Ludwig-Maximilians-Universität München
Lehrstuhl für Datenbanksysteme und Data Mining
Prof. Dr. Thomas Seidl

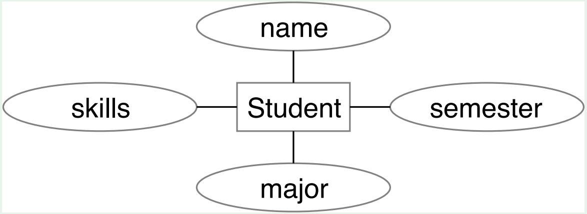
Knowledge Discovery and Data Mining I

Winter Semester 2018/19

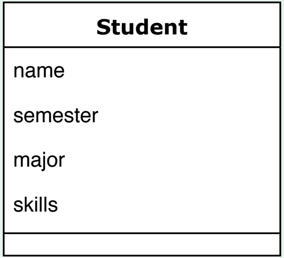
Agenda

Objects and Attributes

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

Overview of (Attribute) Data Types

Simple Data Types

Numeric/metric, Categorical/nominal, ordinal

Composed Data Types

Sets, sequences, vectors

Complex Data Types

- Multimedia: Images, videos, audio, text, documents, web pages, etc.
- Spatial, geometric: Shapes, molecules, geography, etc.
- Structures: Graphs, networks, trees, etc.

Simple Data Types: Numeric Data

Numeric Data

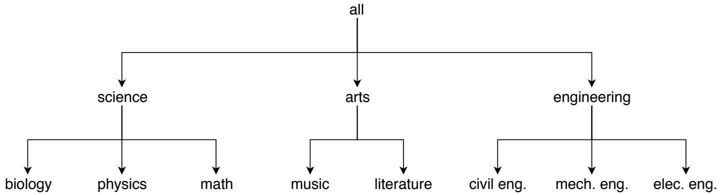
- Numbers: natural, integer, rational, real numbers
- Examples: age, income, shoe size, height, weight
- Comparison: difference
- Example: 3 is more similar to 30 than to 3,000

Simple Data Types: Categorical Data

- "Just identities"
- Examples:
  - occupation = { butcher, hairdresser, physicist, physician, ... }
  - subjects = { physics, biology, math, music, literature, ... }
- Comparison: How to compare values?
  - Trivial metric:

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

  - Generalization hierarchy: Use path length



Generalization: Metric Data

Metric Space

Metric space (O, d) consists of object set O and *metric distance* function $d : O \times O \rightarrow \mathbb{R}^{\geq 0}$ 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 with Euclidean distance

Simple Data Types: Ordinal

Characteristic

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

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

Examples

- Words & lexicographic ordering: *high* $\leq$ *highschool* $\leq$ *highscore*
- (Vague) sizes: *tiny* $\leq$ *small* $\leq$ *medium* $\leq$ *big* $\leq$ *huge*
- Frequencies: *never* $\leq$ *seldom* $\leq$ *rarely* $\leq$ *occasionally* $\leq$ *sometimes* $\leq$ *often* $\leq$ *frequently* $\leq$ *regularly* $\leq$ *usually* $\leq$ *always*

Composed Data Types: Sets

Characteristic

Unordered collection of individual values

Example

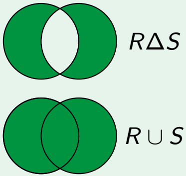
- skills = { Java, C, Python }

Comparison

- Symmetric Set Difference:

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

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



Composed Data Types: Sets

Bitvector Representation

- Given a set S, an ordered base set $B = (b_1, \ldots, b_n)$, create 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

Composed Data Types: Sequences, Vectors

Characteristic

- Put n values of a domain D together
- Order does matter: $I_n \to D$ for an index set $I_n = \{1, \ldots, n\}$

Examples

(Simple) sum	$d_1(o,q) = \sum_{i=1}^{n} \lvert o_i - q_i \rvert$	(Manhattan)
Root of sum of squares	$d_2(o,q) = \sqrt{\sum_{i=1}^{n} (o_i - q_i)^2}$	(Euclidean)
Maximum	$d_3(o,q) = \max_{i=1}^{n} \lvert o_i - q_i \rvert$	(Maximum)
General formula	$d_4(o,q) = \sqrt[p]{\sum_{i=1}^{n} \lvert o_i - q_i \rvert^p}$	(Minkowski)
Weighting of dimensions	$d_5(o,q) = \sqrt[p]{\sum_{i=1}^{n} w_i \cdot \lvert o_i - q_i \rvert^p}$	(Weighted Minkowski)

