Ludwig-Maximilians-Universität München
Lehrstuhl für Datenbanksysteme und Data Mining
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Data Mining Algorithms 1

(Knowledge Discovery and Data Mining 1)

Winter Semester 2024/25

Preliminaries: Data

Preliminaries: Data

- What is data?
  - Representation of real (or artificial) objects, situations, processes, ...
  - Measured by physical sensors $\rightarrow$ temperature, humidity, car traffic, speed, color, ...
  - Recorded from digital systems $\rightarrow$ bank transfers, web browsing, ...
  - Generated by simulations $\rightarrow$ weather forecast, digital mockups, ...
  - Stored and provided by computers $\rightarrow$ e.g., on local disk or on remote server
- How to represent data?
  - Numerical and categorical data types
  - Similarity models $\rightarrow$ allow for pattern mining
  - Data reduction $\rightarrow$ to increase efficiency
- How to present data?
  - Visualization
  - Privacy aspects

Agenda

Data Types – Algebraic View

Ingredients of data types

- Types have identifiers: int, long, float, double, boolean, char, ...
- Types have domains $\mathcal{D}$: $\{1, 2, ...\}, \{true, false\}$, {'hello', 'hi', 'howdy', ...}
- Types have operations: $+$, $-$, mod, div, and, or, not, concat, ...

E.g., operations for comparison, as needed for data mining

- Equality tests $=, \neq : \mathcal{D} \times \mathcal{D} \rightarrow \{true, false\}$
- Distance functions $d : \mathcal{D} \times \mathcal{D} \rightarrow \mathbb{R}_0^+$
- Examples: Euclidean distance, maximum distance, difference value

Data Handling is Expensive – Implementation View

Data need storage space

- Single values need 1 Byte = 8 Bit, 4 Byte = 32 Bit, 8 Byte = 64 Bit
- Big data sets allocate Kilobytes 10^3, Megabytes 10^6, Gigabytes 10^9, Terabytes 10^{12}, Petabytes 10^{15}, Exabytes 10^{18}, Zettabytes 10^{21}, etc
- Data compression helps (partially)

Operations need calculation time

- Calculating the Euclidean distance of two objects from $\mathbb{R}^d$ needs $O(d)$ time
- Mean $\frac{1}{n}\sum_{i=1}^{n} x_i$ of n objects from $\mathbb{R}^d$ needs $O(nd)$ time
- Covariance matrix of n objects $x_i \in \mathbb{R}^d$ needs $O(nd^2)$ time

Overview of Data Types

Simple, basic data types

Numerical data (numbers) or categorical data (symbols)

Composed data types

Vectors, sequences, sets, relations

Complex data types

- Multimedia data: images, videos, audio, text, documents, web pages, etc.
- Spatial data: shapes, geography, trajectories, etc.
- Structures: graphs, networks, trees, etc.

Numeric Data

Simple numeric data

- Numbers: natural, integer, rational, real numbers
- Domain examples: age, income, shoe size, height, weight
- (Dis-)similarity: difference value $d(x, y) = |x - y|$
- Example: 3 is more similar to 30 than 30 is to 3,000

Composed numeric data

- Vectors $x \in \mathbb{R}^d = \mathbb{R} \times \mathbb{R} \times \ldots \times \mathbb{R}$ (d times)
- Examples: geolocation $(lat, lon) \in \mathbb{R}^2$, feature vector $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$
- Comparison by Euclidean distance, Manhattan dist., Earth Movers' dist., etc.

Examples: Comparisons of vectors by L_p-distance functions

Given two vectors $o, q \in \mathbb{R}^n$

Distances based on p-norms:	$d_p(o,q) = \|o-q\|_p = \sqrt[p]{\sum_{i=1}^{n} \lvert o_i - q_i \rvert^p}$
Euclidean distance (aerial, beeline)	$d_2(o,q) = \|o-q\|_2 = \sqrt{\sum_{i=1}^{n} (o_i - q_i)^2}$
Manhattan distance (city blocks)	$d_1(o,q) = \|o-q\|_1 = \sum_{i=1}^{n} \lvert o_i - q_i \rvert$
Maximum distance, $p \to \infty$	$d_\infty(o,q) = \max\{\lvert o_i - q_i \rvert, i = 1..n\}$
Weighted p-distances	$d_{p,w}(o,q) = \sqrt[p]{\sum_{i=1}^{n} w_i \cdot \lvert o_i - q_i \rvert^p}$
To illustrate, draw "circles" around c:	$\{p \in \mathbb{R}^n, d(p,c) = \varepsilon\}$

Generalization: Metric Data

Metric Space

Metric space (O, d) consists of object set O and *metric distance* function $d : O \times O \rightarrow \mathbb{R}_0^+$ which fulfills:

$$\begin{aligned}
\text{Symmetry:} \quad & \forall p, q \in O : d(p, q) = d(q, p) \\
\text{Identity of Indiscernibles:} \quad & \forall p, q \in O : d(p, q) = 0 \iff p = q \\
\text{Triangle Inequality:} \quad & \forall p, q, o \in O : d(p, q) \leq d(p, o) + d(o, q)
\end{aligned}$$

Example: Points in 2D space or in $\mathbb{R}^n$ with Euclidean distance

Counterexamples: do we really want to have metrics in every application?

- non-symmetric: one-way roads on the way from p to q
- non-definite: indiscernible equivalent objects are not necessarily identical
- triangles: sometimes detours maybe preferred

Categorical data

- Symbols, "just identifiers"
- Examples:
  - subjects = { physics, biology, math, music, literature, ... }
  - occupation = { butcher, hairdresser, physicist, physician, ... }
- Similarity measure: How to compare values?

Example: Trivial metric

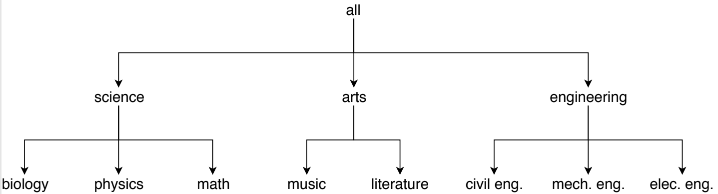
$$d(p, q) = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{else} \end{cases}$$

Categorical data (cont'd)

Explicit similarity matrix, $O \times O \to \mathbb{R}_0^+$

	car	bike	trolley
car	1	0.3	0.1
bike	0.3	1	0.2
trolley	0.1	0.2	1

Path length in generalization hierarchy



Simple Data Types: Ordinal

Characteristic

There is a (total) order $\leq$ on the set of possible data values O:

$$\begin{aligned} \text{Transitivity:} \quad & \forall p, q, o \in O : p \leq q \wedge q \leq o \implies p \leq o \\ \text{Antisymmetry:} \quad & \forall p, q \in O : p \leq q \wedge q \leq p \implies p = q \\ \text{Totality:} \quad & \forall p, q \in O : p \leq q \vee q \leq p \end{aligned}$$

Examples

- Words & lexicographic ordering: $\textit{high} \leq \textit{highschool} \leq \textit{highscore}$
- (Vague) sizes: $\textit{tiny} \leq \textit{small} \leq \textit{medium} \leq \textit{big} \leq \textit{huge}$
- Frequencies, e.g.: $\textit{never} \leq \textit{seldom} \leq \textit{rarely} \leq \textit{occasionally} \leq \textit{sometimes} \leq \textit{often} \leq \textit{frequently} \leq \textit{regularly} \leq \textit{usually} \leq \textit{always}$
- Numbers (finite or infinite sets): $0 \leq 1 \leq 2 \leq \ldots$, or $1.78 \leq 2.35 \leq 3.14 \leq \ldots$

