# Data Mining and Knowledge Discovery

**Part of**
**Jožef Stefan IPS Programme - ICT3**
**and UL Programme - Statistics**

**2015 / 2016**

**Nada Lavrač**

Jožef Stefan Institute
Ljubljana, Slovenia



## Jožef Stefan Institute and IPS

$j = \sigma T^4$

- **Jožef Stefan Institute (JSI, founded in 1949)**
  - named after a distinguished physicist Jožef Stefan (1835-1893)
  - leading national research organization in natural sciences and technology (~700 researchers and students)
- **JSI research areas**
  - information and communication technologies
  - chemistry, biochemistry & nanotechnology
  - physics, nuclear technology and safety
- **Jožef Stefan International Postgraduate School (IPS, founded in 2004)**
  - offers MSc and PhD programs (ICT, nanotechnology, ecotechnology)
  - research oriented, basic + management courses
  - in English



## Jožef Stefan Institute Department of Knowledge Technologies

- **Head:** Nada Lavrač, **Staff:** 30 researchers, 10 students
- **Machine learning & Data mining**
  - ML (decision tree and rule learning, subgroup discovery, …)
  - Text and Web mining
  - Relational data mining - inductive logic programming
  - Equation discovery
- **Other research areas:**
  - Knowledge management
  - Decision support
  - Human language technologies
- **Applications:**
  - Medicine, Bioinformatics, Public Health
  - Ecology, Finance, …



## Course Outline

**I. Introduction**
- Data Mining in a Nutshell
- Predictive and descriptive DM techniques
- Data Mining and KDD process
- DM standards, tools and visualization

(Mladenić et al. Ch. 1 and 11)

**II. Predictive DM Techniques**
- Bayesian classifier (Kononenko Ch. 9.6)
- Decision Tree learning (Mitchell Ch. 3, Kononenko Ch. 9.1)
- Classification rule learning (Kononenko Ch. 9.2)
- Classifier Evaluation (Bramer Ch. 6)

**III. Regression**
(Kononenko Ch. 9.4)

**IV. Descriptive DM**
- Predictive vs. descriptive induction
- Subgroup discovery
- Association rule learning (Kononenko Ch. 9.3)
- Hierarchical clustering (Kononenko Ch. 12.3)

**V. Relational Data Mining**
- RDM and Inductive Logic Programming (Dzeroski & Lavrac Ch. 3, Ch. 4)
- Propositionalization approaches
- Relational subgroup discovery

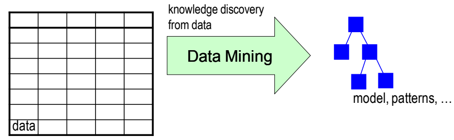


## Part I. Introduction

- Data Mining in a Nutshell
- Predictive and descriptive DM techniques
- Data Mining and the KDD process
- DM standards, tools and visualization



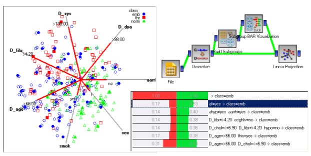
## Basic Data Mining Task




**Input:** transaction data table, relational database, text documents, Web pages
**Goal:** build a classification model, find interesting patterns in data, ...

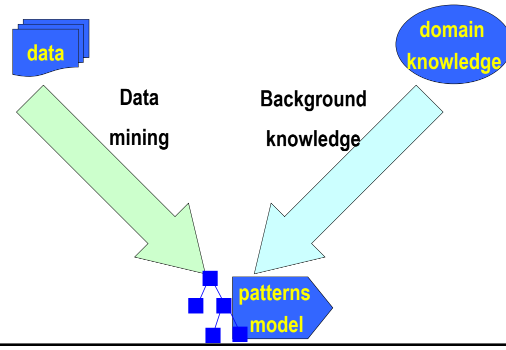
## Data Mining and Machine Learning

- Machine learning techniques
  - classification rule learning
  - subgroup discovery
  - relational data mining and ILP
  - equation discovery
  - inductive databases
- Data mining and decision support integration
- Data mining applications
  - medicine, health care
  - ecology, agriculture
  - knowledge management, virtual organizations



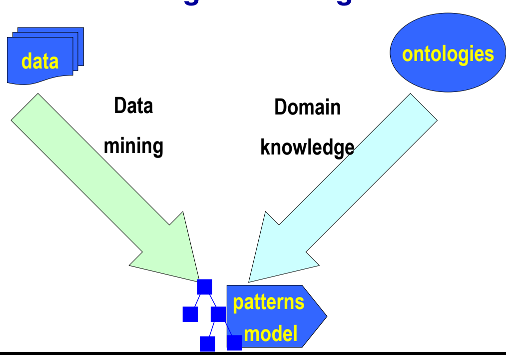


## Relational data mining: domain knowledge = relational database



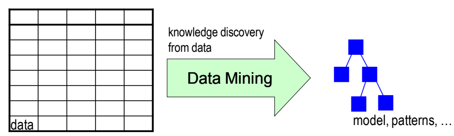



## Semantic data mining: domain knowledge = ontologies

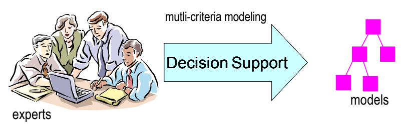





## Basic DM and DS Tasks



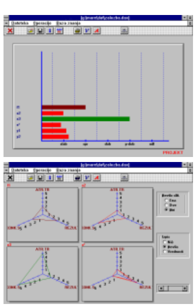

**Input:** transaction data table, relational database, text documents, Web pages
**Goal:** build a classification model, find interesting patterns in data, ...

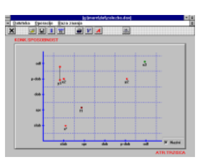


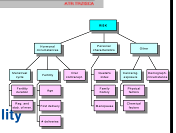

**Input:** expert knowledge about data and decision alternatives
**Goal:** construct decision support model – to support the evaluation and choice of best decision alternatives



## Decision support tools: DEXi



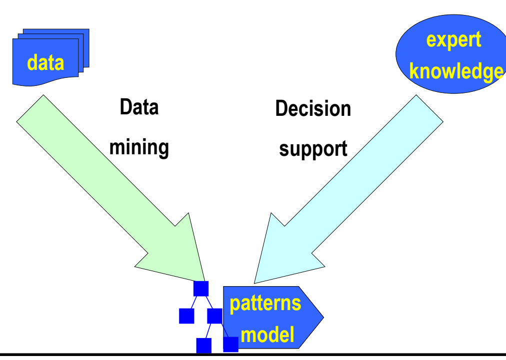




DEXi supports :
- *if-then* analysis
- analysis of stability
- Time analysis
- *how* explanation
- *why* explanation



## DM and DS integration

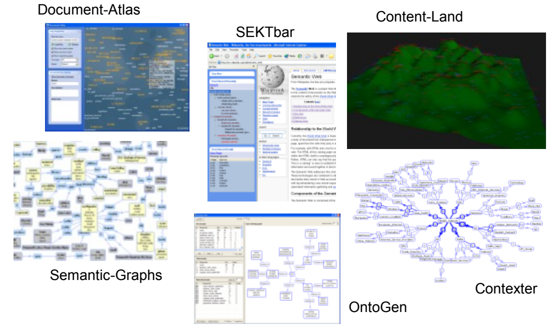


## Basic Text and Web Mining Task


**Input:** text documents, Web pages
**Goal:** text categorization, user modeling, data visualization...

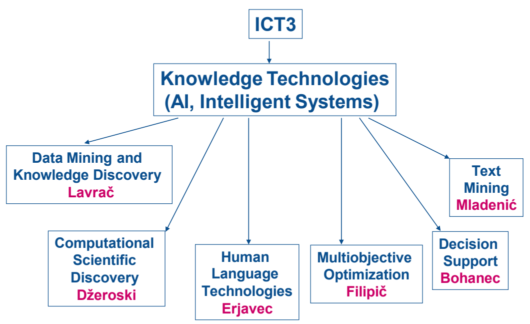


## Text Mining (lectures by D. Mladenić)






## Knowledge Technologies: Main research areas & IPS lectures






**videolectures.net portal**

~ 10,000 lectures

**http//:videolectures.net**



## Selected Publications



## Part I. Introduction

- Data Mining in a Nutshell
- Predictive and descriptive DM techniques
- Data Mining and the KDD process
- DM standards, tools and visualization

## What is DM

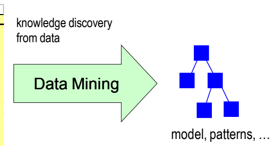
- Extraction of useful information from data: discovering relationships that have not previously been known
- The viewpoint in this course: Data Mining is the application of Machine Learning techniques to solve real-life data analysis problems



## Data Mining in a Nutshell

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | NONE |
| O2 | 23 | myope | no | normal | SOFT |
| O3 | 22 | myope | yes | reduced | NONE |
| O4 | 27 | myope | yes | normal | HARD |
| O5 | 19 | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | SOFT |
| O15 | 43 | hypermetrope | yes | reduced | NONE |
| O16 | 39 | hypermetrope | yes | normal | NONE |
| O17 | 54 | myope | no | reduced | NONE |
| O18 | 62 | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NONE |

data




**Given:** transaction data table, relational database, text documents, Web pages
**Find:** a classification model, a set of interesting patterns



## Data Mining in a Nutshell

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
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| O1 | 17 | myope | no | reduced | NONE |
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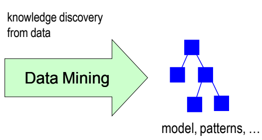
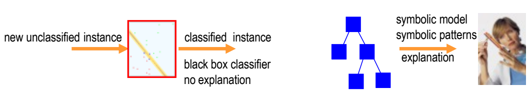
| O17 | 54 | myope | no | reduced | NONE |
| O18 | 62 | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NONE |

data




**Given:** transaction data table, relational database, text documents, Web pages
**Find:** a classification model, a set of interesting patterns





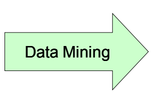

## Simplified example: Learning a classification model from contact lens data

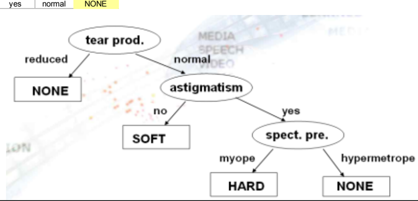
| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | NONE |
| O2 | 23 | myope | no | normal | SOFT |
| O3 | 22 | myope | yes | reduced | NONE |
| O4 | 27 | myope | yes | normal | HARD |
| O5 | 19 | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | SOFT |
| O15 | 43 | hypermetrope | yes | reduced | NONE |
| O16 | 39 | hypermetrope | yes | normal | NONE |
| O17 | 54 | myope | no | reduced | NONE |
| O18 | 62 | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NONE |



## Simplified example: Learning a classification model from contact lens data

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | young | myope | no | reduced | NONE |
| O2 | young | myope | no | normal | SOFT |
| O3 | young | myope | yes | reduced | NONE |
| O4 | young | myope | yes | normal | HARD |
| O5 | young | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | pre-presbyc | hypermetrope | no | normal | SOFT |
| O15 | pre-presbyc | hypermetrope | yes | reduced | NONE |
| O16 | pre-presbyc | hypermetrope | yes | normal | NONE |
| O17 | presbyopic | myope | no | reduced | NONE |
| O18 | presbyopic | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | presbyopic | hypermetrope | yes | normal | NONE |






## Task reformulation: Binary Class Values

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | NO |
| O2 | 23 | myope | no | normal | YES |
| O3 | 22 | myope | yes | reduced | NO |
| O4 | 27 | myope | yes | normal | YES |
| O5 | 19 | hypermetrope | no | reduced | NO |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | YES |
| O15 | 43 | hypermetrope | yes | reduced | NO |
| O16 | 39 | hypermetrope | yes | normal | NO |
| O17 | 54 | myope | no | reduced | NO |
| O18 | 62 | myope | no | normal | NO |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NO |

Binary classes (positive vs. negative examples of Target class)
- for Concept learning – classification and class description
  - for Subgroup discovery – exploring patterns characterizing groups of instances of target class

## Learning from Numeric Class Data

| Person | Age | Spect. presc. | Astigm. | Tear prod. | LensPrice |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | 0 |
| O2 | 23 | myope | no | normal | 8 |
| O3 | 22 | myope | yes | reduced | 0 |
| O4 | 27 | myope | yes | normal | 5 |
| O5 | 19 | hypermetrope | no | reduced | 0 |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | 5 |
| O15 | 43 | hypermetrope | yes | reduced | 0 |
| O16 | 39 | hypermetrope | yes | normal | 0 |
| O17 | 54 | myope | no | reduced | 0 |
| O18 | 62 | myope | no | normal | 0 |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | 0 |

Numeric class values – regression analysis



## Learning from Unlabeled Data

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | NONE |
| O2 | 23 | myope | no | normal | SOFT |
| O3 | 22 | myope | yes | reduced | NONE |
| O4 | 27 | myope | yes | normal | HARD |
| O5 | 19 | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | SOFT |
| O15 | 43 | hypermetrope | yes | reduced | NONE |
| O16 | 39 | hypermetrope | yes | normal | NONE |
| O17 | 54 | myope | no | reduced | NONE |
| O18 | 62 | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NONE |

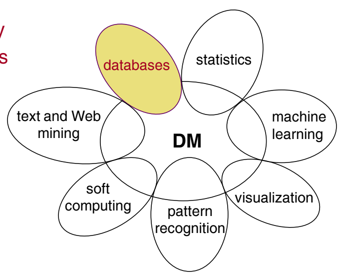
Unlabeled data - clustering: grouping of similar instances
- association rule learning



## Data Mining: Related areas

Database technology and data warehouses

- efficient storage, access and manipulation of data

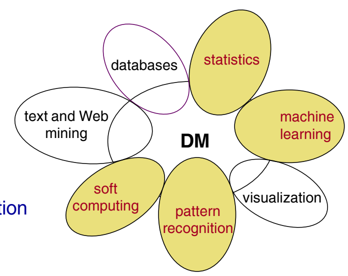





## Related areas

Statistics, machine learning, pattern recognition and soft computing*

- classification techniques and techniques for knowledge extraction from data



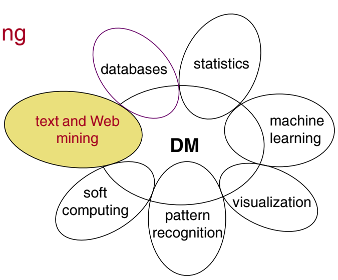

*neural networks, fuzzy logic, genetic algorithms, probabilistic reasoning



## Related areas

Text and Web mining

- Web page analysis
- text categorization
- acquisition, filtering and structuring of textual information
- natural language processing

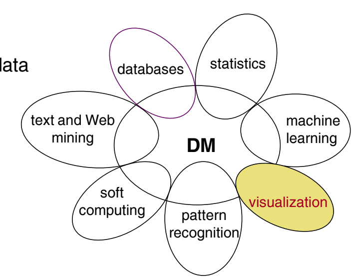





## Related areas

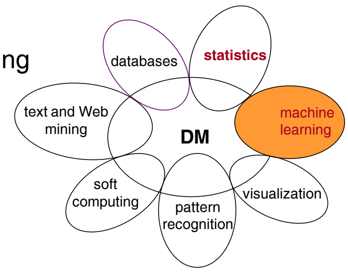
Visualization

- visualization of data and discovered knowledge



## Point of view in this course

Knowledge discovery using machine learning methods






## Data Mining, ML and Statistics

- All three areas have a long tradition of developing inductive techniques for data analysis.
  - reasoning from properties of a data sample to properties of a population
- **DM vs. ML - Viewpoint in this course**:
  - Data Mining is the application of Machine Learning techniques to hard real-life data analysis problems



## Data Mining, ML and Statistics

- All three areas have a long tradition of developing inductive techniques for data analysis.
  - reasoning from properties of a data sample to properties of a population
- **DM vs. Statistics:**
  - **Statistics**
    - Hypothesis testing when certain theoretical expectations about the data distribution, independence, random sampling, sample size, etc. are satisfied
    - Main approach: best fitting all the available data
  - **Data mining**
    - Automated construction of understandable patterns, and structured models
    - Main approach: structuring the data space, heuristic search for decision trees, rules, … covering (parts of) the data space



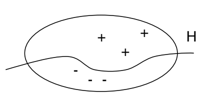
## Part I. Introduction

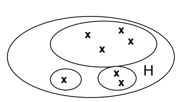
- Data Mining in a Nutshell
- Predictive and descriptive DM techniques
- Data Mining and the KDD process
- DM standards, tools and visualization



## Types of DM tasks

- **Predictive DM:**
  - Classification (learning of rules, decision trees, ...)
  - Prediction and estimation (regression)
  - Predictive relational DM (ILP)
- **Descriptive DM:**
  - description and summarization
  - dependency analysis (association rule learning)
  - discovery of properties and constraints
  - segmentation (clustering)
  - subgroup discovery

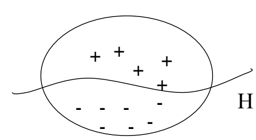


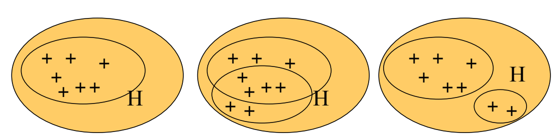



## Predictive vs. descriptive DM

**Predictive DM**




**Descriptive DM**



## Predictive vs. descriptive DM

- **Predictive DM:** Inducing classifiers for solving classification and prediction tasks,
  - Classification rule learning, Decision tree learning, ...
  - Bayesian classifier, ANN, SVM, ...
  - Data analysis through hypothesis generation and testing
- **Descriptive DM:** Discovering interesting regularities in the data, uncovering patterns, ... for solving KDD tasks
  - Symbolic clustering, Association rule learning, Subgroup discovery, ...
  - Exploratory data analysis



## Predictive DM formulated as a machine learning task:

- Given a set of labeled **training examples** (n-tuples of attribute values, labeled by class name)

| | A1 | A2 | A3 | Class |
|---|---|---|---|---|
| example1 | $v_{1,1}$ | $v_{1,2}$ | $v_{1,3}$ | $C_1$ |
| example2 | $v_{2,1}$ | $v_{2,2}$ | $v_{2,3}$ | $C_2$ |

. .

- By performing generalization from examples (induction) find a **hypothesis** (classification rules, decision tree, …) which explains the training examples, e.g. rules of the form:

  $(A_i = v_{i,k})$ & $(A_j = v_{j,l})$ & ... ➔ Class = $C_n$



## Predictive DM - Classification

- data are objects, characterized with attributes - they belong to different classes (discrete labels)
- given objects described with attribute values, induce a model to predict different classes
- decision trees, if-then rules, discriminant analysis, ...



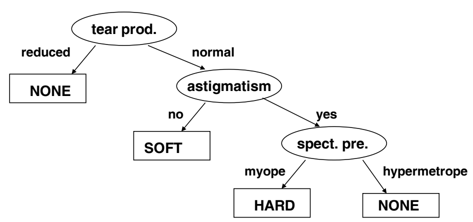
## Data mining example Input: Contact lens data

| | | | | | |
|---|---|---|---|---|---|
| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
| O1 | young | myope | no | reduced | NONE |
| O2 | young | myope | no | normal | SOFT |
| O3 | young | myope | yes | reduced | NONE |
| O4 | young | myope | yes | normal | HARD |
| O5 | young | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | pre-presbyo | hypermetrope | no | normal | SOFT |
| O15 | pre-presbyo | hypermetrope | yes | reduced | NONE |
| O16 | pre-presbyo | hypermetrope | yes | normal | NONE |
| O17 | presbyopic | myope | no | reduced | NONE |
| O18 | presbyopic | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | presbyopic | hypermetrope | yes | normal | NONE |



## Contact lens data: Decision tree

**Type of task:** prediction and classification
**Hypothesis language:** decision trees
(nodes: attributes, arcs: values of attributes, leaves: classes)






## Contact lens data: Classification rules

**Type of task:** prediction and classification
**Hypothesis language:** rules X ➔ C, if X then C
X conjunction of attribute values, C class

tear production=reduced → lenses=NONE
tear production=normal & astigmatism=yes & spect. pre.=hypermetrope → lenses=NONE
tear production=normal & astigmatism=no → lenses=SOFT
tear production=normal & astigmatism=yes & spect. pre.=myope → lenses=HARD
DEFAULT lenses=NONE

## Task reformulation: Concept learning problem
### (positive vs. negative examples of Target class)

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | young | myope | no | reduced | NO |
| O2 | young | myope | no | normal | YES |
| O3 | young | myope | yes | reduced | NO |
| O4 | young | myope | yes | normal | YES |
| O5 | young | hypermetrope | no | reduced | NO |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | pre-presbyc | hypermetrope | no | normal | YES |
| O15 | pre-presbyc | hypermetrope | yes | reduced | NO |
| O16 | pre-presbyc | hypermetrope | yes | normal | NO |
| O17 | presbyopic | myope | no | reduced | NO |
| O18 | presbyopic | myope | no | normal | NO |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | presbyopic | hypermetrope | yes | normal | NO |



## Contact lens data: Classification rules in concept learning

**Type of task:** prediction and classification
**Hypothesis language:** rules X ➔ C, if X then C
X conjunction of attribute values, C target class

Target class: yes

tear production=normal & astigmatism=no → lenses=YES
tear production=normal & astigmatism=yes & spect. pre.=myope → lenses=YES
else NO

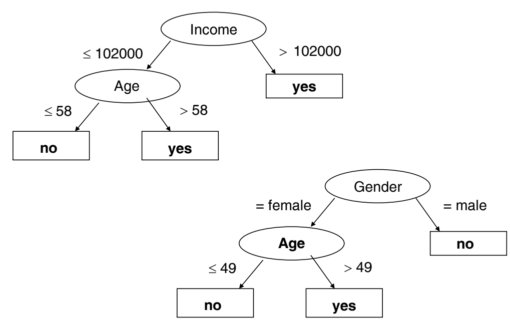


## Illustrative example: Customer data

| Customer | Gender | Age | Income | Spent | BigSpender |
|---|---|---|---|---|---|
| c1 | male | 30 | 214000 | 18800 | yes |
| c2 | female | 19 | 139000 | 15100 | yes |
| c3 | male | 55 | 50000 | 12400 | no |
| c4 | female | 48 | 26000 | 8600 | no |
| c5 | male | 63 | 191000 | 28100 | yes |
| O6-O13 | ... | ... | ... | ... | ... |
| c14 | female | 61 | 95000 | 18100 | yes |
| c15 | male | 56 | 44000 | 12000 | no |
| c16 | male | 36 | 102000 | 13800 | no |
| c17 | female | 57 | 215000 | 29300 | yes |
| c18 | male | 33 | 67000 | 9700 | no |
| c19 | female | 26 | 95000 | 11000 | no |
| c20 | female | 55 | 214000 | 28800 | yes |



## Customer data: Decision trees






## Predictive DM - Estimation

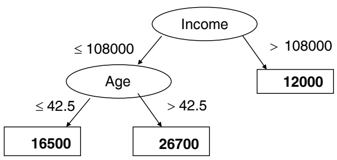
- often referred to as regression
- data are objects, characterized with attributes (discrete or continuous), classes of objects are continuous (numeric)
- given objects described with attribute values, induce a model to predict the numeric class value
- regression trees, linear and logistic regression, ANN, kNN, ...



