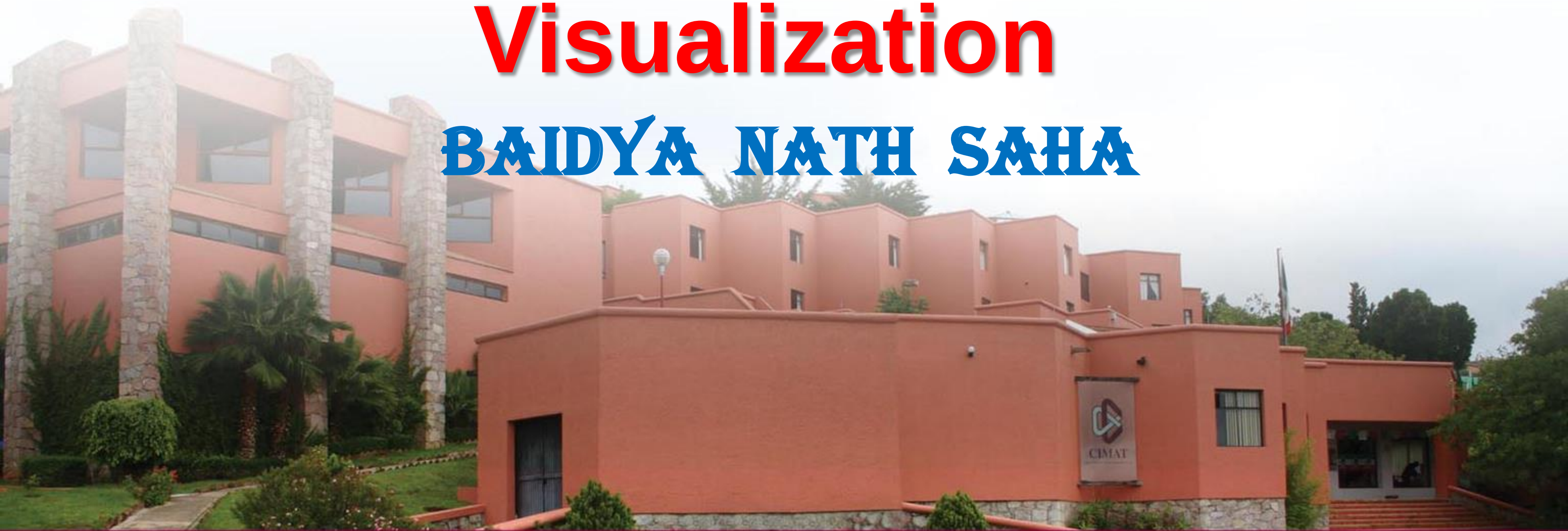
CIMAT Centro de Investigación en Matemáticas, A.C.

CONACYT

Computational Aspects of High Dimensional Large Scale Data Visualization

BAIDYA NATH SAHA



Unidad Monterrey

Outline

- Introduction
- History
- Modern Visualization Techniques and Computational Problems
  - Parallel Co-ordinates, heat map, SOM etc.
  - Space, data ordering, processing
- Conclusion

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What is visualization?

- “any technique for creating images, diagrams, or animations to communicate a message” (Wikipedia)
- “a systematic, rule-based, external, permanent, and graphic representation that depicts information in a way that is conducive to acquiring insights, developing an elaborate understanding, or communicating experiences” (Lengler & Eppler)

Human Visual Perception

- Humans receive input from all five of their senses (sight, touch, hearing, smell, taste), however, Human visual cortex dominates our perception
- Accelerates the identification of hidden patterns in data
  "A picture is worth a thousand words" – Chinese Proverb
- 50% of the human brain is dedicated to visual functions, and images are processed faster than text.
- The brain processes pictures all at once, but processes text in a linear fashion, meaning it takes much longer to obtain information from text.
- Furthermore, it is estimated that 65% of the population are visual learners.

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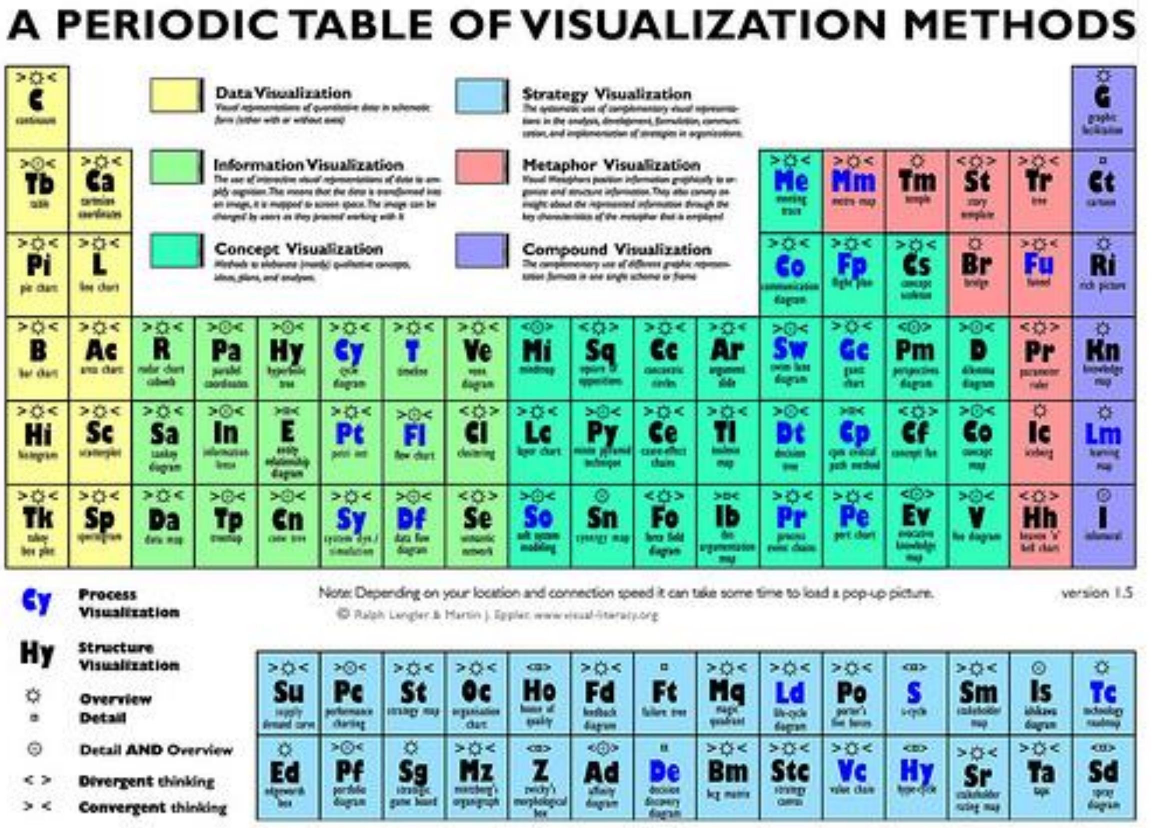
Examples of Information Visualizations

- ❑Pie chart
- ❑Timeline
- ❑Gantt Chart
- ❑Metaphoric, e.g. iceberg
- ❑Cartoon
- ❑Org chart



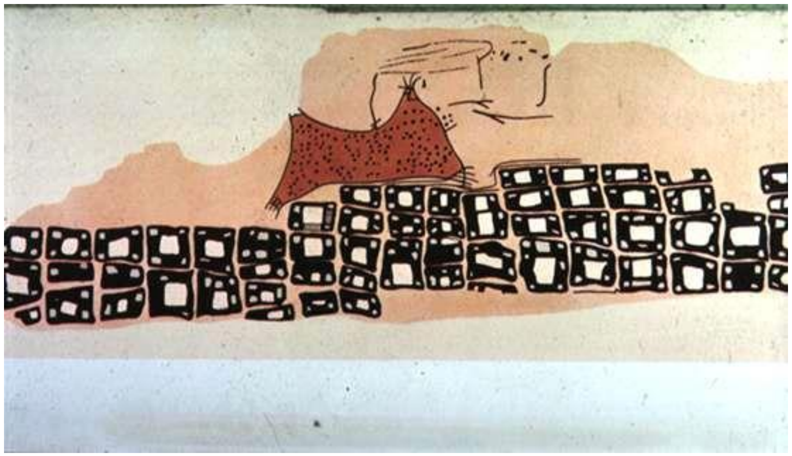
http://www.visual-literacy.org/periodic_table/periodic_table.html

A little history…

- Development of motion - about 100 years
- Mobile sculpture – 20 years
- Video art – 20 years
- Animated maps – begin in the 1930’s, but were not developed until 1959
- Computer animated maps: 1990’s

Maps from the past

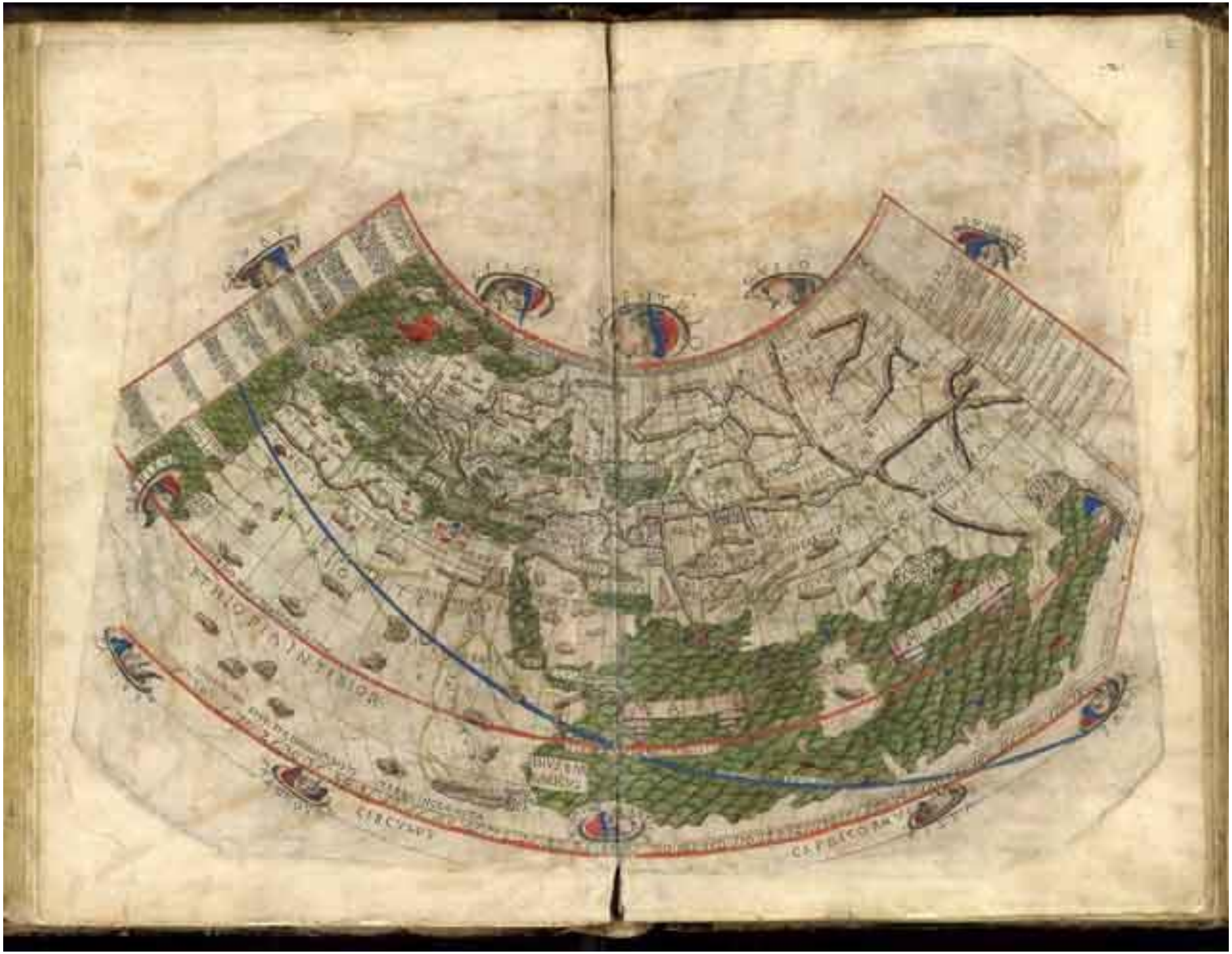
The oldest known map: Konya town,6200 BC



Anaximader's Map of the World

Anaximader's Map of the World

The Ptolemy world map, written circa 150 BCE.