Composed Data Types: Sequences, Vectors

Characteristic

- Given a domain D, a sequence s of length n is a mapping $I_n \to D$ of the index set $I_n = \{1, \ldots, n\}$ into D. Let us write $s \in D^n$ for short.
- The sequence s concatenates n values from D; the order does matter

Examples

- Distances based on p-norms: $d_p(o, q) = \sqrt[p]{\sum_{i=1}^{n} |o_i - q_i|^p}$
- Generalization, with ground distances d_i: $d_p(o, q) = \sqrt[p]{\sum_{i=1}^{n} d_i(o_i, q_i)^p}$
- Note: d_p is metric iff all ground distances $d_i : D_i \times D_i \to \mathbb{R}_0^+$ are metric

Composed Data Types: Sets

Characteristic

Unordered collection of individual values

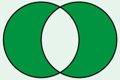
Examples

- skills $= \{$Java, C, Python$\}$, hobbies $= \{\textit{skiing}, \textit{diving}, \textit{hiking}\}$

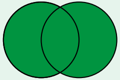
Comparison

- Symmetric Set Difference:

$$\begin{aligned} R \Delta S &= (R - S) \cup (S - R) \\ &= (R \cup S) - (R \cap S) \end{aligned}$$



$R \Delta S$



$R \cup S$

- Jaccard Distance: $d(R, S) = \frac{|R \Delta S|}{|R \cup S|}$

Composed Data Types: Sets

Bitvector Representation

- Given an ordered base set $B = (b_1, \ldots, b_n)$, for any set S create a binary vector $r \in \{0,1\}^n$ with $r_i = 1 \iff b_i \in S$.
- Hamming distance: Sum of different entries (equals cardinality of symmetric set difference)

Example

- Base: B = (Math, Physics, Chemistry, Biology, Music, Arts, English)
- S = {Math, Music, English} = (1,0,0,0,1,0,1)
- R = {Math, Physics, Arts, English} = (1,1,0,0,0,1,1)
- Hamming(R, S) = 3

Complex Data Types

Examples for components of complex data

- Structure: graphs, networks, trees
- Geometry: shapes, contours, routes, trajectories
- Multimedia: images, audio, text, etc.

Similarity models: Approaches

- Direct measures – highly data type dependent
- Feature extraction / feature engineering – explicit vector space embedding with hand-crafted features
- Kernel trick – implicit vector space embedding
- Feature learning – (explicit) vector space embedding learned by deep learning methods, e.g. neural networks

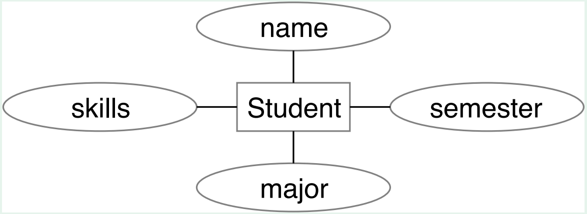
Complex Data Types

Examples for similarity models

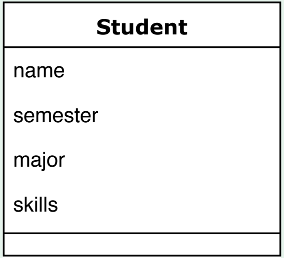
	Direct	Feature extraction	Kernel-based	Feature learning
Graphs	Structural Alignment	Degree Histograms	Label Sequence Kernel	Node embeddings, Spectral Neural Networks
Geometry	Hausdorff Distance	Shape Histograms	Spatial Pyramid Kernel	Convolutionl Neural Networks (CNN)
Sequences	Edit Distance	Symbol Histograms	Cosine Distance	Recurrent neural network (RNN)

Objects and Attributes (Conceptual Modeling)

Entity-Relationship Diagram (ER)



UML Class Diagram

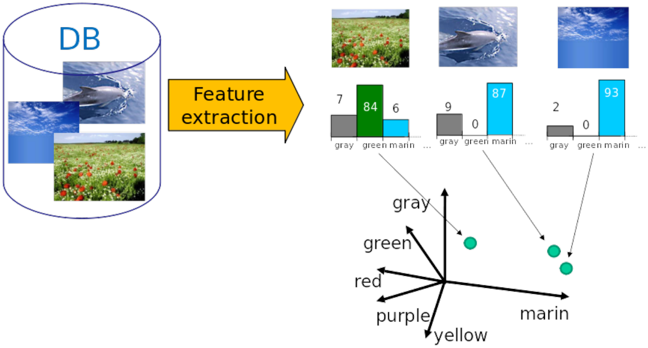


Data Tables (Relational Model)

name	sem	major	skills
Ann	3	CS	Java, C, R
Bob	1	CS	Java, PHP
Charly	4	History	Piano
Debra	2	Arts	Painting

Feature Extraction

- Objects from database DB are mapped to feature vectors



- Feature vector space
  - Points represent objects
  - Distance corresponds to (dis-)similarity

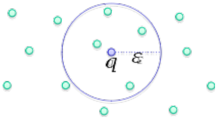
Similarity Queries

- Similarity queries are basic operations in (multimedia) databases
- Given: universe O, database $DB \subseteq O$, distance function d and query object $q \in O$

Range query

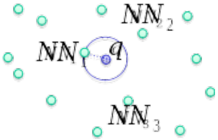
Range query for range parameter $\varepsilon \in \mathbb{R}_0^+$:

$$range(DB, q, d, \varepsilon) = \{o \in DB \mid d(o, q) \leq \varepsilon\}$$



Nearest neighbor query

$$NN(DB, q, d) = \{o \in DB \mid \forall o' \in DB : d(o, q) \leq d(o', q)\}$$



Similarity Queries

k-nearest neighbor query

k-nearest neighbor query for parameter $k \in \mathbb{N}$:

$$NN(DB, q, d, k) \subseteq DB \text{ with } |NN(DB, q, d, k)| = k \text{ and}$$

$$\forall o \in NN(DB, q, d, k), o' \in DB - NN(DB, q, d, k) : d(o, q) \leq d(o', q)$$

Ranking query

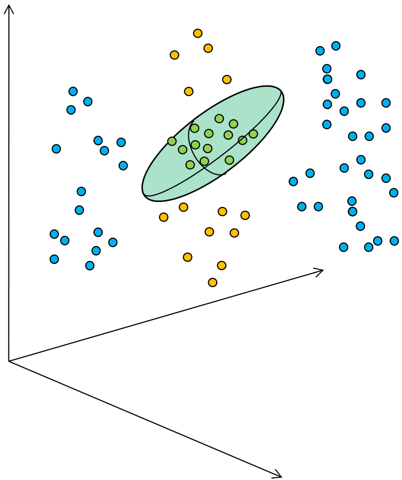
Ranking query (partial sorting query): "get next" functionality for picking database objects in an increasing order w.r.t. their distance to q:

$$\forall i \leq j : d(q, rank_{DB,q,d}(i)) \leq d(q, rank_{DB,q,d}(j))$$

Similarity Search

- Example: Range query $range(DB, q, d, \varepsilon) = \{o \in DB \mid d(o, q) \leq \varepsilon\}$
- Naive search by sequential scan
  - Fetch database objects from secondary storage (e.g. disk): $O(n) time$
  - Check distances individually: $O(n) time$
- Fast search by applying database techniques
  - Filter-refine architecture
    - Filter: Boil database DB down to (small) candidate set $C \subseteq DB$
    - Refine: Apply exact distance calculation to candidates from C only
  - Indexing structures
    - Avoid sequential scans by (hierarchical or other) indexing techniques
    - Data access in time $O(n)$, $O(\log n)$, or even $O(1)$

