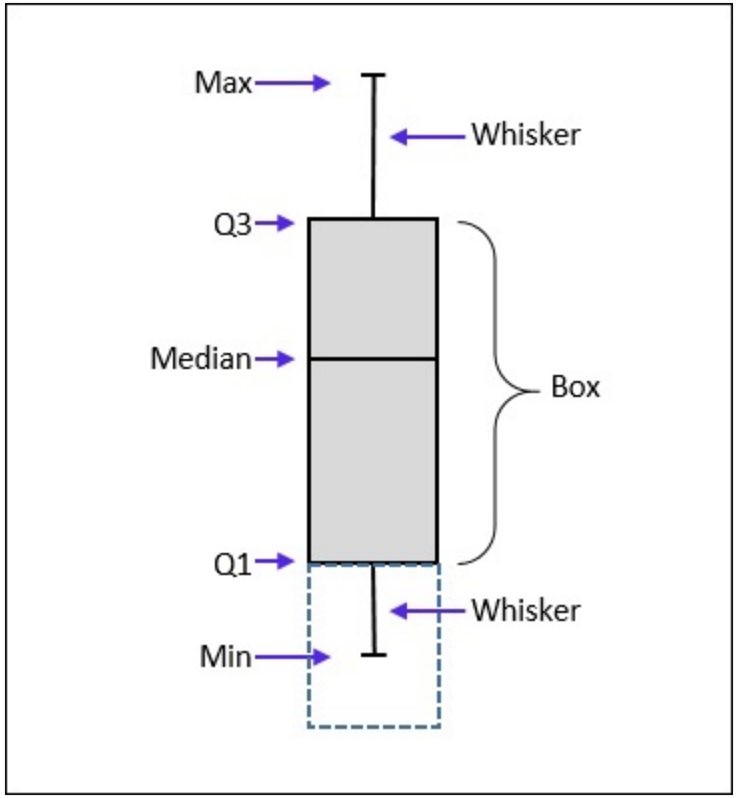
- With 1 degree of freedom, at 0.001 significance level
  - Value needed to reject null hypothesis: 10.828
  - More than that, hence null hypothesis is rejected

Graphic Displays of Basic Statistical Descriptions

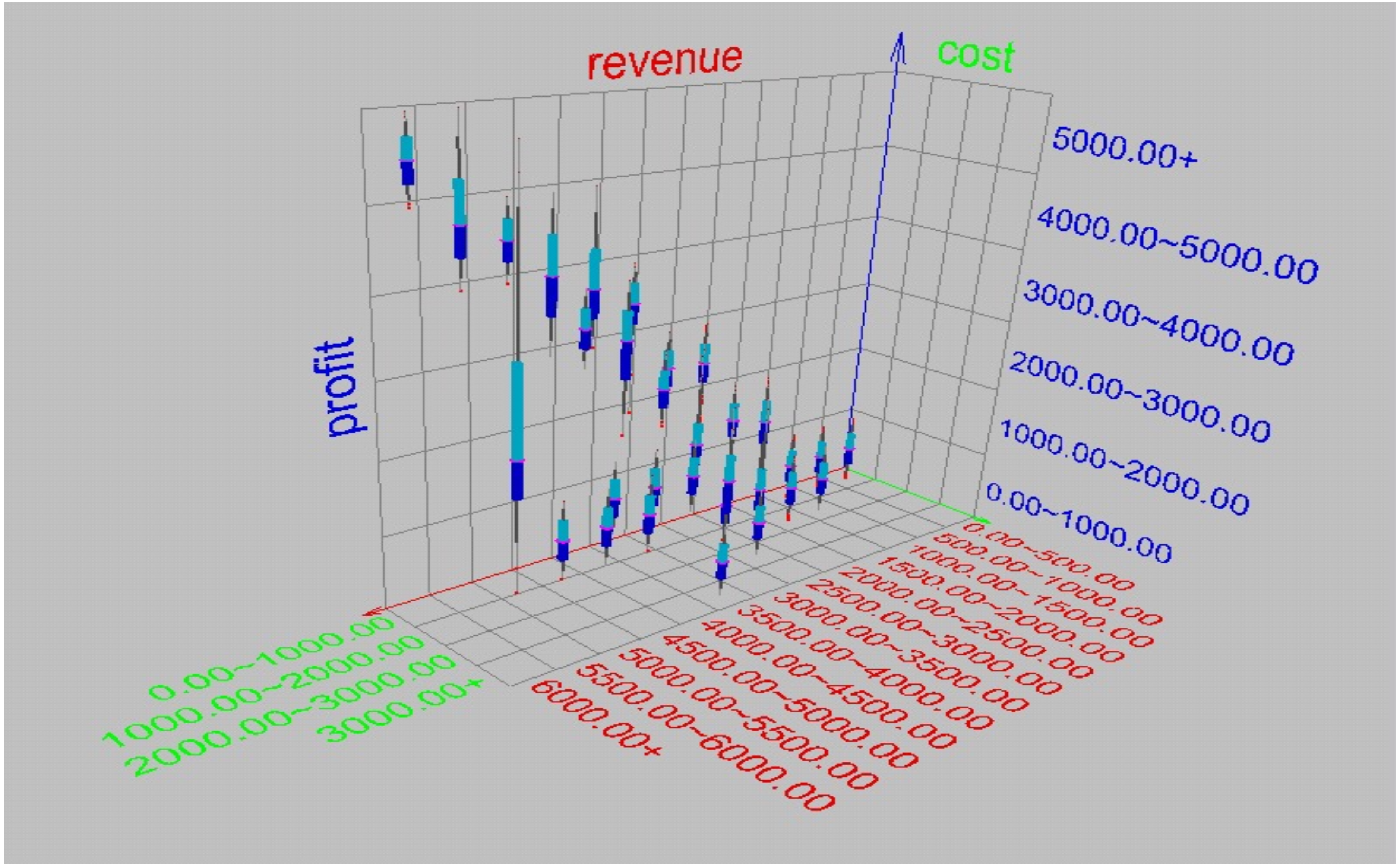
- **Boxplot**: graphic display of five-number summary
- **Histogram**: x-axis are values, y-axis repres. frequencies
- **Quantile plot**: each value x_i is paired with f_i indicating that approximately 100 f_i % of data are $\leq x_i$
- **Quantile-quantile (q-q) plot**: graphs the quantiles of one univariant 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 (25th percentile), Q_3 (75th percentile)
- **Inter-quartile range**: $IQR = Q_3 - Q_1$
- **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 x IQR



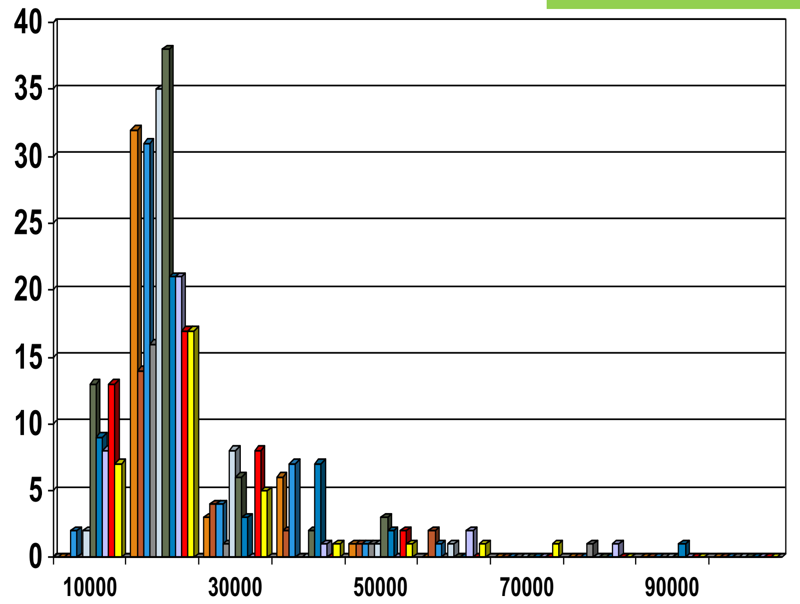
Visualization of Data Dispersion: 3-D Boxplots