Early Representation

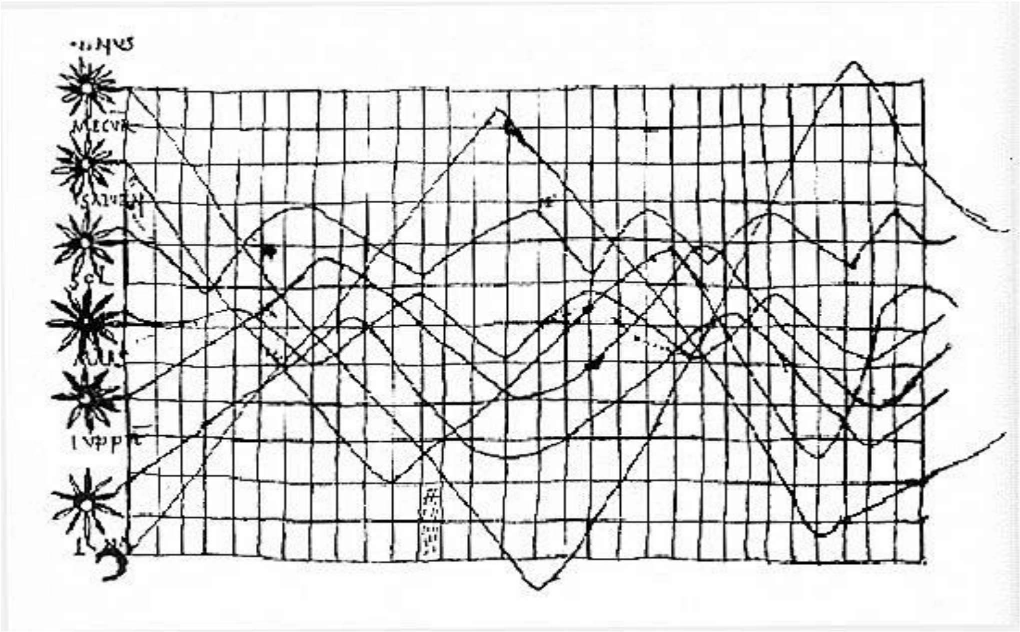
The Cave of Lascaux, France

~15,000 years old

- Tells a story

- Visualization existed before the invention of computers
- Representation of information allowing us to perceive such information visually

Planetary Orbits



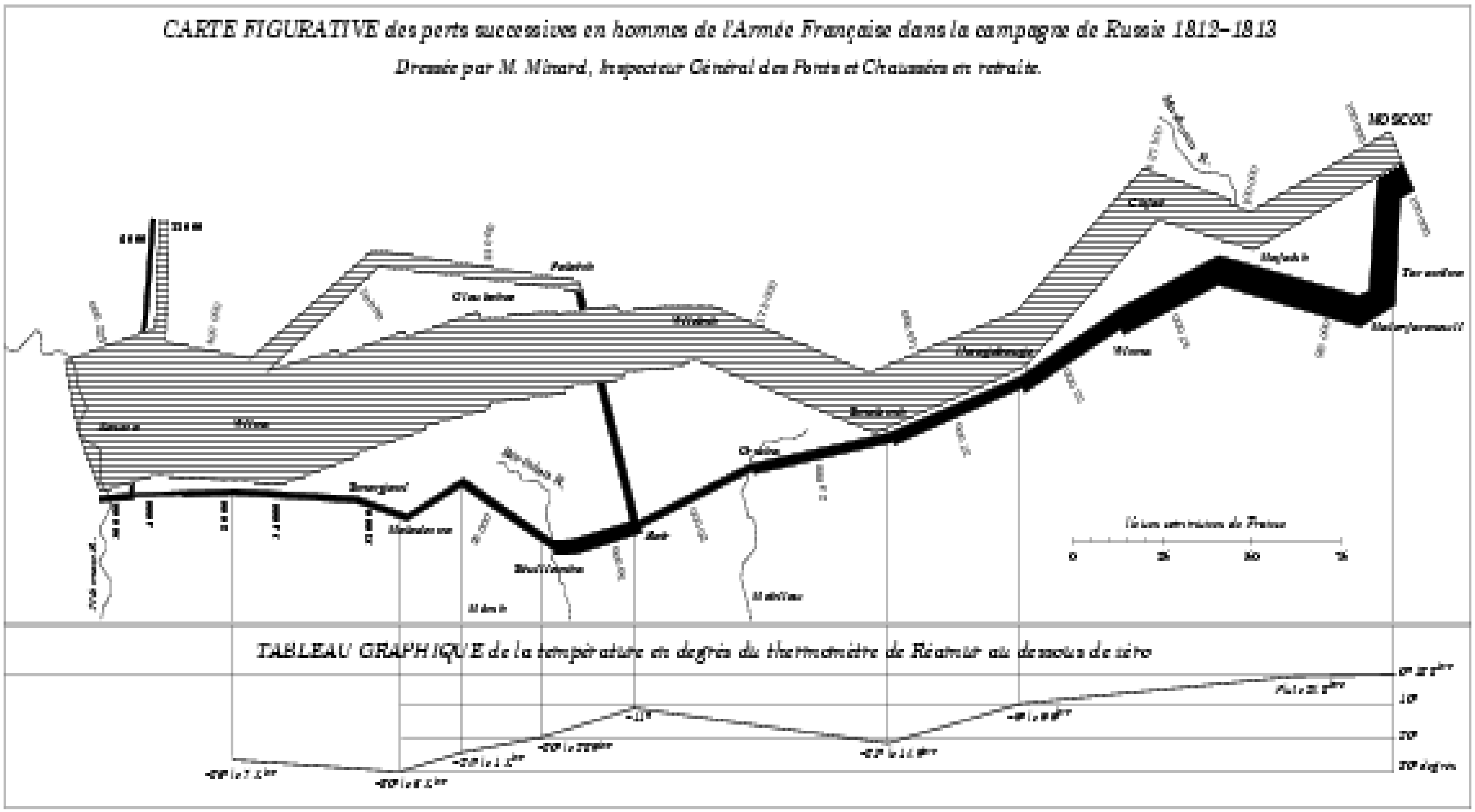
- Tenth century
- Inclinations of the planetary orbits as a function of time.
- Oldest known attempt to show changing values graphically.

Message Communication - Example

- Napolean's 1812 campaign on Russia

- Input data
  - Size of army
    - at the start of the campaign = 442,000
    - at the end of the campaign = 10,000
  - Location of the army (2 dimensions)
  - Direction of the army's movement
  - Temperature and
  - Time

Minard's Drawing



Created in 1861 by French engineer Charles Joseph Minard

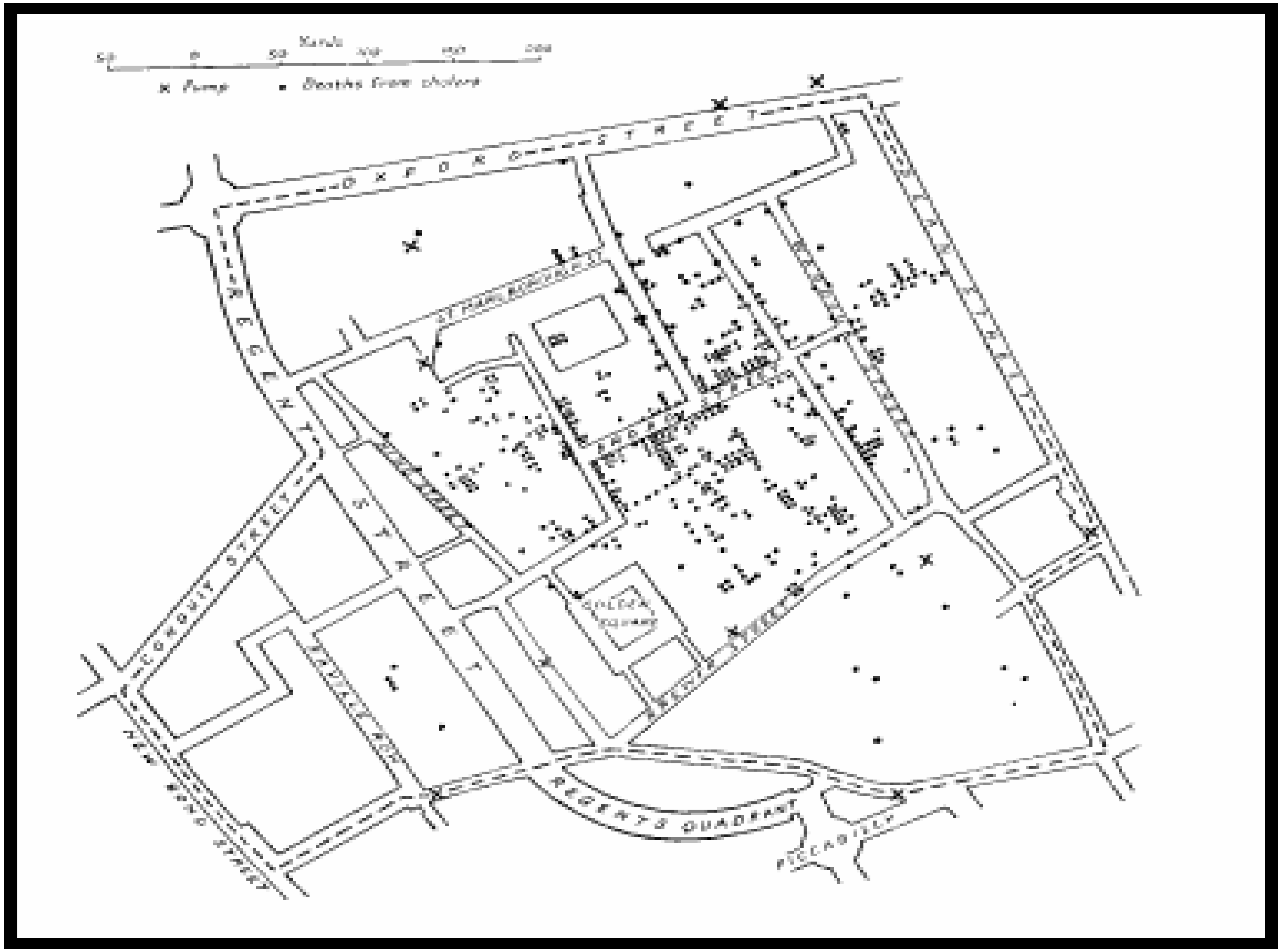
Minard's Drawing (2)

- Considered the best graphic ever produced
  - Inspiration for modern researchers
- Plots all the data corresponding to all the six input variables
- Clearly shows the message underlying the input data
  - Gradual reduction in the size of the army
  - Linked to the gradual fall in temperatures
- Input data is complex
- Yet, most important information abstracted out and presented in a simple graphic

Problem Solving - Example

- London cholera epidemic of 1854
- At that time, two hypotheses of causes of cholera:
  - Cholera is related to miasmas concentrated in the swampy areas of the city
  - Cholera is related to ingestion of contaminated water
- Input Data
  - Locations of deaths due to cholera
  - Locations of water pumps

Dr Snow's Cholera Map



Dots locate deaths due to cholera

Crosses Locate water pumps

Dr Snow's Cholera Map (2)

- Plotting the input data on the map helped Dr Snow
  - to detect the epicentre of the epidemic
  - Close to a pump on Broad Street
- Considered a classic case of visualization helping reasoning with data

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Key points in Visualization

- Visualization can enhance understanding
- Different visualization methods are appropriate to different types of data
- Free online tools such as ManyEyes, Swivel & Google Docs:
  - Make it (fairly) easy to create a visualization
  - Encourage visual literacy
  - Build dialogue and community

Information Visualization (IV)

- Visual presentation of abstractions or relationships underlying input data

- IV has two goals
  - Communication
    - to communicate a rich **message**
  - Problem solving/ reasoning/ analysis
    - to display large amount of information to facilitate reasoning to uncover **new** facts or relationships

- Limited screen sizes pose a serious challenge for using IV on very large data sets

- Therefore the main task is to pack large information into a simple graphic
  - Highlighting all the required (important) information

- **Creative art?**

Gospel like guidelines for IV

As you create graphics keep the following in mind.

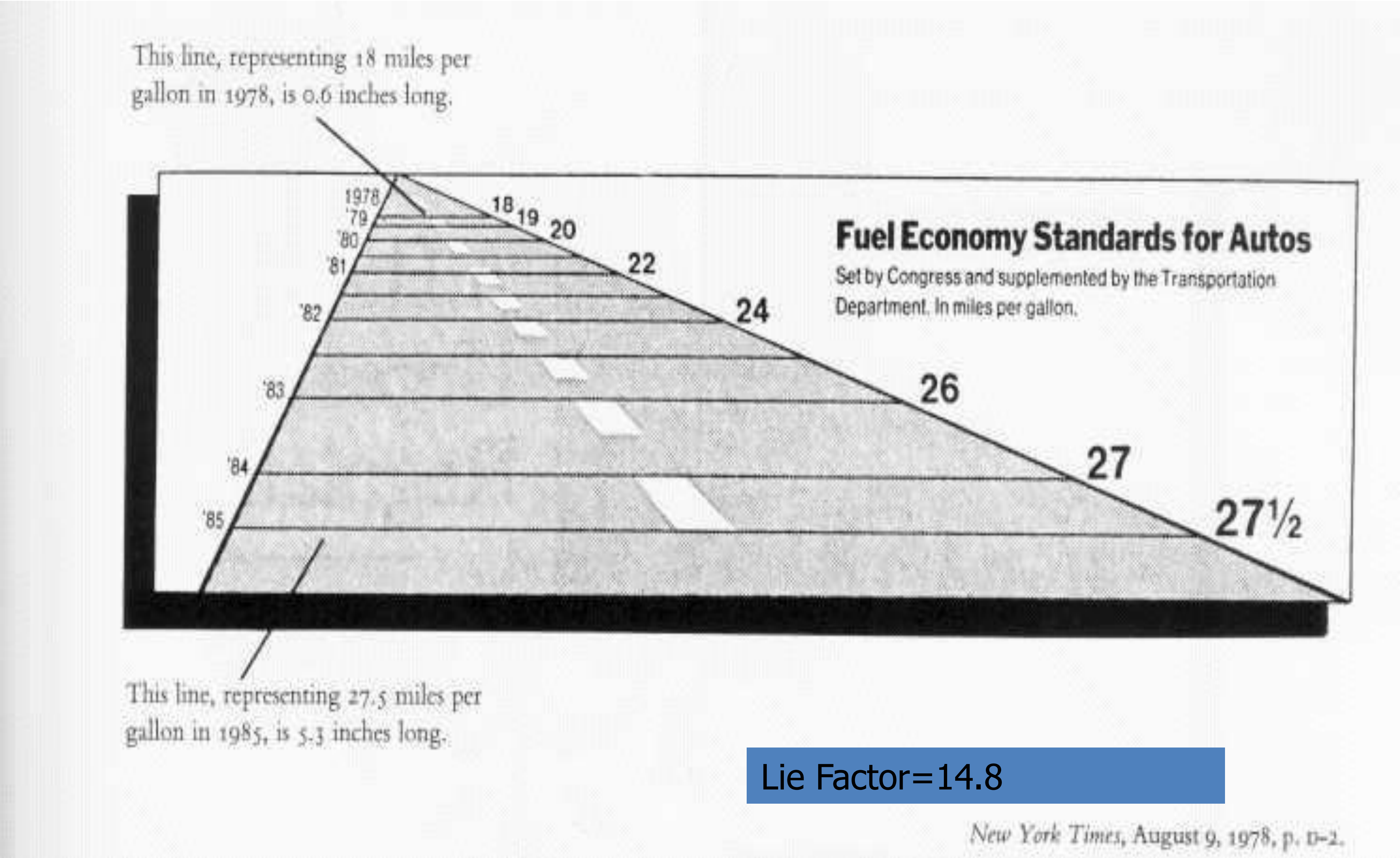
- Avoid distortion of the true story, Don't tell lie.
- Induce the viewer to think about the substance, not the graph.