Filter-Refine Architecture



- Principle of multi-step search:
  1. Fast filter step produces candidate set $C \subset DB$ (by approximate distance function d')
  2. Exact distance function d is calculated on candidate set C only.
- Example: Dimensionality reduction[a]
- ICES criteria for filter quality[b]
  - I ndexable – Index enabled
  - C omplete – No false dismissals
  - E fficient – Fast individual calculation
  - S elective – Small candidate set

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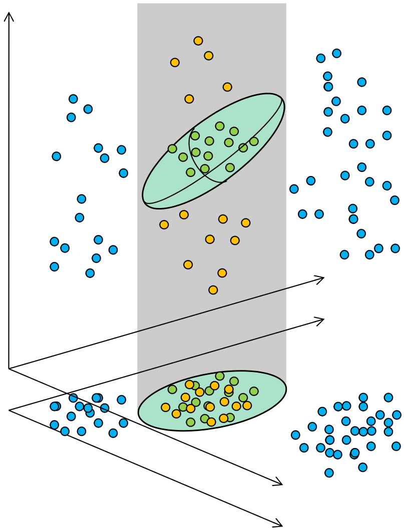
[a] GEMINI: Faloutsos 1996; KNOP: Seidl & Kriegel 1998

[b] Assent, Wenning, Seidl: ICDE 2006

Filter-Refine Architecture



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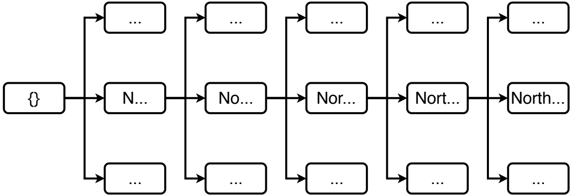
[b] Assent, Wenning, Seidl: ICDE 2006

Indexing: Example

- Example: Phone book
- Indexed using alphabetical order of participants
- Instead of sequential search:
  - Estimate region of query object (interlocutor)
  - Check for correct branch
  - Use next identifier of query object
  - Repeat until query is finished



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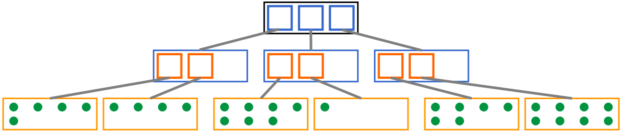
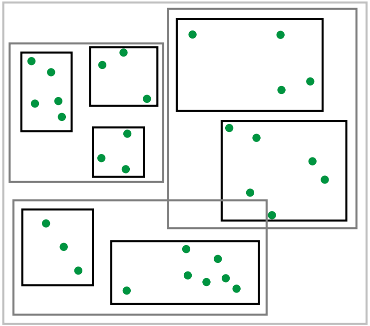
Indexing: Principle

- Organize data in a way that allows for fast access to relevant objects, e.g. by heavy pruning.



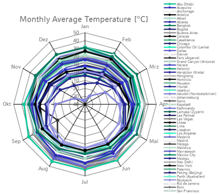


- R-Tree as an example for spatial index structure:
  - Hierarchy of minimum bounding rectangles
  - Disregard subtrees which are not relevant for the current query region

Agenda

Data Visualization

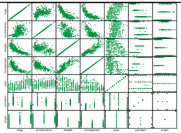
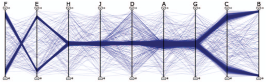
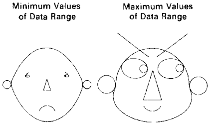
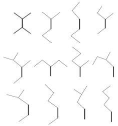
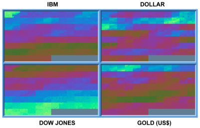
- Patterns in large data sets are hardly perceived from tabular numerical representations
- Data visualization transforms data in visually perceivable representations ("a picture is worth a thousand words")
- Combine capabilities:
  - Computers are good in number crunching (and data visualization by means of computer graphics)
  - Humans are good in visual pattern recognition



Monthly average temperature [°C]

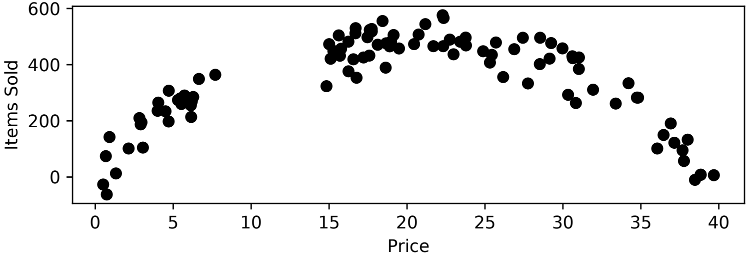
Städte Ø	**Jan**	**Feb**	**Mrz**	**Apr**	**Mai**	**Jun**	**Jul**	**Aug**	**Sep**	**Okt**	**Nov**	**Dez**
Abu Dhabi	25	27	31	36	40	41	42	43	42	37	31	27
Acapulco	32	31	32	32	33	33	33	33	33	33	32	32
Anchorage	-4	-2	0	6	13	17	18	17	13	5	-3	-5
Antalya	15	16	19	22	27	32	35	36	32	27	21	17
Athen	13	14	17	20	26	30	34	34	29	24	18	14
Atlanta	11	13	18	23	26	30	31	31	28	23	17	12
Bangkok	32	33	35	36	35	34	33	33	33	32	32	32
Bogota	20	19	19	19	19	18	18	18	19	19	19	20
Buenos Aires	30	28	26	23	19	16	15	17	19	21	26	29
Caracas	30	28	30	30	31	32	32	32	33	32	31	30
Casablanca	18	18	20	21	22	25	26	27	26	24	21	19
Chicago	0	1	9	16	21	26	29	28	24	17	9	2
Colombo (Sri Lanka)	31	31	32	32	32	31	31	31	31	31	31	31
Dallas	13	16	21	25	29	33	36	36	32	26	19	14
Denver	7	8	14	14	21	28	32	30	25	18	12	6
Faro (Algarve)	16	16	19	21	23	27	29	29	26	23	19	17
Grand Canyon (Arizona)	6	8	13	15	21	27	29	27	25	18	12	6
Harare	27	26	27	26	24	21	22	24	28	29	28	27
Helsinki	-3	-3	2	9	15	20	23	21	17	9	3	0
Heraklion (Kreta)	15	16	18	20	24	27	30	30	27	24	20	17
Hongkong	19	20	23	26	30	32	33	33	32	30	25	21
Honolulu	26	26	27	27	28	30	30	31	30	30	28	27
Houston	16	19	23	27	30	33	34	35	32	28	21	17
Irkutsk	-14	-9	1	9	16	23	24	21	16	7	-4	-13
Istanbul	9	9	13	17	23	27	30	30	26	20	15	11
Jakutsk (Nordostsibirien)	-35	-28	-10	3	14	23	26	21	11	-3	-25	-34
Johannesburg	25	25	24	22	20	17	17	20	24	25	25	25
Kairo	19	20	24	27	32	35	35	35	34	30	25	20
Kapstadt	27	27	26	24	21	18	18	18	19	22	24	26
Kathmandu	18	21	25	28	28	29	28	28	28	26	23	20
Larnaka (Zypern)	17	18	20	23	26	31	33	34	31	28	23	19
Las Palmas	21	20	22	23	24	25	27	28	28	27	24	22
Las Vegas	15	16	23	26	31	38	40	39	35	27	20	14
Lhasa	9	10	13	17	21	24	23	22	21	17	13	10
Lima	26	26	27	24	21	20	19	18	19	20	22	24
Lissabon	14	15	18	20	23	27	28	29	27	22	17	15

Data Visualization Techniques

Type	Idea	Examples
Geometric	Visualization of geometric transformations and projections of the data	 Scatterplots  Parallel Coordinates
Icon-Based	Visualization of data as icons	 Chernoff Faces  Stick Figures
Pixel-oriented	Visualize each attribute value of each data object by one coloured pixel	 Recursive Patterns
Other		Hierarchical Techniques, Graph-based Techniques, Hybrid-Techniques, . . .