## Estimation/regression example: Customer data

| Customer | Gender | Age | Income | Spent |
|---|---|---|---|---|
| c1 | male | 30 | 214000 | 18800 |
| c2 | female | 19 | 139000 | 15100 |
| c3 | male | 55 | 50000 | 12400 |
| c4 | female | 48 | 26000 | 8600 |
| c5 | male | 63 | 191000 | 28100 |
| O6-O13 | ... | ... | ... | ... |
| c14 | female | 61 | 95000 | 18100 |
| c15 | male | 56 | 44000 | 12000 |
| c16 | male | 36 | 102000 | 13800 |
| c17 | female | 57 | 215000 | 29300 |
| c18 | male | 33 | 67000 | 9700 |
| c19 | female | 26 | 95000 | 11000 |
| c20 | female | 55 | 214000 | 28800 |

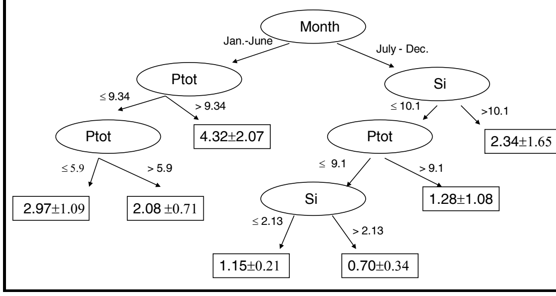
# Customer data: regression tree




**In the nodes one usually has Predicted value +- st. deviation**



# Predicting algal biomass: regression tree






# Descriptive DM: Subgroup discovery example - Customer data

| Customer | Gender | Age | Income | Spent | BigSpender |
|---|---|---|---|---|---|
| c1 | male | 30 | 214000 | 18800 | yes |
| c2 | female | 19 | 139000 | 15100 | yes |
| c3 | male | 55 | 50000 | 12400 | no |
| c4 | female | 48 | 26000 | 8600 | no |
| c5 | male | 63 | 191000 | 28100 | yes |
| O6-O13 | ... | ... | ... | ... | ... |
| c14 | female | 61 | 95000 | 18100 | yes |
| c15 | male | 56 | 44000 | 12000 | no |
| c16 | male | 36 | 102000 | 13800 | no |
| c17 | female | 57 | 215000 | 29300 | yes |
| c18 | male | 33 | 67000 | 9700 | no |
| c19 | female | 26 | 95000 | 11000 | no |
| c20 | female | 55 | 214000 | 28800 | yes |



# Customer data: Subgroup discovery

**Type of task:** description (pattern discovery)
**Hypothesis language:** rules **X ➔ Y,** if X then Y
X is conjunctions of items, Y is target class

Age > 52 & Sex = male ➔ BigSpender = no

Age > 52 & Sex = male & Income ≤ 73250
➔ BigSpender = no



# Descriptive DM: Clustering and association rule learning example - Customer data

| Customer | Gender | Age | Income | Spent | BigSpender |
|---|---|---|---|---|---|
| c1 | male | 30 | 214000 | 18800 | yes |
| c2 | female | 19 | 139000 | 15100 | yes |
| c3 | male | 55 | 50000 | 12400 | no |
| c4 | female | 48 | 26000 | 8600 | no |
| c5 | male | 63 | 191000 | 28100 | yes |
| O6-O13 | ... | ... | ... | ... | ... |
| c14 | female | 61 | 95000 | 18100 | yes |
| c15 | male | 56 | 44000 | 12000 | no |
| c16 | male | 36 | 102000 | 13800 | no |
| c17 | female | 57 | 215000 | 29300 | yes |
| c18 | male | 33 | 67000 | 9700 | no |
| c19 | female | 26 | 95000 | 11000 | no |
| c20 | female | 55 | 214000 | 28800 | yes |



# Descriptive DM: Association rule learning example - Customer data

| Customer | Gender | Age | Income | Spent | BigSpender |
|---|---|---|---|---|---|
| c1 | male | 30 | 214000 | 18800 | yes |
| c2 | female | 19 | 139000 | 15100 | yes |
| c3 | male | 55 | 50000 | 12400 | no |
| c4 | female | 48 | 26000 | 8600 | no |
| c5 | male | 63 | 191000 | 28100 | yes |
| O6-O13 | ... | ... | ... | ... | ... |
| c14 | female | 61 | 95000 | 18100 | yes |
| c15 | male | 56 | 44000 | 12000 | no |
| c16 | male | 36 | 102000 | 13800 | no |
| c17 | female | 57 | 215000 | 29300 | yes |
| c18 | male | 33 | 67000 | 9700 | no |
| c19 | female | 26 | 95000 | 11000 | no |
| c20 | female | 55 | 214000 | 28800 | yes |

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## Customer data: Association rules

**Type of task:** description (pattern discovery)

**Hypothesis language:** rules **X ➔ Y,** if X then Y

X, Y conjunctions of items

1. Age > 52 & BigSpender = no ➔ Sex = male
2. Age > 52 & BigSpender = no ➔
   Sex = male & Income ≤ 73250
3. Sex = male & Age > 52 & Income ≤ 73250 ➔
   BigSpender = no

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## Predictive vs. descriptive DM: Summary from a rule learning perspective

- **Predictive DM:** Induces **rulesets** acting as classifiers for solving classification and prediction tasks
- **Descriptive DM:** Discovers **individual rules** describing interesting regularities in the data
- **Therefore:** Different goals, different heuristics, different evaluation criteria

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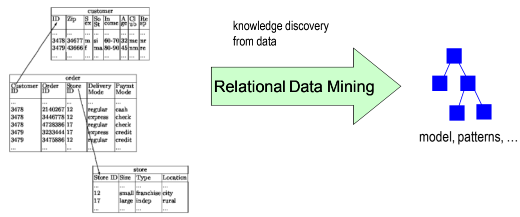
## Relational Data Mining (Inductive Logic Programming) in a Nutshell




customer

| ID | Zip | Sex | So St | Income | Age | Club | Resp |
|---|---|---|---|---|---|---|---|
| ... | ... | ... | ... | ... | ... | ... | ... |
| 3478 | 34677 | m | si | 60-70 | 32 | me | nr |
| 3479 | 43666 | f | ma | 80-90 | 45 | nm | re |
| ... | ... | ... | ... | ... | ... | ... | ... |

order

| Customer ID | Order ID | Store ID | Delivery Mode | Paymt Mode |
|---|---|---|---|---|
| ... | ... | ... | ... | ... |
| 3478 | 2140267 | 12 | regular | cash |
| 3478 | 3446778 | 12 | express | check |
| 3478 | 4728386 | 17 | regular | check |
| 3479 | 3233444 | 17 | express | credit |
| 3479 | 3475886 | 12 | regular | credit |
| ... | ... | ... | ... | ... |

store

| Store ID | Size | Type | Location |
|---|---|---|---|
| ... | ... | ... | ... |
| 12 | small | franchise | city |
| 17 | large | indep | rural |
| ... | ... | ... | ... |

Relational representation of customers, orders and stores.

**Given:** a relational database, a set of tables. sets of logical facts, a graph, …
**Find:** a classification model, a set of interesting patterns

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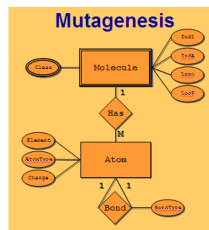
## Relational Data Mining (ILP)

- Learning from multiple tables
- Complex relational problems:
  - temporal data: time series in medicine, trafic control, ...
  - structured data: representation of molecules and their properties in protein engineering, biochemistry, ...

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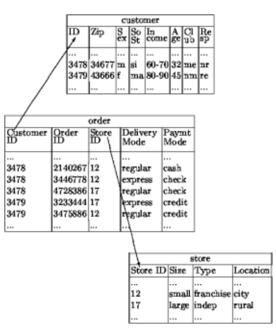
## Relational Data Mining (ILP)


customer

| ID | Zip | Sex | So St | Income | Age | Club | Resp |
|---|---|---|---|---|---|---|---|
| ... | ... | ... | ... | ... | ... | ... | ... |
| 3478 | 34677 | m | si | 60-70 | 32 | me | nr |
| 3479 | 43666 | f | ma | 80-90 | 45 | nm | re |
| ... | ... | ... | ... | ... | ... | ... | ... |

order

| Customer ID | Order ID | Store ID | Delivery Mode | Paymt Mode |
|---|---|---|---|---|
| ... | ... | ... | ... | ... |
| 3478 | 2140267 | 12 | regular | cash |
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| 3479 | 3233444 | 17 | express | credit |
| 3479 | 3475886 | 12 | regular | credit |
| ... | ... | ... | ... | ... |

store

| Store ID | Size | Type | Location |
|---|---|---|---|
| ... | ... | ... | ... |
| 12 | small | franchise | city |
| 17 | large | indep | rural |
| ... | ... | ... | ... |

Relational representation of customers, orders and stores.

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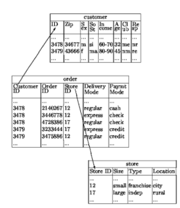

Relational representation of customers, orders and stores.

| ID | Zip | Sex | Soc St | Income | Age | Club | Resp |
|---|---|---|---|---|---|---|---|
| ... | ... | ... | ... | ... | ... | ... | ... |
| 3478 | 34667 | m | si | 60-70 | 32 | me | nr |
| 3479 | 43666 | f | ma | 80-90 | 45 | nm | re |
| ... | ... | ... | ... | ... | ... | ... | ... |

Basic table for analysis

| ID | Zip | Sex | Soc St | Income | Age | Club | Resp |
|---|---|---|---|---|---|---|---|
| ... | ... | ... | ... | ... | ... | ... | ... |
| 3478 | 34667 | m | si | 60-70 | 32 | me | nr |
| 3479 | 43666 | f | ma | 80-90 | 45 | nm | re |
| ... | ... | ... | ... | ... | ... | ... | ... |

**Data table presented as logical facts (Prolog format)**
customer(Id,Zip,Sex,SoSt,In,Age,Club,Re)

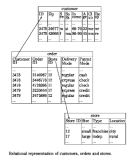
**Prolog facts describing data in Table 2:**
customer(3478,34667,m,si,60-70,32,me,nr).
customer(3479,43666,f,ma,80-90,45,nm,re).

**Expressing a property of a relation:**
customer(_,_,f,_,_,_,_,_).



# Relational Data Mining (ILP)

**Data bases:**
- Name of relation p
- Attribute of p
- n-tuple $< v_1, ..., v_n >$ = row in a relational table
- relation p = set of n-tuples = relational table



**Logic programming:**
- Predicate symbol p
- Argument of predicate p
- Ground fact $p(v_1, ..., v_n)$
- Definition of predicate p
  - Set of ground facts
  - Prolog clause or a set of Prolog clauses

**Example predicate definition:**

good_customer(C) :-
customer(C,_,female,_,_,_,_,_),
order(C,_,_,_,creditcard).



# Part I. Introduction

- Data Mining in a Nutshell
- Predictive and descriptive DM techniques
- Data Mining and the KDD process
- DM standards, tools and visualization



# Data Mining and KDD

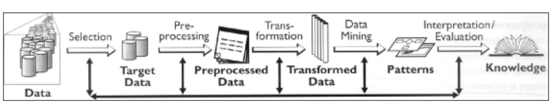
- KDD is defined as "the process of identifying valid, novel, potentially useful and ultimately understandable models/patterns in data." *
- Data Mining (DM) is the key step in the KDD process, performed by using data mining techniques for extracting models or interesting patterns from the data.

*Usama M. Fayyad, Gregory Piatesky-Shapiro, Pedhraic Smyth: The KDD Process for Extracting Useful Knowledge form Volumes of Data. Comm ACM, Nov 96/Vol 39 No 11*



# KDD Process

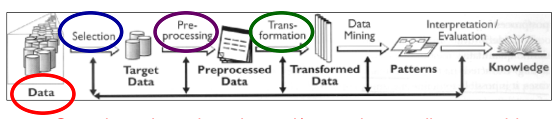
KDD process of discovering useful knowledge from data




- KDD process involves several phases:
  - data preparation
  - data mining (machine learning, statistics)
  - evaluation and use of discovered patterns
- Data mining is the key step, but represents only 15%-25% of the entire KDD process

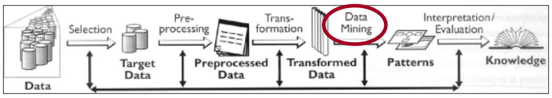


# MEDIANA – analysis of media research data




- Questionnaires about journal/magazine reading, watching of TV programs and listening of radio programs, since 1992, about 1200 questions. Yearly publication: frequency of reading/listening/watching, distribution w.r.t. Sex, Age, Education, Buying power,..
- Data for 1998, about 8000 questionnaires, covering lifestyle, spare time activities, personal viewpoints, reading/listening/watching of media (yes/no/how much), interest for specific topics in media, social status
- good quality, "clean" data
- table of n-tuples (rows: individuals, columns: attributes, in classification tasks selected class)

## MEDIANA – media research pilot study




- Patterns uncovering regularities concerning:
  - Which other journals/magazines are read by readers of a particular journal/magazine ?
  - What are the properties of individuals that are consumers of a particular media offer ?
  - Which properties are distinctive for readers of different journals ?
- Induced models: description (association rules, clusters) and classification (decision trees, classification rules)



## Simplified association rules

**Finding profiles of readers of the Delo daily newspaper**

1. reads_Marketing_magazine 116 ➔
   reads_Delo 95 (0.82)
2. reads_Financial_News (Finance) 223 ➔ reads_Delo 180 (0.81)
3. reads_Views (Razgledi) 201 ➔ reads_Delo 157 (0.78)
4. reads_Money (Denar) 197 ➔ reads_Delo 150 (0.76)
5. reads_Vip 181 ➔ reads_Delo 134 (0.74)

**Interpretation:** Most readers of Marketing magazine, Financial News, Views, Money and Vip read also Delo.



## Simplified association rules

1. reads_Sara 332 ➔ reads_Slovenske novice 211 (0.64)
2. reads_Ljubezenske zgodbe 283 ➔
   reads_Slovenske novice 174 (0.61)
3. reads_Dolenjski list 520 ➔
   reads_Slovenske novice 310 (0.6)
4. reads_Omama 154 ➔ reads_Slovenske novice 90 (0.58)
5. reads_Delavska enotnost 177 ➔
   reads_Slovenske novice 102 (0.58)

Most of the readers of Sara, Love stories, Dolenjska new, Omama in Workers new read also Slovenian news.



## Simplified association rules

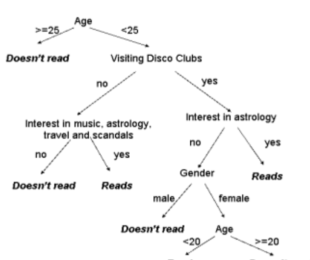
1. reads_Sportske novosti 303 ➔
   reads_Slovenski delnicar 164 (0.54)
2. reads_Sportske novosti 303 ➔
   reads_Salomonov oglasnik 155 (0.51)
3. reads_Sportske novosti 303 ➔
   reads_Lady 152 (0.5)

More than half of readers of Sports news reads also Slovenian shareholders magazine, Solomon advertisements and Lady.



## Decision tree

Finding reader profiles: decision tree for classifying people into readers and non-readers of a teenage magazine Antena.



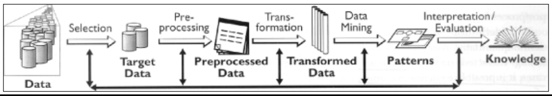



## Part I. Introduction

- Data Mining in a Nutshell
- Predictive and descriptive DM techniques
- Data Mining and the KDD process
- DM standards, tools and visualization

## CRISP-DM

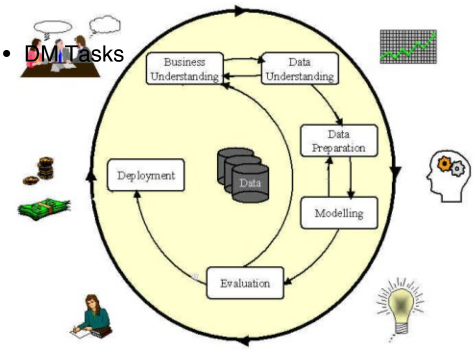
- Cross-Industry Standard Process for DM
- A collaborative, 18-months partially EC founded project started in July 1997
- NCR, ISL (Clementine), Daimler-Benz, OHRA (Dutch health insurance companies), and SIG with more than 80 members
- DM from art to engineering
- Views DM more broadly than Fayyad et al. (actually DM is treated as KDD process):





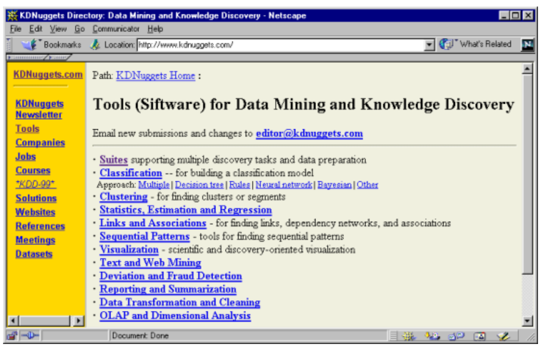

## CRISP Data Mining Process

- DM Tasks





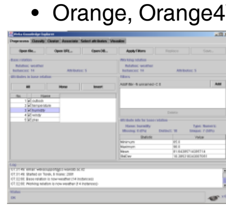

## DM tools

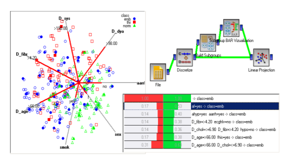





## Public DM tools

- WEKA - Waikato Environment for Knowledge Analysis
- KNIME - Konstanz Information Miner
- R – Bioconductor, …
- Orange, Orange4WS, ClowdFlows





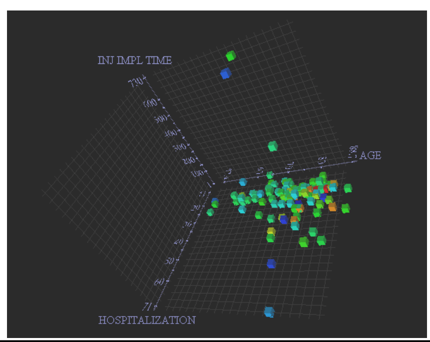


## Visualization

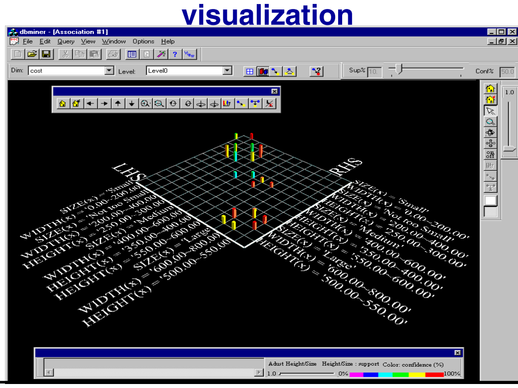
- can be used on its own (usually for description and summarization tasks)
- can be used in combination with other DM techniques, for example
  - visualization of decision trees
  - cluster visualization
  - visualization of association rules
  - subgroup visualization



## Data visualization: Scatter plot

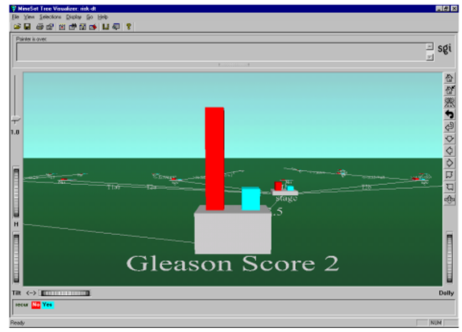


## DB Miner: Association rule visualization



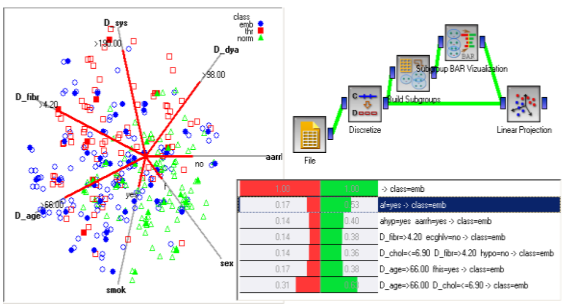


## MineSet: Decision tree visualization






## Orange: Visual programming and subgroup discovery visualization






## Part I: Summary

- KDD is the overall process of discovering useful knowledge in data
  - many steps including data preparation, cleaning, transformation, pre-processing
- Data Mining is the data analysis phase in KDD
  - DM takes only 15%-25% of the effort of the overall KDD process
  - employing techniques from machine learning and statistics
- Predictive and descriptive induction have different goals: classifier vs. pattern discovery
- Many application areas, many powerful tools available



## Part II. Predictive DM techniques

- Naive Bayesian classifier
- Decision tree learning
- Classification rule learning
- Classifier evaluation



## Bayesian methods

- Bayesian methods – simple but powerful classification methods
  - Based on Bayesian formula

$$p(H \mid D) = \frac{p(D \mid H)}{p(D)} p(H)$$

- Main methods:
  - Naive Bayesian classifier
  - Semi-naïve Bayesian classifier
  - Bayesian networks *

* Out of scope of this course

## Naïve Bayesian classifier

- Probability of class, for given attribute values

$$p(c_j \mid v_1 ... v_n) = p(c_j) \cdot \frac{p(v_1 ... v_n \mid c_j)}{p(v_1 ... v_n)}$$

- For all $C_j$ compute probability $p(C_j)$, given values $v_i$ of all attributes describing the example which we want to classify (assumption: conditional independence of attributes, when estimating $p(C_j)$ and $p(C_j \mid v_i)$)

$$p(c_j \mid v_1 ... v_n) \approx p(c_j) \cdot \prod_i \frac{p(c_j \mid v_i)}{p(c_j)}$$

- Output $C_{MAX}$ with maximal posterior probability of class:

$$C_{MAX} = \arg\max_{Cj} p(c_j \mid v_1 ... v_n)$$



## Naïve Bayesian classifier

$$p(c_j \mid v_1 ... v_n) = \frac{p(c_j \cdot v_1 ... v_n)}{p(v_1 ... v_n)} = \frac{p(v_1 ... v_n \mid c_j) \cdot p(c_j)}{p(v_1 ... v_n)} =$$

$$= \frac{\prod_i p(v_i \mid c_j) \cdot p(c_i)}{p(v_1 ... v_n)} = \frac{p(c_j)}{p(v_1 ... v_n)} \prod_i \frac{p(c_j \mid v_i) \cdot p(v_i)}{p(c_j)} =$$

$$= p(c_j) \cdot \frac{\prod p(v_i)}{p(v_1 ... v_n)} \prod_i \frac{p(c_j \mid v_i)}{p(c_j)} \approx p(c_j) \cdot \prod_i \frac{p(c_j \mid v_i)}{p(c_j)}$$