Richard Hamming: "The purpose of computing is insight, not numbers."

- Reveal the data at several layers of detail.
- Encourage the eye to compare different pieces.
- Support the statistical and verbal descriptions of the data.
- Maximize the data-ink ratio (Edward Tufte, www.edwardtufte.com)

Data-ink ratio= data-ink/total ink used on the graphic

Tufte's Principles of Graphical Excellence



(E.R. Tufte, "The Visual Display of Quantitative Information", 2nd edition)

Lie Factor

$$Lie\ \ Factor = \frac{size\ of\ \ effect\ \ shown\ in\ graphic}{size\ of\ \ effect\ \ in\ data} =$$

$$= \frac{\dfrac{(5.3-0.6)}{0.6}}{\dfrac{(27.5-18.0)}{18}} = \frac{7.833}{0.528} = 14.8$$

Tufte requirement: 0.95<Lie Factor<1.05

(E.R. Tufte, "The Visual Display of Quantitative Information", 2nd edition)

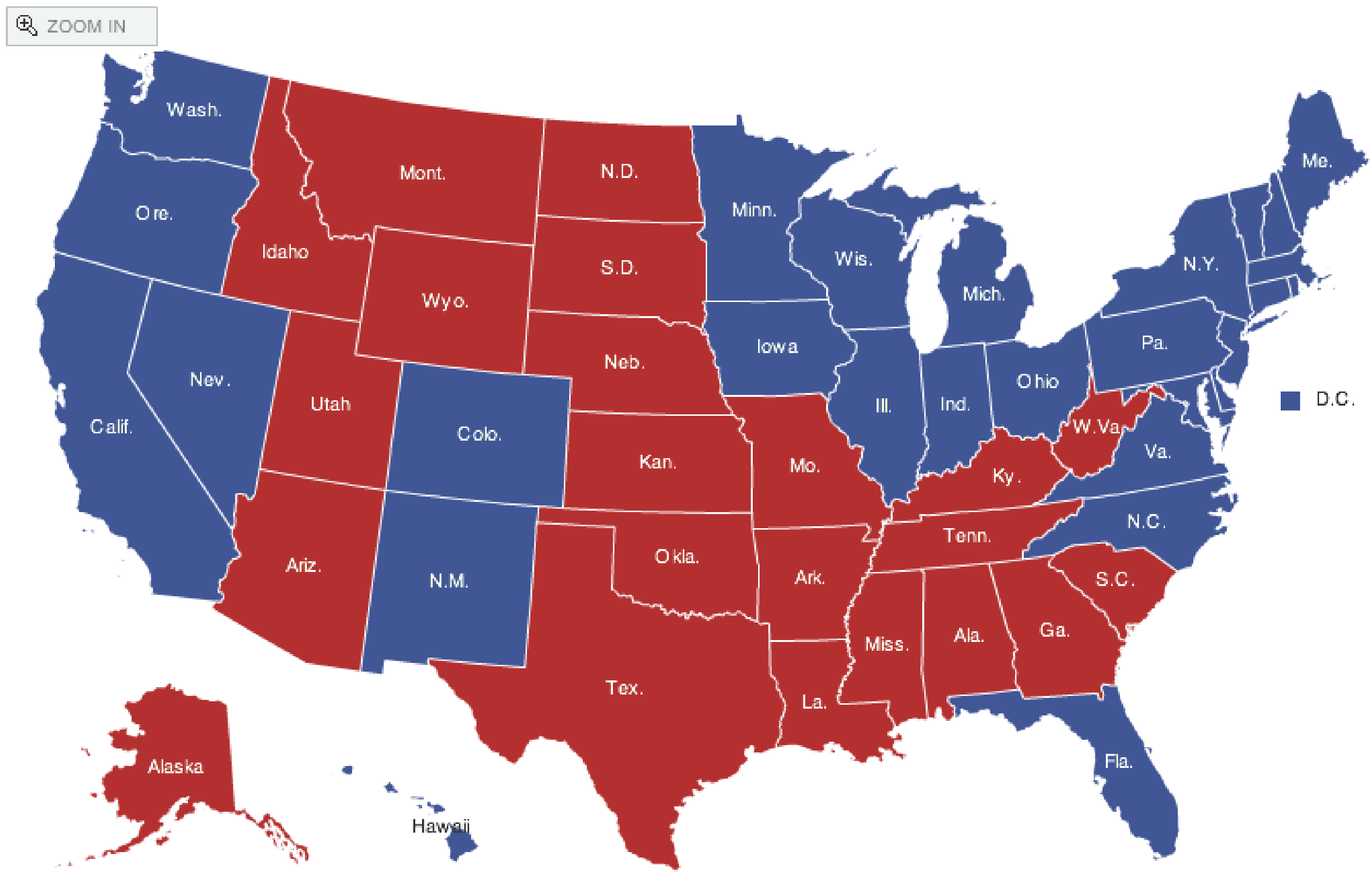
Scientific Visualization

- *Visualization for scientific computing*, shortened to *scientific visualization*, was coined in 1987 and refers to the science or methodology of quickly and effectively displaying scientific data.
  - 1987 NSF report: “Visualization in Scientific Computing”
- Formal name given to the field in computer science that includes user interface, data representation and processing algorithms, visual representations and other sensory presentation such as sound or touch.

- Visual modelling of scientific data using computer graphics
- Examples
  - visualizations of protein docking
  - Molecular structural data is hard to understand without visualization
  - Visualization of brain models

- **Focus** is
  - on modelling (visually) the input data as close to reality as possible
  - Not on presenting abstractions or relationships from the input data

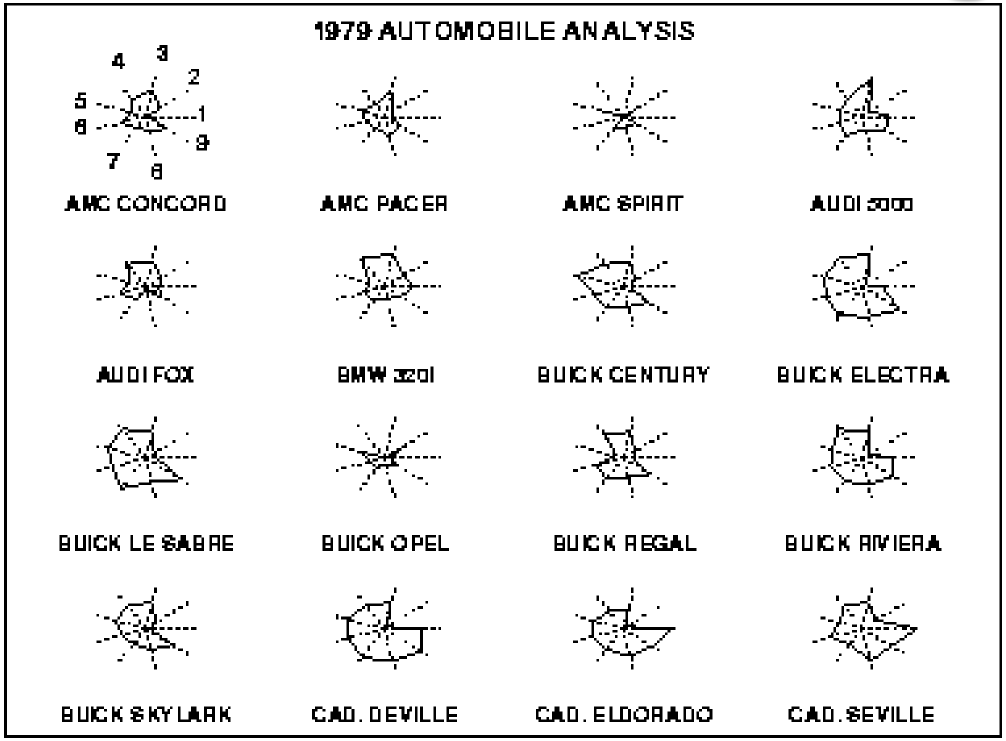
Spatial data: choropleth Maps



- Maps using color shadings to represent numerical values are called chloropleth maps

  http://elections.nytimes.com/2008/results/president/map.html

Using Icons to Encode Information, e.g., Star Plots

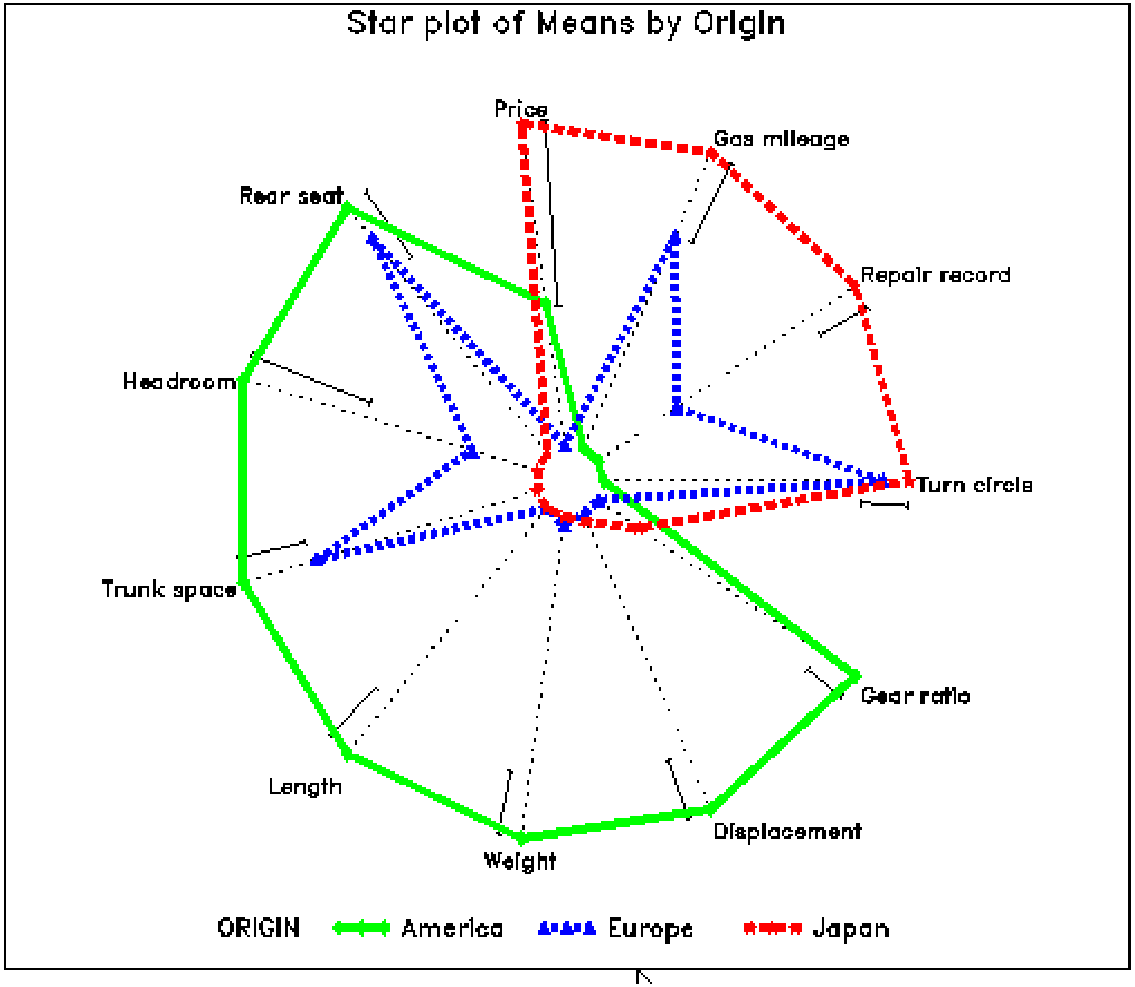


1 Price
2 Mileage (MPG)
3 1978 Repair Record (1 = Worst, 5 = Best)
4 1977 Repair Record (1 = Worst, 5 = Best)
5 Headroom
6 Rear Seat Room
7 Trunk Space
8 Weight
9 Length

- Each star represents a single observation. Star plots are used to examine the relative values for a single data point
- The star plot consists of a sequence of equi-angular spokes, called radii, with each spoke representing one of the variables.