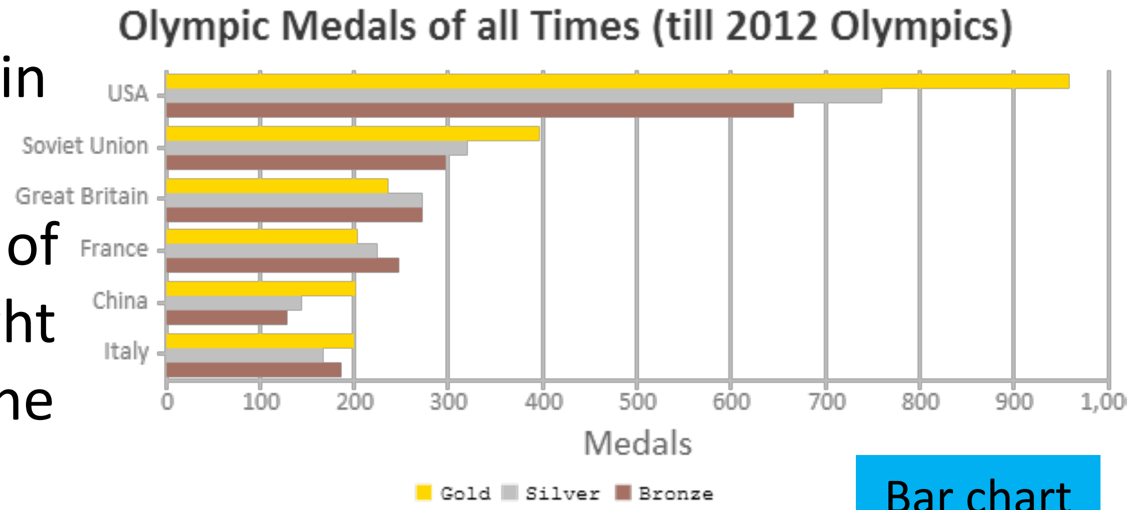


Histogram Analysis

- 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

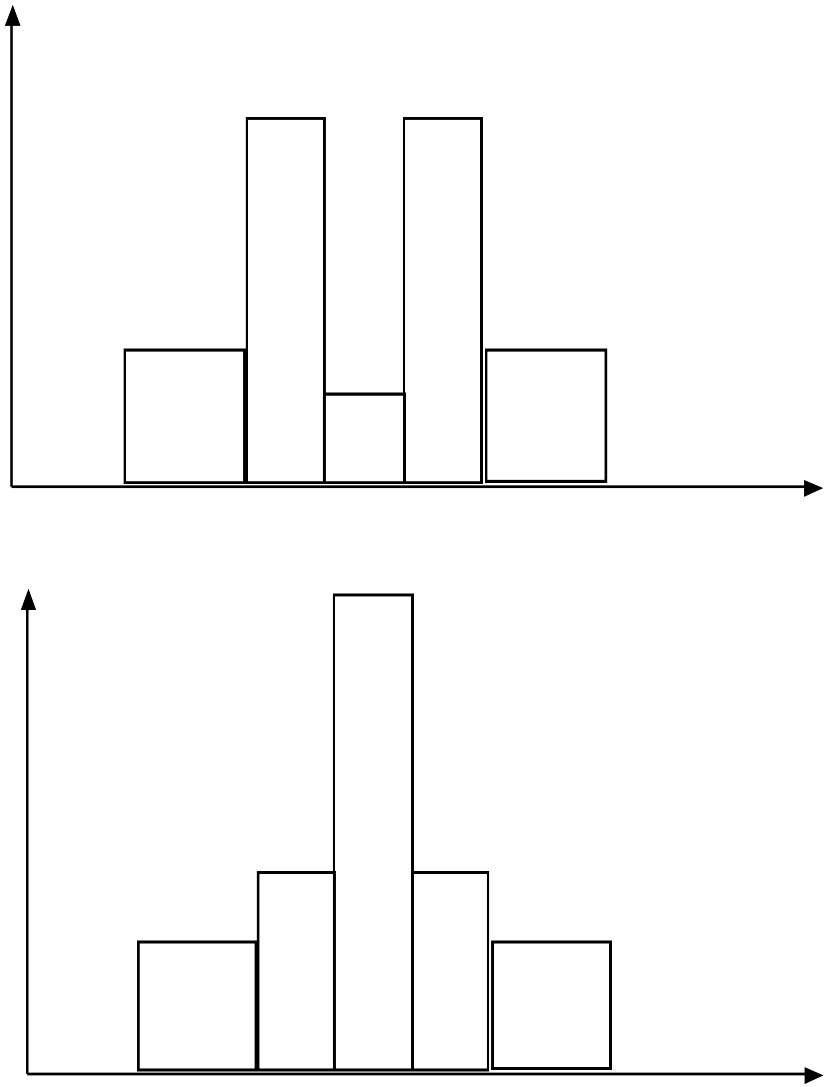
Histogram





Bar chart

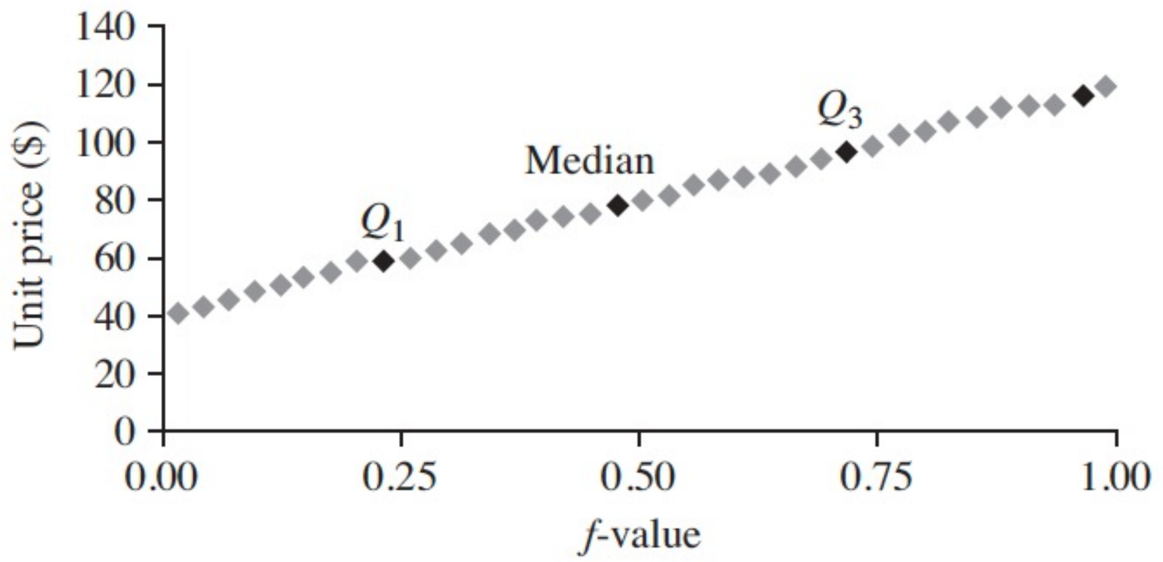
Histograms Often Tell More than Boxplots



- 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

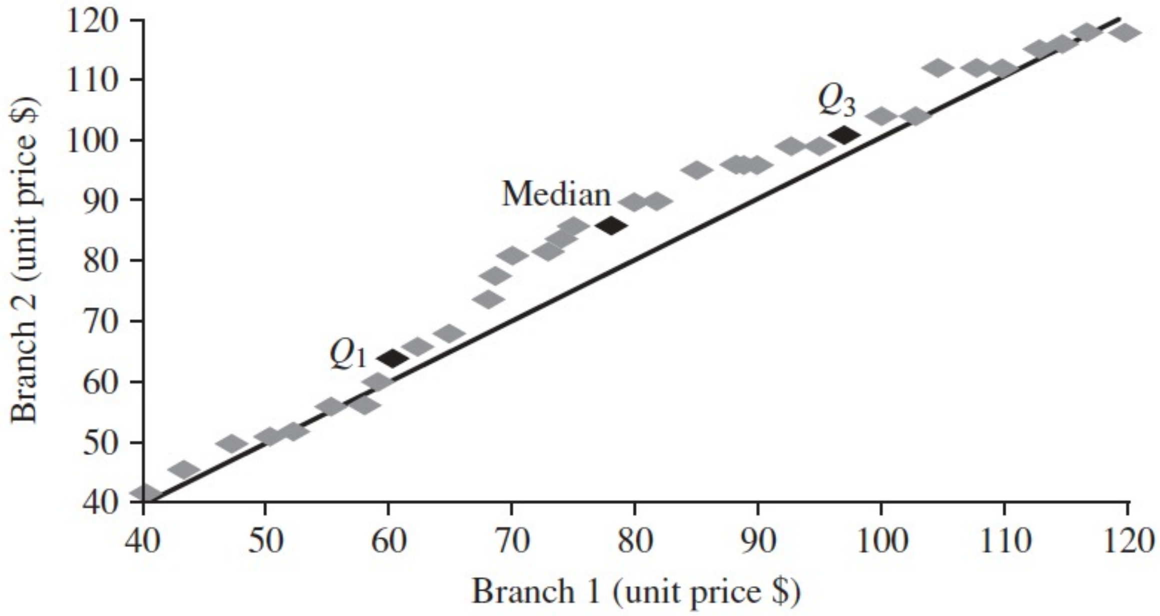
Quantile Plot

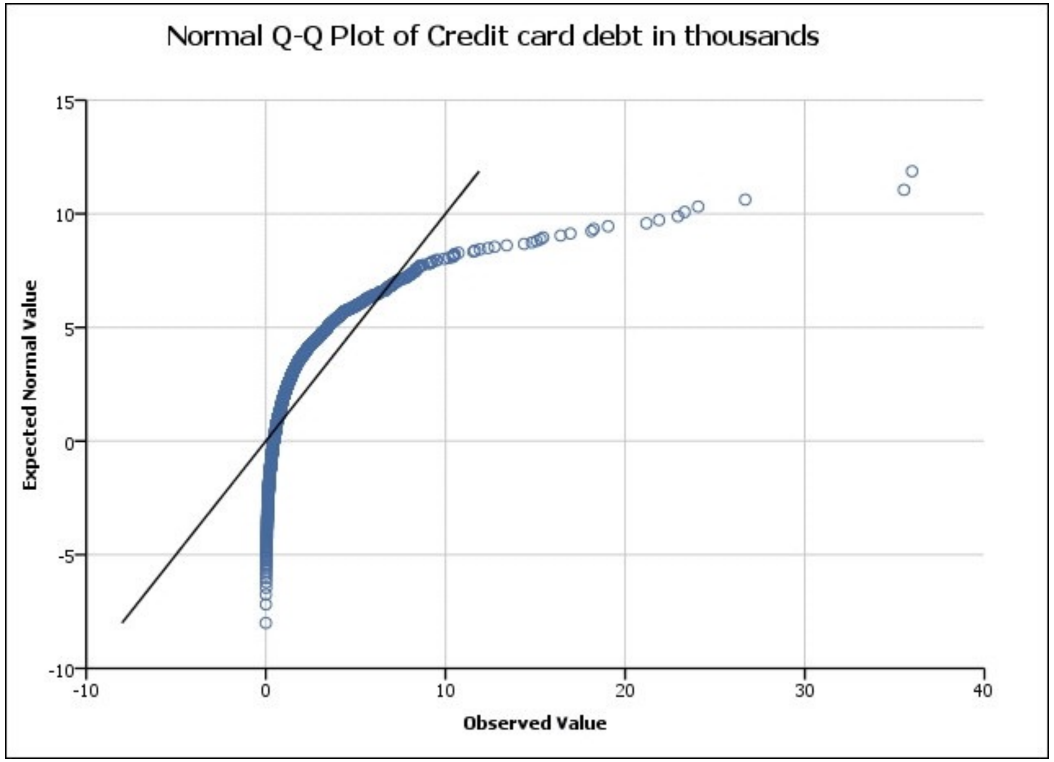
- Displays all of the data (allowing the user to assess both the overall behavior and unusual occurrences)
- Plots **quantile** information
  - For a data x_i data sorted in increasing order, f_i indicates that approximately 100 f_i% of the data are below or equal to the value x_i