Slide credit: Keim, Visual Techniques for Exploring Databases, Tutorial Slides, KDD 1997.

2D Scatterplot



Characteristic

- Designed for two-dimensional data; two axes span the drawing area
- 2D objects are depicted as points in the diagram
- Orthogonal projections of points to axes indicate coordinate values
- Provides a first look at bivariate data to see clusters of points, outliers, etc.

Scatterplot Matrix

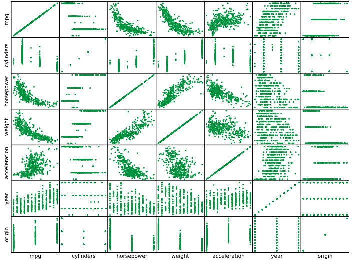
Characteristic

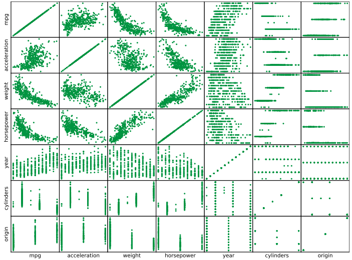
Matrix of scatterplots for pairs of dimensions

Ordering

Ordering of dimensions is important:

- Reordering improves understanding of structures and reduces clutter
- Interestingness of orderings can be evaluated with quality metrics (e.g. Peng et al.)



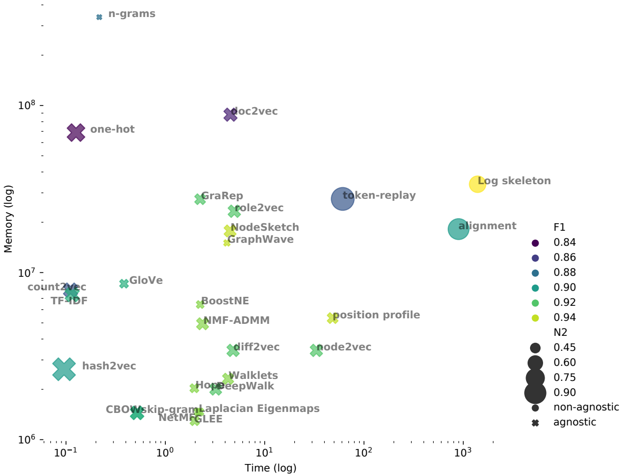


Clutter Reduction in Multi-Dimensional Data Visualization Using Dimension Reordering, IEEE Symp. on Inf. Vis., 2004.

Enhancing Scatterplot

Characteristic

- Using additional formats such as shape and color to represent additional dimensions
- More dimensions lead to higher complexity (information availability vs. interpretability



Trace encoding in process mining: A survey and benchmarking, Engineering Applications of Artificial Intelligence, EAAI, 2003.

Scatterplot Limitations

Limitations

- Scatterplots work well for two dimensions only
- Scatterplot matrices depict pairwise correlations only
- In perspective illustrations of three or more dimensions, projections get ambiguous

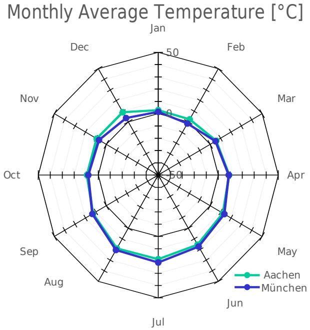
Polygonal Plots

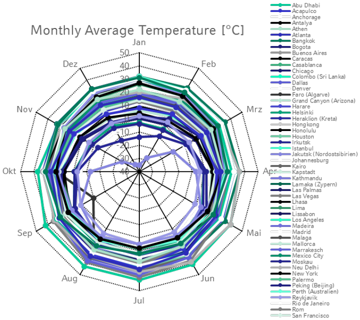
- Depict objects by curves rather than by points
- Coordinates are not indicated by orthogonal projections but by eplicit intersections of polygons with axes
- Example Spiderweb – axes remain connected at origin
- Example Parallel Coordinates – axes are aligned in parallel

Spiderweb Model

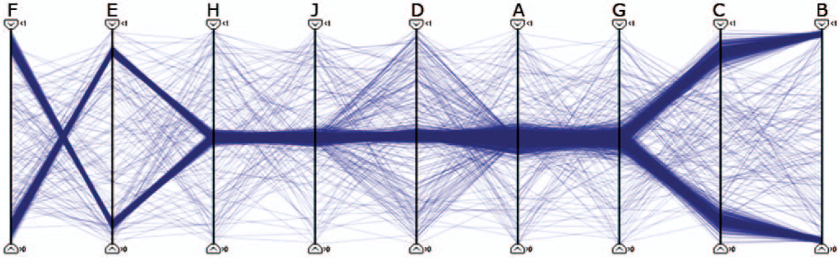
Characteristics

- Illustrate any single object by a polygonal line
- Contract origins of all axes to a global origin point
- Works well for few objects only





Parallel Coordinates



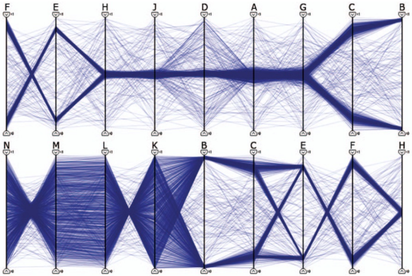
Characteristics

- d-dimensional data space is visualised by d parallel axes
- Each axis is scaled to min-max range
- Object = polygonal line intersecting axis at value in this dimension

Parallel Coordinates (cont'd)

Ordering

- Again, the ordering and orientation of the dimensions is important to reveal correlations
- The farer the attributes the harder their correlations are perceived; coloring helps



- Visualize clusters
- Visualize correlations between dimensions

Bertini et al., Quality Metrics in High-Dimensional Data Visualization: An Overview and Systematization, Trans. on Vis. and Comp. Graph., 2011.

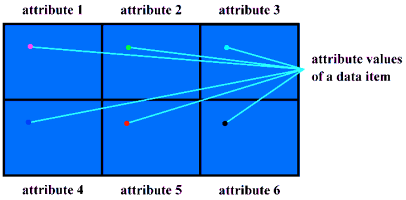
Pixel-Oriented Techniques

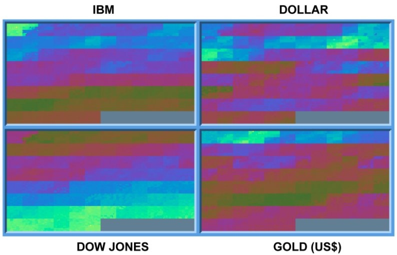
Characteristics

- Each data value is mapped onto a colored pixel
- Each dimension is shown in a separate window

How to arrange the pixel ordering?