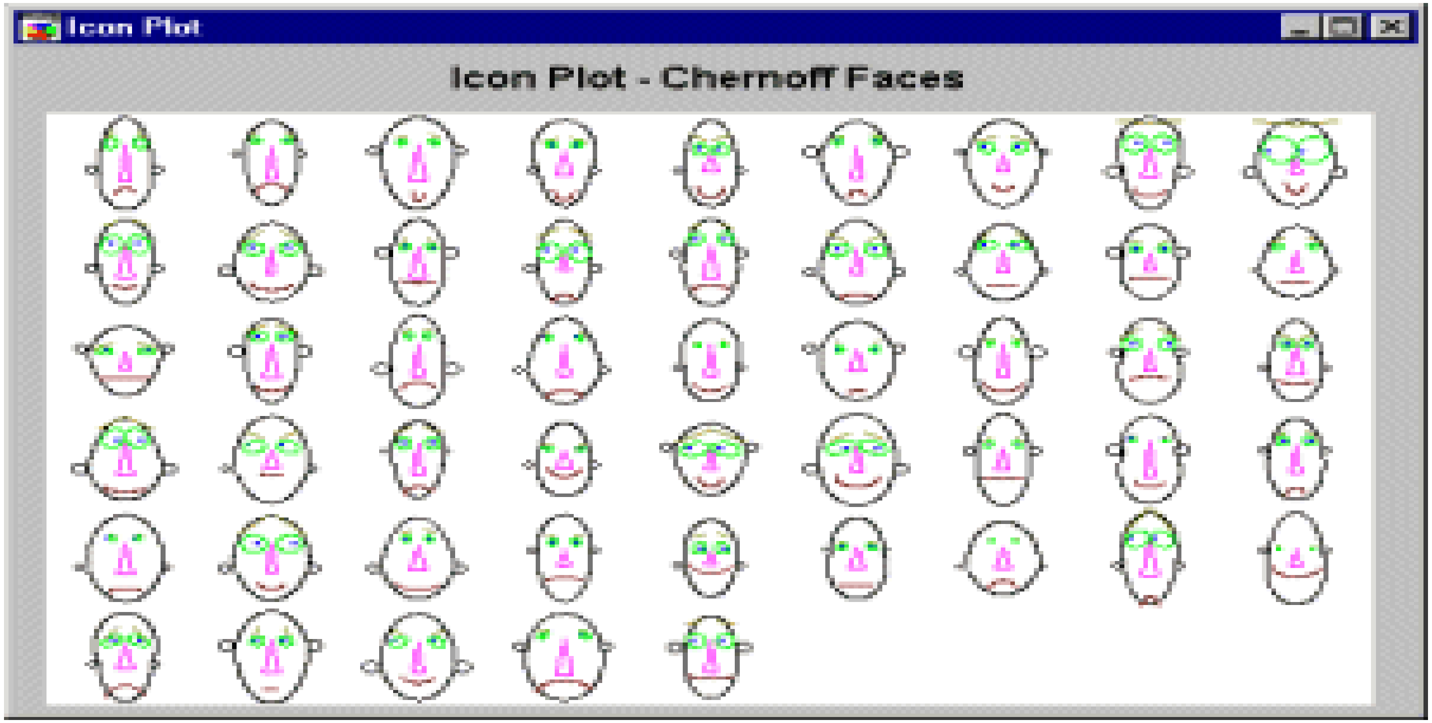
  Useful for small data sets with up to 10 or so variables
- Limitations?
  - Small data sets, small dimensions
  - Ordering of variables may affect perception

Starplots

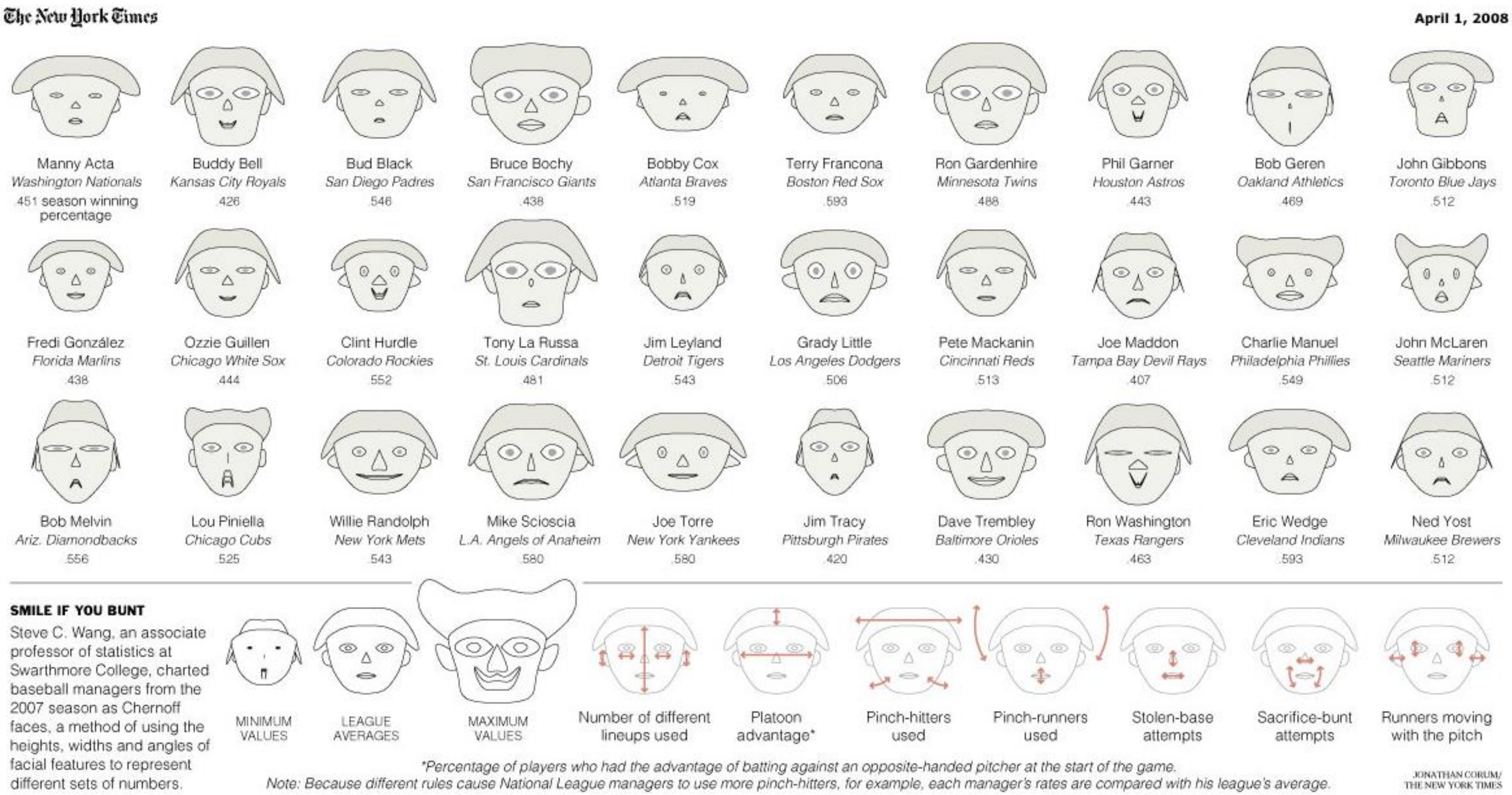

Star plot of Means by Origin
Price
Gas mileage
Repair record
Turn circle
Gear ratio
Displacement
Weight
Length
Trunk space
Headroom
Rear seat
ORIGIN
America
Europe
Japan

Chernoff's Faces

- described by ten facial characteristic parameters: head eccentricity, eye eccentricity, pupil size, eyebrow slant, nose size, mouth shape, eye spacing, eye size, mouth length and degree of mouth opening
- Much derided in statistical circles



Chernoff faces



Chernoff faces

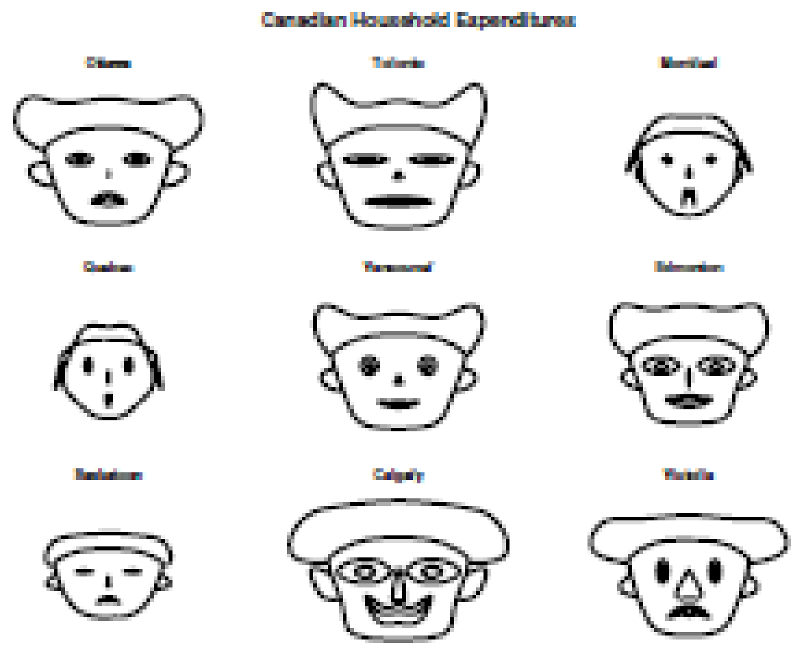


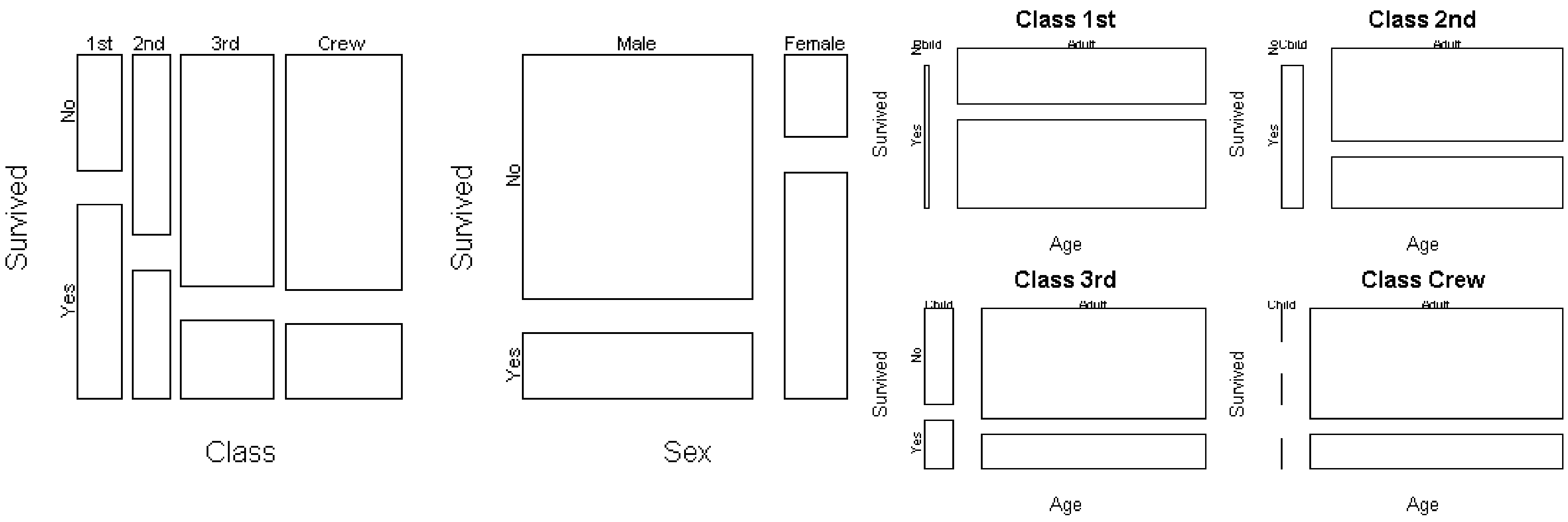
Fig. 9.9 Chernoff faces for household expenditures for nine Canadian cities. Note that food and shelter primarily determine the size of the face. It is great fun to try to match the expression on the face to the character of the city. This shows how exquisitely sensitive we are to facial expressions, underscoring the strength of the method.