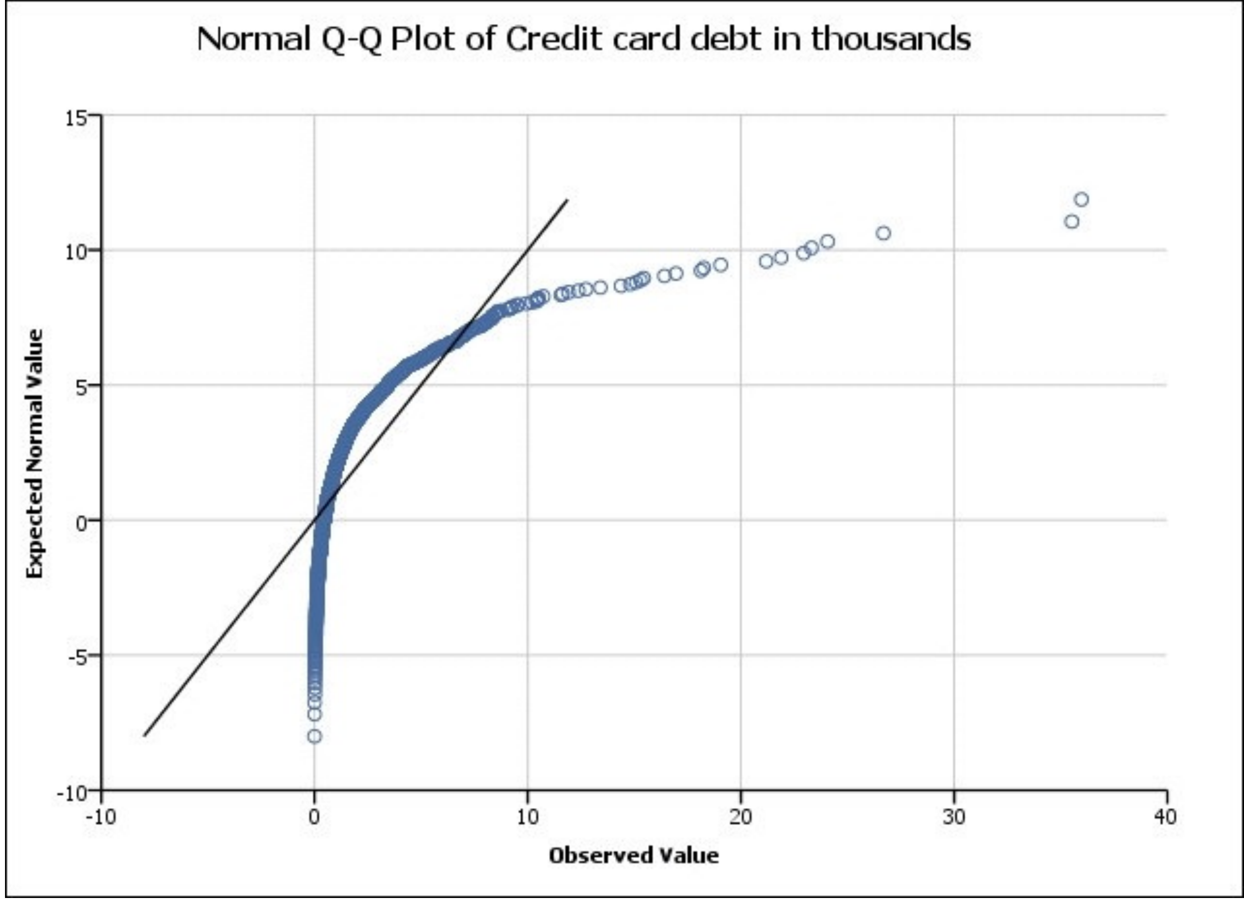


Quantile-Quantile (Q-Q) Plot

- 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

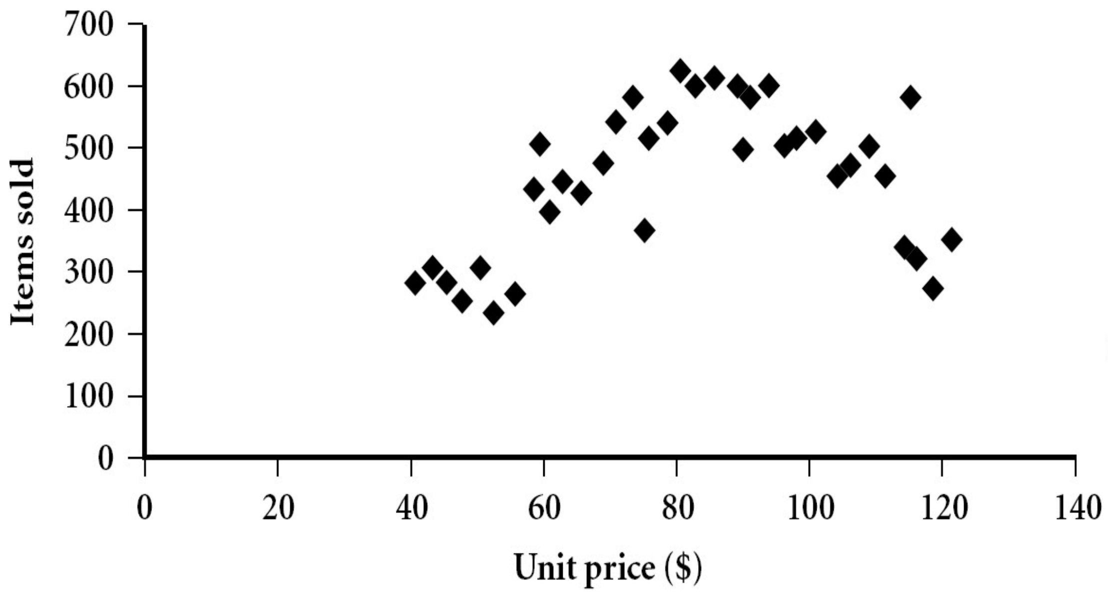


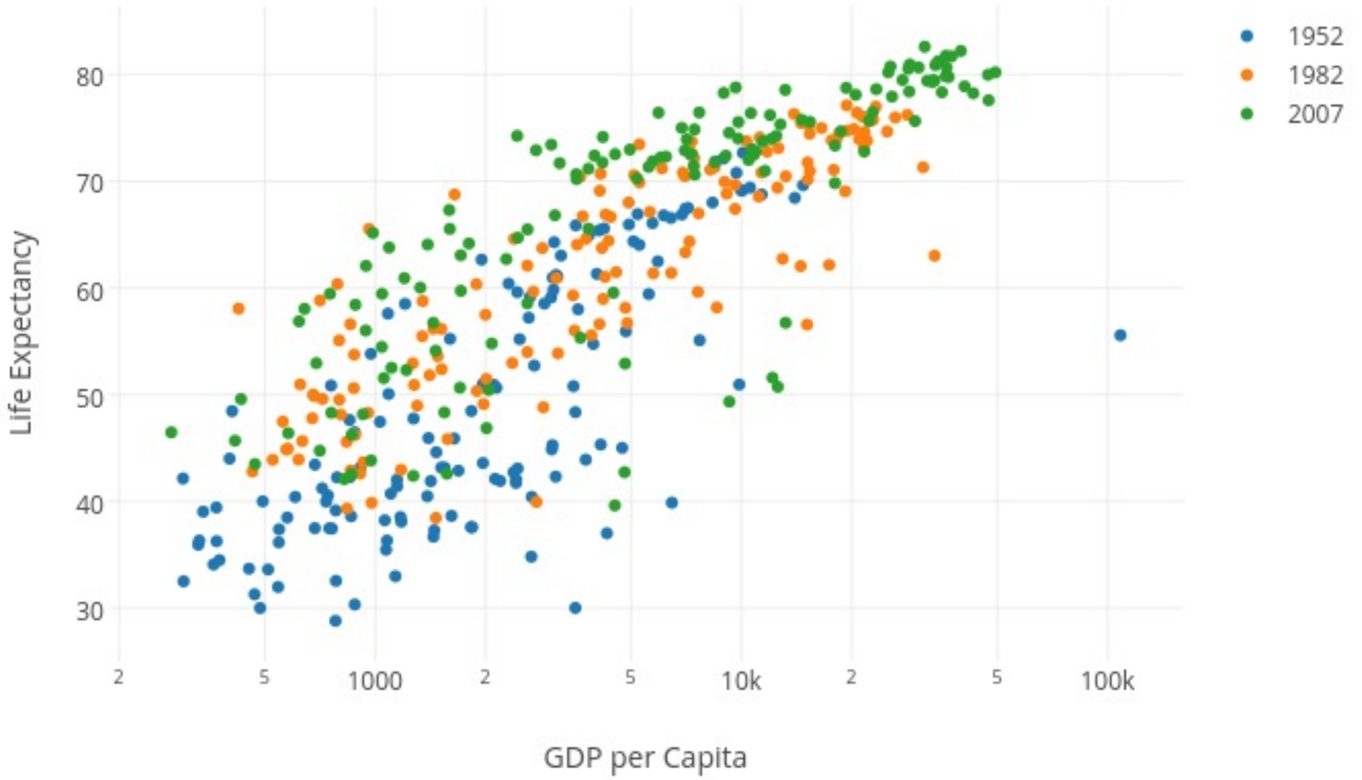



Normal Q-Q Plot of Credit card debt in thousands
Expected Normal Value
Observed Value
15
10
5
0
-5
-10
-10
0
10
20
30
40

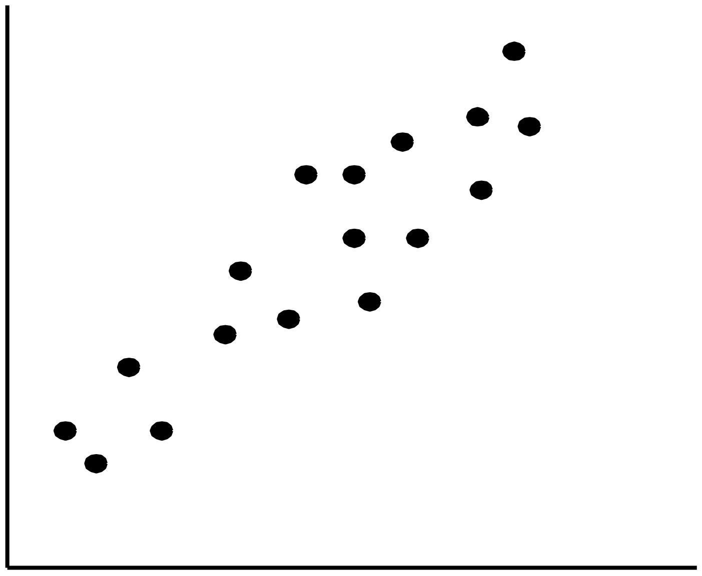
Scatter plot

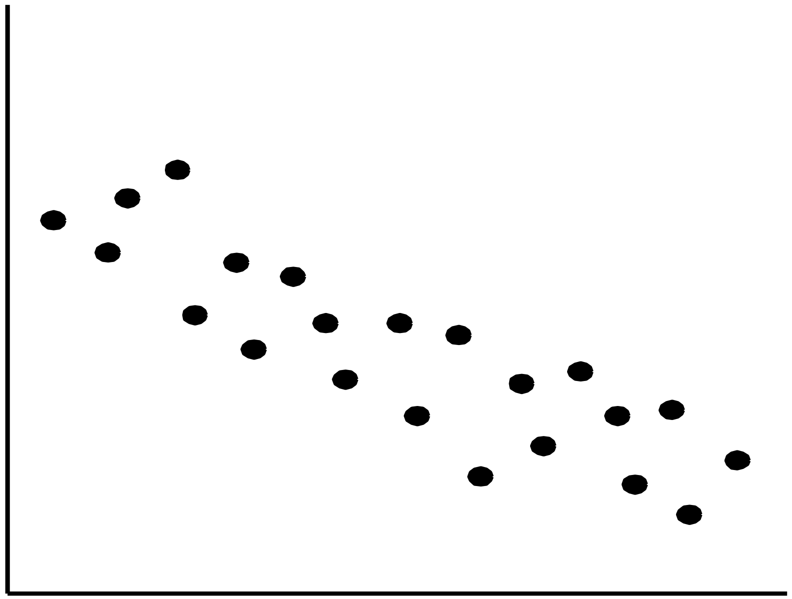
- Provides a first look at bivariate data to see clusters of points, outliers, etc.
- Each pair of values is treated as a pair of coordinates and plotted as points in the plane

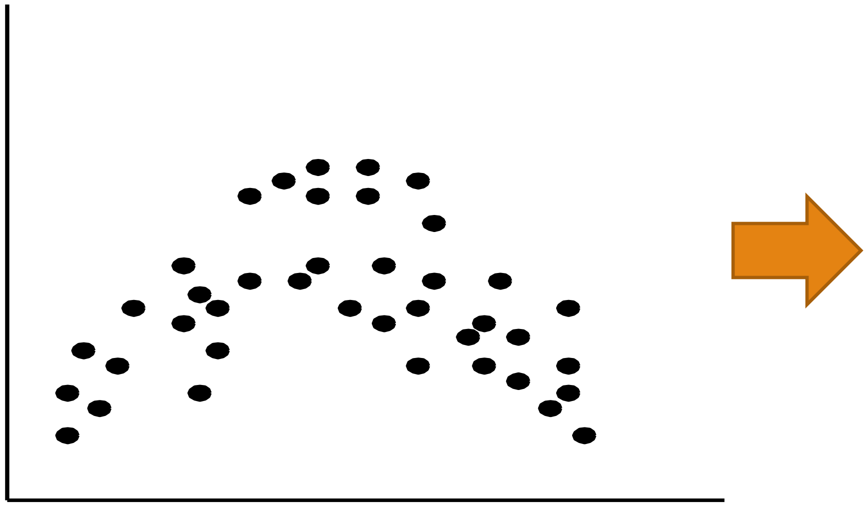




Positively and Negatively Correlated Data

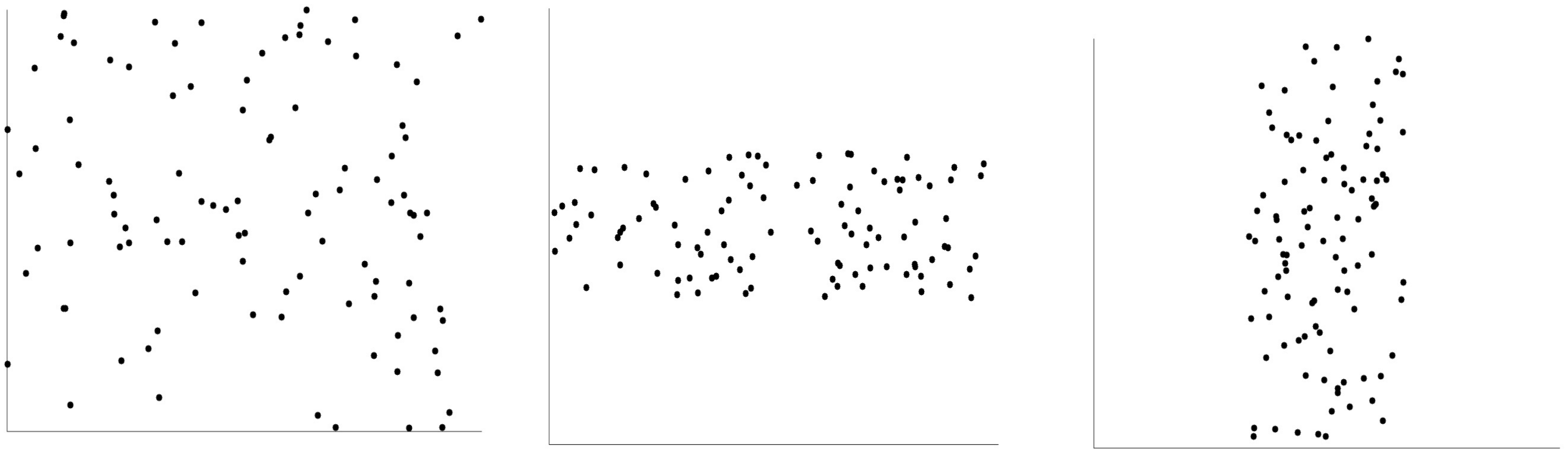






- The left half fragment is positively correlated
- The right half is negative correlated

Uncorrelated Data



Chapter 2. Getting to Know Your Data

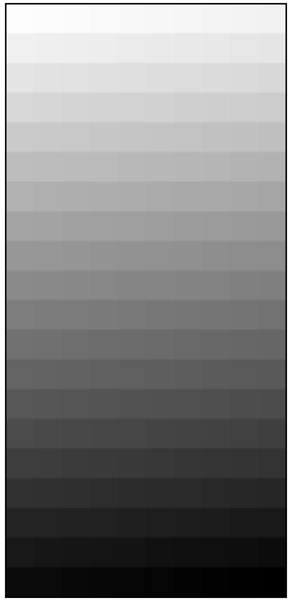
- Data Objects and Attribute Types
- Basic Statistical Descriptions of Data
- Data Visualization
- Measuring Data Similarity and Correlation
- Summary

Data Visualization

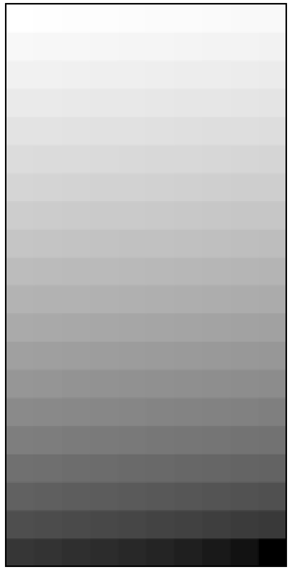
- Why data visualization?
  - Gain insight into an information space by mapping data onto graphical primitives
  - Provide qualitative overview of large data sets
  - Search for patterns, trends, structure, irregularities, relationships among data
  - Help find interesting regions and suitable parameters 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