One strategy: Recursive Patterns iterated line and column-based arrangements





Figures from Keim, Visual Techniques for Exploring Databases, Tutorial Slides, KDD 1997.

Chernoff Faces

Characteristics

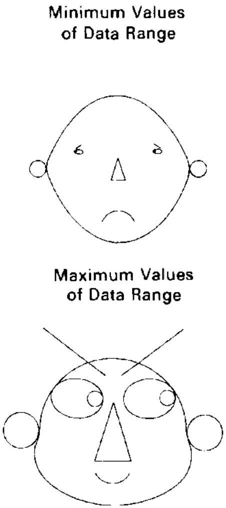
Map d-dimensional space to facial expression, e.g. length of nose = dim 6; curvature of mouth = dim 8

Advantage

Humans can evaluate similarity between faces much more intuitively than between high-dimensional vectors

Disadvantages

- Without dimensionality reduction only applicable to data spaces with up to 18 dimensions
- Which dimension represents what part?



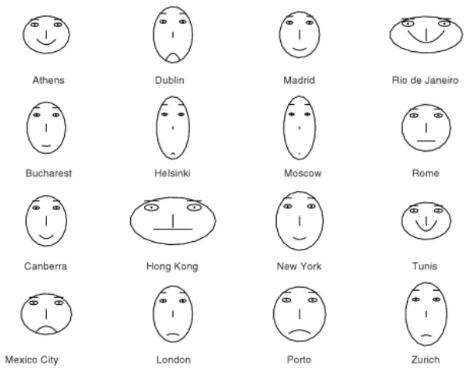
Figures taken from Mazza, Introduction to Information Visualization, Springer, 2009.

Chernoff Faces

Example: Weather Data

City	Precip. average	Temp. average	Temp. max average	Temp. min average	Record max	Record min
Athens	37	17	21	13	42	−3
Bucharest	58	11	16	5	49	−23
Canberra	62	12	19	6	42	−10
Dublin	74	10	12	6	28	−7
Helsinki	63	5	8	1	31	−36
Hong Kong	218	23	25	21	37	2
London	75	10	13	5	35	−13
Madrid	45	13	20	7	40	−10
Mexico City	63	17	23	11	32	−3
Moscow	59	4	8	1	35	−42
New York	118	12	17	8	40	−18
Porto	126	14	18	10	34	−2
Rio de Janeiro	109	25	30	20	43	7
Rome	80	15	20	11	37	−7
Tunis	44	18	23	13	46	−1
Zurich	107	9	12	6	35	−20

Table 4.1 Annual climatic values in Celsius of some world cities. Values from http://www.weatherbase.com.



Figures from Riccardo Mazza, Introduction to Information Visualization, Springer, 2009.

Chernoff Faces

Example: Finance Data

FIGURE 3
Facial Representation of Financial Performance (1 to 5 Years Prior to Failure)

FEDERAL

Date Dimensions	Year to Failure 5	4	3	2	1
1. Return on Assets	0.10	0.11	0.06	0.03	−0.16
2. Debt Service	3.66	3.79	1.55	0.78	−14.11
3. Cash Flows	1.53	1.48	1.39	1.35	0.94
4. Capitalization	0.22	0.20	0.18	0.16	−0.02
5. Current Ratio	71.40	89.10	97.85	96.80	58.21
6. Cash Turnover	24.03	25.92	25.62	27.40	71.26
7. Receivables Turnover	5.25	4.46	4.26	4.36	9.56
8. Inventory Turnover	5.38	4.77	4.57	4.44	5.34
9. Sales per Dollar Working Capital	6.74	6.33	7.02	7.61	−45.77
10. Retained Earning/ Total Assets	0.32	0.30	0.01	−0.01	−0.26
11. Total Assets	0.94	.76	0.39	0.45	0.43

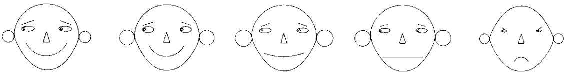


Figure from Huff et al., Facial Representation of Multivariate Data, Journal of Marketing, Vol. 45, 1981, pp. 53-59.

Agenda

Data Reduction

Why data reduction?

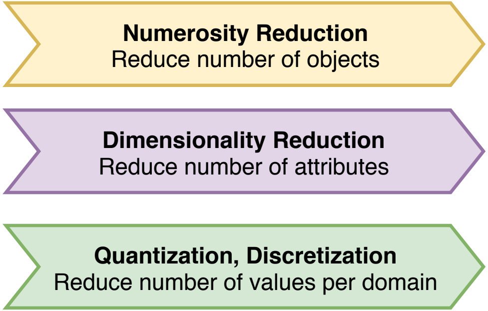
- Better perception of patterns
  - Raw (tabular) data is hard to understand
  - Visualization is limited to (hundreds of) thousands of objects
  - Reduction of data may help to identify patterns
- Computational complexity
  - Big data sets cause prohibitively long runtime for data mining algorithms
  - Reduced data sets are useful the more the algorithms produce (almost) the same analytical results

How to approach data reduction?

- Data aggregation (basic statistics)
- Data generalization (abstraction to higher levels)

Data Reduction Strategies: Three Directions

ID	A1	A2	A3
1	54	56	75
2	87	12	65
3	34	63	76
4	86	23	4



ID	A1	A3
1	L	75
3	XS	76
4	XL	4

Numerosity reduction

Reduce number of objects

- Sampling (loss of data)
- Aggregation (model parameters, e.g., center and spread)

Data Reduction Strategies (cont'd)

Dimensionality reduction

Reduce number of attributes

- Linear methods: feature sub-selection, Principal Components Analysis, Random projections, Fourier transform, Wavelet transform, etc
- Non-linear methods: Multidimensional scaling (force model), Neural embedding

Quantization, discretization

Reduce number of values per domain

- Binning (various types of histograms)
- Generalization along hierarchies (OLAP, attribute-oriented induction)

Data Aggregation

- Aggregation is numerosity reduction ($=$ less tuples)
- Generalization yields duplicates $\rightarrow$ add counting attribute and merge duplicate tuples

Name	Age	Major
Ann	27	CS
Bob	26	CS
Eve	19	CS

Generalization

Name	Age	Major
(any)	Twen	CS
(any)	Twen	CS
(any)	Teen	CS

Aggregation

Age	Major	Count
Twen	CS	2
Teen	CS	1

Basic Aggregates

- Central tendency: Where is the data located? Where is it centered?
  - Examples: mean, median, mode, etc. (see below)
- Variation, spread: How much do the data deviate from the center?
  - Examples: variance / standard deviation, min-max-range, ...

Examples

- Age of students is around 20
- Shoe size is centered around 40
- Recent dates are around 2020
- Average income is in the thousands

Distributive Aggregate Measures

Distributive Measures

The value of a *distributive measure d* on D can be calculated by combining the results of distributed calculations on partitions $D_i \subset D, D = D_1 \cup D_2 \cup \ldots D_n$

Examples

- $count(D_1 \cup D_2) = count(D_1) + count(D_2)$
- $sum(D_1 \cup D_2) = sum(D_1) + sum(D_2)$
- $min(D_1 \cup D_2) = min(min(D_1), min(D_2))$
- $max(D_1 \cup D_2) = max(max(D_1), max(D_2))$

Algebraic Aggregate Measures

Algebraic Measures

An *algebraic measure* on D can be computed by an algebraic function with M arguments (M being a bounded integer), each of which is obtained by applying a distributive aggregate function to the partitions $D_i \subset D, D = D_1 \cup D_2 \cup \ldots D_n$

Examples

- $avg(D_1 \cup D_2) = \frac{sum(D_1 \cup D_2)}{count(D_1 \cup D_2)} = \frac{sum(D_1)+sum(D_2)}{count(D_1)+count(D_2)}$
- Note: *avg* is note distributive, $avg(D_1 \cup D_2) \neq avg(avg(D_1), avg(D_2))$
- $standard\_deviation(D_1 \cup D_2)$

Holistic Aggregate Measures

Holistic Measures

There is no constant bound on the storage size that is needed to calculate and represent sub-aggregates.