Source: Principles and Theory for Data Mining and Machine Learning, Bertrand Clarke et al., Springer, 2012

Mosaic Plots

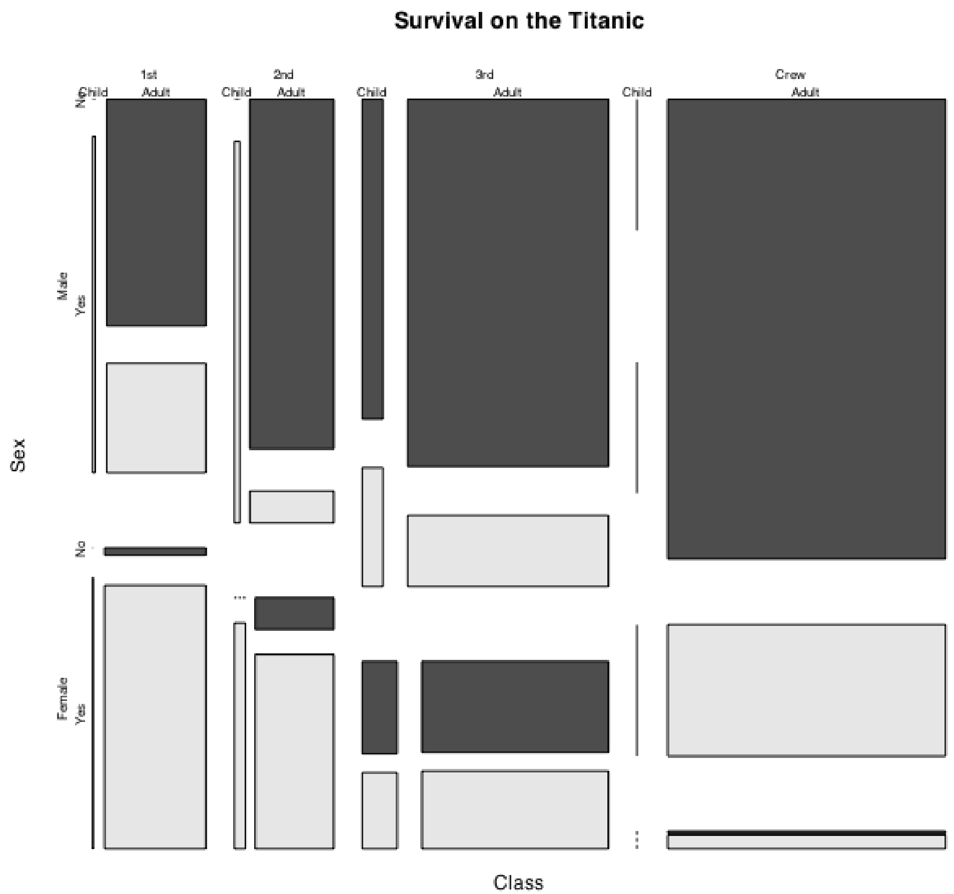
- Very useful for many categorical variables
- sensitive to the order which they are applied

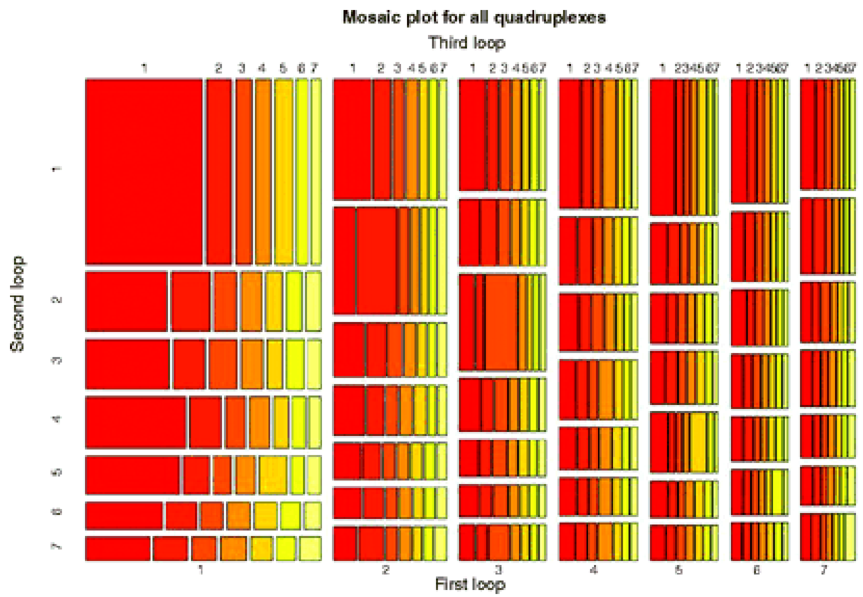
- Titanic Data:



Mosaic plots

Can be effective, but can get out of hand:





Heatmap

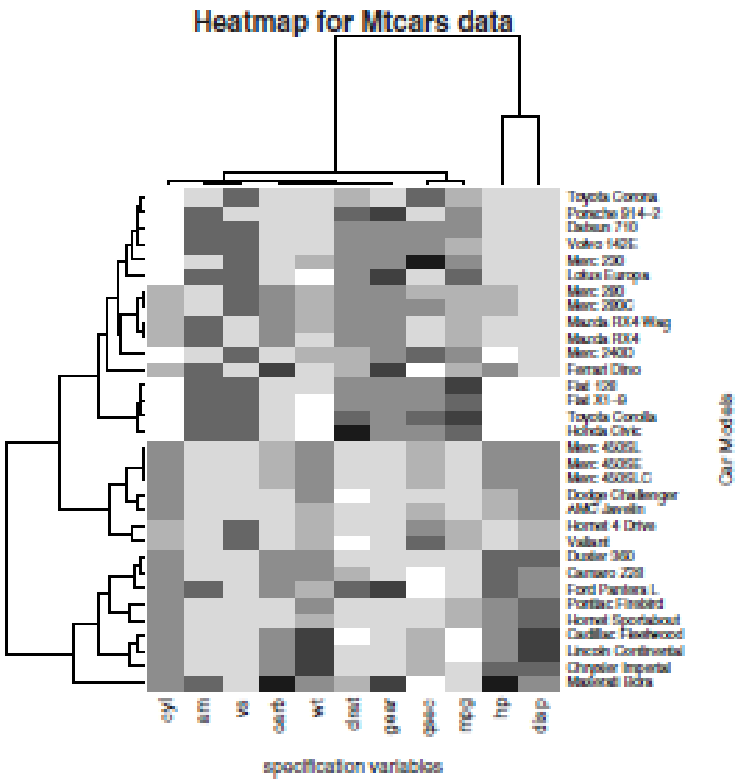


Fig. 9.5 Heatmap for the MTcars data, with clustering on the models and variables done separately. Darker regions correspond to higher values, lighter regions to lower values.

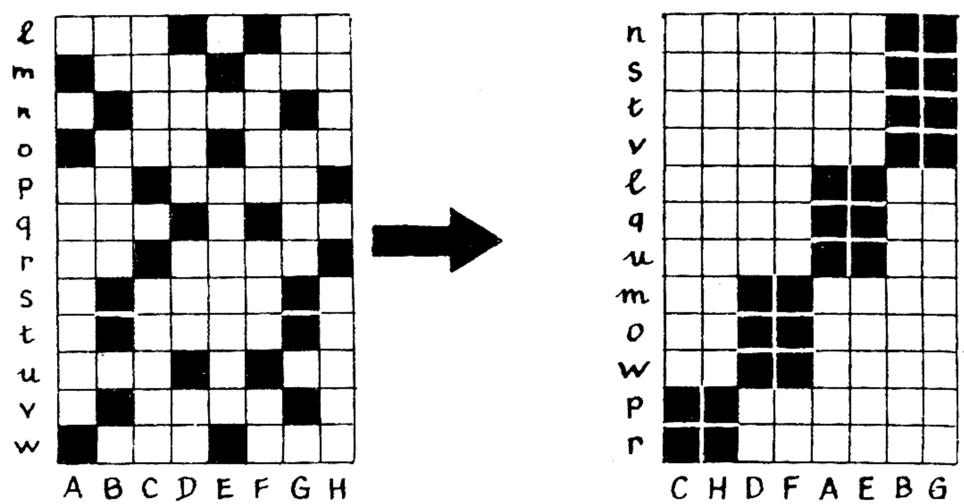
Inventor: Cormac Kinney, 1991,

Source: Principles and Theory for Data Mining and Machine Learning, Bertrand Clarke et al., Springer, 2012

- A heatmap is a matrix of values that have been color coded, usually so that higher values are brighter and lower values are darker, in analogy with temperature.
- The columns and rows of the matrix typically have an interpretation.
- In genomics, The columns and rows represent gene and brighter color represent higher gene expression.

Heatmap

- To rearrange the rows and columns so that two dark blocks place in the main diagonal and two lighter blocks in off the main diagonal is the ideal way to represent a Heat Map



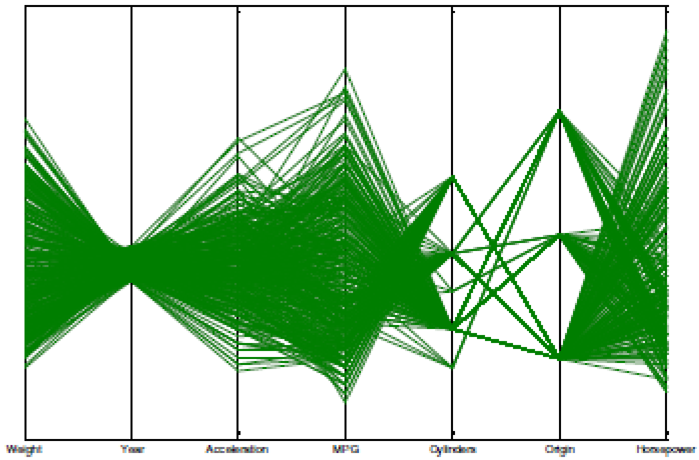
Multi-dimensional data

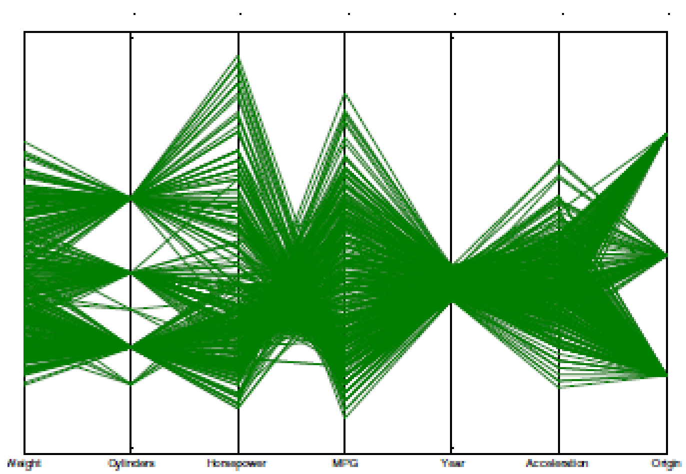
- Two solutions
  - Plot all possible pairs of variables as 2D scatter plots
    - Simple but not helpful to visualize the data as a whole
  - Parallel coordinates
    - A novel way of plotting multi-dimensional data proposed by **Alfred Inselberg**

Parallel Coordinates

- One vertical bar per dimension drawn in parallel
- Each point is represented by a set of lines
- Revolutionary representation for multi-dimensional data
- But users may need long time to learn how to understand the graphs