## Semi-naïve Bayesian classifier

- Naive Bayesian estimation of probabilities (reliable)

$$\frac{p(c_j \mid v_i)}{p(c_j)} \cdot \frac{p(c_j \mid v_k)}{p(c_j)}$$

- Semi-naïve Bayesian estimation of probabilities (less reliable)

$$\frac{p(c_j \mid v_i, v_k)}{p(c_j)}$$



## Probability estimation

- Relative frequency:

$$p(c_j) = \frac{n(c_j)}{N}, \; p(c_j \mid v_i) = \frac{n(c_j, v_i)}{n(v_i)}$$

j = 1. . k, for k classes

- Prior probability: Laplace law

$$p(c_j) = \frac{n(c_j) + 1}{N + k}$$

- m-estimate:

$$p(c_j) = \frac{n(c_j) + m \cdot p_a(c_j)}{N + m}$$



## Probability estimation: intuition

- Experiment with N trials, n successful
- Estimate probability of success of next trial
- **Relative frequency: n/N**
  - reliable estimate when number of trials is large
  - Unreliable when number of trials is small, e.g., 1/1=1
- **Laplace: (n+1)/(N+2), (n+1)/(N+k),** k classes
  - Assumes uniform distribution of classes
- **m-estimate: (n+m.$p_a$)/(N+m)**
  - Prior probability of success $p_a$, parameter m (weight of prior probability, i.e., number of 'virtual' examples )



## Explanation of Bayesian classifier

- Based on information theory
  - Expected number of bits needed to encode a message = optimal code length -log p for a message, whose probability is p (*)
- Explanation based of the sum of information gains of individual attribute values $v_i$ (Kononenko and Bratko 1991, Kononenko 1993)

$$-\log(p(c_j \mid v_1 ... v_n)) =$$

$$= -\log(p(c_j)) - \sum_{i=1}^{n} (-\log p(c_j) + \log(p(c_j \mid v_i))$$

* log p denotes binary logarithm

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## Example of explanation of semi-naïve Bayesian classifier

Hip surgery prognosis

Class = no (“no complications”, most probable class, 2 class problem)

| Attribute value | For decision (bit) | Against (bit) |
|---|---|---|
| Age = 70-80 | 0.07 | |
| Sex = Female | | -0.19 |
| Mobility before injury = Fully mobile | 0.04 | |
| State of health before injury = Other | 0.52 | |
| Mechanism of injury = Simple fall | | -0.08 |
| Additional injuries = None | 0 | |
| Time between injury and operation > 10 days | 0.42 | |
| Fracture classification acc. To Garden = Garden III | | -0.3 |
| Fracture classification acc. To Pauwels = Pauwels III | | -0.14 |
| Transfusion = Yes | 0.07 | |
| Antibiotic profilaxies = Yes | | -0.32 |
| Hospital rehabilitation = Yes | 0.05 | |
| General complications = None | | 0 |
| **Combination:** | 0.21 | |
| Time between injury and examination < 6 hours | | |
| AND Hospitalization time between 4 and 5 weeks | | |
| **Combination:** | 0.63 | |
| Therapy = Artroplastic AND anticoagulant therapy = Yes | | |

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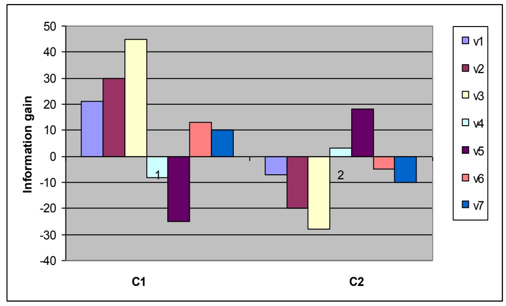
## Visualization of information gains for/against $C_i$

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## Naïve Bayesian classifier

- Naïve Bayesian classifier can be used
  - when we have sufficient number of training examples for reliable probability estimation
- It achieves good classification accuracy
  - can be used as ‘gold standard’ for comparison with other classifiers
- Resistant to noise (errors)
  - Reliable probability estimation
  - Uses all available information
- Successful in many application domains
  - Web page and document classification
  - Medical diagnosis and prognosis, …

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## Improved classification accuracy due to using m-estimate

| | Primary tumor | Breast cancer | thyroid | Rheumatology |
|---|---|---|---|---|
| #instan | 339 | 288 | 884 | 355 |
| #class | 22 | 2 | 4 | 6 |
| #attrib | 17 | 10 | 15 | 32 |
| #values | 2 | 2.7 | 9.1 | 9.1 |
| majority | 25% | 80% | 56% | 66% |
| entropy | 3.64 | 0.72 | 1.59 | 1.7 |

| | Relative freq. | m-estimate |
|---|---|---|
| Primary tumor | 48.20% | 52.50% |
| Breast cancer | 77.40% | 79.70% |
| hepatitis | 58.40% | 90.00% |
| lymphography | 79.70% | 87.70% |

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## Part II. Predictive DM techniques

- Naïve Bayesian classifier
- Decision tree learning
- Classification rule learning
- Classifier evaluation

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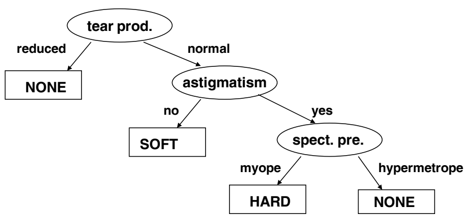
## Illustrative example: Contact lenses data

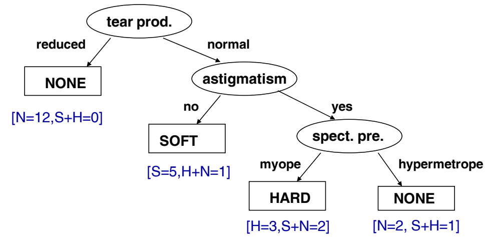
| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | young | myope | no | reduced | NONE |
| O2 | young | myope | no | normal | SOFT |
| O3 | young | myope | yes | reduced | NONE |
| O4 | young | myope | yes | normal | HARD |
| O5 | young | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | pre-presbyc | hypermetrope | no | normal | SOFT |
| O15 | pre-presbyc | hypermetrope | yes | reduced | NONE |
| O16 | pre-presbyc | hypermetrope | yes | normal | NONE |
| O17 | presbyopic | myope | no | reduced | NONE |
| O18 | presbyopic | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | presbyopic | hypermetrope | yes | normal | NONE |

# Decision tree for contact lenses recommendation






# Decision tree for contact lenses recommendation



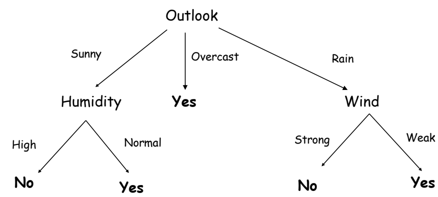



# PlayGolf: Training examples

| Day | Outlook | Temperature | Humidity | Wind | PlayGolf |
|---|---|---|---|---|---|
| D1 | Sunny | Hot | High | Weak | No |
| D2 | Sunny | Hot | High | Strong | No |
| D3 | Overcast | Hot | High | Weak | Yes |
| D4 | Rain | Mild | High | Weak | Yes |
| D5 | Rain | Cool | Normal | Weak | Yes |
| D6 | Rain | Cool | Normal | Strong | No |
| D7 | Overcast | Cool | Normal | Strong | Yes |
| D8 | Sunny | Mild | High | Weak | No |
| D9 | Sunny | Cool | Normal | Weak | Yes |
| D10 | Rain | Mild | Normal | Weak | Yes |
| D11 | Sunny | Mild | Normal | Strong | Yes |
| D12 | Overcast | Mild | High | Weak | Yes |
| D13 | Overcast | Hot | Normal | Weak | Yes |
| D14 | Rain | Mild | High | Strong | No |



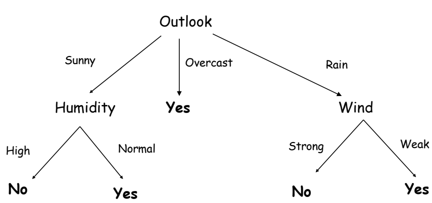
# Decision tree representation for PlayGolf




- each internal node is a test of an attribute
- each branch corresponds to an attribute value
- each path is a conjunction of attribute values
- each leaf node assigns a classification



# Decision tree representation for PlayGolf




Decision trees represent a disjunction of conjunctions of constraints on the attribute values of instances

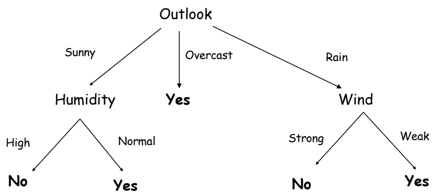
**( Outlook=Sunny $\wedge$ Humidity=Normal )**
**V ( Outlook=Overcast )**
**V ( Outlook=Rain $\wedge$ Wind=Weak )**



# PlayGolf: Other representations

- Logical expression for PlayGolf=Yes:
  - (Outlook=Sunny $\wedge$ Humidity=Normal) $\vee$ (Outlook=Overcast) $\vee$ (Outlook=Rain $\wedge$ Wind=Weak)
- Converting a tree to if-then rules
  - **IF** Outlook=Sunny $\wedge$ Humidity=Normal **THEN** PlayGolf=Yes
  - **IF** Outlook=Overcast **THEN** PlayGolf=Yes
  - **IF** Outlook=Rain $\wedge$ Wind=Weak **THEN** PlayGolf=Yes
  - **IF** Outlook=Sunny $\wedge$ Humidity=High **THEN** PlayGolf=No
  - **IF** Outlook=Rain $\wedge$ Wind=Strong **THEN** PlayGolf=No

## PlayGolf: Using a decision tree for classification




Is Saturday morning OK for playing golf?

Outlook=Sunny, Temperature=Hot, Humidity=High, Wind=Strong

PlayGolf = No, because Outlook=Sunny $\wedge$ Humidity=High



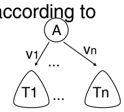
## Appropriate problems for decision tree learning

- Classification problems: classify an instance into one of a discrete set of possible categories (medical diagnosis, classifying loan applicants, …)
- Characteristics:
  - instances described by attribute-value pairs
    (discrete or real-valued attributes)
  - target function has discrete output values
    (boolean or multi-valued, if real-valued then regression trees)
  - disjunctive hypothesis may be required
  - training data may be noisy
    (classification errors and/or errors in attribute values)
  - training data may contain missing attribute values



## Learning of decision trees

- ID3 (Quinlan 1979), CART (Breiman et al. 1984), C4.5, WEKA, ...
  - create the root node of the tree
  - if all examples from S belong to the same class Cj
    - then label the root with Cj
  - else
    - select the 'most informative' attribute **A** with values **v1, v2, … vn**
    - divide training set **S** into **S1,… , Sn** according to values **v1,…,vn**
    - recursively build sub-trees **T1,…,Tn** for **S1,…,Sn**






## Search heuristics in ID3

- Central choice in ID3: Which attribute to test at each node in the tree ? The attribute that is most useful for classifying examples.
- Define a statistical property, called **information gain**, measuring how well a given attribute separates the training examples w.r.t their target classification.
- First define a measure commonly used in information theory, called **entropy**, to characterize the (im)purity of an arbitrary collection of examples.



## Entropy

- **S** - training set, **$C_1$,...,$C_N$** - classes
- **Entropy E(S)** – measure of the impurity of training set S

$$E(S) = -\sum_{c=1}^{N} p_c . \log_2 p_c$$

**$p_c$** - prior probability of class **$C_c$** (relative frequency of **$C_c$** in **S**)

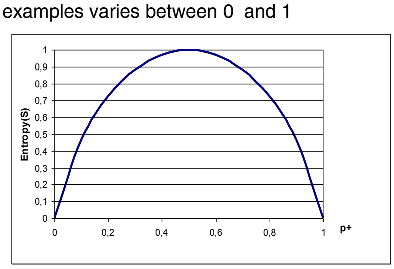
- Entropy in binary classification problems

$$\mathbf{E(S) = - p_+ \log_2 p_+ - p_- \log_2 p_-}$$



## Entropy

- E(S) = $- p_+ \log_2 p_+ - p_- \log_2 p_-$
- The entropy function relative to a Boolean classification, as the proportion **$p_+$** of positive examples varies between 0 and 1



## Entropy – why ?

- **Entropy E(S)** = expected amount of information (in bits) needed to assign a class to a randomly drawn object in S (under the optimal, shortest-length code)
- Why ?
- Information theory: optimal length code assigns $-\log_2 p$ bits to a message having probability p
- So, in binary classification problems, the expected number of bits to encode + or – of a random member of S is:

$$p_+(-\log_2 p_+) + p_-(-\log_2 p_-) = -p_+\log_2 p_+ - p_-\log_2 p_-$$



## PlayGolf: Entropy

- Training set S: 14 examples (9 pos., 5 neg.)
- Notation: S = [9+, 5-]
- $E(S) = -p_+\log_2 p_+ - p_-\log_2 p_-$
- Computing entropy, if probability is estimated by relative frequency

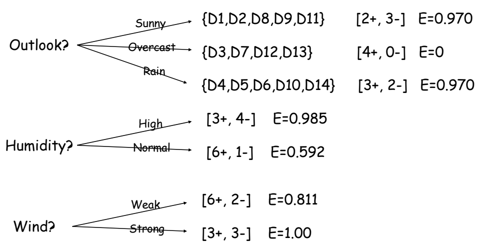
$$E(S) = -\left(\frac{|S_+|}{|S|}\cdot\log\frac{|S_+|}{|S|}\right) - \left(\frac{|S_-|}{|S|}\cdot\log\frac{|S_-|}{|S|}\right)$$

- $E([9+,5-]) = -(9/14)\log_2(9/14) - (5/14)\log_2(5/14)$ $= 0.940$



## PlayGolf: Entropy

- **$E(S) = -p_+\log_2 p_+ - p_-\log_2 p_-$**
- **$E(9+,5-) = -(9/14)\log_2(9/14) - (5/14)\log_2(5/14) = 0.940$**






## Information gain search heuristic

- **Information gain** measure is aimed to minimize the number of tests needed for the classification of a new object
- **Gain(S,A)** – expected reduction in entropy of S due to sorting on A

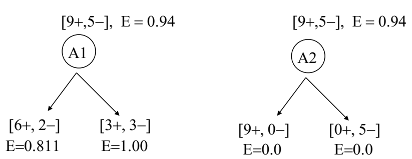
$$Gain(S,A) = E(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} \cdot E(S_v)$$

- **Most informative** attribute: **max Gain(S,A)**



## Information gain search heuristic

- Which attribute is more informative, A1 or A2 ?



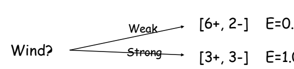

- Gain(S,A1) = 0.94 – (8/14 x 0.811 + 6/14 x 1.00) = 0.048
- Gain(S,A2) = 0.94 – 0 = 0.94 A2 has max Gain



## PlayGolf: Information gain

$$Gain(S,A) = E(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} \cdot E(S_v)$$

- Values(Wind) = {Weak, Strong}




  - S = [9+,5-], E(S) = 0.940
  - $S_{weak}$ = [6+,2-], $E(S_{weak})$ = 0.811
  - $S_{strong}$ = [3+,3-], $E(S_{strong})$ = 1.0
  - **Gain(S,Wind)** = E(S) - (8/14)$E(S_{weak})$ - (6/14)$E(S_{strong})$ = 0.940 - (8/14)x0.811 - (6/14)x1.0=**0.048**

## PlayGolf: Information gain

- **Which attribute is the best?**
  - Gain(S,Outlook)=0.246 *MAX !*
  - Gain(S,Humidity)=0.151
  - Gain(S,Wind)=0.048
  - Gain(S,Temperature)=0.029



## PlayGolf: Information gain

Outlook?
Rain → {D4,D5,D6,D10,D14} [3+, 2-] E > 0 **???**
Overcast → {D3,D7,D12,D13} [4+, 0-] E = 0 **OK - assign class Yes**
Sunny → {D1,D2,D8,D9,D11} [2+, 3-] E > 0 **???**

- Which attribute should be tested here?
  - Gain($S_{sunny}$, Humidity) = 0.97-(3/5)0-(2/5)0 = 0.970 ***MAX !***
  - Gain($S_{sunny}$,Temperature) = 0.97-(2/5)0-(2/5)1-(1/5)0 = 0.570
  - Gain($S_{sunny}$,Wind) = 0.97-(2/5)1-(3/5)0.918 = 0.019



## Probability estimates

- **Relative frequency** :
  - problems with small samples

$$p(Class \mid Cond) = \frac{n(Class.Cond)}{n(Cond)}$$

[6+,1-] (7) = 6/7
[2+,0-] (2) = 2/2 = 1

- **Laplace estimate** :
  - assumes uniform prior distribution of k classes

$$= \frac{n(Class.Cond)+1}{n(Cond)+k} \quad k = 2$$

[6+,1-] (7) = 6+1 / 7+2 = 7/9
[2+,0-] (2) = 2+1 / 2+2 = 3/4



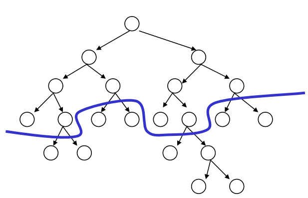
## Heuristic search in ID3

- **Search bias:** Search the space of decision trees from simplest to increasingly complex (greedy search, no backtracking, prefer small trees)
- **Search heuristics:** At a node, select the attribute that is most useful for classifying examples, split the node accordingly
- **Stopping criteria:** A node becomes a leaf
  - if all examples belong to same class $C_j$, label the leaf with $C_j$
  - if all attributes were used, label the leaf with the most common value $C_k$ of examples in the node
- **Extension to ID3:** handling noise - tree pruning



## Pruning of decision trees

- Avoid overfitting the data by tree pruning
- Pruned trees are
  - less accurate on training data
  - more accurate when classifying unseen data





## Handling noise – Tree pruning

Sources of imperfection

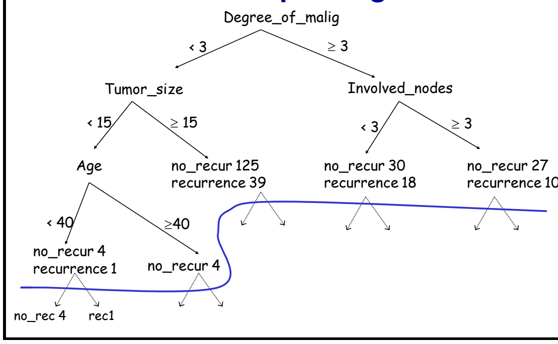
1. Random errors (noise) in training examples
   - erroneous attribute values
   - erroneous classification
2. Too sparse training examples (incompleteness)
3. Inappropriate/insufficient set of attributes (inexactness)
4. Missing attribute values in training examples

## Handling noise – Tree pruning

- Handling imperfect data
  - handling imperfections of type 1-3
    - pre-pruning (stopping criteria)
    - post-pruning / rule truncation
  - handling missing values
- Pruning avoids perfectly fitting noisy data: relaxing the completeness (fitting all +) and consistency (fitting all -) criteria in ID3



## Prediction of breast cancer recurrence: Tree pruning





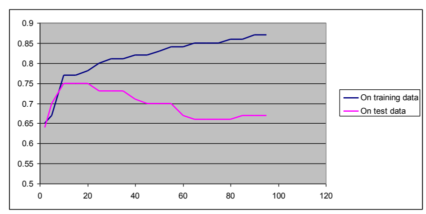

## Accuracy and error

- Accuracy: percentage of correct classifications
  - on the training set
  - on unseen instances
- How accurate is a decision tree when classifying unseen instances
  - An estimate of accuracy on unseen instances can be computed, e.g., by averaging over 4 runs:
    - split the example set into training set (e.g. 70%) and test set (e.g. 30%)
    - induce a decision tree from training set, compute its accuracy on test set
- Error = 1 - Accuracy
- High error may indicate data overfitting



## Overfitting and accuracy

- Typical relation between tree size and accuracy

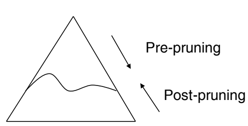



- Question: how to prune optimally?



## Avoiding overfitting

- How can we avoid overfitting?
  - Pre-pruning (forward pruning): stop growing the tree e.g., when data split not statistically significant or too few examples are in a split
  - Post-pruning: grow full tree, then post-prune




- forward pruning considered inferior (myopic)
- post pruning makes use of sub trees



## How to select the “best” tree

- Measure performance over training data (e.g., pessimistic post-pruning, Quinlan 1993)
- Measure performance over separate validation data set (e.g., reduced error pruning, Quinlan 1987)
  - until further pruning is harmful DO:
    - for each node evaluate the impact of replacing a subtree by a leaf, assigning the majority class of examples in the leaf, if the pruned tree performs no worse than the original over the validation set
    - greedily select the node whose removal most improves tree accuracy over the validation set
- MDL: minimize size(tree)+size(misclassifications(tree))

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## Selected decision/regression tree learners

- Decision tree learners
  - ID3 (Quinlan 1979)
  - CART (Breiman et al. 1984)
  - Assistant (Cestnik et al. 1987)
  - C4.5 (Quinlan 1993), C5 (See5, Quinlan)
  - J48 (available in WEKA)
- Regression tree learners, model tree learners
  - M5, M5P (implemented in WEKA)

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## Features of C4.5

- Implemented as part of the WEKA data mining workbench
- Handling noisy data: post-pruning
- Handling incompletely specified training instances: 'unknown' values (**?**)
  - in learning assign conditional probability of value v: p(v|C) = p(vC) / p(C)
  - in classification: follow all branches, weighted by prior prob. of missing attribute values

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## Other features of C4.5

- Binarization of attribute values
  - for continuous values select a boundary value maximally increasing the informativity of the attribute: sort the values and try every possible split (done automaticaly)
  - for discrete values try grouping the values until two groups remain *
- 'Majority' classification in NULL leaf (with no corresponding training example)
  - if an example 'falls' into a NULL leaf during classification, the class assigned to this example is the majority class of the parent of the NULL leaf

* the basic C4.5 doesn't support binarisation of discrete attributes, it supports grouping

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## Part II. Predictive DM techniques

- Naïve Bayesian classifier
- Decision tree learning
- Classification rule learning
- Classifier evaluation

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## Rule Learning in a Nutshell

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | young | myope | no | reduced | NONE |
| O2 | young | myope | no | normal | SOFT |
| O3 | young | myope | yes | reduced | NONE |
| O4 | young | myope | yes | normal | HARD |
| O5 | young | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | pre-presbyc | hypermetrope | no | normal | SOFT |
| O15 | pre-presbyc | hypermetrope | yes | reduced | NONE |
| O16 | pre-presbyc | hypermetrope | yes | normal | NONE |
| O17 | presbyopic | myope | no | reduced | NONE |
| O18 | presbyopic | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | presbyopic | hypermetrope | yes | normal | NONE |

data

knowledge discovery from data

Rule learning

Model: a set of rules

Patterns: individual rules

**Given:** transaction data table, relational database (a set of objects, described by attribute values)
**Find:** a classification model in the form of a set of rules; or a set of interesting patterns in the form of individual rules

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## Rule set representation

- Rule base is a disjunctive set of conjunctive rules
- Standard form of rules:
  IF Condition THEN Class
  Class IF Conditions
  Class ← Conditions

**IF** Outlook=Sunny ∧ Humidity=Normal **THEN** PlayGolf=Yes
**IF** Outlook=Overcast **THEN** PlayGolf=Yes
**IF** Outlook=Rain ∧ Wind=Weak **THEN** PlayGolf=Yes

- Form of CN2 rules:
  IF Conditions THEN MajClass [ClassDistr]
- Rule base: {R1, R2, R3, …, DefaultRule}