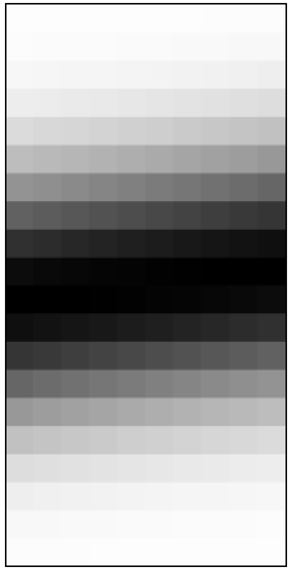
- For a data set of *m* dimensions, create *m* windows on the screen, one for each dimension
- The *m* dimension values of a record are mapped to *m* pixels at the corresponding positions in the windows
- The colors of the pixels reflect the corresponding values



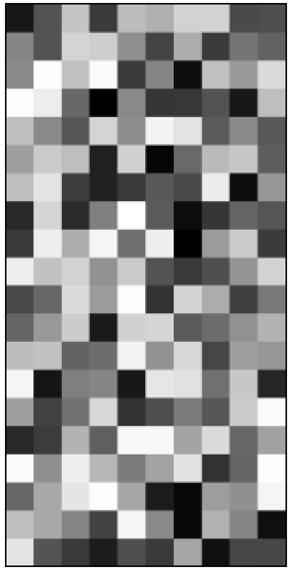
(a) Income



(b) Credit Limit



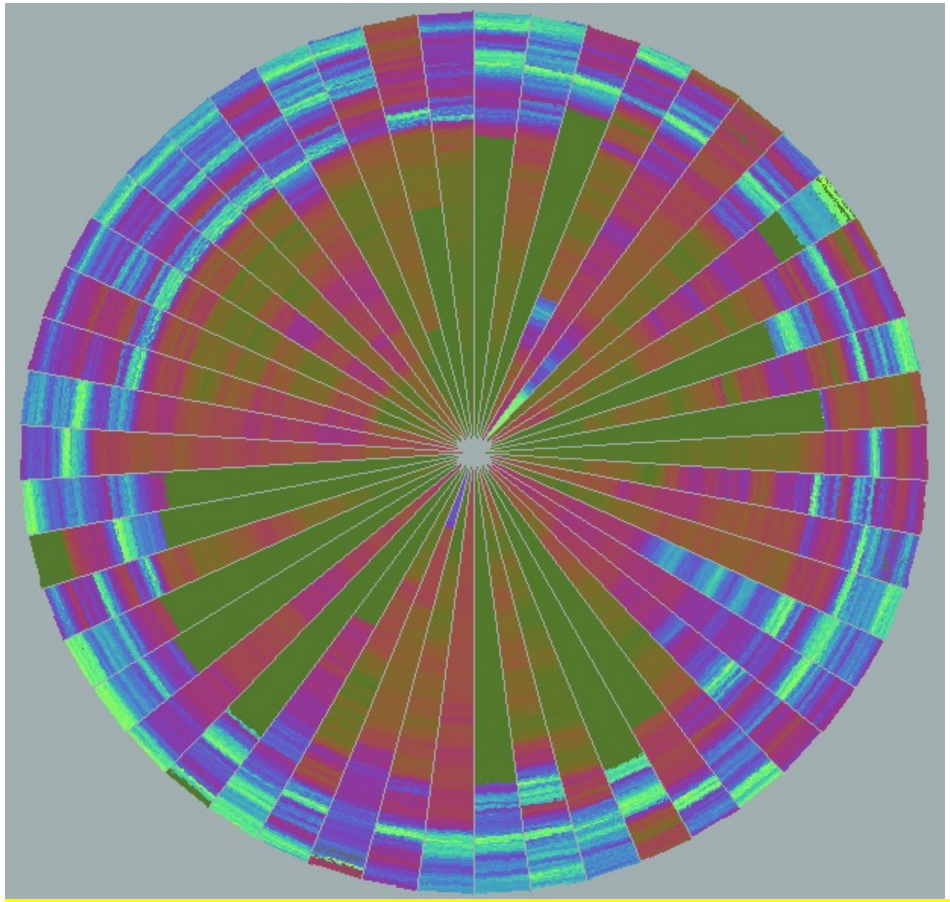
(c) transaction volume



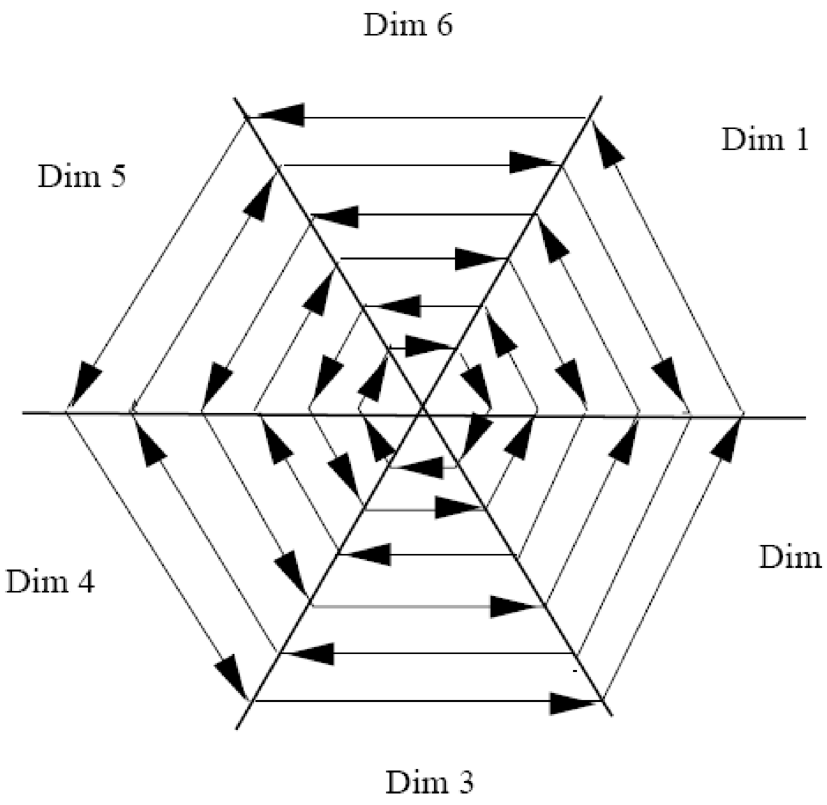
(d) age

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



Representing about 265,000 50-dimensional Data Items with the 'Circle Segments' Technique



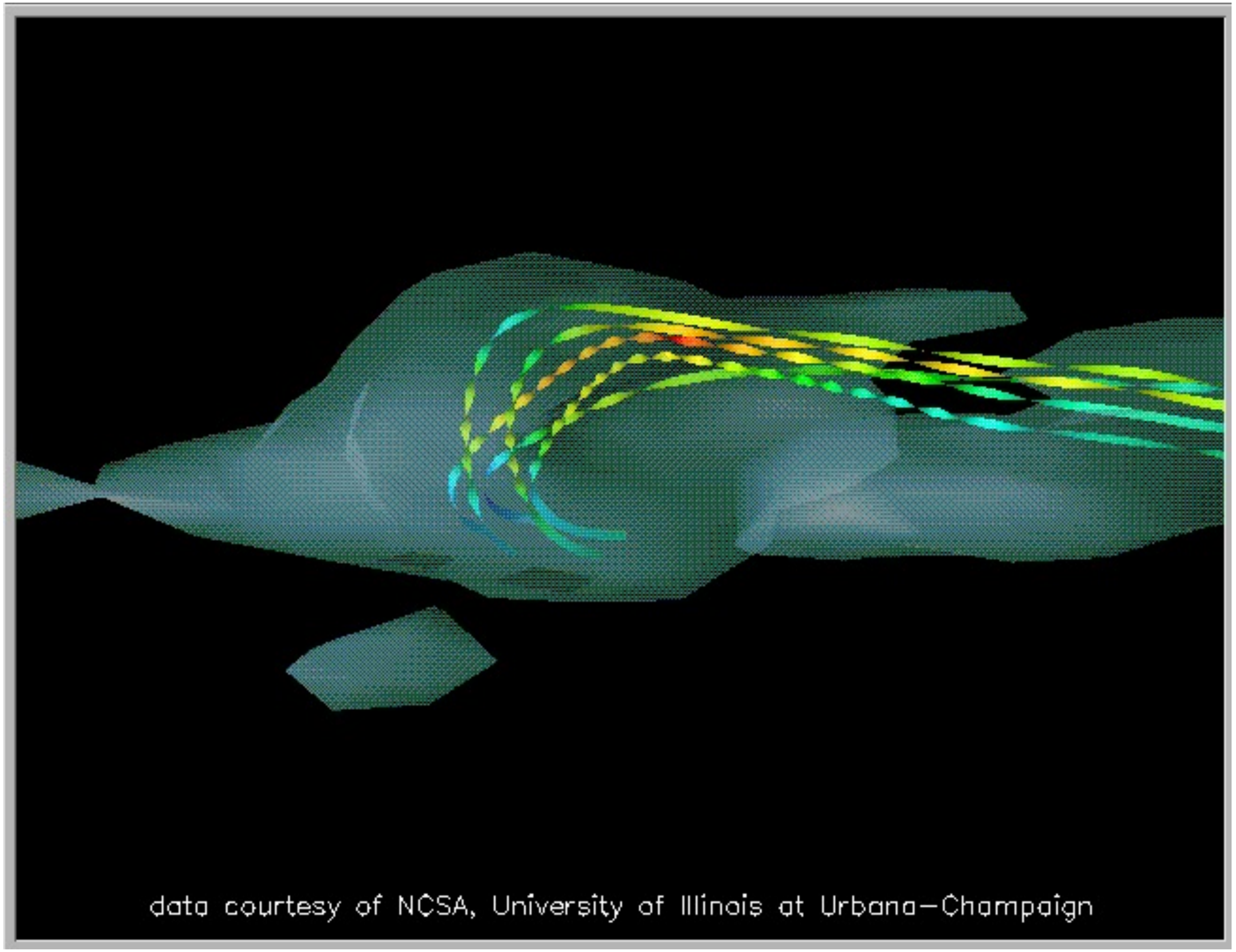
(b) Laying out pixels in circle segment

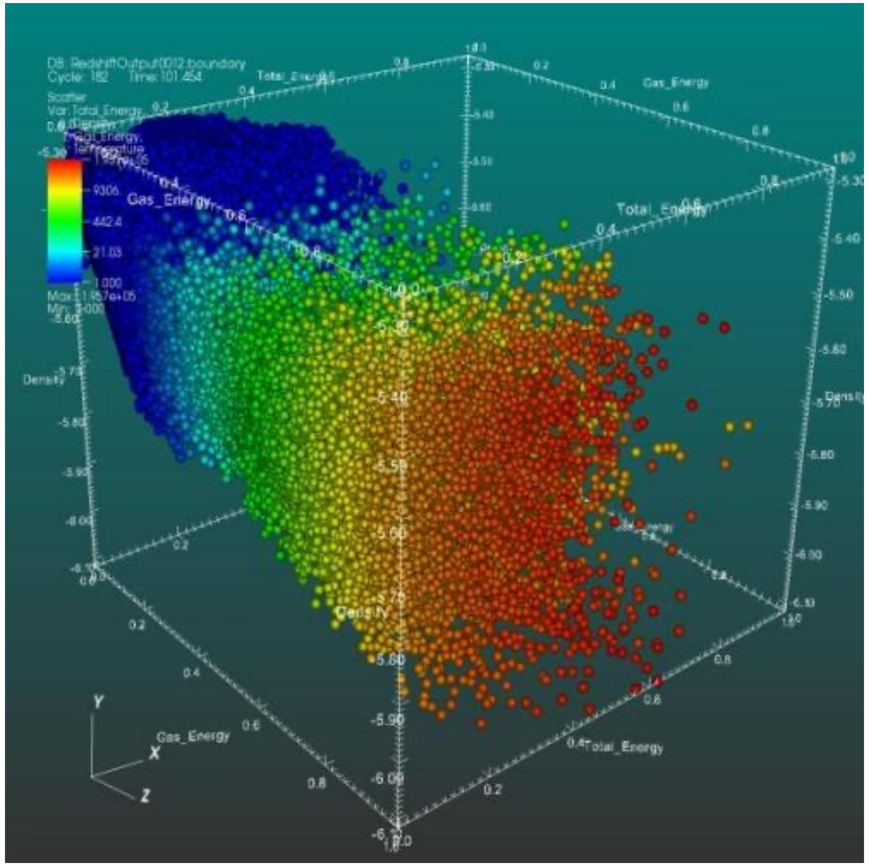
Geometric Projection Visualization Techniques