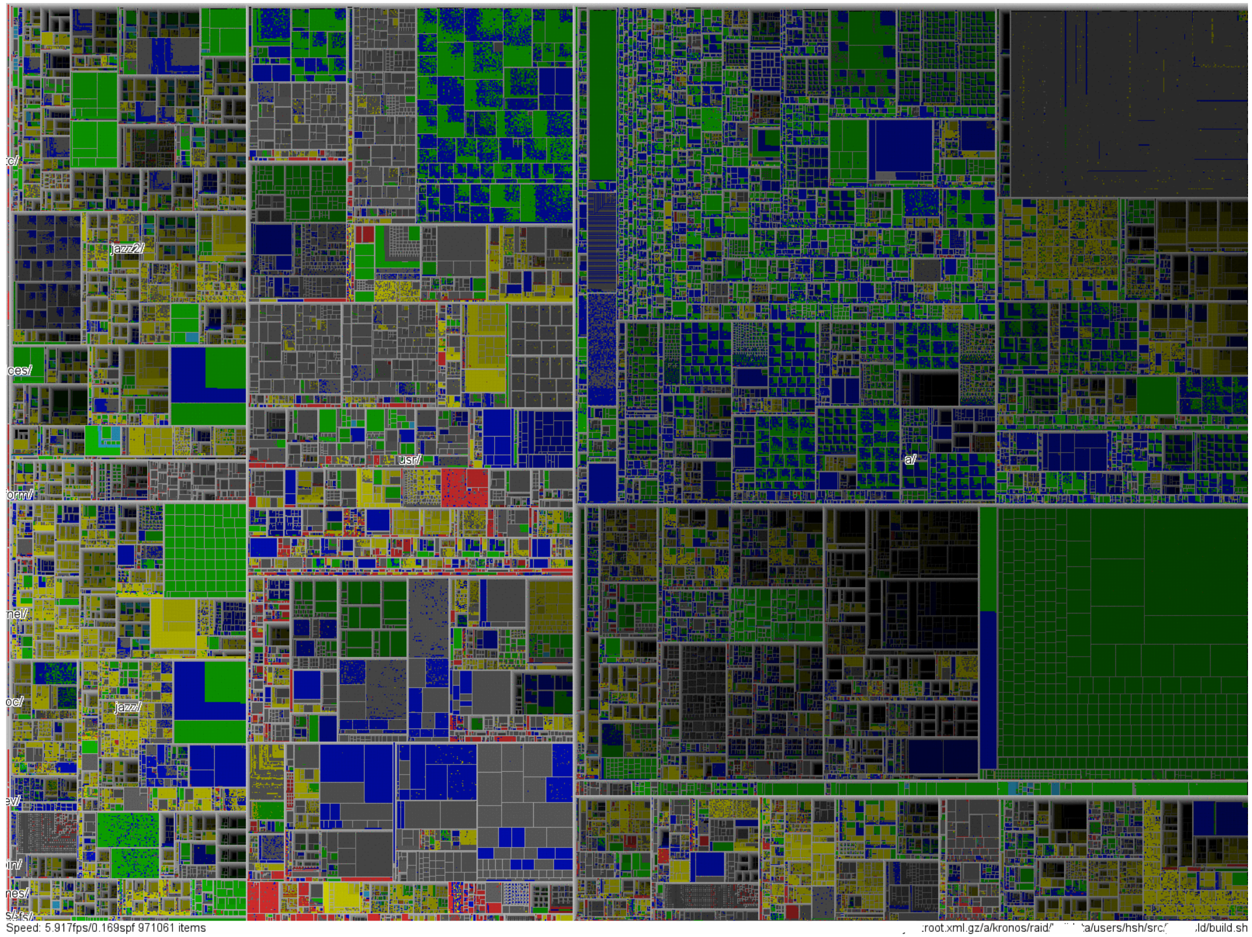
Parallel Coordinates





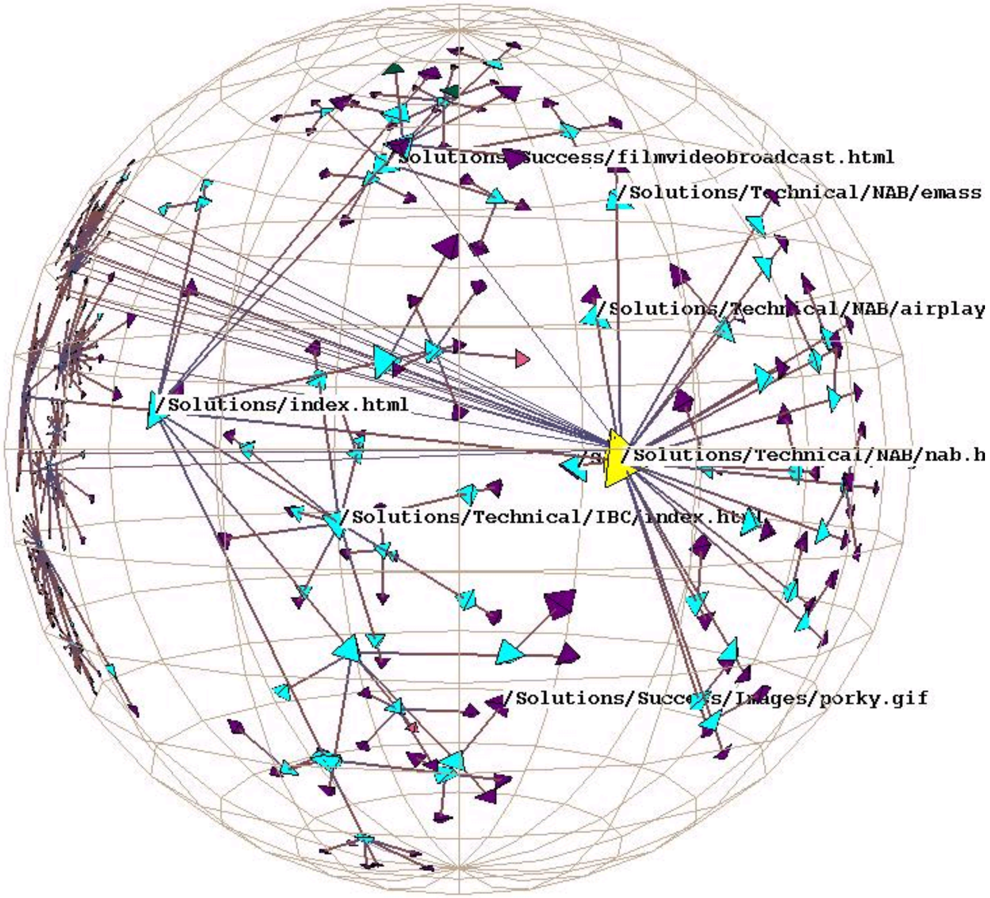
- Reordering of the axes so that crossing angle is minimized increases visualization efficiency

TreeMap of One million items



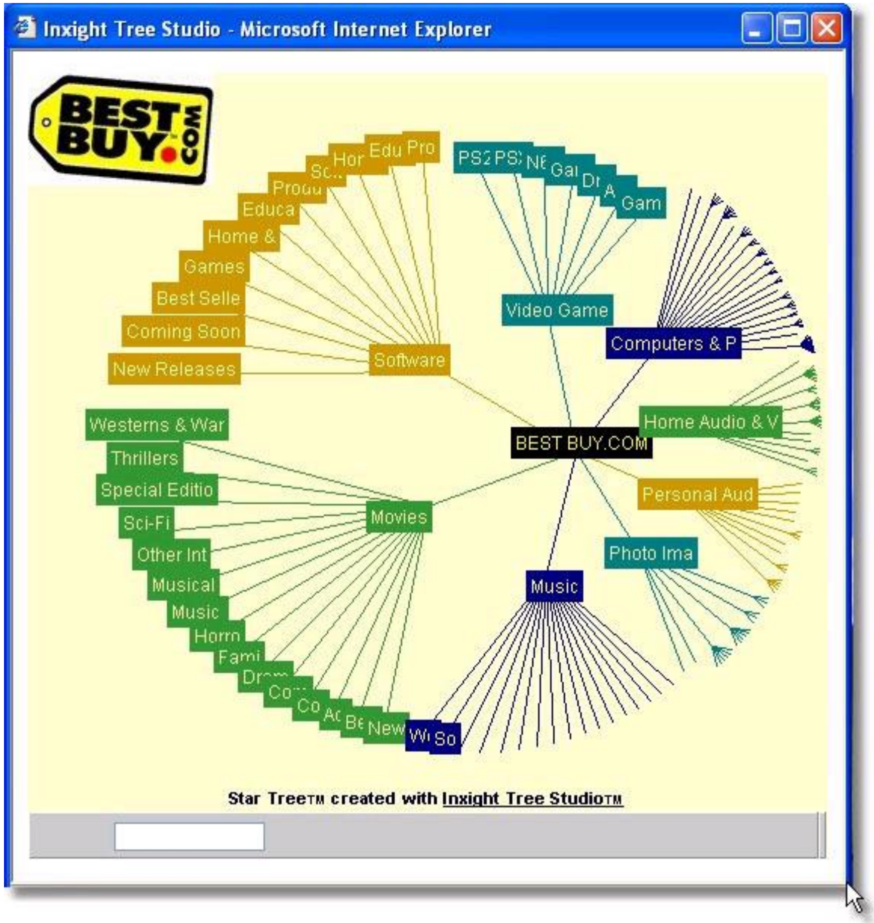
Tree

3-D hyberbolic space (Munzner, 2000)



Visualization of a single Website

StarTree (by InXight



The Curse of Dimensionality

- The term *curse of dimensionality* was coined by **Richard E. Bellman**

$$\boldsymbol{X} \sim \text{MVN}_p\,(\mathbf{0}\ ,\ \mathbf{I})$$

- Gaussian kernel density estimation
- Bandwidth chosen to minimize MSE at the mean
- Suppose want:

$$\left.\frac{E[(\hat{p}(x)-p(x))^2}{p(x)^2} < 0.1\right|_{x=0}$$

- In order to obtain a statistically sound and reliable result, the amount of data needed to support the result often grows exponentially with the dimensionality.

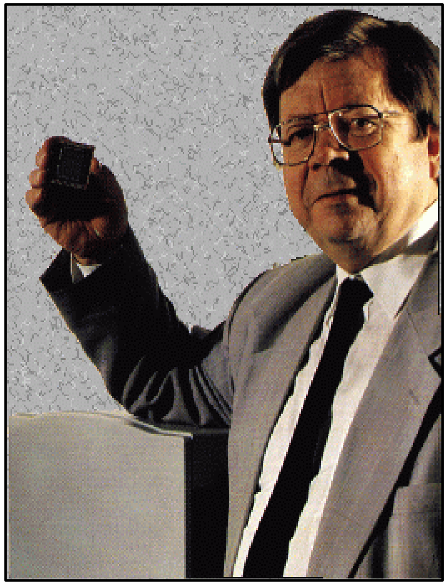
Dimension	# data points
1	4
2	19
3	67
6	2,790
10	842,000

- The volume of the spaces increases very rapidly
- The Availability of the data becomes sparse
- *This sparsity is problematic* for any method that requires statistical significance.
- Organizing and searching data often relies on detecting areas where objects form groups with similar properties
- In high dimensional data however all objects appear to be sparse and dissimilar in many ways.

Self-Organizing Maps

Self-Organizing Maps

- Ideas first introduced by C. von der Malsburg (1973), developed and refined by T. Kohonen (1982)
- Neural network algorithm using unsupervised competitive learning
- Primarily used for organization and visualization of complex data
- Biological basis: 'brain maps'

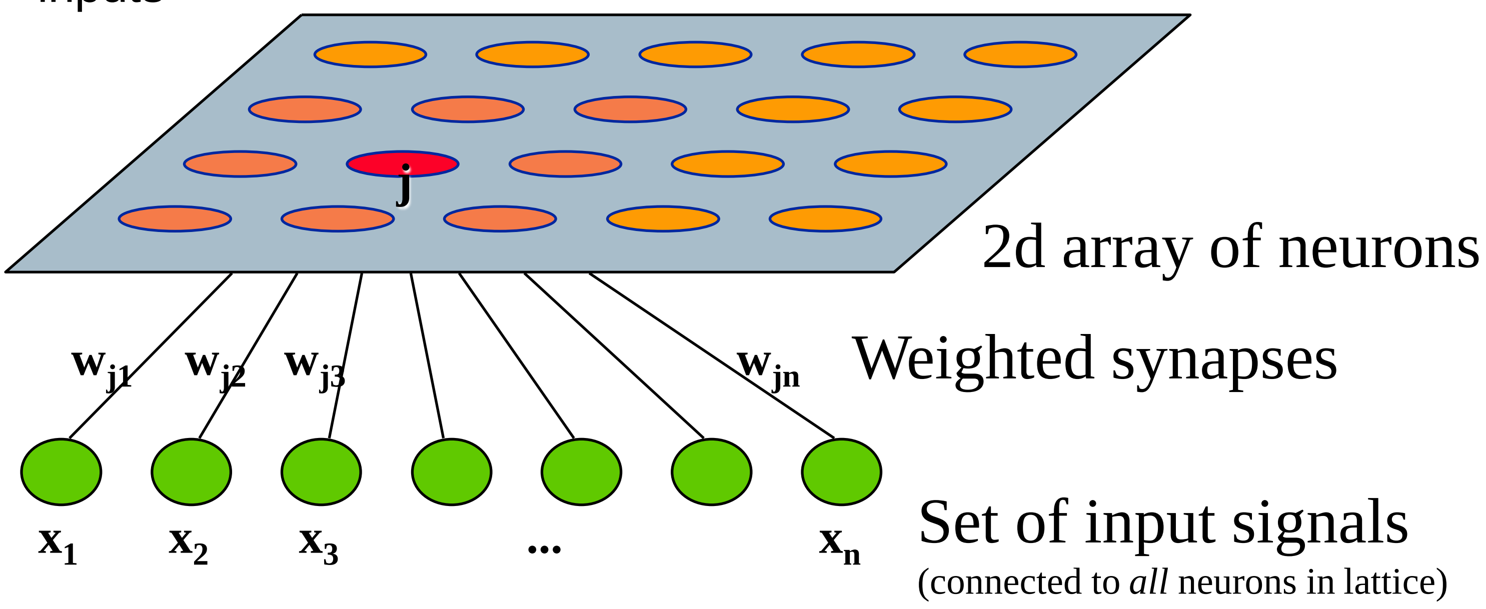


Teuvo Kohonen

Self-Organizing Maps

SOM - Architecture

- Lattice of neurons ('nodes') accepts and responds to set of input signals
- Responses compared; 'winning' neuron selected from lattice
- Selected neuron activated together with 'neighbourhood' neurons
- Adaptive process changes weights to more closely resemble inputs



Self-Organizing Maps

- The brain cells are self organizing themselves in groups, according to incoming information.
- This incoming information is not only received by a single neural cell, but also influences other cells in its neighbourhood. This organisation results in some kind of map, where Neural cells with similar functions are arranged close together.
- SOM mechanism is also based on this principle

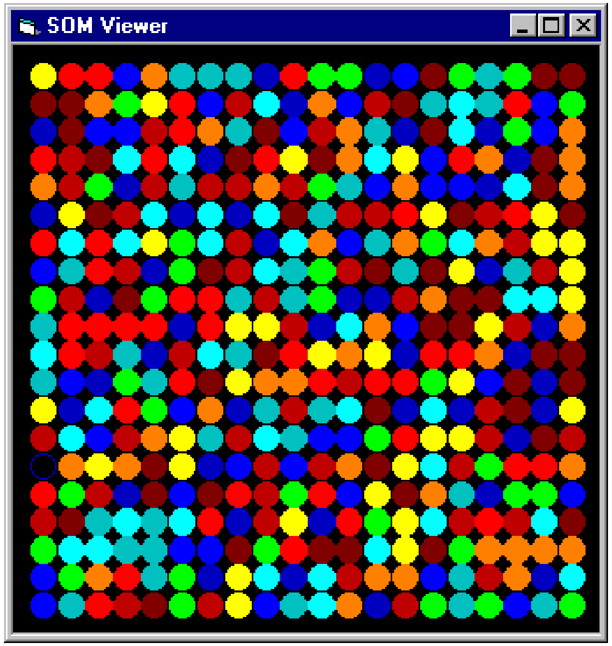
Self-Organizing Maps

SOM – Algorithm Overview

1. Randomly initialise all weights
2. Select input vector **x** = $[x_1, x_2, x_3, \ldots , x_n]$
3. Compare **x** with weights $\mathbf{w}_j$ for each neuron j to determine winner
4. Update winner so that it becomes more like **x**, together with the winner's *neighbours*
5. Adjust parameters: learning rate & 'neighbourhood function'
6. Repeat from (2) until the map has converged (i.e. no noticeable changes in the weights) or pre-defined no. of training cycles have passed