# Data mining example
# Input: Contact lens data

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | young | myope | no | reduced | NONE |
| O2 | young | myope | no | normal | SOFT |
| O3 | young | myope | yes | reduced | NONE |
| O4 | young | myope | yes | normal | HARD |
| O5 | young | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | ore-presbyc | hypermetrope | no | normal | SOFT |
| O15 | ore-presbyc | hypermetrope | yes | reduced | NONE |
| O16 | ore-presbyc | hypermetrope | yes | normal | NONE |
| O17 | presbyopic | myope | no | reduced | NONE |
| O18 | presbyopic | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | presbyopic | hypermetrope | yes | normal | NONE |



# Contact lens data: Classification rules

**Type of task:** prediction and classification
**Hypothesis language:** rules X ➔ C, if X then C
X conjunction of attribute values, C class

tear production=reduced → lenses=NONE
tear production=normal & astigmatism=yes & spect. pre.=hypermetrope → lenses=NONE
tear production=normal & astigmatism=no → lenses=SOFT
tear production=normal & astigmatism=yes & spect. pre.=myope → lenses=HARD
DEFAULT lenses=NONE

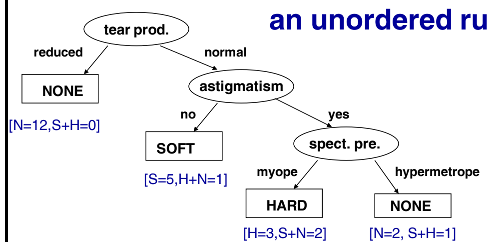


# Rule learning

- Two rule learning approaches:
  - Learn decision tree, convert to rules
  - Learn set/list of rules
    - Learning an unordered set of rules
    - Learning an ordered list of rules
- Heuristics, overfitting, pruning



# Contact lenses: convert decision tree to an unordered rule set

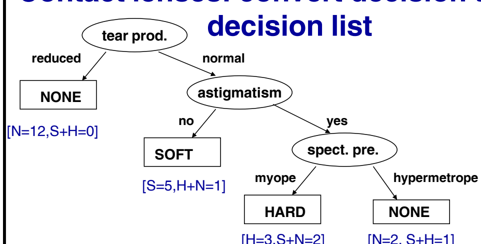



tear production=reduced => lenses=NONE [S=0,H=0,N=12]
tear production=normal & astigmatism=yes & spect. pre.=hypermetrope => lenses=NONE [S=0,H=1,N=2]
tear production=normal & astigmatism=no => lenses=SOFT [S=5,H=0,N=1]
tear production=normal & astigmatism=yes & spect. pre.=myope => lenses=HARD [S=0,H=3,N=2]
DEFAULT lenses=NONE

Order independent rule set (may overlap)



# Contact lenses: convert decision tree to decision list




```
IF tear production=reduced THEN lenses=NONE
 ELSE /*tear production=normal*/
   IF astigmatism=no THEN lenses=SOFT
   ELSE /*astigmatism=yes*/
     IF spect. pre.=myope THEN lenses=HARD
     ELSE /* spect.pre.=hypermetrope*/
       lenses=NONE
```

Ordered (order dependent) rule list



# Converting decision tree to rules, and rule post-pruning (Quinlan 1993)

- Very frequently used method, e.g., in C4.5 and J48
- Procedure:
  - grow a full tree (allowing overfitting)
  - convert the tree to an equivalent set of rules
  - prune each rule independently of others
  - sort final rules into a desired sequence for use

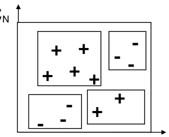
## Concept learning: Task reformulation for rule learning: (pos. vs. neg. examples of Target class)

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | young | myope | no | reduced | NO |
| O2 | young | myope | no | normal | YES |
| O3 | young | myope | yes | reduced | NO |
| O4 | young | myope | yes | normal | YES |
| O5 | young | hypermetrope | no | reduced | NO |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | pre-presbyc | hypermetrope | no | normal | YES |
| O15 | pre-presbyc | hypermetrope | yes | reduced | NO |
| O16 | pre-presbyc | hypermetrope | yes | normal | NO |
| O17 | presbyopic | myope | no | reduced | NO |
| O18 | presbyopic | myope | no | normal | NO |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | presbyopic | hypermetrope | yes | normal | NO |



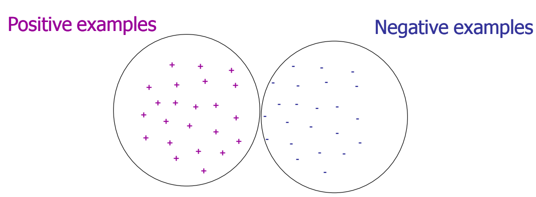
## Original covering algorithm (AQ, Michalski 1969,86)

**Given** examples of N classes $C_1, \ldots, C_N$
**for** each class Ci **do**
- Ei := Pi U Ni (Pi pos., Ni neg.)
- RuleBase(Ci) := empty
- **repeat {learn-set-of-rules}**
  - **learn-one-rule** R covering some positive examples and no negatives
  - add R to RuleBase(Ci)
  - delete from Pi all pos. ex. covered by R
- **until** Pi = empty



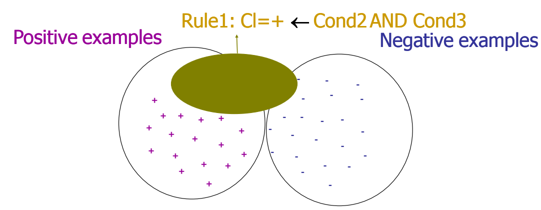


## Covering algorithm



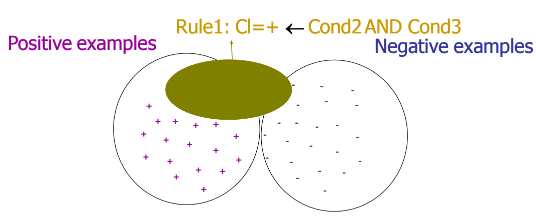



## Covering algorithm



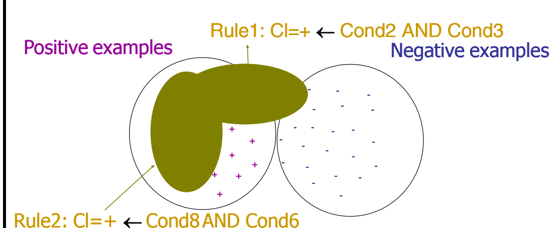



## Covering algorithm






## Covering algorithm



## PlayGolf: Training examples

| Day | Outlook | Temperature | Humidity | Wind | PlayTennis |
|---|---|---|---|---|---|
| D1 | Sunny | Hot | High | Weak | No |
| D2 | Sunny | Hot | High | Strong | No |
| D3 | Overcast | Hot | High | Weak | Yes |
| D4 | Rain | Mild | High | Weak | Yes |
| D5 | Rain | Cool | Normal | Weak | Yes |
| D6 | Rain | Cool | Normal | Strong | No |
| D7 | Overcast | Cool | Normal | Strong | Yes |
| D8 | Sunny | Mild | High | Weak | No |
| D9 | Sunny | Cool | Normal | Weak | Yes |
| D10 | Rain | Mild | Normal | Weak | Yes |
| D11 | Sunny | Mild | Normal | Strong | Yes |
| D12 | Overcast | Mild | High | Weak | Yes |
| D13 | Overcast | Hot | Normal | Weak | Yes |
| D14 | Rain | Mild | High | Strong | No |



## Heuristics for learn-one-rule: PlayGolf example

PlayGolf = yes [9+,5-] (14)
PlayGolf = yes ← Wind=weak [6+,2-] (8)
← Wind=strong [3+,3-] (6)
← Humidity=normal [6+,1-] (7)
← …
PlayGolf = yes ← Humidity=normal
Outlook=sunny [2+,0-] (2)
← …

Estimating **rule accuracy (rule precision)** with the **probability** that a covered example is positive
**A(Class ← Cond) = p(Class| Cond)**

Estimating the **probability** with the **relative frequency** of covered pos. ex. / all covered ex.
[6+,1-] (7) = 6/7, [2+,0-] (2) = 2/2 = 1



## Probability estimates

- **Relative frequency** :
  - problems with small samples

$$p(Class \mid Cond) = \frac{n(Class.Cond)}{n(Cond)}$$

[6+,1-] (7) = 6/7
[2+,0-] (2) = 2/2 = 1

- **Laplace estimate** :
  - assumes uniform prior distribution of k classes

$$= \frac{n(Class.Cond) + 1}{n(Cond) + k} \qquad k = 2$$

[6+,1-] (7) = 6+1 / 7+2 = 7/9
[2+,0-] (2) = 2+1 / 2+2 = 3/4



## Learn-one-rule: search heuristics

- Assume a two-class problem
- Two classes (+,-), learn rules for + class (Cl).
- Search for specializations R' of a rule R = Cl ← Cond from the RuleBase.
- Specializarion R' of rule R = Cl ← Cond
  has the form R' = Cl ← Cond & Cond'
- Heuristic search for rules: find the 'best' Cond' to be added to the current rule R, such that rule accuracy is improved, e.g., such that Acc(R') > Acc(R)
  - where the expected **classification accuracy** can be estimated as A(R) = p(Cl|Cond)

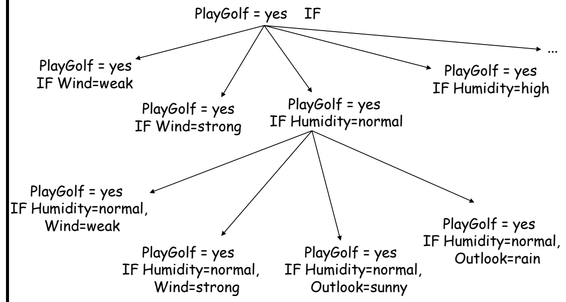


## Learn-one-rule: Greedy vs. beam search

- learn-one-rule by greedy general-to-specific search, at each step selecting the \`best' descendant, no backtracking
  - e.g., the best descendant of the initial rule
    PlayGolf = yes ←
  - is rule PlayGolf = yes ← Humidity=normal
- beam search: maintain a list of k best candidates at each step; descendants (specializations) of each of these k candidates are generated, and the resulting set is again reduced to k best candidates



## Learn-one-rule as search: PlayGolf example



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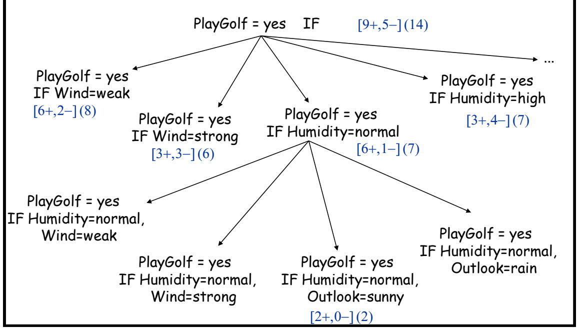
## Learn-one-rule as heuristic search: PlayGolf example

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## What is "high" rule accuracy (rule precision) ?

- Rule evaluation measures:
  - aimed at maximizing classification accuracy
  - minimizing Error = 1 - Accuracy
  - avoiding overfitting
- BUT: Rule accuracy/precision should be traded off against the "default" accuracy/precision of the rule **Cl ←true**
  - 68% accuracy is OK if there are 20% examples of that class in the training set, but bad if there are 80%
- **Relative accuracy** *(relative precision)*
  - RAcc(Cl ←Cond) = p(Cl | Cond) – p(Cl)

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## Weighted relative accuracy

- If a rule covers a single example, its accuracy/precision is either 0% or 100%
  - maximising relative accuracy tends to produce many overly specific rules
- **Weighted relative accuracy**

  **WRAcc(Cl←Cond) = p(Cond) . [p(Cl | Cond) – p(Cl)]**
- WRAcc is a fundamental rule evaluation measure:
  - WRAcc can be used if you want to assess both accuracy and significance
  - WRAcc can be used if you want to compare rules with different heads **and** bodies

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## Learn-one-rule: search heuristics

- Assume two classes (+,-), learn rules for + class (Cl). Search for specializations of one rule R = Cl ← Cond from RuleBase.
- Expected **classification accuracy**: A(R) = p(Cl|Cond)
- **Informativity** (info needed to specify that example covered by Cond belongs to Cl): I(R) = $- \log_2 p(Cl|Cond)$
- **Accuracy gain** (increase in expected accuracy):

  AG(R',R) = p(Cl|Cond') - p(Cl|Cond)
- **Information gain** (decrease in the information needed):

  IG(R',R) = $\log_2 p(Cl|Cond') - \log_2 p(Cl|Cond)$
- **Weighted** measures favoring more general rules: WAG, WIG

  WAG(R',R) =

  p(Cond')/p(Cond) . (p(Cl|Cond') - p(Cl|Cond))
- **Weighted relative accuracy** trades off coverage and relative accuracy WRAcc(R) = p(Cond).(p(Cl|Cond) - p(Cl))

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## Ordered set of rules: if-then-else rules

- rule Class IF Conditions is learned by first determining Conditions and then Class
- **Notice:** mixed sequence of classes C1, …, Cn in RuleBase
- **But: ordered** execution when classifying a new instance: rules are sequentially tried and the first rule that \`fires' (covers the example) is used for classification
- **Decision list {R1, R2, R3, …, D}:** rules Ri are interpreted as **if-then-else** rules
- If no rule fires, then DefaultClass (majority class in $E_{cur}$)

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## Sequential covering algorithm (similar as in Mitchell's book)

- RuleBase := empty
- $E_{cur}$:= E
- **repeat**
  - learn-one-rule R
  - RuleBase := RuleBase U R
  - $E_{cur}$ := $E_{cur}$ - {examples covered and correctly classified by R} **(DELETE ONLY POS. EX.!)**
  - **until** performance(R, $E_{cur}$) < ThresholdR
- RuleBase := sort RuleBase by performance(R,E)
- return RuleBase

## Learn ordered set of rules (CN2, Clark and Niblett 1989)

- RuleBase := empty
- $E_{cur}$:= E
- **repeat**
  - learn-one-rule R
  - RuleBase := RuleBase U R
  - $E_{cur}$ := $E_{cur}$ - {all examples covered by R} **(NOT ONLY POS. EX.!)**
- **until** performance(R, $E_{cur}$) < ThresholdR
- RuleBase := sort RuleBase by performance(R,E)
- RuleBase := RuleBase U DefaultRule($E_{cur}$)



## Learn-one-rule: Beam search in CN2

- Beam search in CN2 learn-one-rule algo.:
  - construct BeamSize of best rule bodies (conjunctive conditions) that are statistically significant
  - BestBody - min. entropy of examples covered by Body
  - construct best rule R := Head $\leftarrow$ BestBody by adding majority class of examples covered by BestBody in rule Head
- performance (R, $E_{cur}$) : - Entropy($E_{cur}$)
  - performance(R, $E_{cur}$) < ThresholdR (neg. num.)
  - Why? Ent. > t is bad, Perf. = -Ent < -t is bad



## Variations

- Sequential vs. simultaneous covering of data (as in TDIDT): choosing between attribute-values vs. choosing attributes
- Learning rules vs. learning decision trees and converting them to rules
- Pre-pruning vs. post-pruning of rules
- What statistical evaluation functions to use
- Probabilistic classification



## Probabilistic classification

- In the ordered case of standard CN2 rules are interpreted in an `IF-THEN-ELSE` fashion, and the first fired rule assigns the class.
- In the unordered case all rules are tried and all rules which fire are collected. If a clash occurs, a probabilistic method is used to resolve the clash.
- A simplified example:
  1. tear production=reduced => lenses=NONE [S=0,H=0,N=12]
  2. tear production=normal & astigmatism=yes & spect. pre.=hypermetrope => lenses=NONE [S=0,H=1,N=2]
  3. tear production=normal & astigmatism=no => lenses=SOFT [S=5,H=0,N=1]
  4. tear production=normal & astigmatism=yes & spect. pre.=myope => lenses=HARD [S=0,H=3,N=2]
  5. DEFAULT lenses=NONE

Suppose we want to classify a person with normal tear production and astigmatism. Two rules fire: rule 2 with coverage [S=0,H=1,N=2] and rule 4 with coverage [S=0,H=3,N=2]. The classifier computes total coverage as [S=0,H=4,N=4], resulting in probabilistic classification into class H with probability 0.5 and N with probability 0.5. In this case, the clash can not be resolved, as both probabilities are equal.



## Part II. Predictive DM techniques

- Naïve Bayesian classifier
- Decision tree learning
- Classification rule learning
- Classifier evaluation



## Classifier evaluation

- Accuracy and Error
- n-fold cross-validation
- Confusion matrix
- ROC

## Evaluating hypotheses

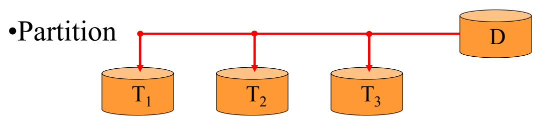
- **Use of induced hypotheses**
  - discovery of new patterns, new knowledge
  - classification of new objects
- **Evaluating the quality of induced hypotheses**
  - Accuracy, Error = 1 - Accuracy
  - classification accuracy on testing examples = percentage of correctly classified instances
    - split the example set into training set (e.g. 70%) to induce a concept, and test set (e.g. 30%) to test its accuracy
    - more elaborate strategies: 10-fold cross validation, leave-one-out, ...
  - comprehensibility (compactness)
  - information contents (information score), significance



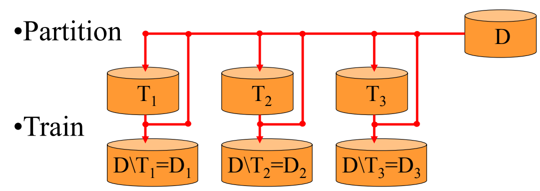
## n-fold cross validation

- A method for accuracy estimation of classifiers
- Partition set D into n disjoint, almost equally-sized folds $T_i$ where $U_i T_i = D$
- **for** i = 1, ..., n **do**
  - form a training set out of n-1 folds: Di = D\$T_i$
  - induce classifier $H_i$ from examples in Di
  - use fold $T_i$ for testing the accuracy of $H_i$
- Estimate the accuracy of the classifier by averaging accuracies over 10 folds $T_i$

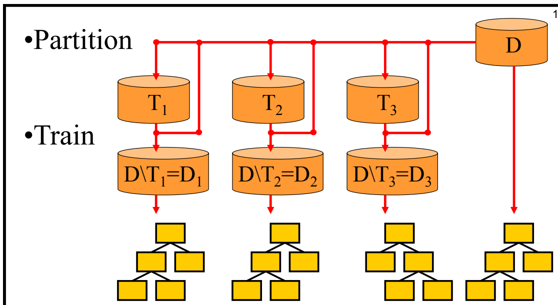




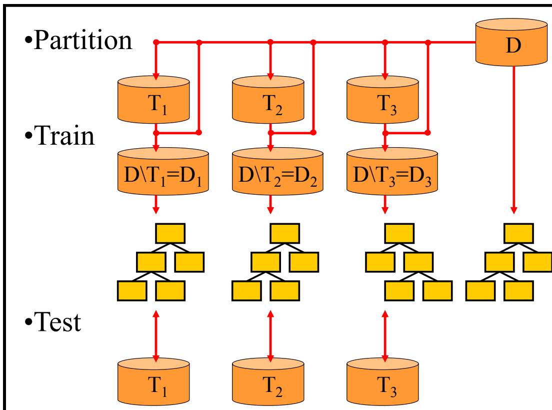






## Confusion matrix and rule (in)accuracy

- Accuracy of a classifier is measured as TP+TN / N.
- Suppose two rules are both 80% accurate on an evaluation dataset, are they always equally good?
  - e.g., Rule 1 correctly classifies 40 out of 50 positives and 40 out of 50 negatives; Rule 2 correctly classifies 30 out of 50 positives and 50 out of 50 negatives
  - on a test set which has more negatives than positives, Rule 2 is preferable;
  - on a test set which has more positives than negatives, Rule 1 is preferable; unless…
  - …the proportion of positives becomes so high that the ‘always positive’ predictor becomes superior!
- Conclusion: classification accuracy is not always an appropriate rule quality measure



## Confusion matrix

[redacted]

- also called ***contingency table***

Classifier 1

| | Predicted positive | Predicted negative | |
|---|---|---|---|
| Positive examples | **40** | **10** | 50 |
| Negative examples | **10** | **40** | 50 |
| | 50 | 50 | 100 |

Classifier 2

| | Predicted positive | Predicted negative | |
|---|---|---|---|
| Positive examples | **30** | **20** | 50 |
| Negative examples | **0** | **50** | 50 |
| | 30 | 70 | 100 |



## ROC space

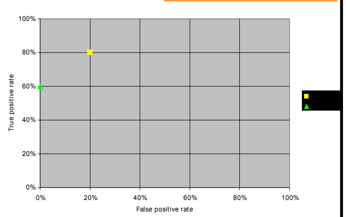
- ***True positive rate*** = #true pos. / #pos.
  - $TPr_1$ = 40/50 = 80%
  - $TPr_2$ = 30/50 = 60%
- ***False positive rate*** = #false pos. / #neg.
  - $FPr_1$ = 10/50 = 20%
  - $FPr_2$ = 0/50 = 0%
- ***ROC space*** has
  - FPr on X axis
  - TPr on Y axis

Classifier 1

| | Predicted positive | Predicted negative | |
|---|---|---|---|
| Positive examples | 40 | 10 | 50 |
| Negative examples | 10 | 40 | 50 |
| | 50 | 50 | 100 |

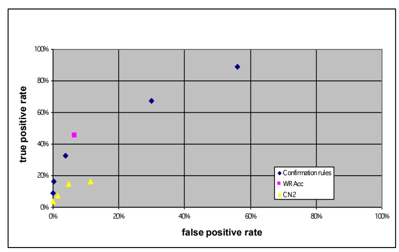
Classifier 2

| | Predicted positive | Predicted negative | |
|---|---|---|---|
| Positive examples | 30 | 20 | 50 |
| Negative examples | 0 | 50 | 50 |
| | 30 | 70 | 100 |



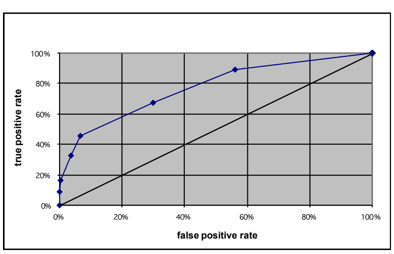



## The ROC space






## The ROC convex hull






## Summary of evaluation

- 10-fold cross-validation is a standard classifier evaluation method used in machine learning
- ROC analysis is very natural for rule learning and subgroup discovery
  - can take costs into account
  - here used for evaluation
  - also possible to use as search heuristic

## Part III. Numeric prediction

- Baseline
- Linear Regression
- Regression tree
- Model Tree
- kNN

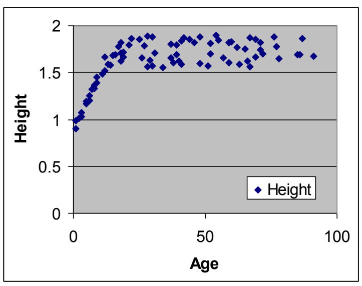


| Regression | Classification |
|---|---|
| **Data**: attribute-value description | |
| **Target variable**: Continuous | **Target variable**: Categorical (nominal) |
| **Evaluation**: cross validation, separate test set, … | |
| **Error**: MSE, MAE, RMSE, … | **Error**: 1-accuracy |
| **Algorithms**: Linear regression, regression trees,… | **Algorithms**: Decision trees, Naïve Bayes, … |
| **Baseline predictor**: Mean of the target variable | **Baseline predictor**: Majority class |