Complex Data Types

Components

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

Similarity models: Approaches

- Direct measures – highly data type dependent
- Feature engineering – explicit vector space embedding with hand-crafted features
- Feature learning – explicit vector space embedding learned by machine learning model, e.g. neural network
- Kernel trick – implicit vector space embedding

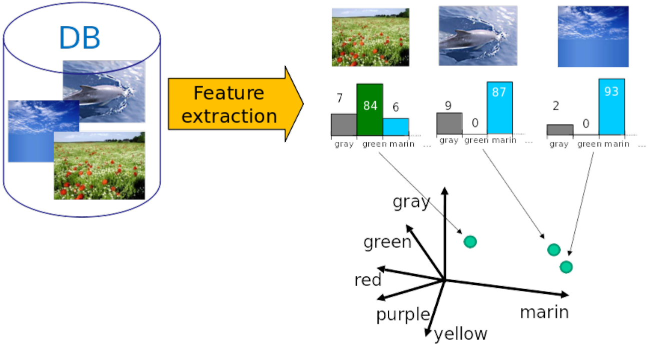
Complex Data Types

Examples for similarity models

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

Feature Extraction

- Objects from database DB are mapped to feature vectors



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

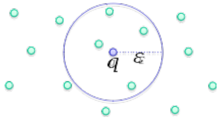
Similarity Queries

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

Range query

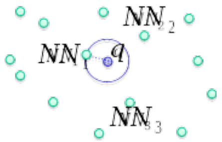
Range query for range parameter $\epsilon \in \mathbb{R}_0^+$:

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



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 $k \in \mathbb{N}$:

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

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

Ranking query

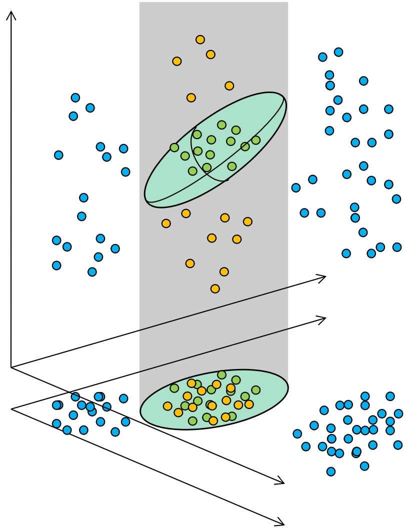
Ranking query (partial sorting query): "get next" functionality for picking database objects in an increasing order w.r.t. their distance to q:

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

Similarity Search

- Example: Range query $range(DB, q, d, \epsilon) = \{o \in DB \mid d(o, q) \leq \epsilon\}$
- Naive search by sequential scan
  - Fetch database objects from secondary storage (e.g. disk): $O(n)$
  - Check distances individually: $O(n)$
- 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 (fast) $O(n)$, $O(\log n)$ 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[b] criteria for filter quality
  - I ndexable – Index enabled
  - C omplete – No false dismissals
  - E fficient – Fast individual calculation
  - S elective – Small candidate set

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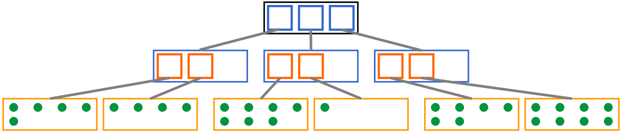
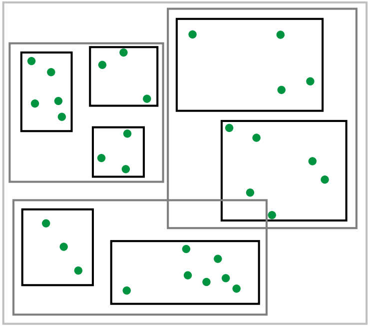
[a] GEMINI: Faloutsos 1996; KNOP: Seidl & Kriegel 1998

[b] Assent, Wenning, Seidl: ICDE 2006

Indexing

- 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

Indexing

- 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