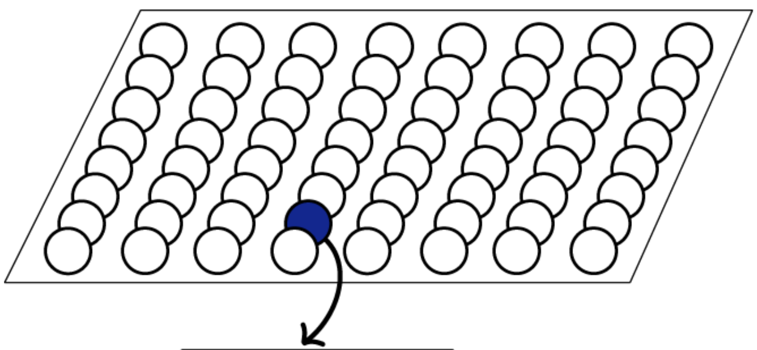
Initialization

(i)Randomly initialize the weight vectors $\mathbf{w}_j$ for all nodes j



Input vector

(ii) Choose an input vector **x** from the training set



Dokumentenkarten	1
Tiere	0
Texte	1
Michael	1
Schuhmacher	1
Dokumentenvektoren	1

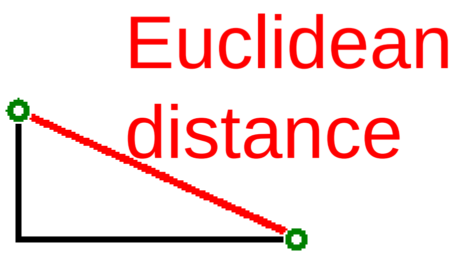
Finding a Winner

(iii) Find the best-matching neuron w(**x**), usually the neuron whose weight vector has smallest Euclidean distance from the input vector **x**

The winning node is that which is in some sense ‘closest’ to the input vector

‘Euclidean distance’ is the straight line distance between the data points, if they were plotted on a (multi-dimensional) graph

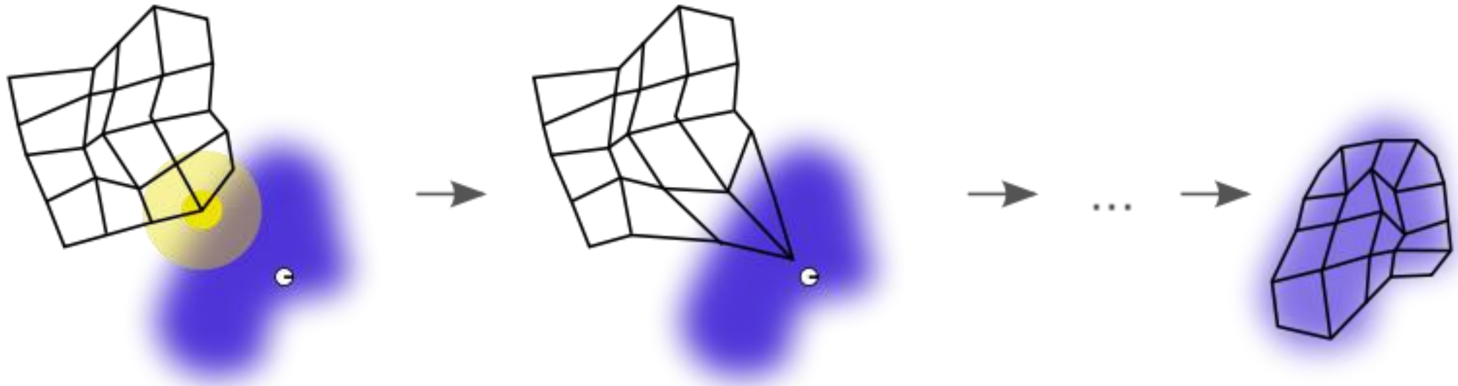
Euclidean distance between two vectors **a** and **b**, **a** = $(a_1,a_2,\ldots,a_n)$, **b** = $(b_1,b_2,\ldots b_n)$, is calculated as:



$$d_{\mathbf{a},\mathbf{b}} = \sqrt{\sum_i (a_i - b_i)^2}$$

Learning the SOM

- Determine the winner (the neuron of which the weight vector has the smallest distance to the input vector)
- Move the weight vector *w* of the winning neuron towards the input *i*



Weight Update

SOM Weight Update Equation

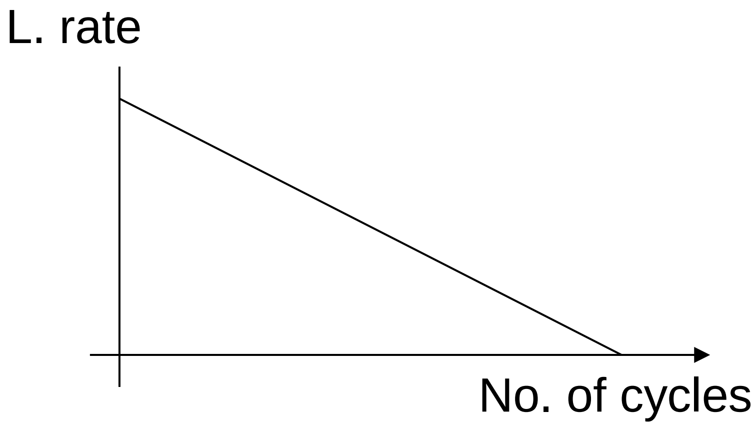
$$\mathbf{w}_j(t+1) = \mathbf{w}_j(t) + \mu(t)\, \lambda_{\omega(\mathbf{x})}(j,t)\, [\mathbf{x} - \mathbf{w}_j(t)]$$

"The weights of every node are updated at each cycle by adding

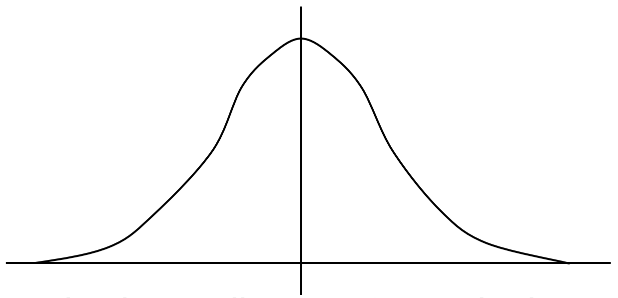
Current learning rate × Degree of neighbourhood with respect to winner × Difference between current weights and input vector

to the current weights"

Example of $\mu(t)$



Example of $\lambda_{\omega(\mathbf{x})}(j,t)$

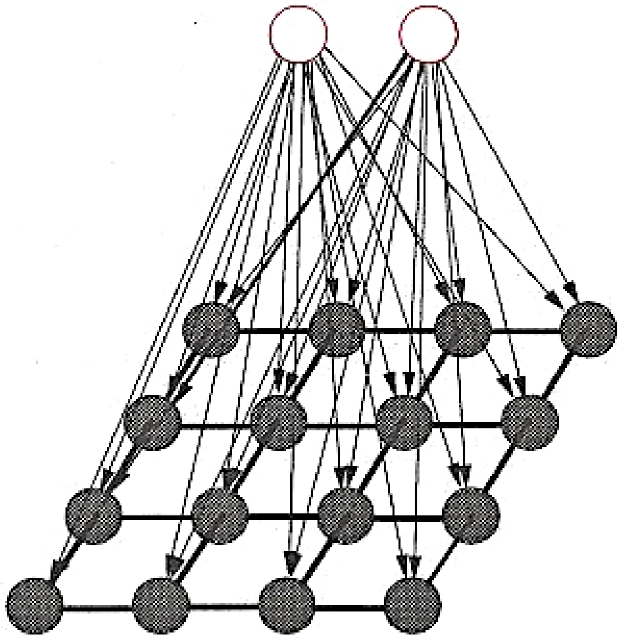


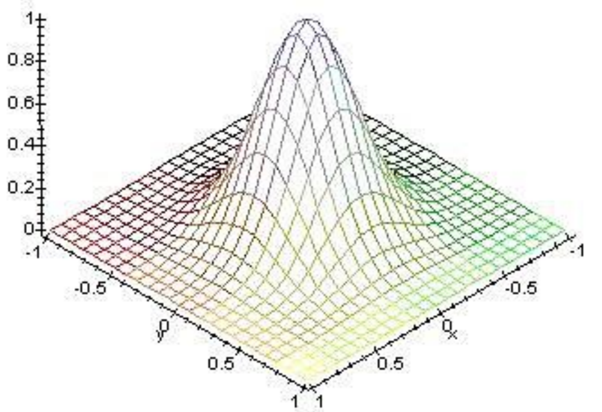
–x-axis shows distance from winning node

–y-axis shows 'degree of neighbourhood' (max. 1)

Self Organizing Map

- Neighborhood function to preserve topological properties of the input space
- Neighbors share the prize (postcode lottery principle)





Self Organizing Map

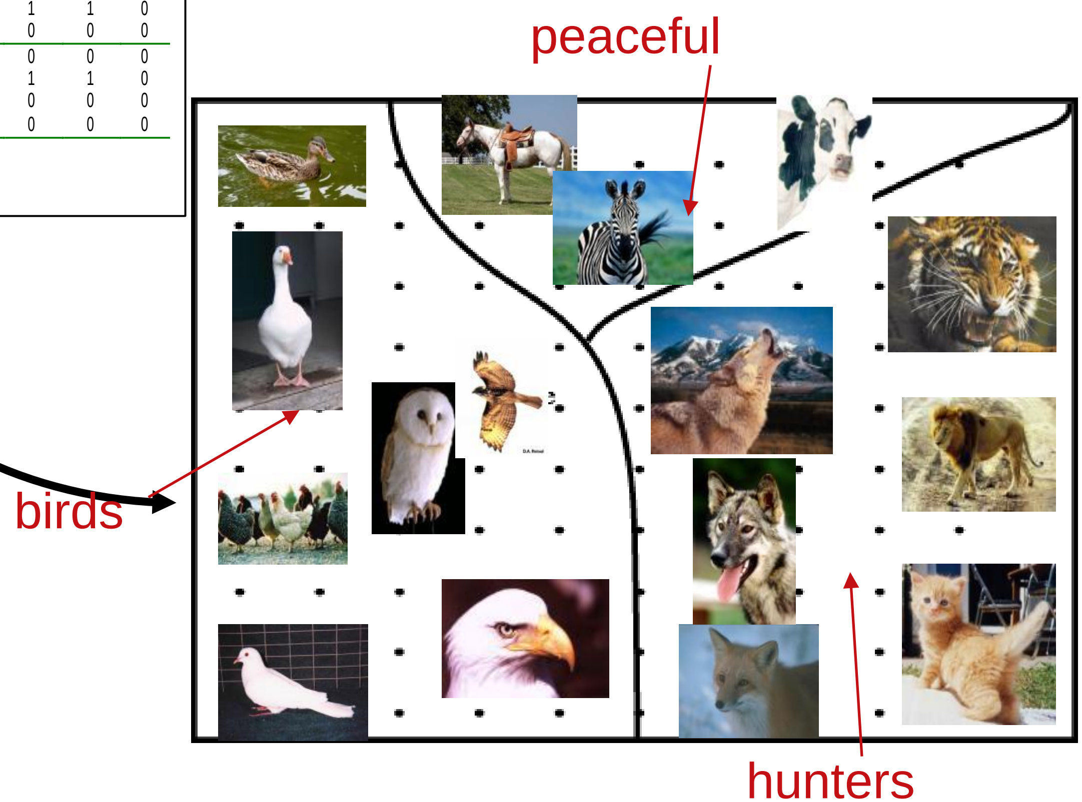
- Input: high-dimension input space
- Output: low dimensional (typically 2 or 3)
  - network topology
- Training
  - Starting with a large learning rate and neighborhood size, both are gradually decreased to facilitate convergence
- After learning, neurons with similar weights tend to cluster on the map

Example: Self-Organizing Maps

Animal names and their attributes

		Dove	Hen	Duck	Goose	Owl	Hawk	Eagle	Fox	Dog	Wolf	Cat	Tiger	Lion	Horse	Zebra	Cow
is	Small	1	1	1	1	1	1	0	0	0	0	1	0	0	0	0	0
	Medium	0	0	0	0	0	0	1	1	1	1	0	0	0	0	0	0
	Big	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1
has	2 legs	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
	4 legs	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1
	Hair	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1
	Hooves	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1
	Mane	0	0	0	0	0	0	0	0	0	1	0	0	1	1	1	0
	Feathers	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0
likes to	Hunt	0	0	0	0	1	1	1	1	0	1	1	1	1	0	0	0
	Run	0	0	0	0	0	0	0	0	1	1	0	1	1	1	1	0
	Fly	1	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0
	Swim	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0

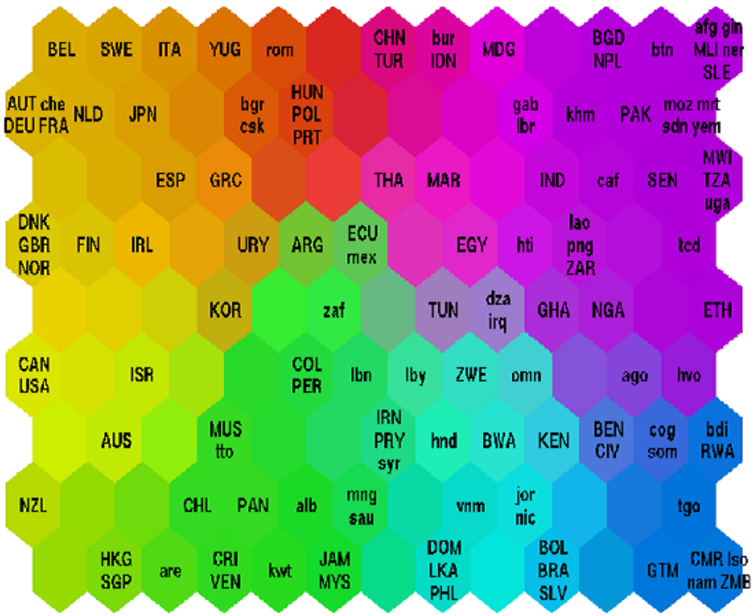
A grouping according to similarity has emerged