## Example

- data about 80 people: Age and Height




| Age | Height |
|---|---|
| 3 | 1.03 |
| 5 | 1.19 |
| 6 | 1.26 |
| 9 | 1.39 |
| 15 | 1.69 |
| 19 | 1.67 |
| 22 | 1.86 |
| 25 | 1.85 |
| 41 | 1.59 |
| 48 | 1.60 |
| 54 | 1.90 |
| 71 | 1.82 |
| … | … |



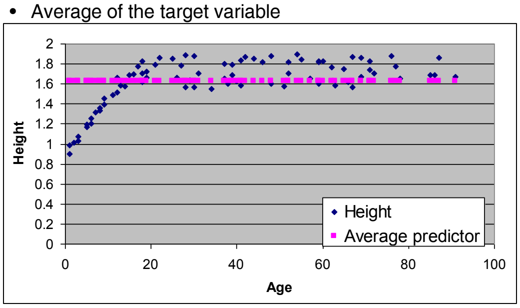
## Test set

| Age | Height |
|---|---|
| 2 | 0.85 |
| 10 | 1.4 |
| 35 | 1.7 |
| 70 | 1.6 |



## Baseline numeric model

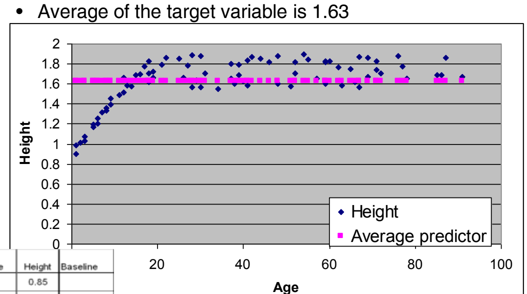
- Average of the target variable






## Baseline numeric predictor

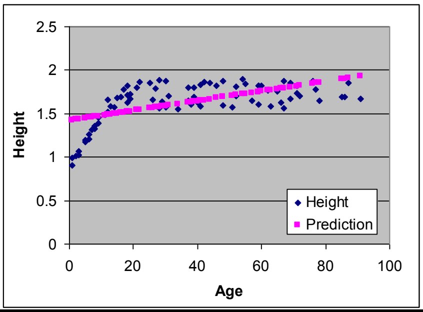
- Average of the target variable is 1.63




| Age | Height | Baseline |
|---|---|---|
| 2 | 0.85 | |
| 10 | 1.4 | |
| 35 | 1.7 | |
| 70 | 1.6 | |

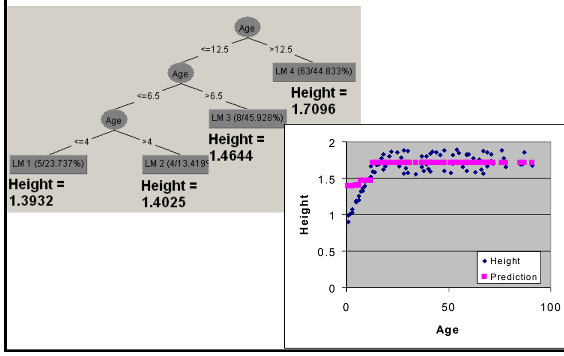
# Linear Regression Model

Height = 0.0056 * Age + 1.4181

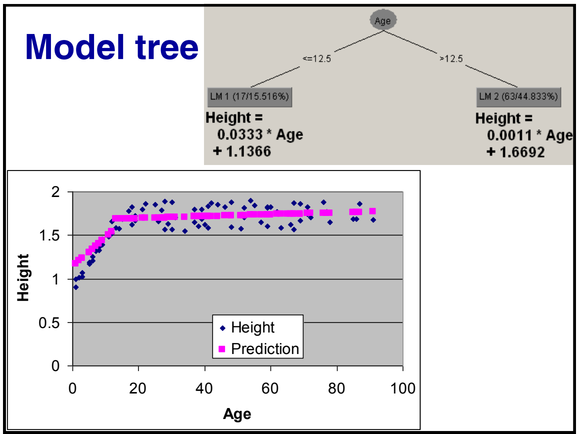





# Regression tree



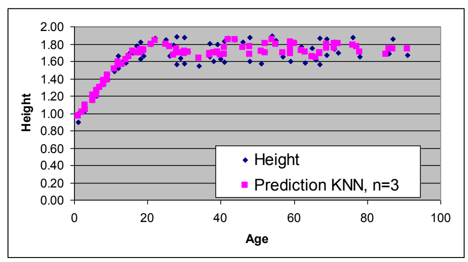

# Model tree






# kNN – K nearest neighbors

- Looks at K closest examples (by age) and predicts the average of their target variable
- K=3






# Which predictor is the best?

| Age | Height | Baseline | Linear regression | Regression tree | Model tree | kNN |
|---|---|---|---|---|---|---|
| 2 | 0.85 | 1.63 | 1.43 | 1.39 | 1.20 | 1.01 |
| 10 | 1.4 | 1.63 | 1.47 | 1.46 | 1.47 | 1.51 |
| 35 | 1.7 | 1.63 | 1.61 | 1.71 | 1.71 | 1.67 |
| 70 | 1.6 | 1.63 | 1.81 | 1.71 | 1.75 | 1.81 |



# Evaluating numeric prediction

| Performance measure | Formula |
|---|---|
| mean-squared error | $\frac{(p_1-a_1)^2+\ldots+(p_n-a_n)^2}{n}$ |
| root mean-squared error | $\sqrt{\frac{(p_1-a_1)^2+\ldots+(p_n-a_n)^2}{n}}$ |
| mean absolute error | $\frac{\lvert p_1-a_1\rvert+\ldots+\lvert p_n-a_n\rvert}{n}$ |
| relative squared error | $\frac{(p_1-a_1)^2+\ldots+(p_n-a_n)^2}{(a_1-\bar{a})^2+\ldots+(a_n-\bar{a})^2}$, where $\bar{a}=\frac{1}{n}\sum_i a_i$ |
| root relative squared error | $\sqrt{\frac{(p_1-a_1)^2+\ldots+(p_n-a_n)^2}{(a_1-\bar{a})^2+\ldots+(a_n-\bar{a})^2}}$ |
| relative absolute error | $\frac{\lvert p_1-a_1\rvert+\ldots+\lvert p_n-a_n\rvert}{\lvert a_1-\bar{a}\rvert+\ldots+\lvert a_n-\bar{a}\rvert}$ |
| correlation coefficient | $\frac{S_{PA}}{\sqrt{S_P S_A}}$, where $S_{PA}=\frac{\sum_i(p_i-\bar{p})(a_i-\bar{a})}{n-1}$, $S_p=\frac{\sum_i(p_i-\bar{p})^2}{n-1}$, and $S_A=\frac{\sum_i(a_i-\bar{a})^2}{n-1}$ |

# Course Outline





# Part IV. Descriptive DM techniques

- Predictive vs. descriptive induction
- Subgroup discovery
- Association rule learning
- Hierarchical clustering



# Predictive vs. descriptive induction

- **Predictive induction:** Inducing classifiers for solving classification and prediction tasks,
  - Classification rule learning, Decision tree learning, ...
  - Bayesian classifier, ANN, SVM, ...
  - Data analysis through hypothesis generation and testing
- **Descriptive induction:** Discovering interesting regularities in the data, uncovering patterns, ... for solving KDD tasks
  - Symbolic clustering, Association rule learning, Subgroup discovery, ...
  - Exploratory data analysis



# Descriptive DM

- Often used for preliminary explanatory data analysis
- User gets feel for the data and its structure
- Aims at deriving descriptions of characteristics of the data
- Visualization and descriptive statistical techniques can be used



# Descriptive DM

- **Description**
  - Data description and summarization: describe elementary and aggregated data characteristics (statistics, …)
  - Dependency analysis:
    - describe associations, dependencies, …
    - discovery of properties and constraints
- **Segmentation**
  - Clustering: separate objects into subsets according to distance and/or similarity (clustering, SOM, visualization, ...)
  - Subgroup discovery: find unusual subgroups that are significantly different from the majority (deviation detection w.r.t. overall class distribution)



# Predictive vs. descriptive induction: A rule learning perspective

- **Predictive induction:** Induces **rulesets** acting as classifiers for solving classification and prediction tasks
- **Descriptive induction:** Discovers **individual rules** describing interesting regularities in the data

- **Therefore:** Different goals, different heuristics, different evaluation criteria

# Supervised vs. unsupervised learning: A rule learning perspective

- **Supervised learning:** Rules are induced from labeled instances (training examples with class assignment) - usually used in **predictive induction**

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | NONE |
| O2 | 23 | myope | no | normal | SOFT |
| O3 | 22 | myope | yes | reduced | NONE |
| O4 | 27 | myope | yes | normal | HARD |
| O5 | 19 | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | SOFT |
| O15 | 43 | hypermetrope | yes | reduced | NONE |
| O16 | 39 | hypermetrope | yes | normal | NONE |
| O17 | 54 | myope | no | reduced | NONE |
| O18 | 62 | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NONE |



# Supervised vs. unsupervised learning: A rule learning perspective

- **Supervised learning:** Rules are induced from labeled instances (training examples with class assignment) - usually used in **predictive induction**
- **Unsupervised learning:** Rules are induced from unlabeled instances (training examples with no class assignment) - usually used in **descriptive induction**

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | ~~NONE~~ |
| O2 | 23 | myope | no | normal | ~~SOFT~~ |
| O3 | 22 | myope | yes | reduced | ~~NONE~~ |
| O4 | 27 | myope | yes | normal | ~~HARD~~ |
| O5 | 19 | hypermetrope | no | reduced | ~~NONE~~ |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | ~~SOFT~~ |
| O15 | 43 | hypermetrope | yes | reduced | ~~NONE~~ |
| O16 | 39 | hypermetrope | yes | normal | ~~NONE~~ |
| O17 | 54 | myope | no | reduced | ~~NONE~~ |
| O18 | 62 | myope | no | normal | ~~NONE~~ |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | ~~NONE~~ |



# Supervised vs. unsupervised learning: A rule learning perspective

- **Supervised learning:** Rules are induced from labeled instances (training examples with class assignment) - usually used in **predictive induction**
- **Unsupervised learning:** Rules are induced from unlabeled instances (training examples with no class assignment) - usually used in **descriptive induction**
- **Exception: Subgroup discovery**

  Discovers **individual rules** describing interesting regularities in the data from **labeled** examples



# Task reformulation: Binary Class Values

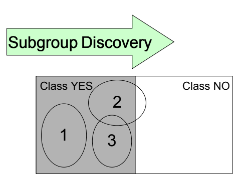
| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | NO |
| O2 | 23 | myope | no | normal | YES |
| O3 | 22 | myope | yes | reduced | NO |
| O4 | 27 | myope | yes | normal | YES |
| O5 | 19 | hypermetrope | no | reduced | NO |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | YES |
| O15 | 43 | hypermetrope | yes | reduced | NO |
| O16 | 39 | hypermetrope | yes | normal | NO |
| O17 | 54 | myope | no | reduced | NO |
| O18 | 62 | myope | no | normal | NO |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NO |

Binary classes (positive vs. negative examples of Target class)
- for Concept learning – classification and class description
- for Subgroup discovery – exploring patterns characterizing groups of instances of target class



# Subgroup Discovery

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | NO |
| O2 | 23 | myope | no | normal | YES |
| O3 | 22 | myope | yes | reduced | NO |
| O4 | 27 | myope | yes | normal | YES |
| O5 | 19 | hypermetrope | no | reduced | NO |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | YES |
| O15 | 43 | hypermetrope | yes | reduced | NO |
| O16 | 39 | hypermetrope | yes | normal | NO |
| O17 | 54 | myope | no | reduced | NO |
| O18 | 62 | myope | no | normal | NO |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NO |




- A task in which individual interpretable patterns in the form of rules are induced from data, labeled by a predefined property of interest.
- SD algorithms learn several independent rules that describe groups of target class examples
  - subgroups must be large and significant



# Part IV. Descriptive DM techniques

- Predictive vs. descriptive induction
- Subgroup discovery
- Association rule learning
- Hierarchical clustering

# Subgroup Discovery

**Task definition (Kloesgen, Wrobel 1997)**

**Given:** a population of individuals and a target class label (the property of individuals we are interested in)

**Find:** population subgroups that are statistically most `interesting', e.g., are as large as possible and have most unusual statistical (distributional) characteristics w.r.t. the target class (property of interest)

# Subgroup interestingness

**Interestingness criteria:**

– As large as possible
– Class distribution as different as possible from the distribution in the entire data set
– Significant
– Surprising to the user
– Non-redundant
– Simple
– Useful - actionable

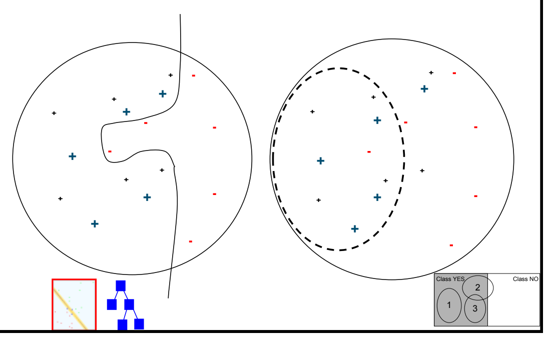


# Classification versus Subgroup Discovery

- **Classification (predictive induction) - constructing sets of classification rules**
  – aimed at learning a model for classification or prediction
  – rules are dependent
- **Subgroup discovery (descriptive induction) – constructing individual subgroup describing rules**
  – aimed at finding interesting patterns in target class examples
    - large subgroups (high target class coverage)
    - with significantly different distribution of target class examples (high TP/FP ratio, high significance, high WRAcc)
  – each rule (pattern) is an independent chunk of knowledge



# Classification versus Subgroup discovery






# Subgroup discovery task

**Task definition for a use case of finding and characterizing population subgroups with high risk for coronary heart disease (CHD)**

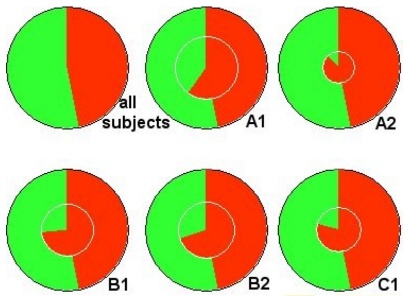
– **Given:** a population of individuals and a property of interest (target class, e.g. CHD)
– **Find:** `most interesting' descriptions of population subgroups
  - are as large as possible (high target class coverage)
  - have most unusual distribution of the target property (high TP/FP ratio, high significance)



# Subgroup Discovery: Medical Use Case

- **Find and characterize population subgroups with high risk for coronary heart disease (CHD)** (Gamberger, Lavrač, Krstačić)
- **A1** for males: **principal risk factors**
  CHD ← pos. fam. history & age > 46
- **A2** for females: **principal risk factors**
  CHD ← bodyMassIndex > 25 & age >63
- **A1, A2** (anamnestic info only), **B1, B2** (an. and physical examination), **C1** (an., phy. and ECG)
- **A1: supporting factors** (found by statistical analysis): psychosocial stress, as well as cigarette smoking, hypertension and overweight

## Subgroup visualization



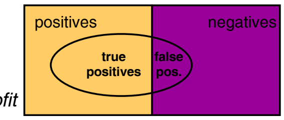

Subgroups of patients with CHD risk

[Gamberger, Lavrač & Wettschereck, IDAMAP2002]



## Subgroups vs. classifiers

- Classifiers:
  - Classification rules aim at pure subgroups
  - A set of rules forms a domain model
- Subgroups:
  - Rules describing subgroups aim at significantly higher proportion of positives
  - Each rule is an independent chunk of knowledge
- Link
  - SD can be viewed as cost-sensitive classification
  - Instead of *FNcost* we aim at increased *TPprofit*






## Classification Rule Learning for Subgroup Discovery: Deficiencies

- Only first few rules induced by the covering algorithm have sufficient support (coverage)
- Subsequent rules are induced from smaller and strongly biased example subsets (pos. examples not covered by previously induced rules), which hinders their ability to detect population subgroups
- 'Ordered' rules are induced and interpreted sequentially as a **if-then-else** decision list



## CN2-SD: Adapting CN2 Rule Learning to Subgroup Discovery

- Weighted covering algorithm
- Weighted relative accuracy (WRAcc) search heuristics, with added example weights
- Probabilistic classification
- Evaluation with different interestingness measures



## CN2-SD: CN2 Adaptations

- General-to-specific search (beam search) for best rules
- Rule quality measure:
  - CN2: Laplace: Acc(Class ← Cond) =
    = p(Class|Cond) = $(n_c+1)/(n_{rule}+k)$
  - CN2-SD: Weighted Relative Accuracy
    WRAcc(Class ← Cond) =
    p(Cond) (p(Class|Cond) - p(Class))
- Weighted covering approach (example weights)
- Significance testing (likelihood ratio statistics)
- Output: Unordered rule sets (probabilistic classification)

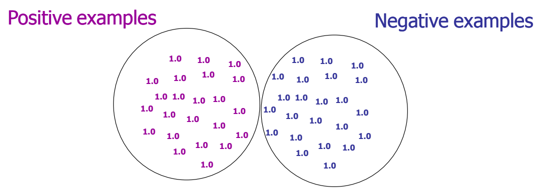


## CN2-SD: Weighted Covering

- Standard covering approach:
  covered examples are deleted from current training set

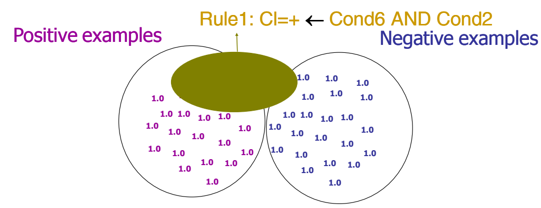
- Weighted covering approach:
  - weights assigned to examples
  - covered pos. examples are re-weighted:
    in all covering loop iterations, store count i how many times (with how many rules induced so far) a pos. example has been covered: w(e,i), w(e,0)=1
    - **Additive weights:** `w(e,i) = 1/(i+1)`
      **`w(e,i)` – pos. example e being covered `i` times**

# Subgroup Discovery



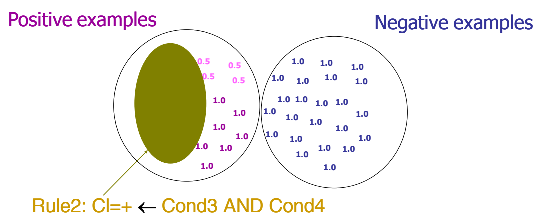



# Subgroup Discovery



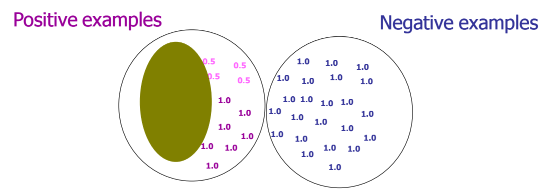



# Subgroup Discovery






# Subgroup Discovery



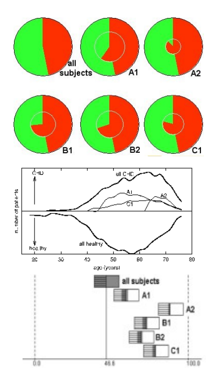


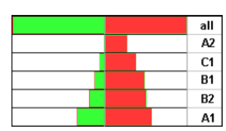

# CN2-SD: Weighted WRAcc Search Heuristic

- **Weighted relative accuracy (WRAcc) search heuristics, with added example weights**
  WRAcc(Cl ← Cond) = p(Cond) (p(Cl|Cond) - p(Cl))
  increased coverage, decreased # of rules, approx. equal accuracy (PKDD-2000)
- In WRAcc computation, probabilities are estimated with relative frequencies, adapt:
  WRAcc(Cl ← Cond) = p(Cond) (p(Cl|Cond) - p(Cl)) =
  n'(Cond)/N' ( n'(Cl.Cond)/n'(Cond) - n'(Cl)/N' )
  - N' : sum of weights of examples
  - n'(Cond) : sum of weights of all covered examples
  - n'(Cl.Cond) : sum of weights of all correctly covered examples



# Subgroup visualization




**The CHD task:** Find, characterize and visualize population subgroups with high CHD risk (large enough, distributionally unusual, most actionable)

## Induced subgroups and their statistical characterization

**Subgroup A2 for femle patients:**

High-CHD-risk **IF**
body mass index over 25 kg/m$^2$ (typically 29)
**AND**
age over 63 years

**Supporting characteristics** (computed using ℵ2 statistical significance test) are: positive family history and hypertension. Women in this risk group typically have slightly increased LDL cholesterol values and normal but decreased HDL cholesterol values.