- 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

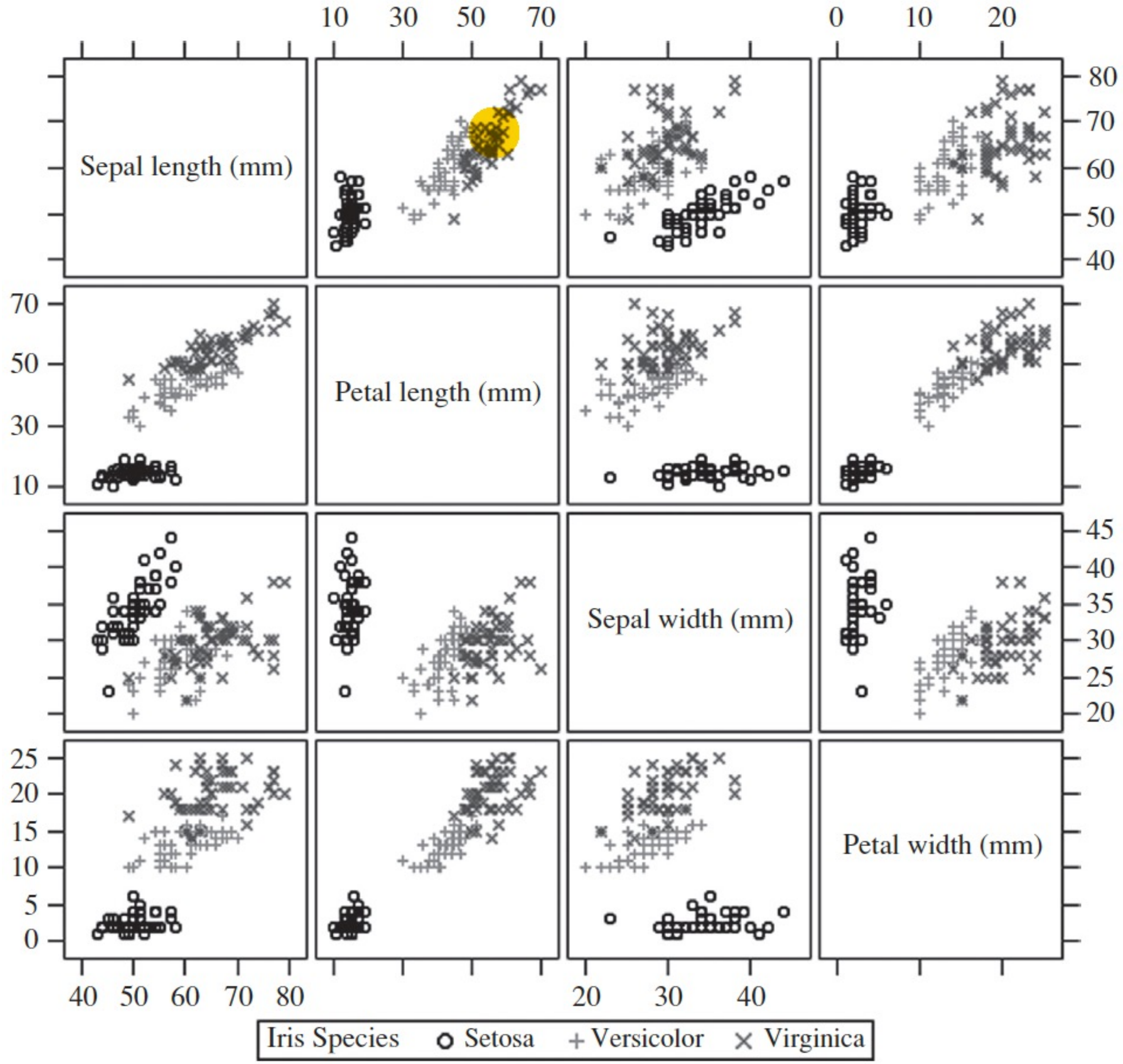
Ribbons with Twists Based on Vorticity





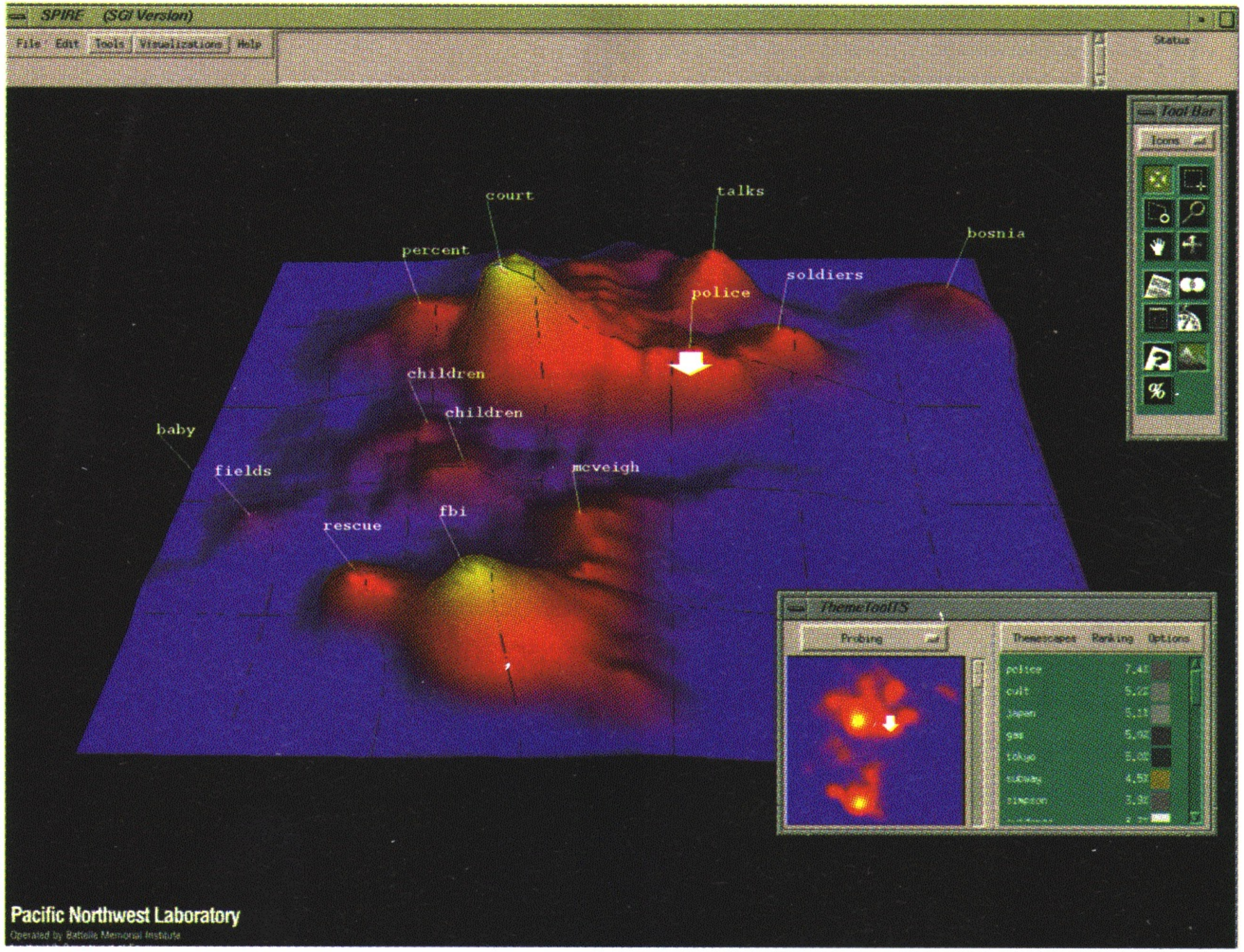
From Wiki: Scatter plot: A 3D scatter plot to visualize multivariate data

Scatterplot Matrices



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

Landscapes



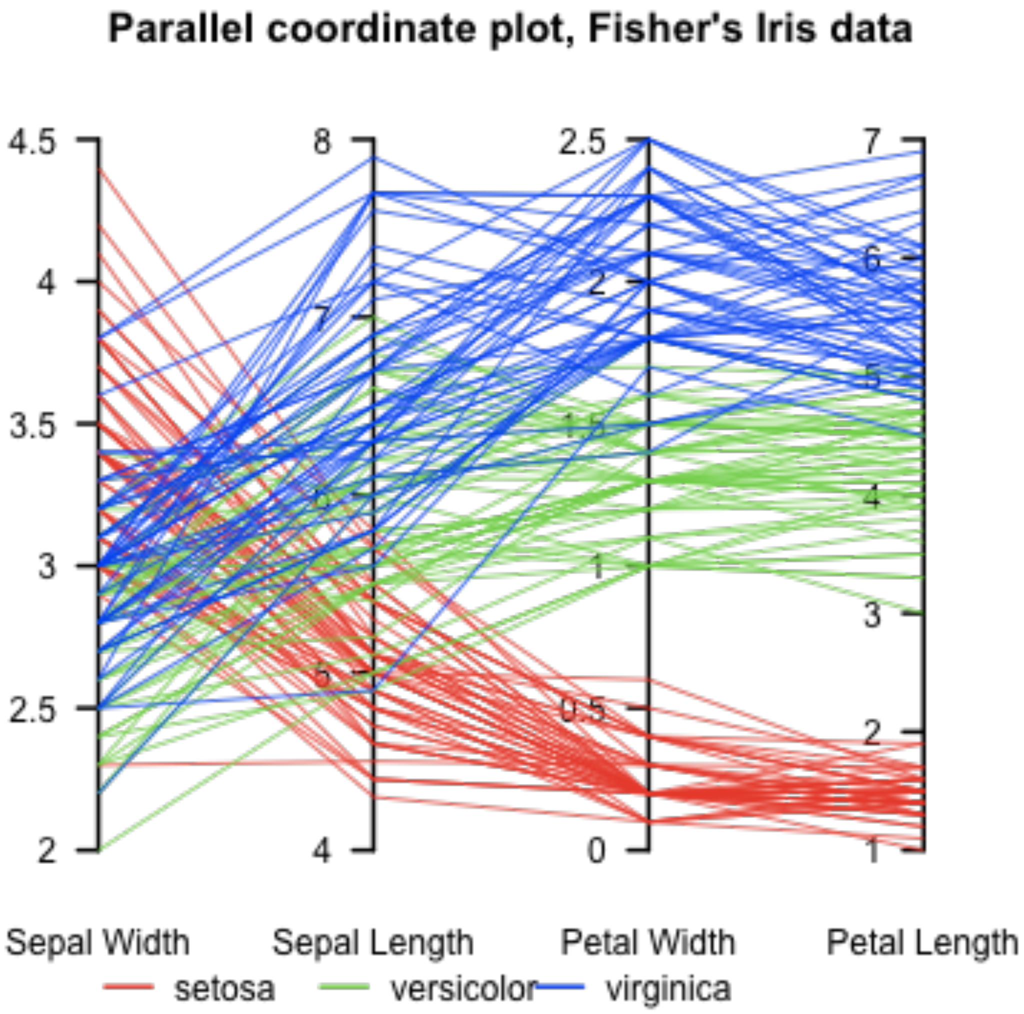
Used by permission of B. Wright, Visible Decisions Inc.