[Teuvo Kohonen 2001] Self-Organizing Maps; Springer;

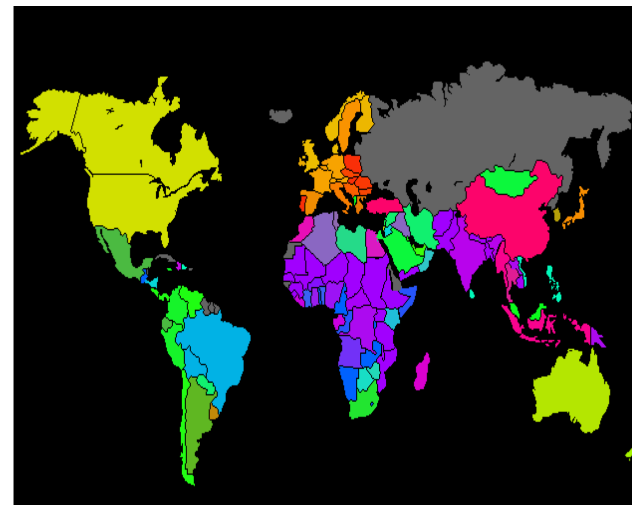
Self-Organizing Maps

SOM – Result Example
Classifying World Poverty



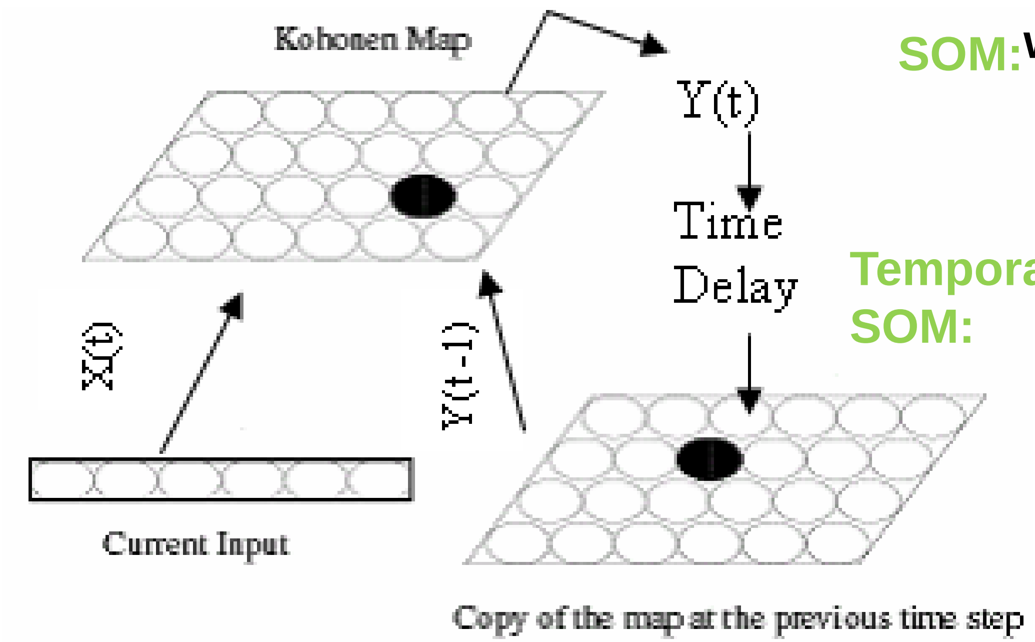
The Country Names

AFG	Afghanistan	GTM	Guatemala	NZL	New Zealand
AGO	Angola	HKG	Hong Kong	OAN	Taiwan, China
ALB	Albania	HND	Honduras	OMN	Oman
ARE	United Arab Emirates	HTI	Haiti	PAK	Pakistan
ARG	Argentina	HUN	Hungary	PAN	Panama
AUS	Australia	HVO	Burkina Faso	PER	Peru
AUT	Austria	IDN	Indonesia	PHL	Philippines
BDI	Burundi	IND	India	PNG	Papua New Guinea
BEL	Belgium	IRL	Ireland	POL	Poland
BEN	Benin	IRN	Iran, Islamic Rep.	PRT	Portugal
BGD	Bangladesh	IRQ	Iraq	PRY	Paraguay
BGR	Bulgaria	ISR	Israel	ROM	Romania
BOL	Bolivia	ITA	Italy	RWA	Rwanda
BRA	Brazil	JAM	Jamaica	SAU	Saudi Arabia
BTN	Bhutan	JOR	Jordan	SDN	Sudan
BUR	Myanmar	JPN	Japan	SEN	Senegal
BWA	Botswana	KEN	Kenya	SGP	Singapore
CAF	Central African Rep.	KHM	Cambodia	SLE	Sierra Leone
CAN	Canada	KOR	Korea, Rep.	SLV	El Salvador
CHE	Switzerland	KWT	Kuwait	SOM	Somalia
CHL	Chile	LAO	Lao PDR	SWE	Sweden
CHN	China	LBN	Lebanon	SYR	Syrian Arab Rep.
CIV	Cote d'Ivoire	LBR	Liberia	TCD	Chad
CMR	Cameroon	LBY	Libya	TGO	Togo
COG	Congo	LKA	Sri Lanka	THA	Thailand
COL	Colombia	LSO	Lesotho	TTO	Trinidad and Tobago
CRI	Costa Rica	MAR	Morocco	TUN	Tunisia
CSK	Czechoslovakia	MDG	Madagascar	TUR	Turkey
DEU	Germany	MEX	Mexico	TZA	Tanzania
DNK	Denmark	MLI	Mali	UGA	Uganda
DOM	Dominican Rep.	MNG	Mongolia	URY	Uruguay
DZA	Algeria	MOZ	Mozambique	USA	United States
ECU	Ecuador	MRT	Mauritania	VEN	Venezuela
EGY	Egypt, Arab Rep.	MUS	Mauritius	VNM	Viet Nam
ESP	Spain	MWI	Malawi	YEM	Yemen, Rep.
ETH	Ethiopia	MYS	Malaysia	YUG	Yugoslavia
FIN	Finland	NAM	Namibia	ZAF	South Africa
FRA	France	NER	Niger	ZAR	Zaire
GAB	Gabon	NGA	Nigeria	ZMB	Zambia
GBR	United Kingdom	NIC	Nicaragua	ZWE	Zimbabwe
GHA	Ghana	NLD	Netherlands		
GIN	Guinea	NOR	Norway		
GRC	Greece	NPL	Nepal		



'Poverty map' based on 39 indicators describing various quality-of-life factors, such as state of health, nutrition, educational services, etc,) from World Bank statistics (1992)

Temporal SOM



SOM: $w_j(t+1) = w_j(t) + \mu(t)\, \lambda_{\omega(x)}(j,t)\, [x(t) - w_j(t)]$

Temporal SOM:

$$y_j(t) = (1-\alpha)\, y_j(t-1) + \alpha\, [x(t) - w_j(t)]$$

$$w_j(t+1) = w_j(t) + \mu(t)\, \lambda_{\omega(x)}(j,t)\, y_j(t)$$

$[x(t) - w_j(t)]$ is called quantization error

$y_j(t)$ is called recursive of the neuron j at time t

α is the leaking coefficient (value is between 0 and 1)

Recursive SOM architecture. The original SOM algorithm is used
recursively, on both the input vector X(t) and the representation derived at
the previous time step, y(t-1)

Self-Organizing Maps

- Advantages
  - SOM is Algorithm that projects high-dimensional data onto a two-dimensional map.
  - The projection preserves the topology of the data so that similar data items will be mapped to nearby locations on the map.
  - SOM still have many practical applications in pattern recognition, speech analysis, industrial and medical diagnostics, data mining
- Disadvantages
  - Large quantity of good quality representative training data required
  - No generally accepted measure of ‘quality’ of a SOM

    e.g. Average quantization error (how well the data is classified)

Outline

- Introduction
- History
- Modern Visualization and Computational Problems

  - Parallel Co-ordinates, heat map, SOM etc.

  - Space, data ordering, processing

- Conclusion

Conclusion

- The advent of computer capacity and power push the envelope of computational sciences and scientific visualization (SciVis).
- SciVis has revolutionized the way we do sciences.
- SciVis provides scientists a process to probe into enormously large data sets, perceive incredible details of the domain, and discover unexpected insights.
- Challenging issues in SciVis evolve, but we will continue to face them, solve the problems, and face future challenges.

Scientists make music from DNA

By Daniel Woolls
The Associated Press

MADRID, Spain – Imagine the human genome as music. Unravel DNA's double helix, picture its components lined up like piano keys and assign a note to each. Run your finger along the keys.

Spanish scientists did that just for fun and recorded what they call an audio version of the blueprint for life.

The team at Madrid's Ramon y Cajal Hospital was intrigued by music's lure – how it can make toddlers dance and adults cry – and looked for hints in the genetic material that makes us what we are. They also had some microbial genes wax melodic.

The end product is *Genoma Music*, a 10-tune CD due out in February. "It's a way to bring science and music closer together," said Dr. Aurora Sanchez Sousa, a piano-playing microbiologist who specializes in fungi.

DNA, or deoxyribonucleic acid, is composed of long strings of molecules called nucleotides, which are distinguished by which of four nitrogen-containing bases they contain: adenine, guanine, thymine or cytosine, represented as A, G, T and C. These became the musical notes.

French-born composer Richard Krull turned DNA sequences – a snippet of a gene might look like AGCGTATACGAGT – into sheet music. He arbitrarily assigned tones of the eight-note, do-re-mi scale to each letter. Thymine became re, for instance. Guanine is so, adenine la and cytosine do.

Played solo on percussion, classical guitar or the other instruments used on the CD, the sequences would sound cute but rudimentary, the musical equivalent of PacMan in an era of Microsoft Xbox.

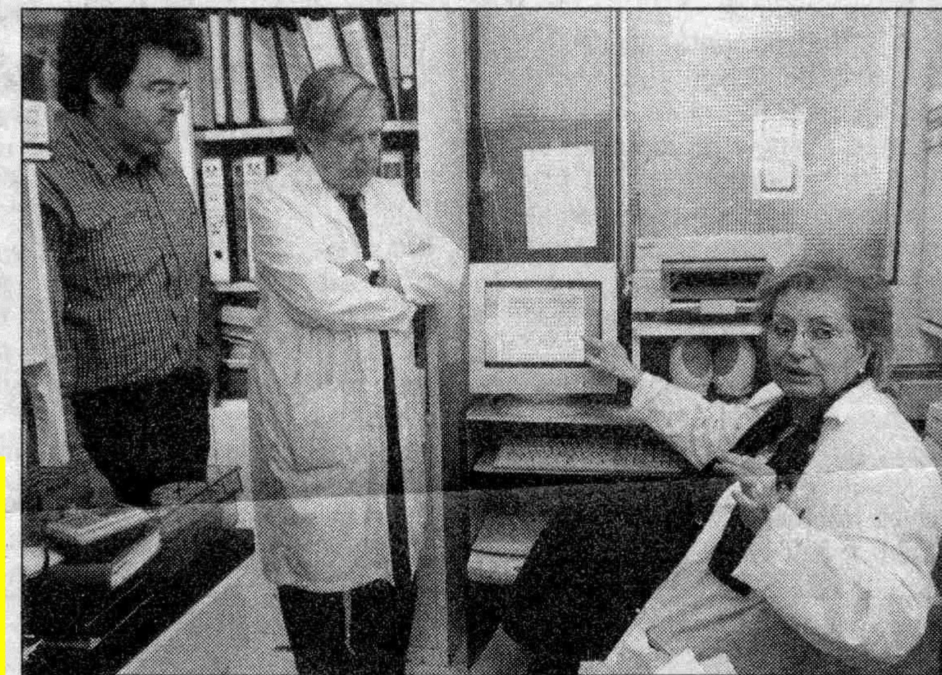
So the alphabet soup of bases served as just that, base lines to accompany melodies composed by Mr. Krull and his scientific colleague. They say the melodies were influenced, even dictated, by the mood and rhythm of the underlying genetic code.

In general, the genome music is an easy-listening sound that is vaguely New Age. One of the prettiest songs is based on Connexin 26, a human gene that causes deafness when it mutates. The DNA skeleton is expressed with tinkling bells and a flute melody does the rest.

Another song draws on a yeast gene known as SLT2. Dr. Sanchez Sousa, the main author of the project, is fond of the sequence because it features a stretch in which one triplet of nitrogen bases appears several times in rapid succession – a repetitive phenomenon that has a musical equivalent called ostinato.

"This is a very sad part, but a beautiful one," Dr. Sanchez Sousa said, wearing a white lab coat and waving her arms like a musical conductor as she played the segment for a visitor.

Her team's plans for future music include having the hospital choir sing a vocal piece based on DNA from a bacteria.



The Associated Press/PAUL WHITE

Dr. Aurora Sanchez Sousa (right) points to some sheet music that has been translated from the DNA code into easy-listening music, inside the Ramon y Cajal hospital in Madrid, Spain.

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