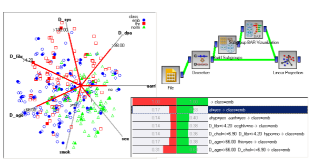
## SD algorithms in the Orange DM Platform

- **SD Algorithms in Orange**
  - SD (Gamberger & Lavrač, JAIR 2002
  - APRIORI-SD (Kavšek & Lavrač, AAI 2006
  - CN2-SD (Lavrač et al., JMLR 2004): Adapting CN2 classification rule learner to Subgroup Discovery
    - Weighted covering algorithm
    - Weighted relative accuracy (WRAcc) search heuristics, with added example weights



## SD algorithms in Orange and Orange4WS

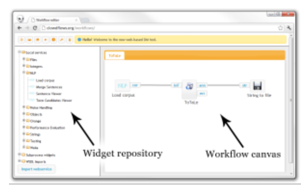
- **Orange**
  - classification and subgroup discovery algorithms
  - data mining workflows
  - visualization
  - developed at FRI, Ljubljana
- **Orange4WS** (Podpečan 2010)
  - Web service oriented
  - supports workflows and other Orange functionality
  - includes also
    - WEKA algorithms
    - relational data mining
    - semantic data mining with ontologies
  - Web-based platform is under construction

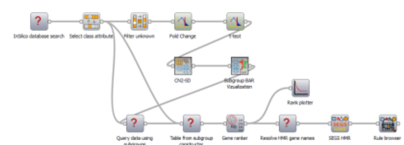




## Current platform and workflow developments

- CrowdFlows browser-based DM platform (Kranjc et al. 2012)
- Semantic Subgroup Discovery workflows (Vavpetič et al., 2012)





## Part IV. Descriptive DM techniques

- Predictive vs. descriptive induction
- Subgroup discovery
- Association rule learning
- Hierarchical clustering



## Association Rule Learning

**Rules: X =>Y, if X then Y**

X and Y are itemsets (records, conjunction of items), where items/features are binary-valued attributes)

**Given:** Transactions
itemsets (records)

| | i1 | i2 | ..................... | i50 |
|---|---|---|---|---|
| t1 | 1 | 1 | | 0 |
| t2 | 0 | 1 | | 0 |
| ... | ... | ... | ..................... | ... |

**Find:** A set of association rules in the form X =>Y

**Example:** Market basket analysis

beer & coke => peanuts & chips (0.05, 0.65)

- Support: Sup(X,Y) = #XY/#D = p(XY)
- Confidence: Conf(X,Y) = #XY/#X = Sup(X,Y)/Sup(X) = = p(XY)/p(X) = p(Y|X)

# Association Rule Learning: Examples

- Market basket analysis
  - beer & coke ⇒ peanuts & chips (5%, 65%)
    (IF beer AND coke THEN peanuts AND chips)
  - Support 5%: 5% of all customers buy all four items
  - Confidence 65%: 65% of customers that buy beer and coke also buy peanuts and chips
- Insurance
  - mortgage & loans & savings ⇒ insurance (2%, 62%)
  - Support 2%: 2% of all customers have all four
  - Confidence 62%: 62% of all customers that have mortgage, loan and savings also have insurance



# Association rule learning

- **X ⇒ Y** . . . IF X THEN Y, where X and Y are itemsets
- intuitive meaning: transactions that contain X tend to contain Y
- **Items** - binary attributes (features) m,f,headache, muscle pain, arthrotic, arthritic, spondylotic, spondylitic, stiff_less_1_hour
- **Example transactions** – itemsets formed of patient records

| | i1 | i2 ...... | ... i50 |
|---|---|---|---|
| t1 | 1 | 0 | 0 |
| t2 | 0 | 1 | 0 |
| ... | ... | ... | ... |

- **Association rules**
  spondylitic ⇒ arthritic & stiff_gt_1_hour [5%, 70%]
  arthrotic & spondylotic ⇒ stiff_less_1_hour [20%, 90%]



# Association Rule Learning

**Given:** a set of transactions D

**Find:** all association rules that hold on the set of transactions that have

- user defined minimum support, i.e., support > MinSup, and
- user defined minimum confidence, i.e., confidence > MinConf

It is a form of exploratory data analysis, rather than hypothesis verification



# Searching for the associations

- Find all large itemsets
- Use the large itemsets to generate association rules
- If XY is a large itemset, compute
  r =support(XY) / support(X)
- If r > MinConf, then X ⇒ Y holds
  (support > MinSup, as XY is large)



# Large itemsets

- Large itemsets are itemsets that appear in at least MinSup transaction
- All subsets of a large itemset are large itemsets (e.g., if A,B appears in at least MinSup transactions, so do A and B)
- This observation is the basis for very efficient algorithms for association rules discovery (linear in the number of transactions)



# Association rules vs. Classification rules

**Association rules**

- Exploration of dependencies
- Different combinations of dependent and independent attributes
- Complete search (all rules found)

**Classification rules**

- Focused prediction
- Predict one attribute (class) from the others
- Heuristic search (subset of rules found)

## Part IV. Descriptive DM techniques

- Predictive vs. descriptive induction
- Subgroup discovery
- Association rule learning
- Hierarchical clustering



## Hierarchical clustering

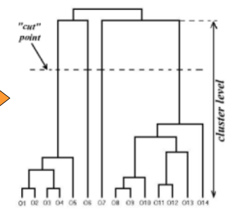
- Algorithm (agglomerative hierarchical clustering):

**Each instance is a cluster;**

**repeat**
  **find** ***nearest*** **pair** ***$C_i$*** **in** ***$C_j$*****;**
  ***fuse*** ***$C_i$*** **in** ***$C_j$*** **in a new cluster**
    ***$C_r = C_i \cup C_j$*****;**
  **determine** ***dissimilarities*** **between**
    ***$C_r$*** **and other clusters;**

**until one cluster left;**

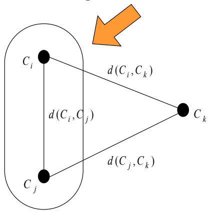
- Dendogram:






## Hierarchical clustering

- Fusing the nearest pair of clusters

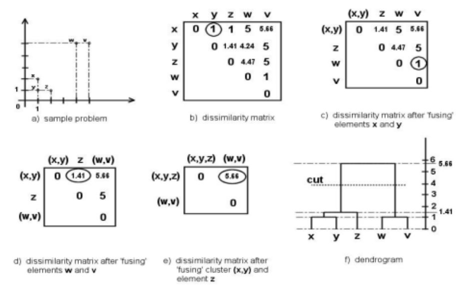



- Minimizing intra-cluster similarity
- Maximizing inter-cluster similarity

- Computing the dissimilarities from the "new" cluster

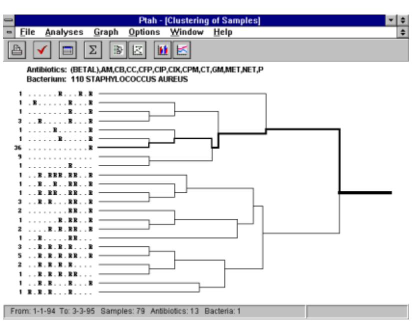


## Hierarchical clustering: example






## Results of clustering




A dendogram of resistance vectors

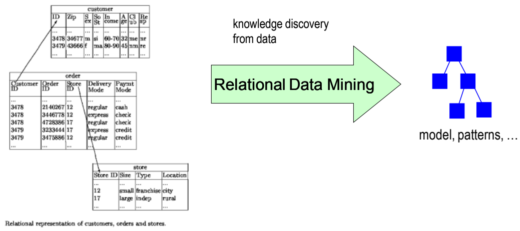
[Bohanec et al., "PTAH: A system for supporting nosocomial infection therapy", IDAMAP book, 1997]



## Part V: Relational Data Mining

- What is RDM
- Propositionalization techniques
- Semantic Data Mining
- Inductive Logic programming
- Learning as search in Inductive Logic Programming

# Relational Data Mining (Inductive Logic Programming) in a nutshell

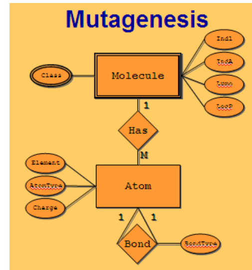



**Given:** a relational database, a set of tables. sets of logical facts, a graph, …
**Find:** a classification model, a set of interesting patterns



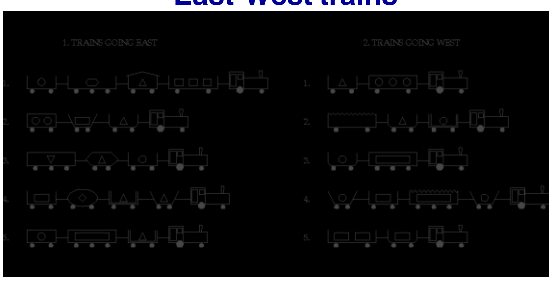
# Relational Data Mining (ILP)

- Learning from multiple tables
  - patient records connected with other patient and demographic information
- Complex relational problems:
  - temporal data: time series in medicine, ...
  - structured data: representation of molecules and their properties in protein engineering, biochemistry, ...



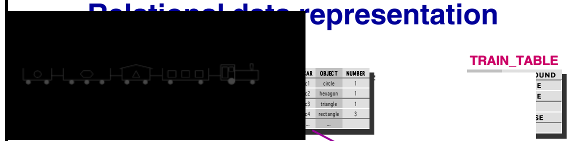



# Sample ILP problem: East-West trains





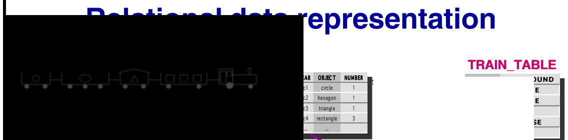
# [redacted]representation




| CAR | TRAIN | SHAPE | LENGTH | ROOF | WHEELS |
|---|---|---|---|---|---|
| c1 | t1 | rectangle | short | none | 2 |
| c2 | t1 | rectangle | long | none | 3 |
| c3 | t1 | rectangle | short | peaked | 2 |
| c4 | t1 | rectangle | long | none | 2 |
| ... | ... | ... |  |  | ... |



# [redacted]representation




| CAR | TRAIN | SHAPE | LENGTH | ROOF | WHEELS |
|---|---|---|---|---|---|
| c1 | t1 | rectangle | short | none | 2 |
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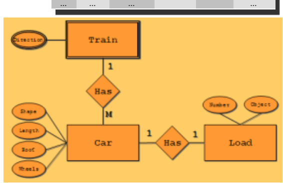
| c4 | t1 | rectangle | long | none | 2 |
| ... | ... | ... |  |  | ... |






# Part V: Relational Data Mining

- What is RDM
- Propositionalization techniques
- Semantic Data Mining
- Inductive Logic programming
- Learning as search in Inductive Logic Programming

## [redacted]on in a nutshell

[redacted]

TRAIN_TABLE

| CAR | TRAIN | SHAPE | LENGTH | ROOF | WHEELS |
|---|---|---|---|---|---|
| c1 | t1 | rectangle | short | none | 2 |
| c2 | t1 | rectangle | long | none | 3 |
| c3 | t1 | rectangle | short | peaked | 2 |
| c4 | t1 | rectangle | long | none | 2 |
| ... | ... | ... | | | ... |

**Transform** a multi-relational (**multiple-table**) representation to a propositional representation (**single table**)

Proposed in ILP systems
LINUS (Lavrac et al. 1991, 1994),
1BC (Flach and Lachiche 1999), …



## Propositionalization in a nutshell

**Main propositionalization step: first-order feature construction**

f1(T):-hasCar(T,C),clength(C,short).
f2(T):-hasCar(T,C), hasLoad(C,L), loadShape(L,circle)
f3(T) :- ….

TRAIN_TABLE

| LOAD | CAR | OBJECT | NUMBER |
|---|---|---|---|
| l1 | c1 | circle | 1 |
| l2 | c2 | hexagon | 1 |
| l3 | c3 | triangle | 1 |
| l4 | c4 | rectangle | 3 |
| ... | ... | ... | |

| CAR | TRAIN | SHAPE | LENGTH | ROOF | WHEELS |
|---|---|---|---|---|---|
| c1 | t1 | rectangle | short | none | 2 |
| c2 | t1 | rectangle | long | none | 3 |
| c3 | t1 | rectangle | short | peaked | 2 |
| c4 | t1 | rectangle | long | none | 2 |
| ... | ... | ... | | | ... |

**Propositional learning:**

t(T) ← f1(T), f4(T)

PROPOSITIONAL TRAIN_TABLE

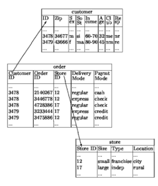
| train(T) | f1(T) | f2(T) | f3(T) | f4(T) | f5(T) |
|---|---|---|---|---|---|
| t1 | t | t | f | t | t |
| t2 | t | t | t | t | t |
| t3 | f | f | t | f | f |
| t4 | t | f | t | f | f |
| … | … | … | | | … |

**Relational interpretation:**

eastbound(T) ←
hasShortCar(T),hasClosedCar(T).

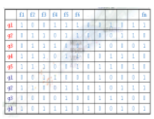


## Relational Data Mining through Propositionalization



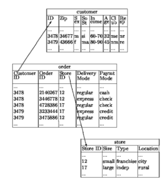
Step 1

Propositionalization





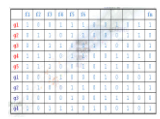
## Relational Data Mining through Propositionalization



Step 1

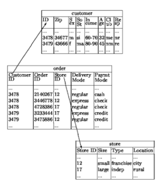
Propositionalization

1. constructing relational features
2. constructing a propositional table



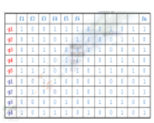


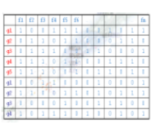
## Relational Data Mining through Propositionalization



Step 1

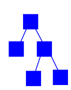
Propositionalization





Step 2

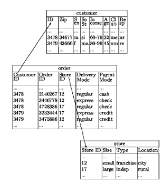
Data Mining



model, patterns, …

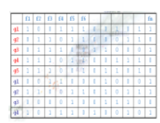


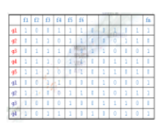
## Relational Data Mining through Propositionalization



Step 1

Propositionalization





Step 2

Data Mining

```
target(A) :-
   'Doctor'(A), 'Italy'(A).

target(A) :-
   'Public'(A), 'Gold'(A).

target(A) :-
   'Poland'(A), 'Deposit'(A), 'Gold'(A).

target(A) :-
   'Germany'(A), 'Insurance'(A).

target(A) :-
   'Service'(A), 'Germany'(A).
```

patterns (set of rules)

# RSD Lessons learned

Efficient propositionalization can be applied to individual-centered, multi-instance learning problems:

- one free global variable (denoting an individual, e.g. molecule M)
- one or more structural predicates: (e.g. has_atom(M,A)), each introducing a new existential local variable (e.g. atom A), using either the global variable (M) or a local variable introduced by other structural predicates (A)
- one or more utility predicates defining properties of individuals or their parts, assigning values to variables

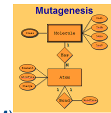
feature121(M):- hasAtom(M,A), atomType(A,21)
feature235(M):- lumo(M,Lu), lessThr(Lu,-1.21)
mutagenic(M):- feature121(M), feature235(M)



# Relational Data Mining in Orange4WS

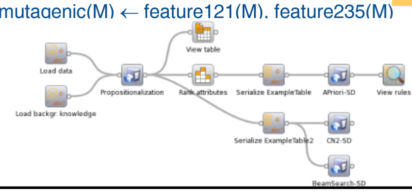
- service for propositionalization through efficient first-order feature construction (Železny and Lavrač, MLJ 2006)

  f121(M):- hasAtom(M,A), atomType(A,21)
  f235(M):- lumo(M,Lu), lessThr(Lu,1.21)




- subgroup discovery using CN2-SD

  mutagenic(M) ← feature121(M), feature235(M)








# Part V: Relational Data Mining

- What is RDM
- Propositionalization techniques
- Semantic Data Mining
- Inductive Logic programming
- Learning as search in Inductive Logic Programming



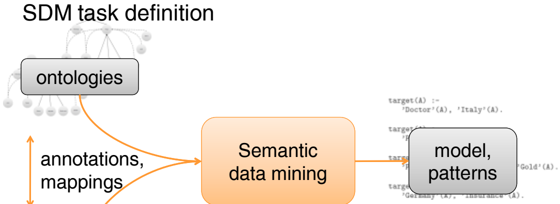
# What is Semantic Data Mining

- Ontology-driven (semantic) data mining is an emerging research topic
- Semantic Data Mining (SDM) - a new term denoting:
  - the new challenge of mining semantically annotated resources, with ontologies used as background knowledge to data mining
  - approaches with which semantic data are mined



# What is Semantic Data Mining

SDM task definition




**Given:**

- transaction data table, relational database, text documents, Web pages, …
- one or more domain ontologies

**Find:** a classification model, a set of patterns



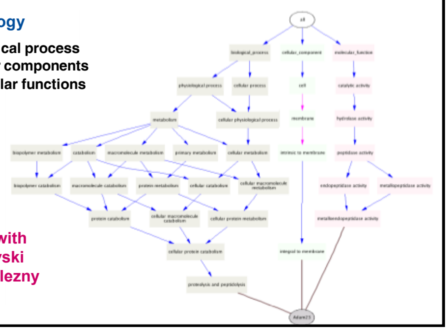
# Semantic Data Mining in Orange4WS

- Exploiting semantics in data mining
  - Using **domain ontologies** as background knowledge for data mining
- Semantic data mining technology: a two-step approach
  - Using propositionalization through first-order feature construction
  - Using subgroup discovery for rule learning
- Implemented in the SEGS algorithm

## Using domain ontologies (e.g. Gene Ontology) as background knowledge for Data Mining

**Gene Ontology**

**12093 biological process**
**1812 cellular components**
**7459 molecular functions**



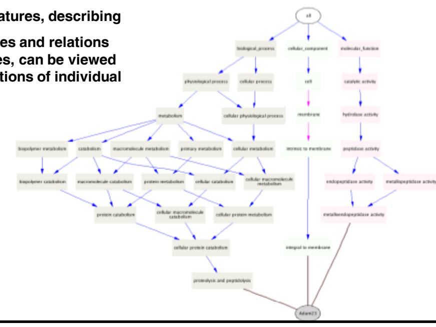
**Joint work with Igor Trajkovski and Filip Zelezny**



## Using domain ontologies (e.g. Gene Ontology) as background knowledge for Data Mining

**First-order features, describing**

**gene properties and relations between genes, can be viewed as generalisations of individual genes**





## First order feature construction

First order features with support > *min_support*

f(7,A):-function(A,'GO:0046872').
f(8,A):-function(A,'GO:0004871').
f(11,A):-process(A,'GO:0007165').
f(14,A):-process(A,'GO:0044267').
f(15,A):-process(A,'GO:0050874').
f(20,A):-function(A,'GO:0004871'), process(A,'GO:0050874').
f(26,A):-component(A,'GO:0016021').
f(29,A):- function(A,'GO:0046872'), component(A,'GO:0016020')
f(122,A):-interaction(A,B),function(B,'GO:0004872').
f(223,A):-interaction(A,B),function(B,'GO:0004871'), process(B,'GO:0009613').
f(224,A):-interaction(A,B),function(B,'GO:0016787'), component(B,'GO:0043231').

existential



## Propositionalization

diffexp g1 (gene64499)
diffexp g2 (gene2534)
diffexp g3 (gene5199)
diffexp g4 (gene1052)
diffexp g5 (gene6036)
….

random g1 (gene7443)
random g2 (gene9221)
random g3 (gene2339)
random g4 (gene9657)
random g5 (gene19679)
….

| | f1 | f2 | f3 | f4 | f5 | f6 | … | | | | … | fn |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| g1 | 1 | 0 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 0 | 1 | 1 |
| g2 | 0 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 0 | 1 | 1 | 0 |
| g3 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 1 |
| g4 | 1 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 1 | 1 | 1 | 0 |
| g5 | 1 | 1 | 1 | 0 | 0 | 1 | 0 | 1 | 1 | 0 | 1 | 0 |
| g1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 |
| g2 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 1 | 0 | 1 | 1 | 1 |
| g3 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 1 | 1 | 0 | 0 |
| g4 | 1 | 0 | 1 | 1 | 1 | 0 | 1 | 0 | 0 | 1 | 0 | 1 |



## Propositional learning: subgroup discovery

| | f1 | f2 | f3 | f4 | f5 | f6 | … | | | | … | fn |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| g1 | 1 | 0 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 0 | 1 | 1 |
| g2 | 0 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 0 | 1 | 1 | 0 |
| g3 | 0 | 1 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 1 |
| g4 | 1 | 1 | 1 | 0 | 1 | 1 | 0 | 0 | 1 | 1 | 1 | 0 |
| g5 | 1 | 1 | 1 | 0 | 0 | 1 | 0 | 1 | 1 | 0 | 1 | 0 |
| g1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 |
| g2 | 1 | 1 | 0 | 0 | 1 | 1 | 0 | 1 | 0 | 1 | 1 | 1 |
| g3 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 1 | 1 | 0 | 0 |
| g4 | 1 | 0 | 1 | 1 | 1 | 0 | 1 | 0 | 0 | 1 | 0 | 1 |

Over-expressed

IF

f2 and f3

[4,0]

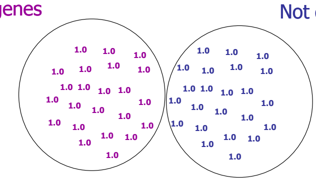
diffexp(A) :- interaction(A,B) & function(B,'GO:0004871')



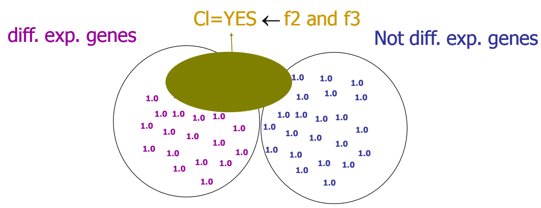
## Subgroup Discovery

diff. exp. genes

Not diff. exp. genes



## Subgroup Discovery




In RSD (using propositional learner CN2-SD):

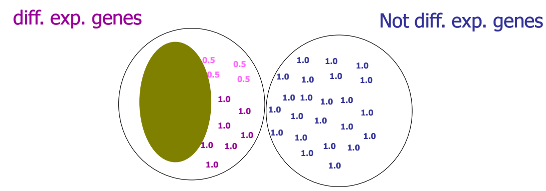
Quality of the rules = Coverage x Precision

*Coverage = sum of the covered weights

*Precision = purity of the covered genes



## Subgroup Discovery




RSD naturally uses gene weights in its procedure for repetitive subgroup generation, via its heuristic rule evaluation: weighted relative accuracy



## Semantic Data Mining in two steps

- **Step 1:** **Construct relational logic features** of genes such as
  **interaction(g, G) & function(G, protein_binding)**
  *(g interacts with another gene whose functions include protein binding)*
  and **propositional table construction** with features as attributes
- **Step 2:** Using these features to **discover and describe subgroups of genes** that are differentially expressed (e.g., belong to class DIFF.EXP. of top 300 most differentially expressed genes) in contrast with RANDOM genes (randomly selected genes with low differential expression).
- Sample subgroup description:

```
diffexp(A) :- interaction(A,B) AND
              function(B,'GO:0004871') AND
              process(B,'GO:0009613')
```



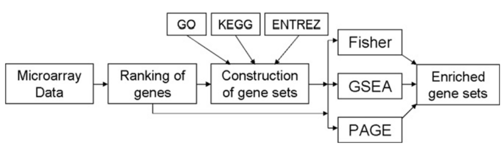
## Summary: SEGS, using the RSD approach

- The SEGS approach enables to discover new medical knowledge from the combination of gene expression data with public gene annotation databases
- The SEGS approach proved effective in several biomedical applications (JBI 2008, …)
  - The work on semantic data mining - using ontologies as background knowledge for subgroup discovery with SEGS - was done in collaboration with I.Trajkovski, F. Železny and J. Tolar
- Recent work: Semantic subgroup discovery implemented in Orange4WS



## Semantic subgroup discovery with SEGS

- SEGS workflow is implemented in the Orange4WS data mining environment

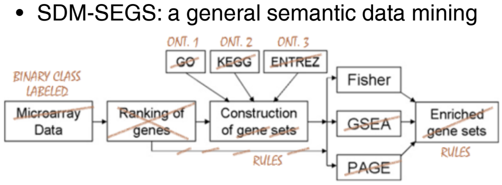



- SEGS is also implemented also as a Web applications
  (Trajkovski et al., IEEE TSMC 2008, Trajkovski et al., JBI 2008)



## From SEGS to SDM-SEGS: Generalizing SEGS

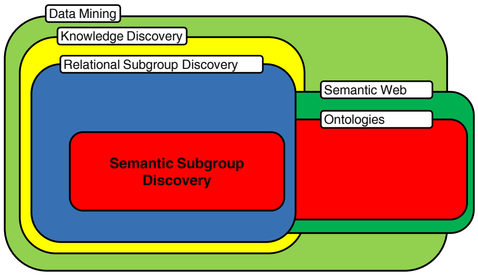
- SDM-SEGS: a general semantic data mining




- Discovers subgroups both for ranked and labeled data
- Exploits input ontologies in OWL format
- Is also implemented in Orange4WS

## Semantic Data Mining

- Semantic subgroup discovery (Vavpetič et al., 2012)






## Part V: Relational Data Mining

- What is RDM
- Propositionalization techniques
- Semantic Data Mining
- Inductive Logic programming
- Learning as search in Inductive Logic Programming



## Sample ILP problem: Logic programming

$E^+$ = `{sort([2,1,3],[1,2,3])}`
$E^-$ = `{sort([2,1],[1]),sort([3,1,2],[2,1,3])}`