news articles visualized as a landscape

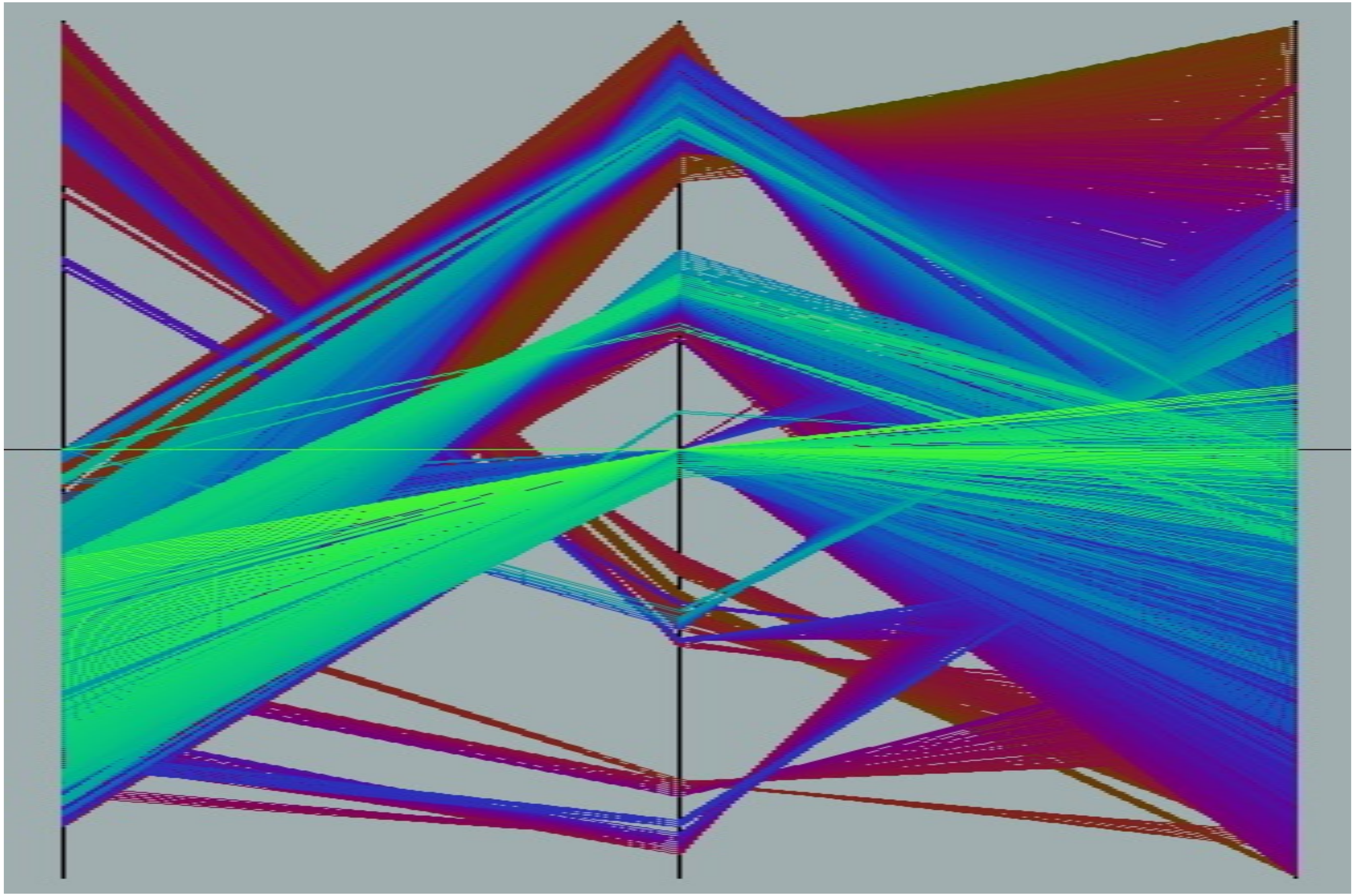
- Visualization of the data as perspective landscape
- The data needs to be transformed into a (possibly artificial) 2D spatial representation which preserves the characteristics of the data

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

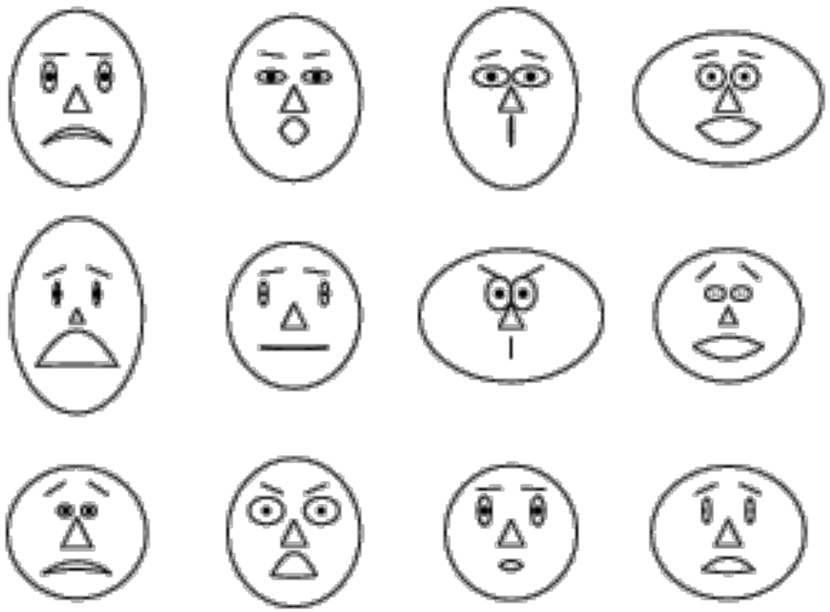


Icon-Based Visualization Techniques

- 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

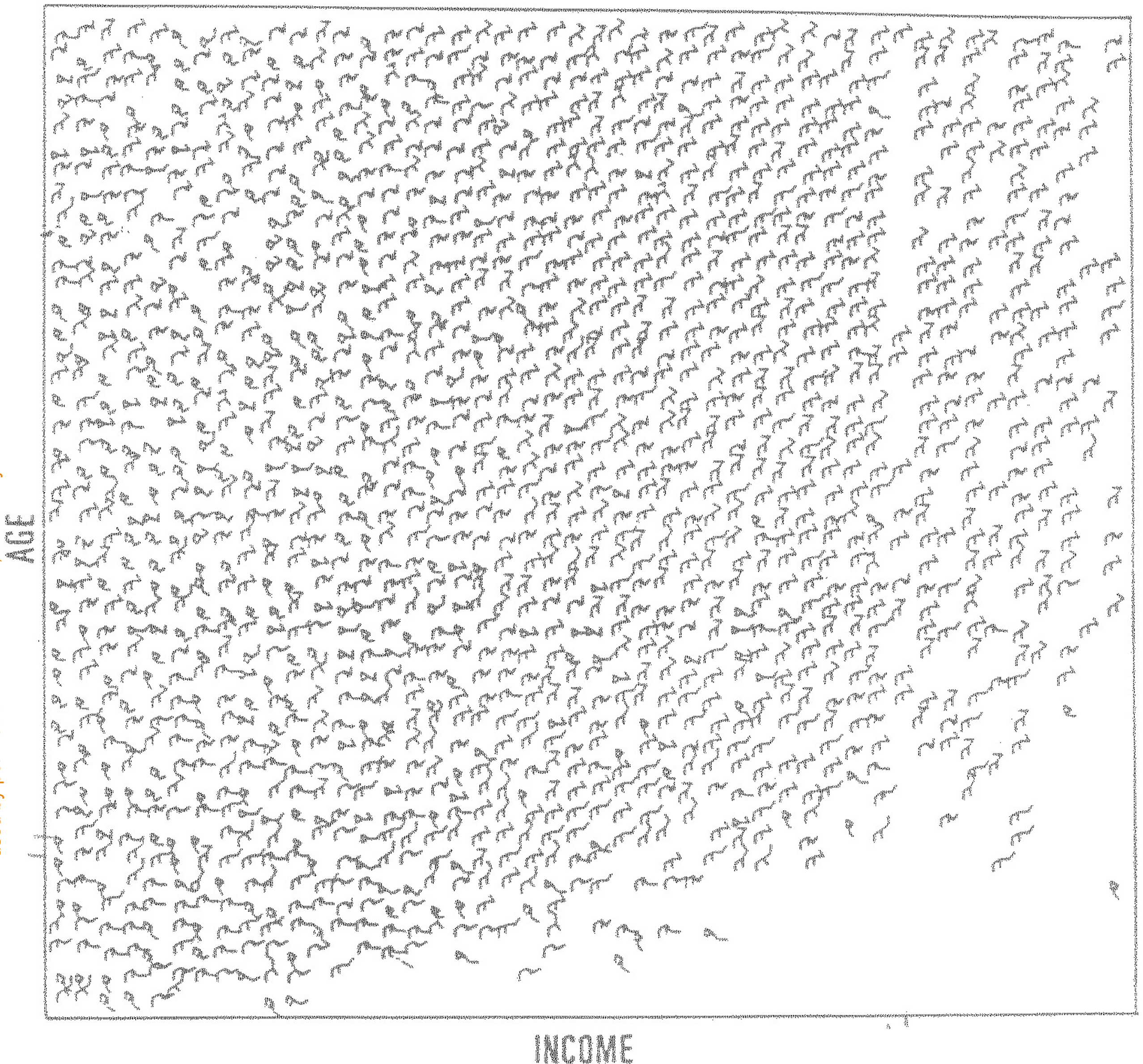
Chernoff Faces

- 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]()

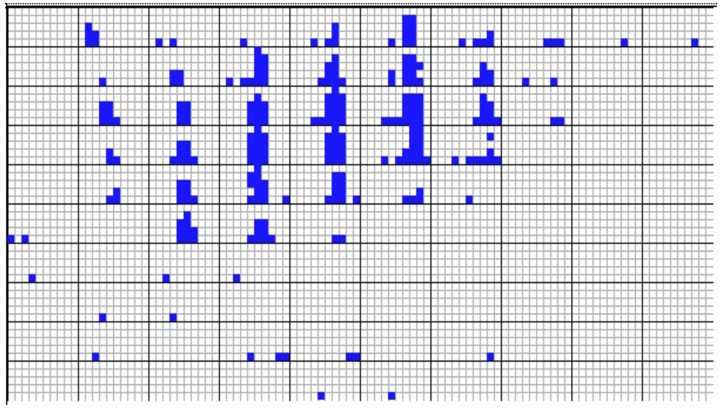
Stick Figure

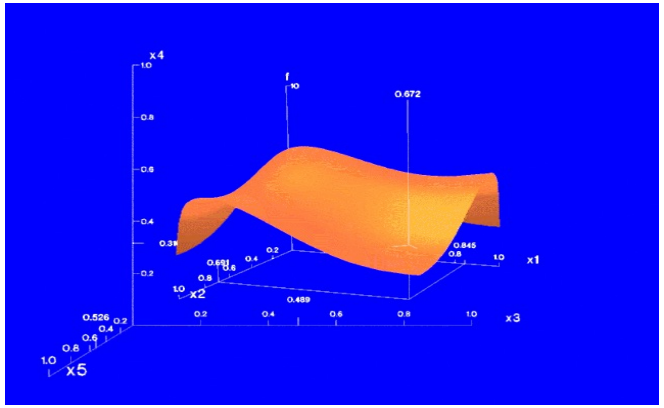


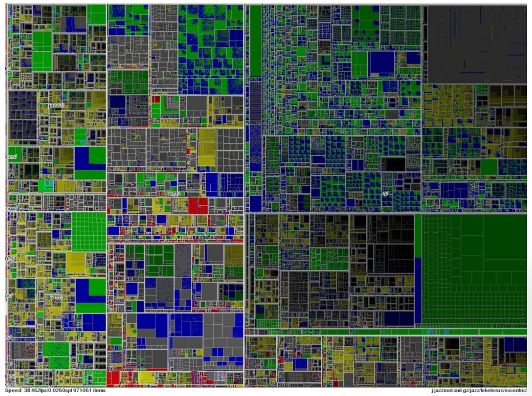
- A census data figure showing age, income, gender, education, etc.
- A 5-piece stick figure (1 body and 4 limbs w. different angle/length)

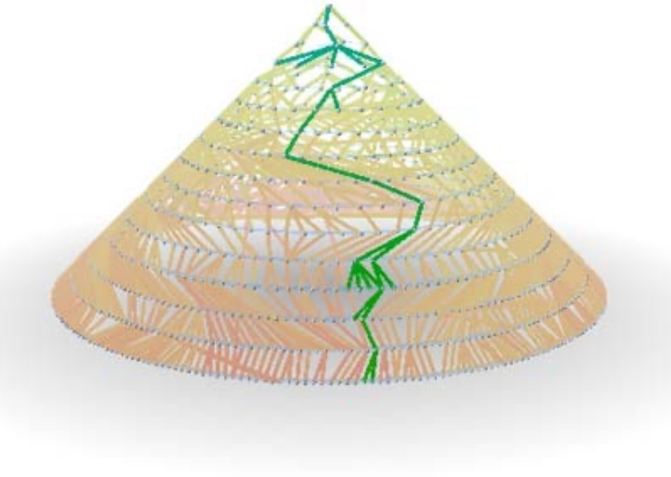
Hierarchical Visualization Techniques

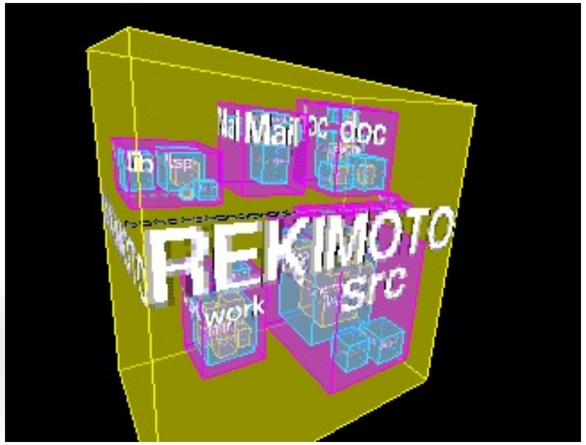
- Visualization of the data using a hierarchical partitioning into subspaces
- Methods
  - Dimensional Stacking
  - Worlds-within-Worlds
  - Tree-Map
  - Cone Trees
  - InfoCube





