Data Mining
and Knowledge Discovery

Part of
Jožef Stefan IPS “ICT” Programme
and “Statistics” Programme

2010 / 2011

Nada Lavrač

Jožef Stefan Institute

Ljubljana, Slovenia

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, Kononenko & Kukar Ch. 1)

II. Predictive DM Techniques
- Bayesian classifier (Kononenko Ch. 9.6)
- Decision Tree learning (Mitchell Ch. 3, Kononenko Ch. 9.1)
- Classification rule learning (Berthold book Ch. 7, 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

Introductory seminar lecture

X. JSI & Department of Knowledge Technologies

I. Introduction: First generation data mining

- 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, Kononenko & Kukar Ch. 1)

XX. Selected data mining techniques: Advanced subgroup discovery techniques and applications

XXX. Recent advances: Cross-context link discovery

Jožef Stefan Institute

- **Jožef Stefan Institute (JSI, founded in 1949)**
  - named after a distinguished physicist Jožef Stefan (1835-1893)

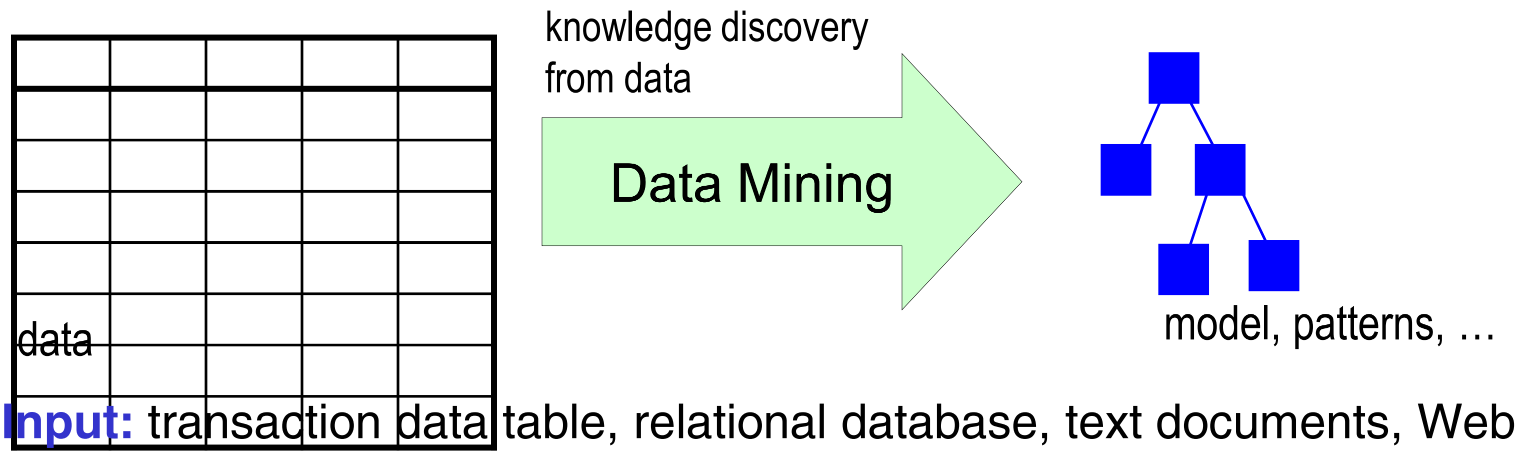
    $j = \sigma T^4$

  - 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

Department of Knowledge Technologies

- **Head:** Nada Lavrač, **Staff:** 40 researchers, 15 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:**
  - Semantic Web and Ontologies
  - Knowledge management
  - Decision support
  - Human language technologies
- **Applications:**
  - Medicine, Bioinformatics, Public Health
  - Ecology, Finance, …