Examples

- *median*: value in the middle of a sorted series of values (=50% quantile)

$$median(D_1 \cup D_2) \neq simple\_function(median(D_1), median(D_2))$$

- *mode*: value that appears most often in a set of values
- *rank*: k-smallest / k-largest value (cf. quantiles, percentiles)

Measuring the Central Tendency

Mean – (weighted) arithmetic mean

Well-known measure for central tendency ("average").

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

Mid-range

Average of the largest and the smallest values in a data set:

$$(max + min)/2$$

- Both are algebraic measures
- Applicable to numerical data only (sum, scalar multiplication)

  What about categorical data?

Measuring the Central Tendency (cont'd)

Median

- Middle value of sorted values (if their count is odd)
- For even number of values: average of the middle two values (numeric case), or one of the two middle values (non-numeric case)
- Applicable to ordinal data only, as a (total) order is required
- Median is a holistic measure

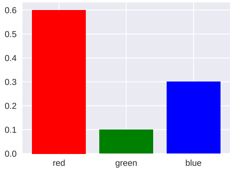
Examples

- never, never, never, rarely, <u>rarely</u>, often, usually, usually, always
- tiny, small, big, big, <u>big</u>, <u>big</u>, big, big, huge, huge
- tiny, tiny, small, <u>medium</u>, <u>big</u>, big, large, huge

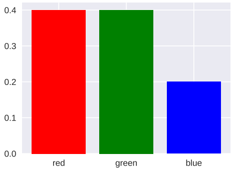
What if there is no ordering?

Measuring the Central Tendency

Unimodal



Bimodal



Mode

- Value that occurs most frequently in the data
- Example: *blue*, red, *blue*, yellow, green, *blue*, red
- Unimodal, bimodal, trimodal, . . . : There are 1, 2, 3, . . . modes in the data (multi-modal in general), cf. mixture models
- There is no mode if each data value occurs only once
- Well suited for categorical (i.e., non-numerical) data

Measuring the Dispersion of Data

Variance

- The variance measures the spread around the mean of numerical data:

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

- The single pass calculation (sum of squares and square of sum in parallel) is faster than the two-pass method but numerically less robust in case of big numbers.
- Variance is zero if and only if all the values are equal
- Standard deviation is equal to the square root of the variance
- Both the standard deviation and the variance are algebraic measures

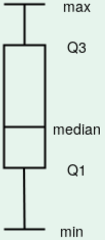
Boxplot Analysis

Boxplots comprise a five-number summary of a dataset

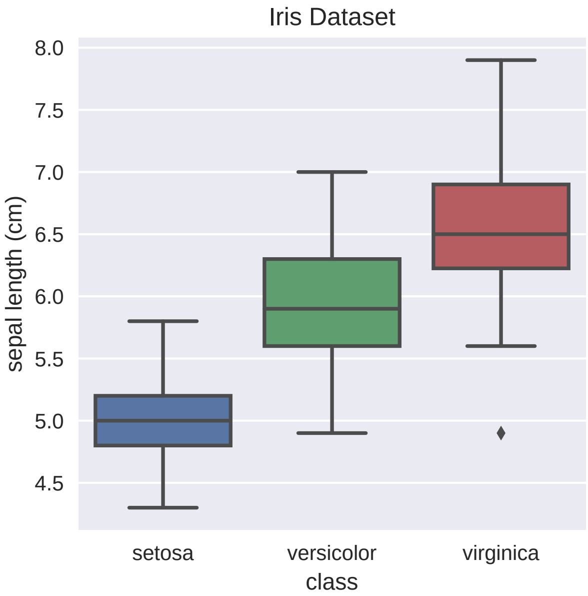
- Minimum, first quartile, median, third quartile, maximum
- These are the 0%, 25%, 50%, 75%, 100% quantiles of the data
- Also called "25-percentile", etc.

Boxplot illustration

- The box ranges from the first to the third quartile
- Height: inter-quartile range (IQR) = Q3 - Q1
- The median is marked by a line within the box
- Whiskers at minimum and maximum value
- Outliers: usually values more than $1.5 \cdot IQR$ below Q1 or above Q3

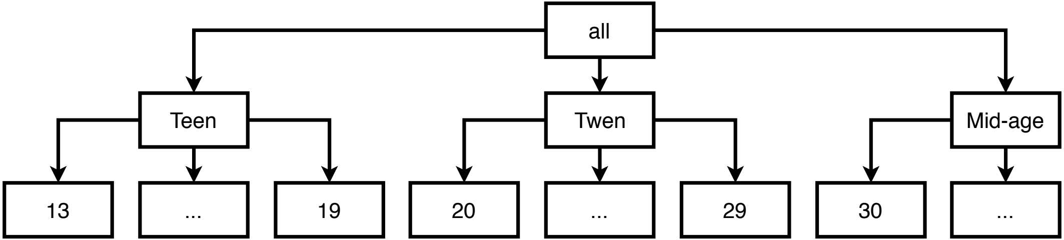


Boxplot Example



Data Generalization

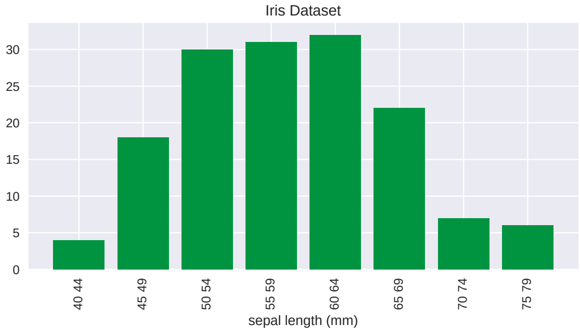
- Quantization may use generalization
  - E.g., group age (7 bits $\rightarrow$ 128 values) to age_range (4 bits $\rightarrow$ 16 values only)
- Dimensionality reduction is a borderline case of quantization
  - Dropping age corresponds to reduction zero bits
  - Corresponds to generalization of age to "all" = "any age" = no information



Data Generalization

- How to group the values of an attribute into partitions?
- Overall data (no partitioning, i.e., single partition)
  - Overall mean, overall variance: too coarse (overgeneralization)
- Different techniques to form groups for aggregation
  - Binning – histograms, based on value ranges
  - Generalization – abstraction based on generalization hierarchies
  - Clustering (see later) – based on object similarity

Binning Techniques: Histograms



- Histograms use binning to approximate data distributions
- Divide data into bins and store a representative (sum, average, median) for each bin

Equi-width Histograms

- Divide the range into N intervals of equal size (uniform grid)
- If A and B are the lowest and highest values of the attribute, the width of intervals will be $(B - A)/N$