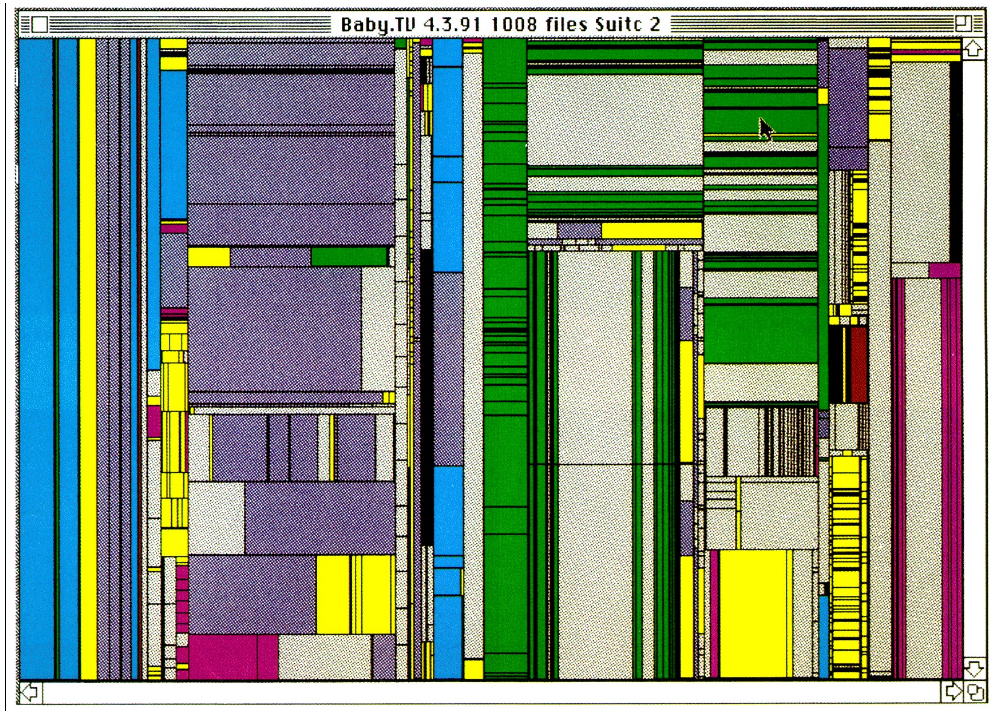




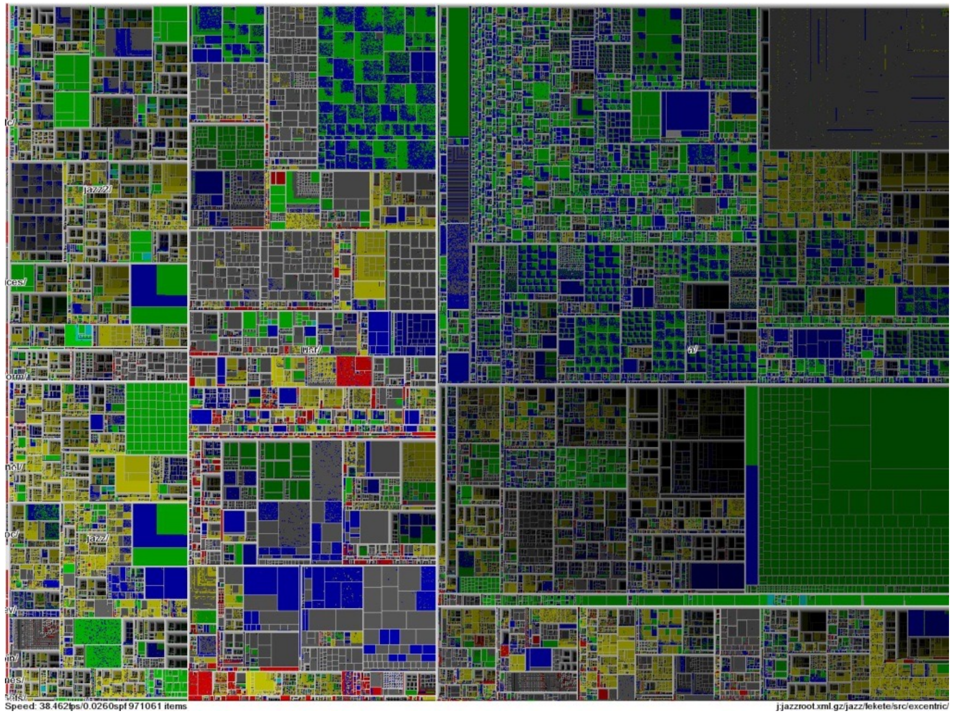


Tree-Map

- 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)

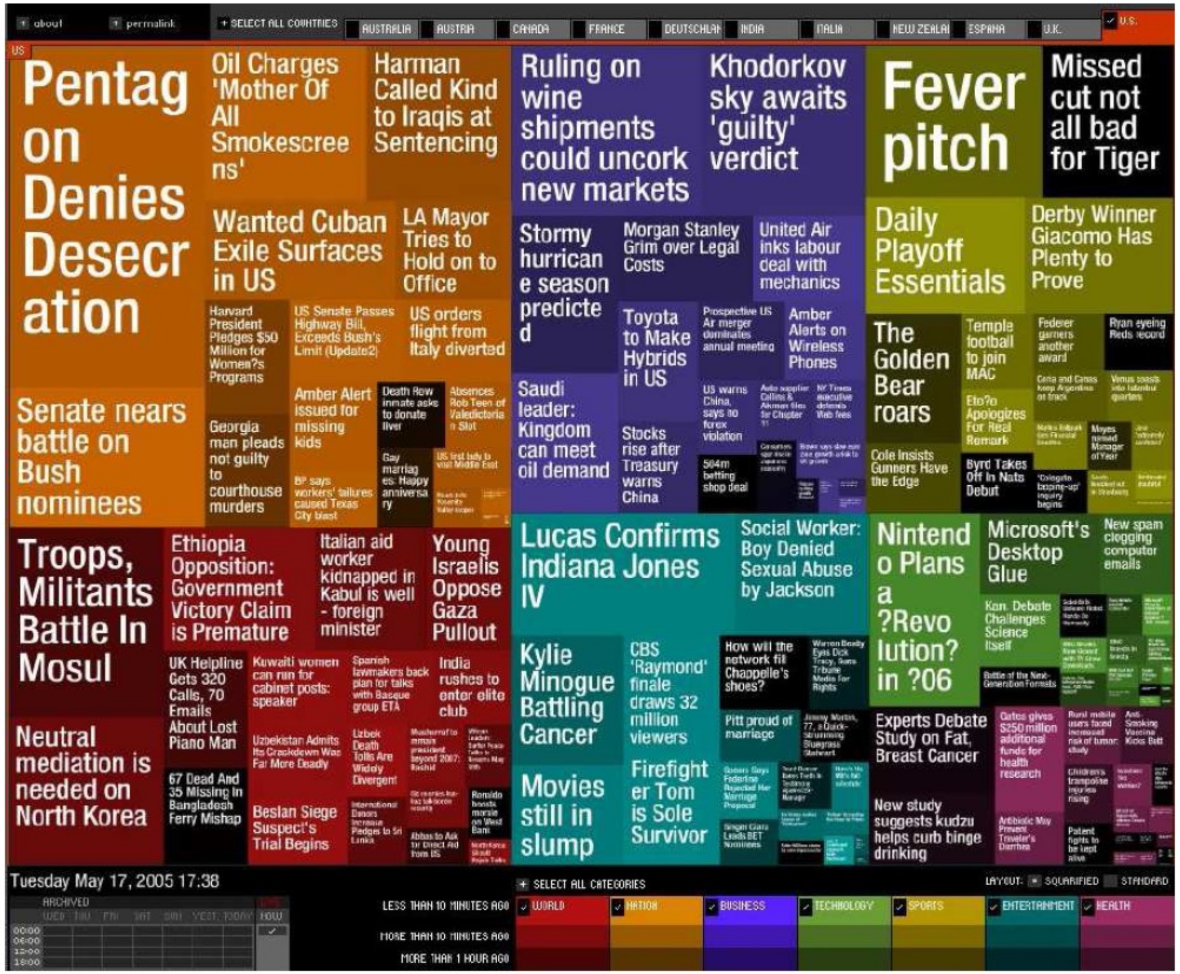


Schneiderman@UMD: Tree-Map of a File System



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

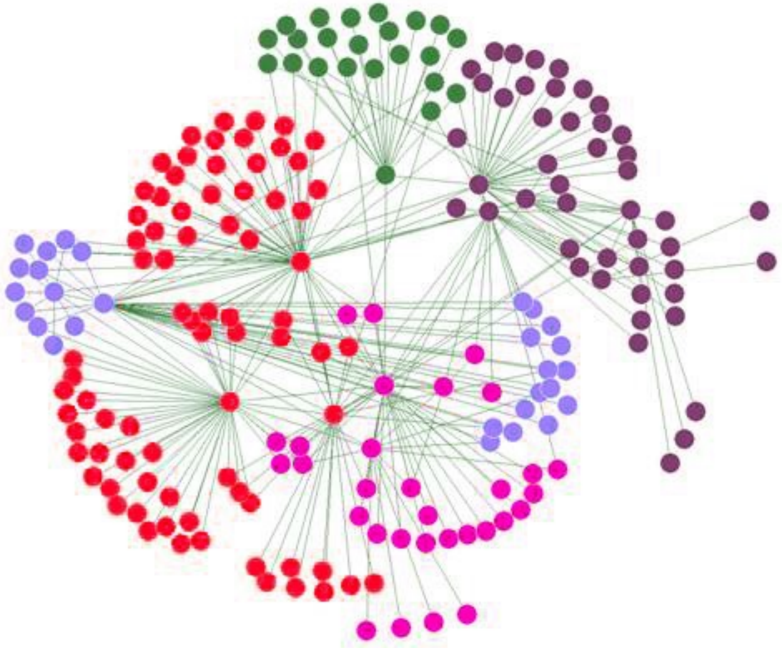
Newsmap: Tree-Maps for News



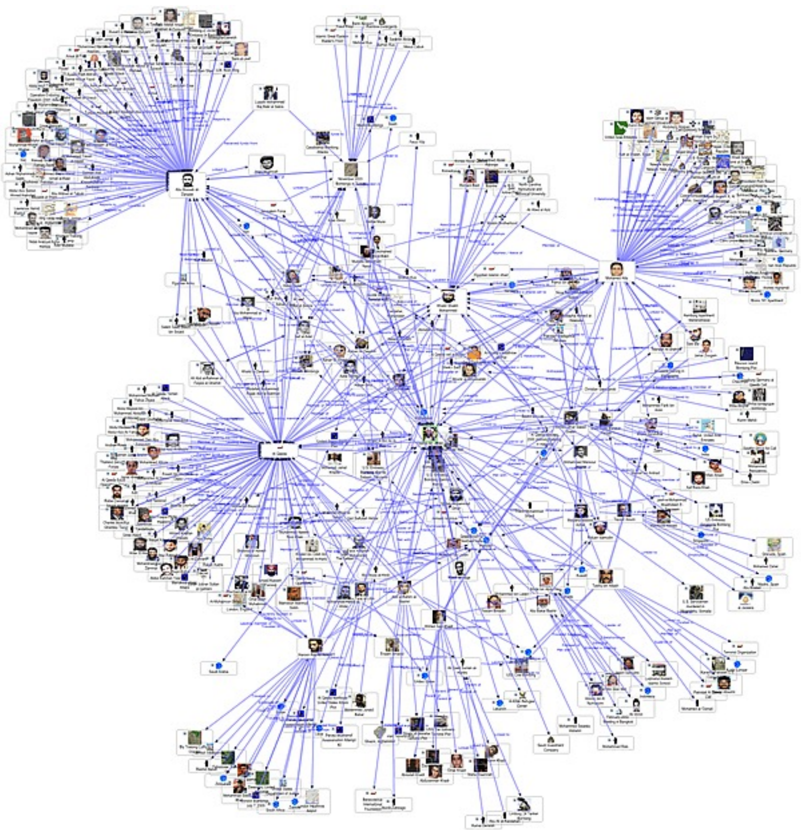
Google News Stories in 2005

Visualizing Complex Data and Relations: Social Networks

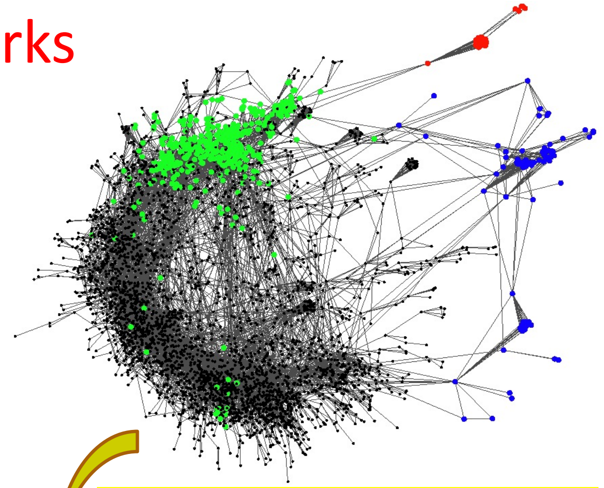
- Visualizing non-numerical data: social and information networks