$B$: definitions of `permutation/2` and `sorted/1`

- **Predictive ILP**

```
sort(X,Y) ← permutation(X,Y), sorted(Y).
```

- **Descriptive ILP**

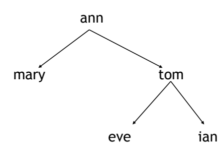
```
sorted(Y) ← sort(X,Y).
permutation(X,Y) ← sort(X,Y)
sorted(X) ← sort(X,X)
```



## Sample ILP problem: Knowledge discovery

$E^+$ = `{daughter(mary,ann),daughter(eve,tom)}`
$E^-$ = `{daughter(tom,ann),daughter(eve,ann)}`

$B$ = `{mother(ann,mary), mother(ann,tom), father(tom,eve), father(tom,ian), female(ann), female(mary), female(eve), male(pat),male(tom), parent(X,Y) ← mother(X,Y), parent(X,Y) ← father(X,Y)}`






## Sample relational problem: Knowledge discovery

- $E^+$ = `{daughter(mary,ann),daughter(eve,tom)}`
  $E^-$ = `{daughter(tom,ann),daughter(eve,ann)}`
- $B$ = `{mother(ann,mary),mother(ann,tom),father(tom,eve), father(tom,ian),female(ann),female(mary),female(eve), male(pat),male(tom),parent(X,Y)←mother(X,Y), parent(X,Y)←father(X,Y)}`

- **Predictive ILP -** Induce a definite clause

```
daughter(X,Y) ← female(X), parent(Y,X).
```

or a set of definite clauses

```
daughter(X,Y) ← female(X), mother(Y,X).
daughter(X,Y) ← female(X), father(Y,X).
```

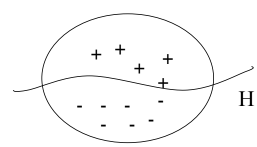
- **Descriptive ILP -** Induce a set of (general) clauses

```
← daughter(X,Y), mother(X,Y).
female(X)← daughter(X,Y).
mother(X,Y); father(X,Y) ← parent(X,Y).
```

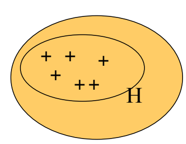


## Basic Relational Data Mining and ILP learning tasks

**Predictive RDM**

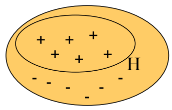



**Descriptive RDM**



# Predictive ILP

- **Given:**
  - **A set of observations**
    - **positive examples $E^+$**
    - **negative examples $E^-$**
  - **background knowledge $B$**
  - **hypothesis language $L_H$**
  - **covers relation**
- **Find:**
  **A hypothesis $H \in L_H$, such that (given $B$) $H$ covers all positive and no negative examples**

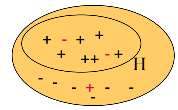



- **In logic, find $H$ such that**
  - **$\forall e \in E^+ : B \wedge H \models e$ ($H$ is complete)**
  - **$\forall e \in E^- : B \wedge H \not\models e$ ($H$ is consistent)**
- **In ILP, $E$ are ground facts, $B$ and $H$ are (sets of) definite clauses**



# Predictive ILP

- **Given:**
  - A set of observations
    - positive examples $E^+$
    - negative examples $E^-$
  - background knowledge $B$
  - hypothesis language $L_H$
  - covers relation
  - quality criterion
- **Find:**
  A hypothesis $H \in L_H$, such that (given $B$) $H$ is optimal w.r.t. some quality criterion, e.g., max. predictive accuracy $A(H)$

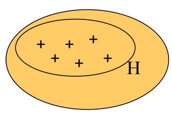



(instead of finding a hypothesis $H \in L_H$, such that (given $B$) $H$ covers all positive and no negative examples)



# Descriptive ILP

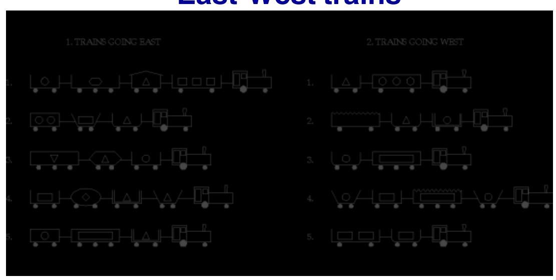
- **Given:**
  - A set of observations
    (positive examples $E^+$)
  - background knowledge $B$
  - hypothesis language $L_H$
  - covers relation
- **Find:**
  Maximally specific hypothesis $H \in L_H$, such that (given $B$) $H$ covers all positive examples




- In logic, **find** $H$ such that $\forall c \in H$, $c$ is true in some preferred model of $B \cup E$ (e.g., least Herbrand model $M(B \cup E)$)
- **In ILP, $E$ are ground facts, $B$ are (sets of) general clauses**



# Sample problem: East-West trains






# RDM knowledge representation (database)

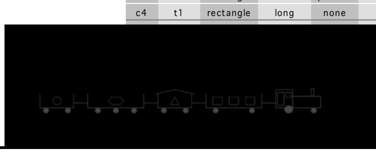
LOAD_TABLE

| LOAD | CAR | OBJECT | NUMBER |
|---|---|---|---|
| l1 | c1 | circle | 1 |
| l2 | c2 | hexagon | 1 |
| l3 | c3 | triangle | 1 |
| l4 | c4 | rectangle | 3 |
| ... | ... | ... | |

TRAIN_TABLE

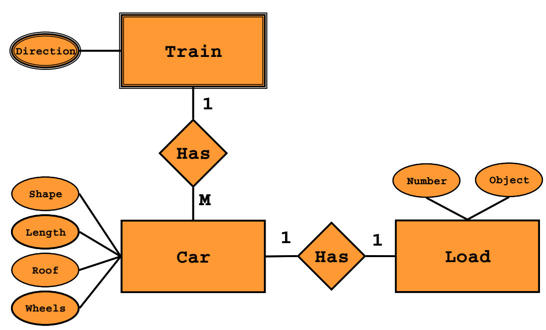
CAR_TABLE

| CAR | TRAIN | SHAPE | LENGTH | ROOF | WHEELS |
|---|---|---|---|---|---|
| c1 | t1 | rectangle | short | none | 2 |
| c2 | t1 | rectangle | long | none | 3 |
| c3 | t1 | rectangle | short | peaked | 2 |
| c4 | t1 | rectangle | long | none | 2 |
| | | | | | ... |

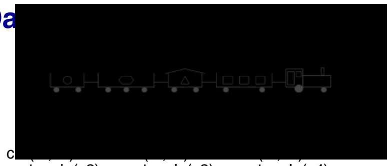




# ER diagram for East-West trains



## ILP representation:
## Da



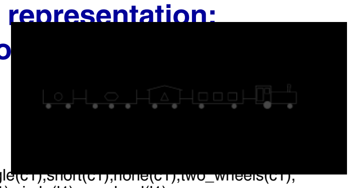
- Example:
  eastbound(t1).
- Background theory:

| | | | |
|---|---|---|---|
| car(t1,c1). | c | | |
| rectangle(c1). | rectangle(c2). | rectangle(c3). | rectangle(c4). |
| short(c1). | long(c2). | short(c3). | long(c4). |
| none(c1). | none(c2). | peaked(c3). | none(c4). |
| two_wheels(c1). | three_wheels(c2). | two_wheels(c3). | two_wheels(c4). |
| load(c1,l1). | load(c2,l2). | load(c3,l3). | load(c4,l4). |
| circle(l1). | hexagon(l2). | triangle(l3). | rectangle(l4). |
| one_load(l1). | one_load(l2). | one_load(l3). | three_loads(l4). |

- Hypothesis (predictive ILP):
  eastbound(T) :- car(T,C),short(C),not none(C).



## ILP representation:
## Datalo



- Example:
  eastbound(t1):-
  car(t1,c1),rectangle
  load(c1,l1),circle(l1),one_load(l1),
  car(t1,c2),rectangle(c2),long(c2),none(c2),three_wheels(c2),
  load(c2,l2),hexagon(l2),one_load(l2),
  car(t1,c3),rectangle(c3),short(c3),peaked(c3),two_wheels(c3),
  load(c3,l3),triangle(l3),one_load(l3),
  car(t1,c4),rectangle(c4),long(c4),none(c4),two_wheels(c4),
  load(c4,l4),rectangle(l4),three_load(l4).
- Background theory: empty
- Hypothesis:
  eastbound(T):-car(T,C),short(C),not none(C).



## ILP represe

- Example:
  eastbound([c(rectangle
  c(rectangle,long,none,3,l(hexagon,1)),
  c(rectangle,short,peaked,2,l(triangle,1)),
  c(rectangle,long,none,2,l(rectangle,3))]).
- Background theory: member/2, arg/3
- Hypothesis:
  eastbound(T):-member(C,T),arg(2,C,short), not arg(3,C,none).



## Propositionalization in ILP (LINUS)

- **Example: learning family relationships**

| Training examples | | Background knowledge | |
|---|---|---|---|
| daughter(sue,eve). | (+) | parent(eve,sue). | female(ann). |
| daughter(ann,pat). | (+) | parent(ann,tom). | female(sue). |
| daughter(tom,ann). | (-) | parent(pat,ann). | female(eve). |
| daughter(eve,ann). | (-) | parent(tom,sue). | |

- **Transformation to propositional form:**

| Class | Variables | | Propositional features | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | X | Y | f(X) | f(Y) | p(X,X) | p(X,Y) | p(Y,X) | p(Y,Y) | X=Y |
| ⊕ | sue | eve | true | true | false | false | true | false | false |
| ⊕ | ann | pat | true | false | false | false | true | false | false |
| ⊖ | tom | ann | false | true | false | false | true | false | false |
| ⊖ | eve | ann | true | true | false | false | false | false | false |

- **Result of propositional rule learning:**
  Class = ⊕ if (female(X) = true) $\wedge$ (parent(Y,X) = true
- **Transformation to program clause form:**
  daughter(X,Y) $\leftarrow$ female(X),parent(Y,X)



## First-order feature construction

- All the expressiveness of ILP is in the features
- Given a way to construct (or choose) first-order features, body construction in ILP becomes propositional
  – idea: learn non-determinate clauses with LINUS by saturating background knowledge (performing systematic feature construction in a given language bias)



## Declarative bias for first-order feature construction

- In ILP, features involve interactions of local variables
- Features should define properties of individuals (e.g. trains, molecules) or their parts (e.g., cars, atoms)
- Feature construction in LINUS, using the following language bias:
  – one free global variable (denoting an individual, e.g. train)
  – one or more structural predicates: (e.g., has_car(T,C)) ,each introducing a new existential local variable (e.g. car, atom), using either the global variable (train, molecule) or a local variable introduced by other structural predicates (car, load)
  – one or more utility predicates defining properties of individuals or their parts: no new variables, just using variables
  – all variables should be used
  – parameter: max. number of predicates forming a feature

## Sample first-order features

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- The following rule has two features 'has a short car' and 'has a closed car':
  eastbound(T):-hasCar(T,C1),clength(C1,short),
  hasCar(T,C2),not croof(C2,none).
- The following rule has one feature 'has a short closed car':
  eastbound(T):-hasCar(T,C),clength(C,short),
  not croof(C,none).
- Equivalent representation:

  eastbound(T):-hasShortCar(T),hasClosedCar(T).

  hasShortCar(T):-hasCar(T,C),clength(C,short).

  hasClosedCar(T):-hasCar(T,C),not croof(C,none).

## LINUS revisited

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- Standard LINUS:
  - transforming an ILP problem to a propositional problem
  - apply background knowledge predicates
- Revisited LINUS:
  - Systematic first-order feature construction in a given language bias
- Too many features?
  - use a relevancy filter (Gamberger and Lavrac)

## LINUS revisited: Example: East-West trains

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**Rules induced by CN2, using 190 first-order features with up to two utility predicates:**

eastbound(T):-
hasCarHasLoadSingleTriangle(T),
not hasCarLongJagged(T),
not hasCarLongHasLoadCircle(T).

westbound(T):-
not hasCarEllipse(T),
not hasCarShortFlat(T),
not hasCarPeakedTwo(T).

**Meaning:**

eastbound(T):-
hasCar(T,C1),hasLoad(C1,L1),lshape(L1,tria),lnumber(L1,1),
not (hasCar(T,C2),clength(C2,long),croof(C2,jagged)),
not (hasCar(T,C3),hasLoad(C3,L3),clength(C3,long),lshape(L3,circ)).

westbound(T):-
not (hasCar(T,C1),cshape(C1,ellipse)),
not (hasCar(T,C2),clength(C2,short),croof(C2,flat)),
not (hasCar(T,C3),croof(C3,peak),cwheels(C3,2)).

## Relational Data Mining in Orange4WS and ClowdFlows

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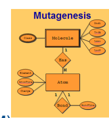
- service for propositionalization through efficient first-order feature construction (Železny and Lavrač, MLJ 2006)

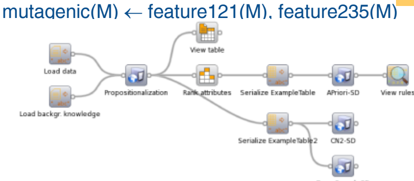
  f121(M):- hasAtom(M,A), atomType(A,21)

  f235(M):- lumo(M,Lu), lessThr(Lu,1.21)




- subgroup discovery using CN2-SD

  mutagenic(M) ← feature121(M), feature235(M)

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## Part V: Relational Data Mining

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- What is RDM
- Propositionalization techniques
- Semantic Data Mining
- Inductive Logic programming
- Learning as search in Inductive Logic Programming

## Learning as search

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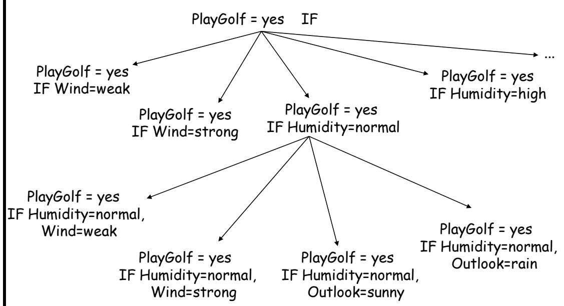
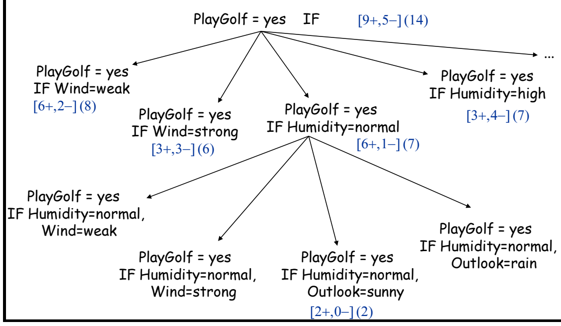
- **Structuring the state space**: Representing a partial order of hypotheses (e.g. rules) as a graph
  - nodes: concept descriptions (hypotheses/rules)
  - arcs defined by specialization/generalization operators : an arc from parent to child exists if-and-only-if parent is a proper most specific generalization of child
- **Specialization operators**: e.g., adding conditions: s(A=a2 & B=b1) = {A=a2 & B=b1 & D=d1, A=a2 & B=b1 & D=d2}
- **Generalization operators**: e.g., dropping conditions: g(A=a2 & B=b1) = {A=a2, B=b1}
- **Partial order of hypotheses defines a lattice (called a refinement graph)**

## Learn-one-rule as search - Structuring the hypothesis space: PlayGolf example





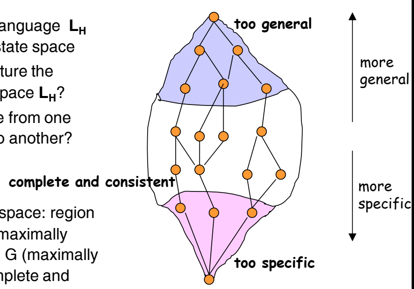

## Learn-one-rule as heuristic search: PlayGolf example






## Learning as search (Mitchell's version space model)

- Hypothesis language $\mathbf{L_H}$ defines the state space
- How to structure the hypothesis space $\mathbf{L_H}$?
- How to move from one hypothesis to another?

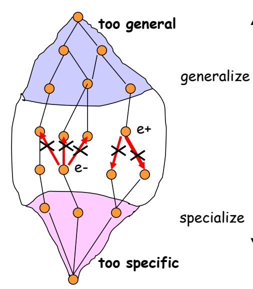



- The version space: region between S (maximally specific) and G (maximally general) complete and consistent concept descriptions



## Learning as search

- Search/move by applying generalization and specialization
- **Prune generalizations**:
  - if H covers example e then all generalizations of H will also cover e (prune using neg. ex.)
- **Prune specializations:**
  - if H does not cover example e, no specialization will cover e (prune using if H pos. ex.)






## Learning as search: Learner's ingredients

- structure of the search space (specialization and generalization operators)
- search strategy
  - depth-first
  - breath-first
  - heuristic search (best first, hill-climbing, beam search)
- search heuristics
  - measure of attribute 'informativity'
  - measure of 'expected classification accuracy' (relative frequency, Laplace estimate, m-estimate), ...
- stopping criteria (consistency, completeness, statistical significance, …)



## Learn-one-rule: search heuristics

- Assume a two-class problem
- Two classes (+,-), learn rules for + class (Cl).
- Search for specializations R' of a rule R = Cl ← Cond from the RuleBase.
- Specializarion R' of rule R = Cl ← Cond

  has the form R' = Cl ← Cond & Cond'
- Heuristic search for rules: find the 'best' Cond' to be added to the current rule R, such that rule accuracy is improved, e.g., such that Acc(R') > Acc(R)
  - where the expected **classification accuracy** can be estimated as A(R) = p(Cl|Cond)

## Learn-one-rule – Search strategy: Greedy vs. beam search

- learn-one-rule by greedy general-to-specific search, at each step selecting the `best' descendant, no backtracking
  - e.g., the best descendant of the initial rule
    PlayGolf = yes ←
  - is rule PlayGolf = yes ← Humidity=normal
- beam search: maintain a list of k best candidates at each step; descendants (specializations) of each of these k candidates are generated, and the resulting set is again reduced to k best candidates



## ILP as search of program clauses

- An ILP learner can be described by
  - the **structure of the space of clauses**
    - based on the generality relation
    - Let C and D be two clauses.
      C is more general than D (C |= D) iff
      covers(D) ⊆ covers(C)
    - Example: p(X,Y) ← r(Y,X) is more general than
      p(X,Y) ← r(Y,X), q(X)
  - its **search strategy**
    - uninformed search (depth-first, breadth-first, iterative deepening)
    - heuristic search (best-first, hill-climbing, beam search)
  - its **heuristics**
    - for directing search
    - for stopping search (quality criterion)



## ILP as search of program clauses

- **Semantic generality**
  Hypothesis $H_1$ is semantically more general than $H_2$ w.r.t. background theory $B$ if and only if $B \cup H_1 \models H_2$
- **Syntactic generality or θ-subsumption**
  (most popular in ILP)
  - Clause $c_1$ $\theta$-subsumes $c_2$ ($c_1 \geq_\theta c_2$)
    if and only if $\exists\theta: c_1\theta \subseteq c_2$
  - Hypothesis $H_1 \geq \theta H_2$
    if and only if $\forall c_2 \in H_2$ exists $c_1 \in H_1$ such that $c_1 \geq \theta\, c_2$
- **Example**
  c1 = daughter(X,Y) ← parent(Y,X)
  c2 = daughter(mary,ann) ← female(mary),
  parent(ann,mary),
  parent(ann,tom).
  c1 $\theta$-subsumes $c_2$ under $\theta$ = {X/mary,Y/ann}

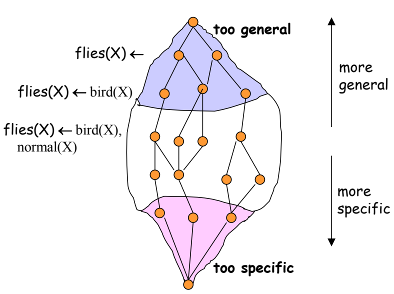


## The role of subsumption in ILP

- Generality ordering for hypotheses
- Pruning of the search space:
  - generalization
    - if C covers a neg. example then its generalizations need not be considered
  - specialization
    - if C doesn't cover a pos. example then its specializations need not be considered
- Top-down search of refinement graphs
- Bottom-up search of the hypo. space by
  - building least general generalizations, and
  - inverting resolutions



## Structuring the hypothesis space





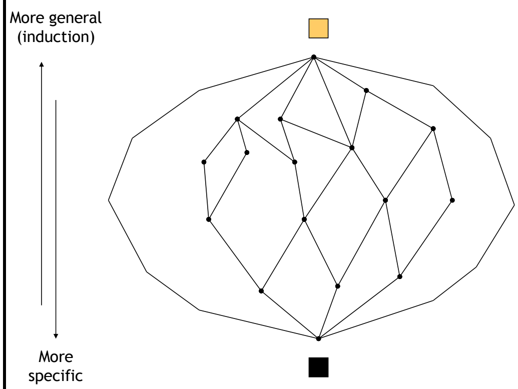

## Two strategies for learning

- General-to-specific
  - if Θ-subsumption is used then refinement operators
- Specific-to-general search
  - if Θ-subsumption is used then lgg-operator or generalization operator

# ILP as search of program clauses

- Two strategies for learning
  - Top-down search of refinement graphs
  - Bottom-up search
    - building least general generalizations
    - inverting resolution (CIGOL)
    - inverting entailment (PROGOL)

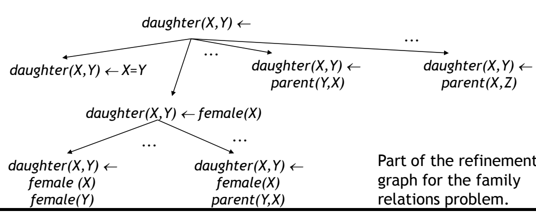







# Generality ordering of clauses

| Training examples | | Background knowledge | |
|---|---|---|---|
| daughter(mary,ann). | ⊕ | parent(ann,mary). | female(ann.). |
| daughter(eve,tom). | ⊕ | parent(ann,tom). | female(mary). |
| daughter(tom,ann). | ⊖ | parent(tom,eve). | female(eve). |
| daughter(eve,ann). | ⊖ | parent(tom,ian). | |

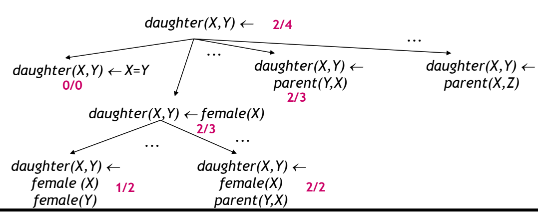



Part of the refinement graph for the family relations problem.