Benefits

- Most straightforward
- Easy to understand

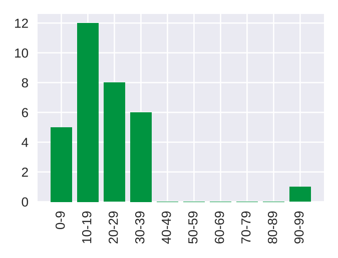
Limitations

- Outliers may dominate presentation
- Skewed data is not handled well

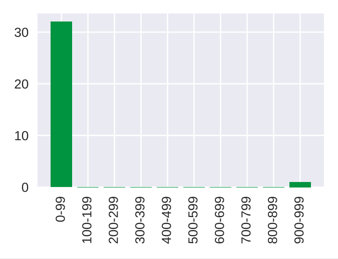
Equi-width Histograms

Example

- Sorted data, 10 bins: 5, 7, 8, 8, 9, 11, 13, 13, 14, 14, 14, 15, 17, 17, 17, 18, 19, 23, 24, 25, 26, 26, 26, 27, 28, 32, 34, 36, 37, 38, 39, 97



- Insert 999



Equi-height Histograms

Divide the range into N intervals, each containing approx. the same number of samples (*quantile-based approach*)

Benefits

- Good data scaling
- Less prone to outliers

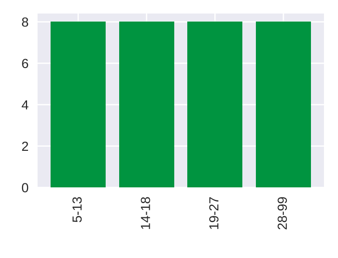
Limitations

- Key information in bin boundaries (somehow subtle)
- If any value occurs often, the equal frequency criterion might not be met (intervals have to be disjoint!)

Equi-height Histograms

Example

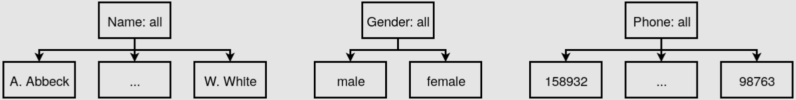
- Same data, 4 bins: 5, 7, 8, 8, 9, 11, 13, 13, 14, 14, 14, 15, 17, 17, 17, 18, 19, 23, 24, 25, 26, 26, 26, 27, 28, 32, 34, 36, 37, 38, 39, 97



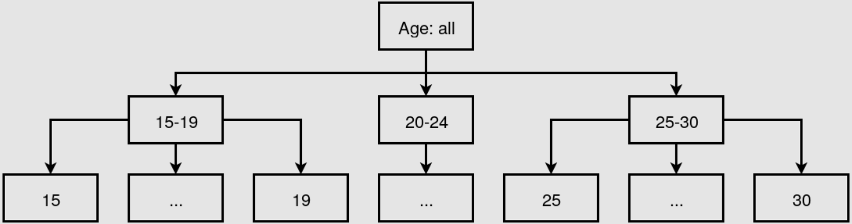
- Median = 50%-quantile
  - More robust against outliers (cf. value 999 from above)
  - Four bin example is strongly related to boxplot

Concept Hierarchies: Examples

Flat groups (i.e., no serious hierarchies)

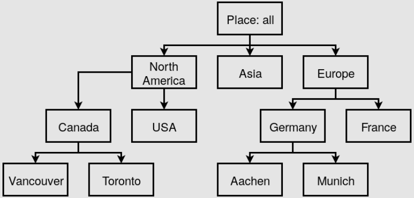


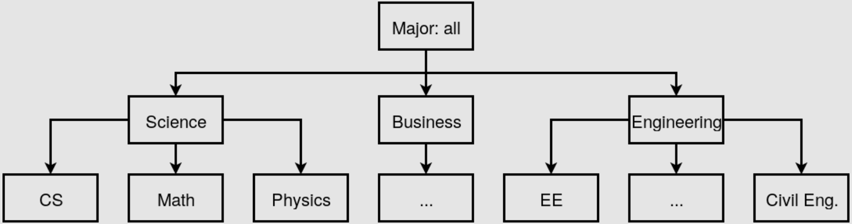
Hierarchies by subgrouping



Concept Hierarchies: Examples

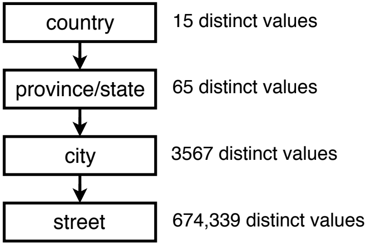
Hierarchies from schema information





Concept Hierarchy for Categorical Data

- Concept hierarchies can be specified by (expert) users
- Heuristically generate a hierarchy for a set of (related) attributes
  - based on the number of distinct values per attribute in the attribute set
  - The attribute with the most distinct values is placed at the lowest level of the hierarchy

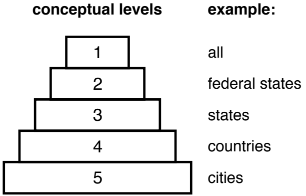


- Fails for counter examples: 20 distinct years, 12 months, 7 days_of_week, but not "year $<$ month $<$ days_of_week" with the latter on top

Summarization-based Aggregation

Data Generalization

A process which abstracts a large set of task-relevant data in a database from low conceptual levels to higher ones.



- Approaches:
  - Data-cube approach (OLAP / Roll-up) – manual
  - Attribute-oriented induction (AOI) – automated

Basic OLAP (Online Analytical Processing) Operations

Roll up

Summarize data by climbing up hierarchy or by dimension reduction.

Drill down

Reverse of roll-up. From higher level summary to lower level summary or detailed data, or introducing new dimensions.

Slice and dice

Selection on one (slice) or more (dice) dimensions.

Pivot (rotate)

Reorient the cube, visualization, 3D to series of 2D planes.

Example: Roll up / Drill down

Query

```sql
SELECT country, quarter, some_agg_fnc(...)
FROM business
GROUP BY country, quarter
```

Roll-Up

```sql
SELECT continent, quarter, some_agg_fnc(...)
FROM business
GROUP BY continent, quarter
```

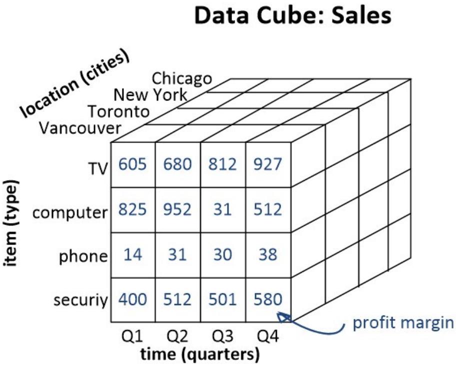
```sql
SELECT country, some_agg_fnc(...)
FROM business
GROUP BY country
```

Drill-Down

```sql
SELECT city, quarter, some_agg_fnc(...)
FROM business
GROUP BY city, quarter
```

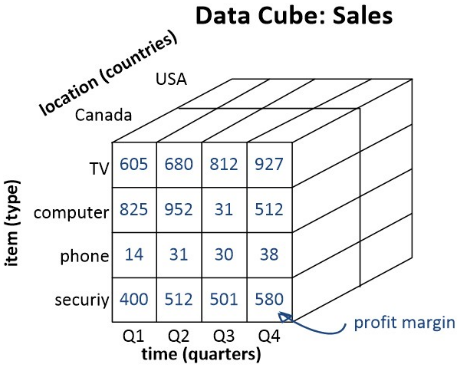
```sql
SELECT country, quarter, product, some_agg_fnc(...)
FROM business
GROUP BY country, quarter, product
```