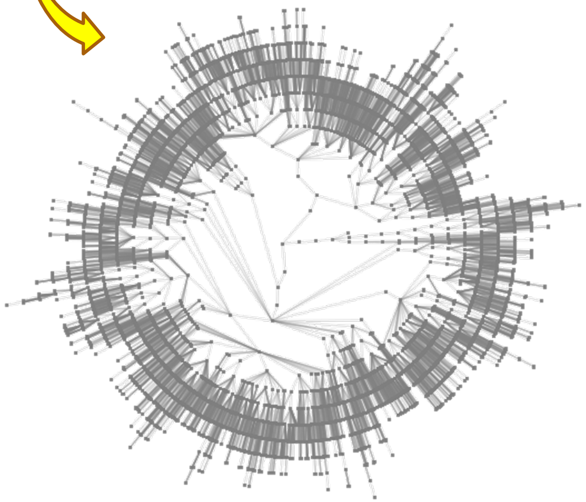
A typical network structure



A social network



organizing
information networks



Text Data: Tag Clouds

Chapter 2. Getting to Know Your Data

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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, ∞) , 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

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

- 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

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

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

Proximity Measure for Binary Attributes

- A contingency table for binary data

Object j (columns), Object i (rows)

	1	0	sum
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: $d(i, j) = \frac{r+s}{q+r+s}$

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

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

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

Jack (rows) vs. Mary (columns):

	1	0	$\sum_{row}$
1	2	0	2
0	1	3	4
$\sum_{col}$	3	3	6

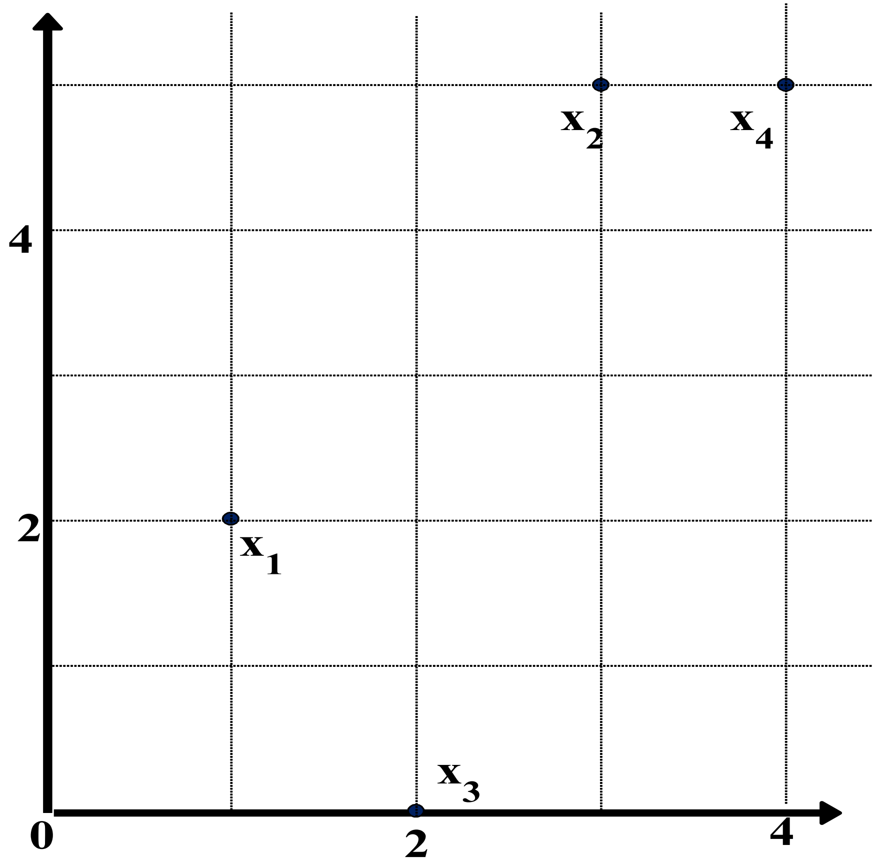
Jack (rows) vs. Jim (columns):

	1	0	$\sum_{row}$
1	1	1	2
0	1	3	4
$\sum_{col}$	2	4	6

Jim (rows) vs. Mary (columns):

	1	0	$\sum_{row}$
1	1	1	2
0	2	2	4
$\sum_{col}$	3	3	6

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

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

where $i = (x_{i1}, x_{i2}, \ldots, x_{il})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jl})$ 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 ≠ j, and d(i, i) = 0 (Positivity)
  - 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
- 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

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

- p = 2: (L_2 norm) Euclidean distance

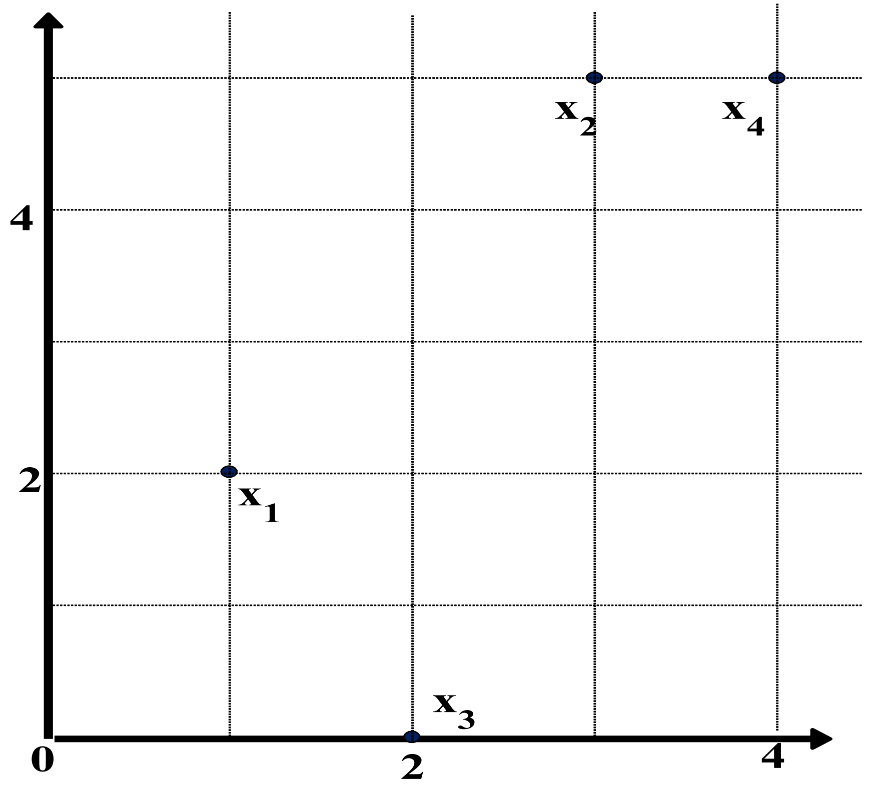
$$d(i,j) = \sqrt{|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \cdots + |x_{il} - x_{jl}|^2}$$

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

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

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

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

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

where

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

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

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: $r_{if} \in \{1, ..., M_f\}$
  - 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(freshman, senior) = 1, d(junior, 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

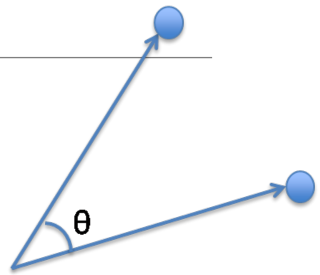
- Other vector objects: Gene features in micro-arrays
- Applications: Information retrieval, biologic taxonomy, gene feature mapping, etc.
- Cosine measure: If d_1 and d_2 are two vectors (e.g., term-frequency vectors), then

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

where • 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) d_2 = (3, 0, 2, 0, 1, 1, 0, 1, 0, 1)

  - First, calculate vector dot product

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

  - Then, calculate $||d_1||$ and $||d_2||$

$$\| d_1 \| = \sqrt{5\times5+0\times0+3\times3+0\times0+2\times2+0\times0+0\times0+2\times2+0\times0+0\times0} = 6.481$$

$$\| d_2 \| = \sqrt{3\times3+0\times0+2\times2+0\times0+1\times1+1\times1+0\times0+1\times1+0\times0+1\times1} = 4.12$$

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

KL Divergence: Comparing Two Probability Distributions

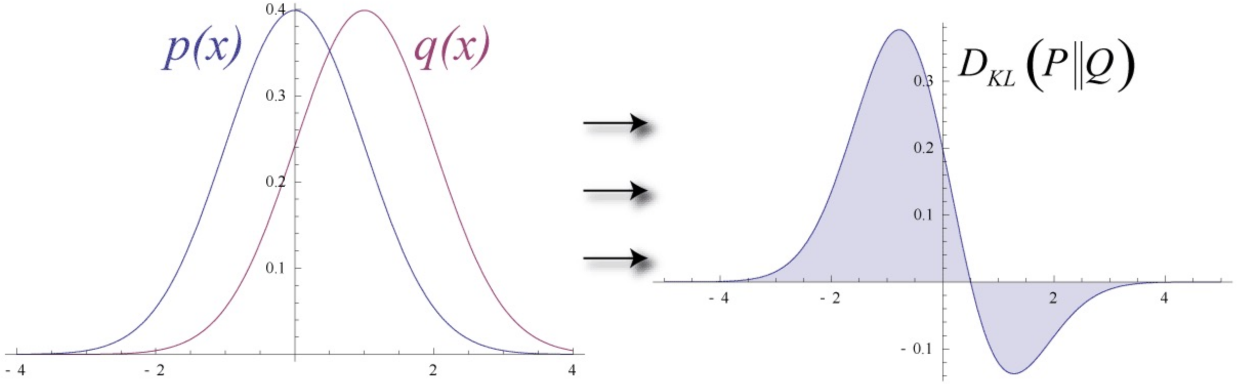
- *The Kullback-Leibler (KL) divergence:* Measure the difference between two probability distributions over the same variable *x*
  - From information theory, closely related to *relative entropy*, *information divergence*, and *information for discrimination*
- $D_{KL}(p(x) \,||\, q(x))$: divergence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

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

Discrete form

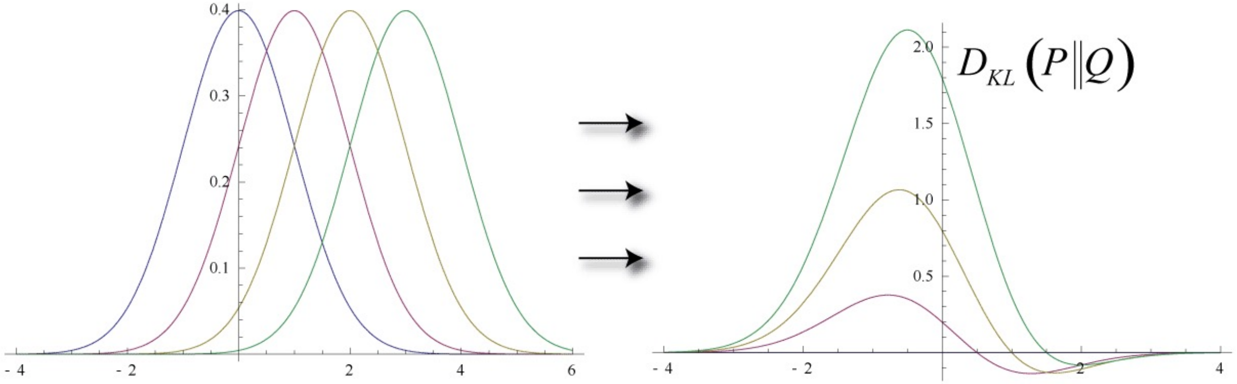
$$D_{KL}(p(x)||q(x)) = \int_{-\infty}^{\infty} p(x) \ln \frac{p(x)}{q(x)} dx$$

Continuous form



Original Gaussian PDF's

KL Area to be Integrated



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

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*)

$$\begin{aligned} D_{KL}(p(x)\|q(x)) &= E_{p(x)}\left[\log \frac{p(x)}{q(x)}\right] \\ &= E_{p(x)}\left[\log \frac{1}{q(x)}\right] - E_{p(x)}\left[\log \frac{1}{p(x)}\right] \end{aligned}$$

- 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*.

More on KL Divergence

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

- 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.

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?
  - $lim_{p \to 0}\, p \log p = 0$
  - when p != 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

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

- 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

Chapter 2. Getting to Know Your Data

- Data Objects and Attribute Types
- Basic Statistical Descriptions of Data
- Data Visualization
- Measuring Data Similarity and Correlation
- 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 and correlation
- Above steps are the beginning of data preprocessing
- Many methods have been developed but still an active area of research

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