# Greedy search of the best clause

| Training examples | | Background knowledge | |
|---|---|---|---|
| daughter(mary,ann). | ⊕ | parent(ann,mary). | female(ann.). |
| daughter(eve,tom). | ⊕ | parent(ann,tom). | female(mary). |
| daughter(tom,ann). | ⊖ | parent(tom,eve). | female(eve). |
| daughter(eve,ann). | ⊖ | parent(tom,ian). | |






# FOIL

- Language: function-free normal programs recursion, negation, new variables in the body, no functors, no constants (original)
- Algorithm: covering
- Search heuristics: weighted info gain
- Search strategy: hill climbing
- Stopping criterion: encoding length restriction
- Search space reduction: types, in/out modes determinate literals
- Ground background knowledge, extensional coverage
- Implemented in C



# Part V: Summary

- RDM extends DM by allowing multiple tables describing structured data
- Complexity of representation and therefore of learning is determined by one-to-many links
- Many RDM problems are individual-centred and therefore allow strong declarative bias

# Advanced Topics

- Text mining: An introduction
- Document clustering and outlier detection
- Wordification approach to relational data mining

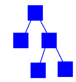
# Background: Data mining

| Person | Age | Spect. presc. | Astigm. | Tear prod. | Lenses |
|---|---|---|---|---|---|
| O1 | 17 | myope | no | reduced | NONE |
| O2 | 23 | myope | no | normal | SOFT |
| O3 | 22 | myope | yes | reduced | NONE |
| O4 | 27 | myope | yes | normal | HARD |
| O5 | 19 | hypermetrope | no | reduced | NONE |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 35 | hypermetrope | no | normal | SOFT |
| O15 | 43 | hypermetrope | yes | reduced | NONE |
| O16 | 39 | hypermetrope | yes | normal | NONE |
| O17 | 54 | myope | no | reduced | NONE |
| O18 | 62 | myope | no | normal | NONE |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 56 | hypermetrope | yes | normal | NONE |

data

knowledge discovery from data

Data Mining



model, patterns, clusters, …

**Given:** transaction data table, a set of text documents, …

**Find:** a classification model, a set of interesting patterns

# Data mining: Task reformulation

| Person | Young | Myope | Astigm. | Reuced tea | Lenses |
|---|---|---|---|---|---|
| O1 | 1 | 1 | 0 | 1 | NO |
| O2 | 1 | 1 | 0 | 0 | YES |
| O3 | 1 | 1 | 1 | 1 | NO |
| O4 | 1 | 1 | 1 | 0 | YES |
| O5 | 1 | 0 | 0 | 1 | NO |
| O6-O13 | ... | ... | ... | ... | ... |
| O14 | 0 | 0 | 0 | 0 | YES |
| O15 | 0 | 0 | 1 | 1 | NO |
| O16 | 0 | 0 | 1 | 0 | NO |
| O17 | 0 | 1 | 0 | 1 | NO |
| O18 | 0 | 1 | 0 | 0 | NO |
| O19-O23 | ... | ... | ... | ... | ... |
| O24 | 0 | 0 | 1 | 0 | NO |

Binary features and class values

# Text mining: Words/terms as binary features

| Document | Word1 | Word2 | … | WordN | Class |
|---|---|---|---|---|---|
| d1 | 1 | 1 | 0 | 1 | NO |
| d2 | 1 | 1 | 0 | 0 | YES |
| d3 | 1 | 1 | 1 | 1 | NO |
| d4 | 1 | 1 | 1 | 0 | YES |
| d5 | 1 | 0 | 0 | 1 | NO |
| d6-d13 | … | … | … | … | … |
| d14 | 0 | 0 | 0 | 0 | YES |
| d15 | 0 | 0 | 1 | 1 | NO |
| d16 | 0 | 0 | 1 | 0 | NO |
| d17 | 0 | 1 | 0 | 1 | NO |
| d18 | 0 | 1 | 0 | 0 | NO |
| d19-d23 | … | … | … | … | … |
| d24 | 0 | 0 | 1 | 0 | NO |

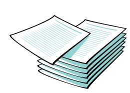
Instances = documents
Words and terms = Binary features

# Text Mining from unlabeled data

| Document | Word1 | Word2 | … | WordN | ~~Class~~ |
|---|---|---|---|---|---|
| d1 | 1 | 1 | 0 | 1 | ~~NO~~ |
| d2 | 1 | 1 | 0 | 0 | ~~YES~~ |
| d3 | 1 | 1 | 1 | 1 | ~~NO~~ |
| d4 | 1 | 1 | 1 | 0 | ~~YES~~ |
| d5 | 1 | 0 | 0 | 1 | ~~NO~~ |
| d6-d13 | … | … | … | … | ~~…~~ |
| d14 | 0 | 0 | 0 | 0 | ~~YES~~ |
| d15 | 0 | 0 | 1 | 1 | ~~NO~~ |
| d16 | 0 | 0 | 1 | 0 | ~~NO~~ |
| d17 | 0 | 1 | 0 | 1 | ~~NO~~ |
| d18 | 0 | 1 | 0 | 0 | ~~NO~~ |
| d19-d23 | … | … | … | … | ~~…~~ |
| d24 | 0 | 0 | 1 | 0 | ~~NO~~ |

Unlabeled data - clustering: grouping of similar instances
- association rule learning

# Text mining



Step 1

BoW vector construction

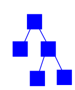
| Document | Word1 | Word2 | … | WordN | Class |
|---|---|---|---|---|---|
| d1 | 1 | 1 | 0 | 1 | NO |
| d2 | 1 | 1 | 0 | 0 | YES |
| d3 | 1 | 1 | 1 | 1 | NO |
| d4 | 1 | 1 | 1 | 0 | YES |
| d5 | 1 | 0 | 0 | 1 | NO |
| d6-d13 | ... | ... | ... | ... | ... |
| d14 | 0 | 0 | 0 | 0 | YES |
| d15 | 0 | 0 | 1 | 1 | NO |
| d16 | 0 | 0 | 1 | 0 | NO |
| d17 | 0 | 1 | 0 | 1 | NO |
| d18 | 0 | 1 | 0 | 0 | NO |
| d19-d23 | ... | ... | ... | ... | ... |
| d24 | 0 | 0 | 1 | 0 | NO |

1. BoW features construction
2. Table of BoW vectors construction

| Document | Word1 | Word2 | … | WordN | Class |
|---|---|---|---|---|---|
| d1 | 1 | 1 | 0 | 1 | NO |
| d2 | 1 | 1 | 0 | 0 | YES |
| d3 | 1 | 1 | 1 | 1 | NO |
| d4 | 1 | 1 | 1 | 0 | YES |
| d5 | 1 | 0 | 0 | 1 | NO |
| d6-d13 | ... | ... | ... | ... | ... |
| d14 | 0 | 0 | 0 | 0 | YES |
| d15 | 0 | 0 | 1 | 1 | NO |
| d16 | 0 | 0 | 1 | 0 | NO |
| d17 | 0 | 1 | 0 | 1 | NO |
| d18 | 0 | 1 | 0 | 0 | NO |
| d19-d23 | ... | ... | ... | ... | ... |
| d24 | 0 | 0 | 1 | 0 | NO |

Step 2

Data Mining



model, patterns, clusters,

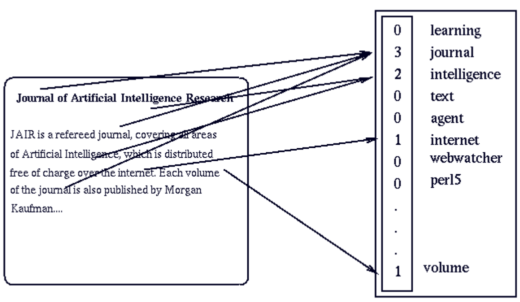
## Text Mining

- Feature construction
  - StopWords elimination
  - Stemming or lemmatization
  - Term construction by frequent N-Grams construction
  - Terms obtained from thesaurus (e.g., WordNet)
- BoW vector construction
- Mining of BoW vector table
  - Feature selection, Document similarity computation
  - Text mining: Categorization, Clustering, Summarization, …

## Stemming and Lemmatization

- Different forms of the same word usually problematic for text data analysis
  - because they have different spelling and similar meaning (e.g. learns, learned, learning,…)
  - usually treated as completely unrelated words
- Stemming is a process of transforming a word into its stem
  - cutting off a suffix (eg., smejala -> smej)
- Lemmatization is a process of transforming a word into its normalized form
  - replacing the word, most often replacing a suffix (eg., smejala -> smejati)

## Bag-of-Words document representation




## Word weighting

- In bag-of-words representation each word is represented as a separate variable having numeric weight.
- The most popular weighting schema is normalized word frequency TFIDF:

$$tfidf(w) = tf \cdot \log\left(\frac{N}{df(w)}\right)$$

- Tf(w) – term frequency (number of word occurrences in a document)
- Df(w) – document frequency (number of documents containing the word)
- N – number of all documents
- Tfidf(w) – relative importance of the word in the document

The word is more important if it appears several times in a target document

The word is more important if it appears in less documents

## Cosine similarity between document vectors

- Each document D is represented as a vector of TF-IDF weights
- Similarity between two vectors is estimated by the similarity between their vector representations (cosine of the angle between the two vectors):

$$Similarity\ (D_1, D_2) = \frac{\sum_i x_{1i} x_{2i}}{\sqrt{\sum_j x_j^2}\sqrt{\sum_k x_k^2}}$$

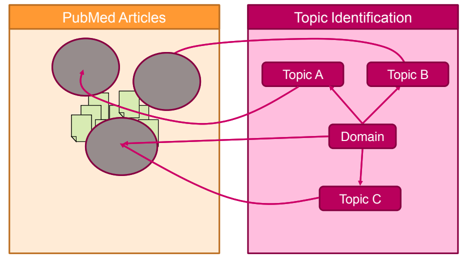
## Advanced Topics

- Text mining: An introduction
- Document clustering and outlier detection
- Wordification approach to relational data mining

## Document clustering

- Clustering is a process of finding natural groups in data in a unsupervised way (no class labels pre-assigned to documents)
- Document similarity is used
- Most popular clustering methods:
  - K-Means clustering
  - Agglomerative hierarchical clustering
  - EM (Gaussian Mixture)
  - …

## Document clustering with OntoGen ontogen.ijs.si




Slide adapted from D. Mladenić, JSI

## Using OntoGen for clustering PubMed articles on autism

Work by Petrič et al. 2009


www.ontogen.si
Fortuna, Mladenić, Grobelnik 2006

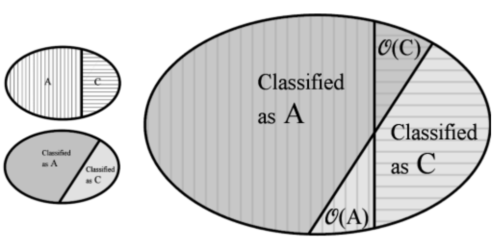
## K-Means clustering in OntoGen

OntoGen uses k-Means clustering for semi-automated topic ontology construction

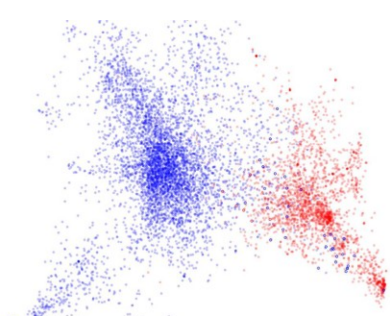
- Given:
  - set of documents (eg., word-vectors with TFIDF),
  - distance measure (eg., cosine similarity)
  - K - number of groups
- For each group initialize its centroid with a random document
- While not converging
  - each document is assigned to the nearest group (represented by its centroid)
  - for each group calculate new centroid (group mass point, average document in the group)

## Detecting outlier documents

- By classification noise detection on a domain pair dataset, assuming two separate document corpora A and C




## Outlier detection for cross-domain knowledge discovery

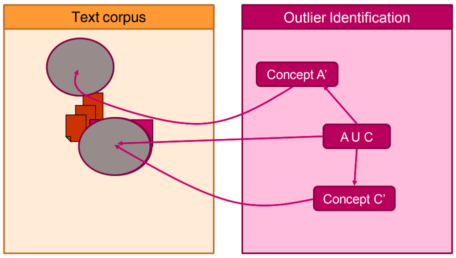


*2-dimensional projection of documents (about autism (red) and calcineurin (blue). Outlier documents are bolded for the user to easily spot them.*

***Our research has shown that most domain bridging terms appear in outlier documents.***

(Lavrač, Sluban, Grčar, Juršič 2010)

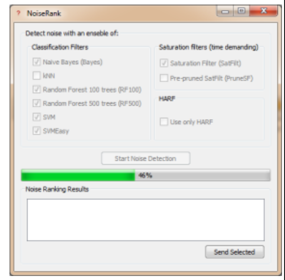
## Using OntoGen for outlier document identification




Slide adapted from D. Mladenić, JSI

## NoiseRank: Ensemble-based noise and outlier detection

- Misclassified document detection by an ensemble of diverse classifiers (e.g., Naive Bayes, Random Forest, SVM, … classifiers)
- Ranking of misclassified documents by "voting" of classifiers



## NoiseRank on news articles

Articles on Kenyan elections: local vs. Western media

```
Rank | Class | ID | Detected by:
-------------------------------------------------------------------
 1.     WE    352  __Bayes____RF100____RF500_____SVM____SVMEasy__SatFilt_
-------------------------------------------------------------------
 2.     LO     25  __Bayes____RF100____RF500_____SVM____SVMEasy_
 3.     LO    101  __Bayes____RF100____RF500_____SVM____SVMEasy_
 4.     LO    173  __Bayes____RF100____RF500_____SVM____SVMEasy_
 5.     WE    348  __Bayes____RF100____RF500_____SVM____SVMEasy_
 6.     WE    326  __Bayes____RF100____RF500_____SVM____SVMEasy_
 7.     WE    357  __Bayes____RF100____RF500_____SVM____SatFilt_
 8.     WE    410  __Bayes____RF100____RF500_____SVM____SVMEasy_
-------------------------------------------------------------------
 9.     LO     21  __RF100____RF500_____SVM____SVMEasy_
10.     LO      4  __Bayes____RF500_____SVM____SVMEasy_
11.     LO     68  __RF100____RF500_____SVM____SVMEasy_
12.     LO    162  __Bayes____RF500_____SVM____SVMEasy_
13.     WE    358  __Bayes____RF100____RF500_____SVM___
14.     WE    464  __RF100____RF500_____SVM____SVMEasy_
-------------------------------------------------------------------
15.     LO    153  __Bayes_____SVM____SVMEasy_
16.     LO    201  __RF100____RF500___SatFilt_
17.     WE    238  __RF100____RF500_____SVM___
18.     WE    364  __Bayes____RF500_____SVM___
19.     WE    370  __Bayes____RF100_____SVM___
20.     WE    379  __RF100____RF500___SVMEasy_
```

## NoiseRank on news articles

- **Article 352: Out of topic** The article was later indeed removed from the corpus used for further linguistic analysis, since it is not about Kenya(ns) or the socio-political climate but about British tourists or expatriates' misfortune.
- **Article 173: Guest journalist** Wrongly classified because it could be regarded as a "Western article" among the local Kenyan press. The author does not have the cultural sensitivity or does not follow the editorial guidelines requiring to be careful when mentioning words like tribe in negative contexts. One could even say that he has a kind of "Western" writing style.

## Advanced Topics

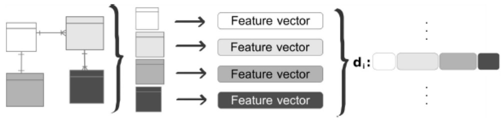
- Text mining: An introduction
- Document clustering and outlier
- Wordification approach to relational data mining

## Motivation

- Develop a RDM technique inspired by **text mining**
- Using a large number of simple, easy to understand features (**words**)
- Improved **scalability**, handling large datasets
- Used as a preprocessing step to propositional learners

## Wordification Methodology

- Transform a relational database to a document corpus
  - For each individual (row) in the main table, concatenate words generated for the main table with words generated for the other tables, linked through external keys




## Wordification Methodology

- One individual of the main data table in the relational database ~ one text document
- Features (attribute values) ~ the words of this document
- Individual words (called **word-items** or **witems**) are constructed as combinations of:

$$[table\ name]\_[attribute\ name]\_[value]$$

- **n-grams** are constructed to model feature dependencies:

$$[witem_1]\_[witem_2]\_\ ...\ \_[witem_n]$$

## Wordification Methodology

- Transform a relational database to a document corpus
- Construct BoW vectors with TF-IDF weights on words
  (optional: Perform feature selection)
- Apply text mining or propositional learning on BoW table

## Wordification

**TRAIN**

| trainID | eastbound |
|---|---|
| t1 | east |
| ... | ... |
| t5 | west |
| ... | ... |

**CAR**

| carID | shape | roof | wheels | train |
|---|---|---|---|---|
| c11 | rectangle | none | 2 | t1 |
| c12 | rectangle | peaked | 3 | t1 |
| ... | ... | ... | ... | ... |
| c51 | rectangle | none | 2 | t5 |
| c52 | hexagon | flat | 2 | t5 |
| ... | ... | ... | ... | ... |

**t1:** [car_roof_none, car_shape_rectangle, car_wheels_2,
car_roof_none__car_shape_rectangle,
car_roof_none__car_wheels_2,
car_shape_rectangle__car_wheels_2,
car_roof_peaked, car_shape_rectangle,
car_wheels_3, car_roof_peaked__car_shape_rectangle,
car_roof_peaked__car_wheels_3,
car_shape_rectangle__car_wheels_3], **east**

## Wordification

**t1:** [car_roof_none, car_shape_rectangle, car_wheels_2,
car_roof_none__car_shape_rectangle, car_roof_none__car_wheels_2,
car_shape_rectangle__car_wheels_2, car_roof_peaked, car_shape_rectangle,
car_wheels_3, car_roof_peaked__car_shape_rectangle,
car_roof_peaked__car_wheels_3, car_shape_rectangle__car_wheels_3], **east**

**t5:** [car_roof_none, car_shape_rectangle, car_wheels_2,
car_roof_none__car_shape_rectangle, car_roof_none__car_wheels_2,
car_shape_rectangle__car_wheels_2, car_roof_flat, car_shape_hexagon,
car_wheels_2, car_roof_flat__car_shape_hexagon,
car_roof_flat__car_wheels_2, car_shape_hexagon__car_wheels_2], **west**

TF-IDF calculation for BoW vector construction:

| | car_shape_rectangle | car_roof_peaked | car_wheels_3 | car_roof_peaked__car_shape_rectangle | car_shape_rectangle__car_wheels_3 | ... | class |
|---|---|---|---|---|---|---|---|
| t1 | 0.000 | 0.693 | 0.693 | 0.693 | 0.693 | ... | east |
| ... | ... | ... | ... | ... | ... | ... | ... |
| t5 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | ... | west |
| ... | ... | ... | ... | ... | ... | ... | ... |

## TF-IDF weights

- No explicit use of existential variables in features, TF-IDF instead
- The weight of a word indicates how relevant is the feature for the given individual
- The TF-IDF weights can then be used either for filtering words with low importance or for using them directly by a propositional learner (e.g. J48)

## Experiments

- Cross-validation experiments on 8 relational datasets: Trains (in two variants), Carcinogenesis, Mutagenesis with 42 and 188 examples, IMDB, and Financial.
- Results (using J48 for propositional learning)

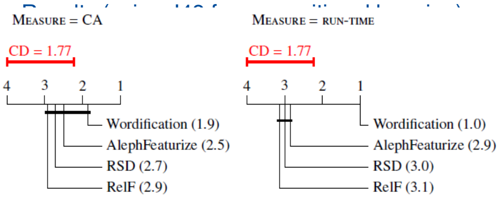

## Experiments

- Cross-validation experiments on 8 relational datasets: Trains (in two variants), Carcinogenesis, Mutagenesis with 42 and 188 examples, IMDB, and Financial.

- Results (using J48 for propositional learning)
  - first applying Friedman test to rank the algorithms,
  - then post-hoc test Nemenyi test to compare multiple algorithms to each other


## Experiments

- Cross-validation experiments on 8 relational datasets: Trains (in two variants), Carcinogenesis, Mutagenesis with 42 and 188 examples, IMDB, and Financial.


## Experiments

| Domain | Algorithm | J48-Accuracy[%] | J48-AUC | Run-time[s] |
|---|---|---|---|---|
| Trains without position | Wordification | 55.00 | 0.51 | **0.11** |
| | RelF | 65.00 | 0.65 | 1.04 |
| | RSD | 65.00 | 0.68 | 0.53 |
| | AlephFeaturize | **75.00** | **0.82** | 0.40 |
| Trains | Wordification | **95.00** | **0.91** | **0.12** |
| | RelF | 65.00 | 0.62 | 1.06 |
| | RSD | 50.00 | 0.53 | 0.47 |
| | AlephFeaturize | 85.00 | 0.74 | 0.38 |
| Mutagenesis42 | Wordification | **97.62** | **0.93** | **0.39** |
| | RelF | 80.95 | 0.59 | 2.11 |
| | RSD | **97.62** | **0.93** | 2.63 |
| | AlephFeaturize | **97.62** | **0.93** | 2.07 |
| Mutagenesis188 | Wordification | **95.74** | 0.90 | **1.65** |
| | RelF | 75.53 | 0.79 | 7.76 |
| | RSD | 94.15 | **0.91** | 10.10 |
| | AlephFeaturize | 87.23 | 0.88 | 19.27 |
| IMDB | Wordification | **84.34** | **0.79** | **1.23** |
| | RelF | 79.52 | 0.73 | 32.49 |
| | RSD | 73.49 | 0.47 | 4.33 |
| | AlephFeaturize | 73.49 | 0.47 | 4.96 |
| Carcinogenesis | Wordification | **61.09** | **0.62** | **1.79** |
| | RelF | 54.71 | 0.53 | 16.44 |
| | RSD | 58.05 | 0.56 | 9.29 |
| | AlephFeaturize | 55.32 | 0.49 | 104.70 |
| Financial | Wordification | 86.75 | 0.48 | **4.65** |
| | RelF | **97.00** | **0.91** | 260.93 |
| | RSD | 86.75 | 0.48 | 533.68 |
| | AlephFeaturize | 86.75 | 0.48 | 525.86 |

## Use Case: IMDB

- **IMDB subset:** Top 250 and bottom 100 movies
- Movies, actors, movie genres, directors, director genres
- Wordification methodology applied
- Association rules learned on BoW vector table

## Use Case: IMDB

goodMovie ← director_genre_drama, movie_genre_thriller, director_name_AlfredHitchcock. (Support: 5.38% Confidence: 100.00%)

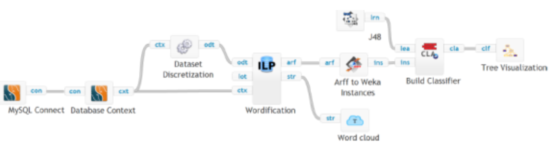
movie_genre_drama ← goodMovie, actor_name_RobertDeNiro. (Support: 3.59% Confidence: 100.00%)

director_name_AlfredHitchcock ← actor_name_AlfredHitchcock. (Support: 4.79% Confidence: 100.00%)

director_name_StevenSpielberg ← goodMovie, movie_genre_adventure, actor_name_TedGrossman. (Support: 1.79% Confidence: 100.00%)

# Wordification implemented in ClowdFlows

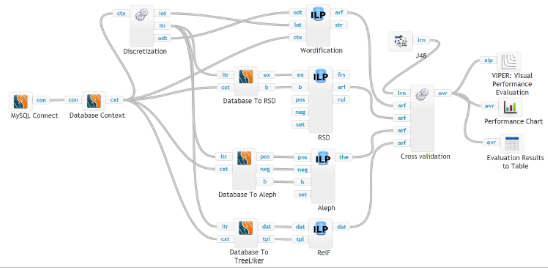
- Propositionalization through wordification, available at http://clowdflows.org/workflow/1455/






# Evaluation implemented in ClowdFlows

- Wordification and propositionalization algorithms comparison, available at http://clowdflows.org/workflow/1456/




# Summary

- Wordification methodology
- Implemented in ClowdFlows
- Allows for solving non-standard RDM tasks, including RDM clustering, **word cloud visualization**, **association rule learning**, topic ontology construction, outlier detection, …