Example: Roll up and Drill-Down in a Data Cube



Roll Up $\Longrightarrow$

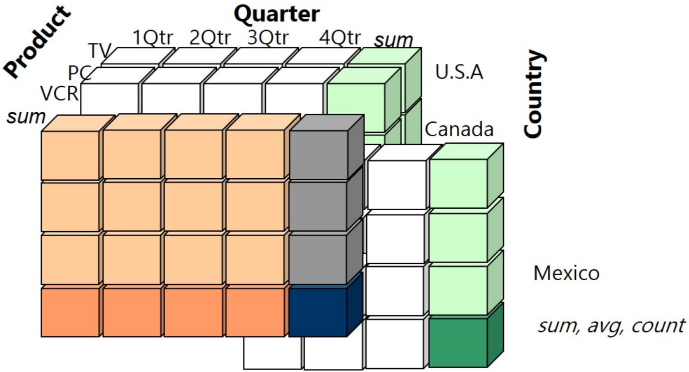
Drill-Down $\Longleftarrow$



Example: Slice Operation

```
SELECT income
FROM   time t, product p, country c
WHERE  p.name = 'VCR'
```

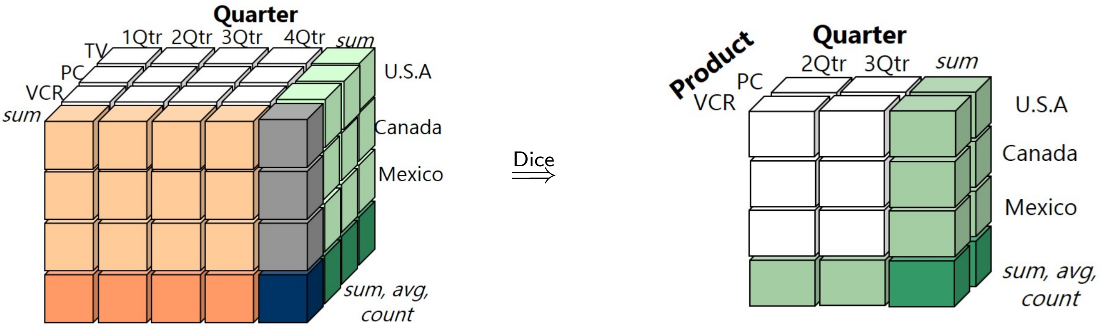
VCR dimension is chosen



Example: Dice Operation

```
SELECT income
FROM   time t, product p, country c
WHERE  p.name = 'VCR' OR p.name = 'PC' AND t.quarter BETWEEN 2 AND 3
```

sub-data cube over PC, VCR and quarters 2 and 3 is extracted



Example: Pivot (rotate)

year	17			18			19		
product	TV	PC	VCR	TV	PC	VCR	TV	PC	VCR
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

$\downarrow$ Pivot (rotate) $\downarrow$

product	TV			PC			VCR		
year	17	18	19	17	18	19	17	18	19
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

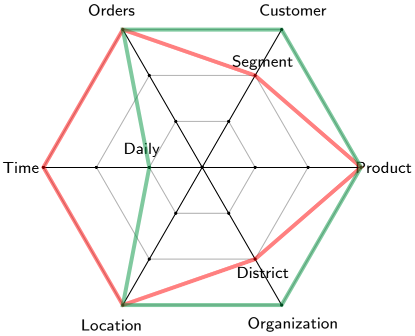
Further OLAP Operations

Other operations

- *Drill across:* involving (across) more than one fact table
- *Drill through:* through the bottom level of the cube to its back-end relational tables (using SQL)

Specifying Generalizations by Star-Nets

- Each circle is called a *footprint*
- Footprints represent the granularities available for OLAP operations



Discussion of OLAP-based Generalization

- Strength
  - Efficient implementation of data generalization
  - Computation of various kinds of measures, e.g., count, sum, average, max
  - Generalization (and specialization) can be performed on a data cube by roll-up (and drill-down)
- Limitations
  - Handles only dimensions of simple non-numeric data and measures of simple aggregated numeric values
  - Lack of intelligent analysis, does not suggest which dimensions should be used and what levels the generalization should aim at

Attribute-Oriented Induction (AOI)

- More automated approach than OLAP
- Apply aggregation by merging identical, generalized tuples and accumulating their respective counts.
- Builds on *data focusing:* task-relevant data, including dimensions, resulting in the *initial relation*
- Generates a *generalization plan:* decide for either *attribute removal* or *attribute generalization*

Attribute-Oriented Induction (AOI)

Three choices for each attribute: keep it, remove it, or generalize it

Attribute Removal

Remove attribute A in the following cases:

- There is a large set of distinct values for A but there is no generalization operator (concept hierarchy) on A, or
- A's higher level concepts are expressed in terms of other attributes (e.g. *street* is covered by *city*, *state*, *country*).

Attribute Generalization

If there is a large set of distinct values for A, and there exists a set of generalization operators (i.e., a concept hierarchy) on A, then select an operator and generalize A.

Attribute Oriented Induction: Example

Name	Gender	Major	Birth place	Birth data	Residence	Phone	GPA
Jim Woodman	M	CS	Vancouver, BC, Canada	8-12-81	3511 Main St., Richmond	687-4598	3.67
Scott Lachance	M	CS	Montreal, Que, Canada	28-7-80	345 1st Ave., Richmond	253-9106	3.70
Laura Lee	F	Physics	Seattle, WA, USA	25-8-75	125 Austin Ave., Burnaby	420-5232	3.83
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

- Name: large number of distinct values, no hierarchy – removed
- Gender: only two distinct values – retained
- Major: many values, hierarchy exists – generalized to Sci., Eng., Biz.
- Birth_place: many values, hierarchy – generalized, e.g., to country
- Birth_date: many values – generalized to age (or age_range)
- Residence: many streets and numbers – generalized to city
- Phone number: many values, no hierarchy – removed
- Grade_point_avg (GPA): hierarchy exists – generalized to good, . . .
- Count: additional attribute to aggregate base tuples

Attribute Oriented Induction: Example

- Initial Relation:

Name	Gender	Major	Birth place	Birth data	Residence	Phone	GPA
Jim Woodman	M	CS	Vancouver, BC, Canada	8-12-81	3511 Main St., Richmond	687-4598	3.67
Scott Lachance	M	CS	Montreal, Que, Canada	28-7-80	345 1st Ave., Richmond	253-9106	3.70
Laura Lee	F	Physics	Seattle, WA, USA	25-8-75	125 Austin Ave., Burnaby	420-5232	3.83
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

- Prime Generalized Relation:

Gender	Major	Birth region	Age Range	Residence	GPA	Count
M	Science	Canada	20-25	Richmond	Very good	16
F	Science	Foreign	25-30	Burnaby	Excellent	22
⋮	⋮	⋮	⋮	⋮	⋮	⋮

- Crosstab for generalized relation:

	Canada	Foreign	Total
M	16	14	30
F	10	22	32
Total	26	36	62

Attribute Generalization Control

- Two common approaches
  - *Attribute-threshold control:* default or user-specified, typically 2-8 values
  - *Generalized relation threshold control:* control the size of the final relation/rule, e.g., 10-30 tuples
- Tradeoff: how many distinct values for an attribute?
  - *Overgeneralization:* values are too high-level
  - *Undergeneralization:* level not sufficiently high
  - Both yield tuples of poor usefulness

Strategies for Next Attribute Selection

- Aiming at *minimal degree of generalization*
  - Choose attribute that reduces the number of tuples the most
  - Useful heuristic: choose attribute with highest number of distinct values.
- Aiming at *similar degree of generalization* for all attributes
  - Choose the attribute currently having the least degree of generalization
- *User-controlled*
  - Domain experts may specify appropriate priorities for the selection of attributes