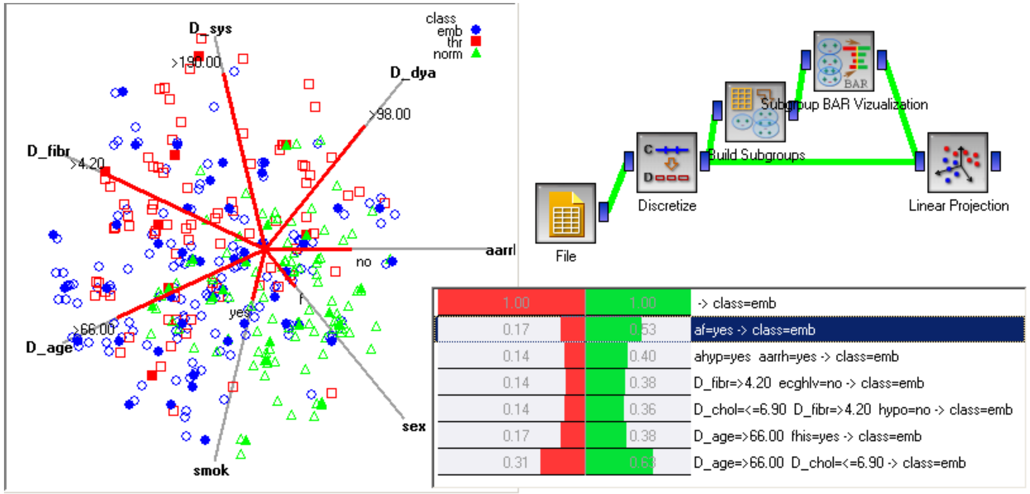
Basic Data Mining Task



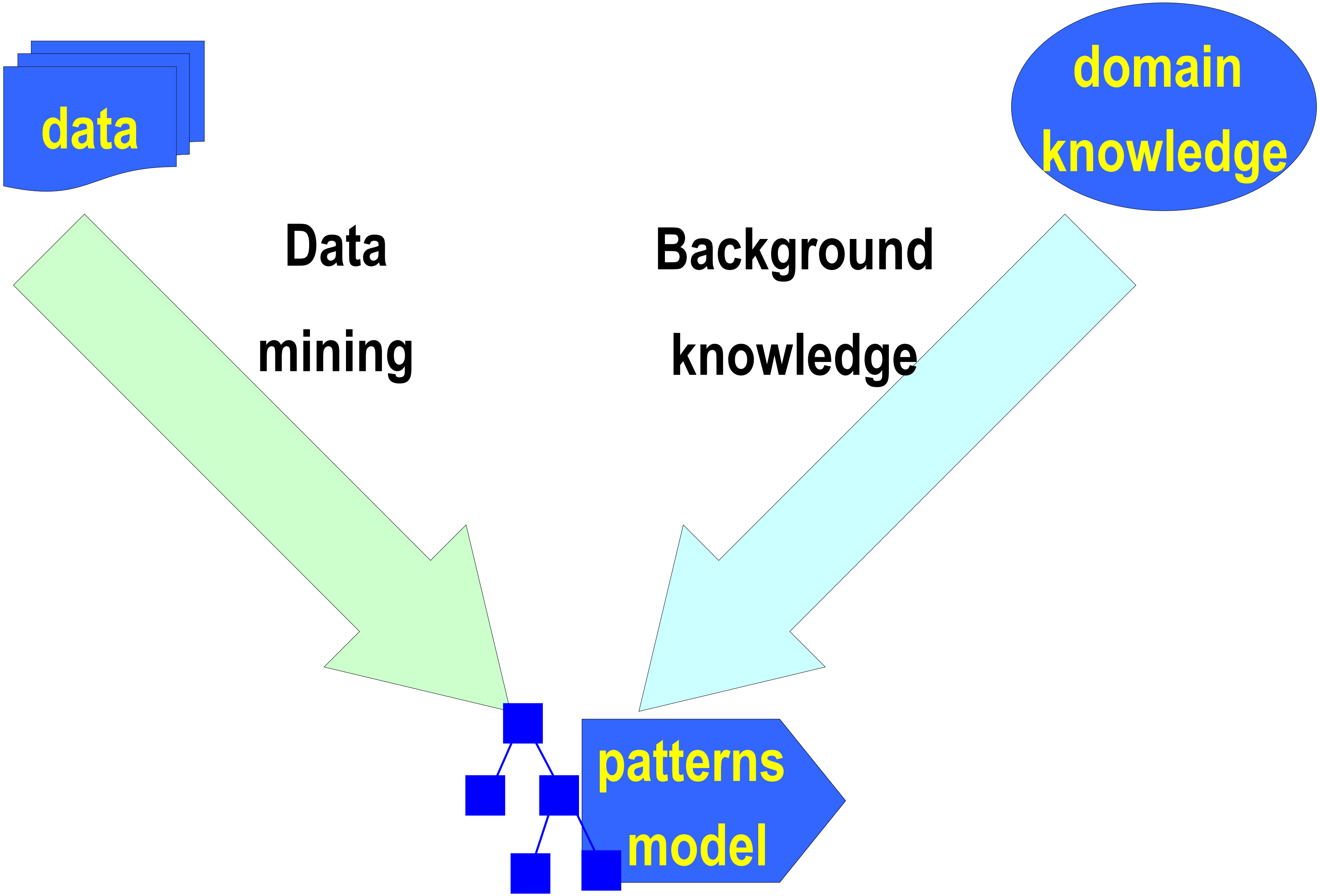
Input: transaction data table, relational database, text documents, Web pages
Goal: build a classification model, find interesting patterns in data, ...

Data Mining and Machine Learning

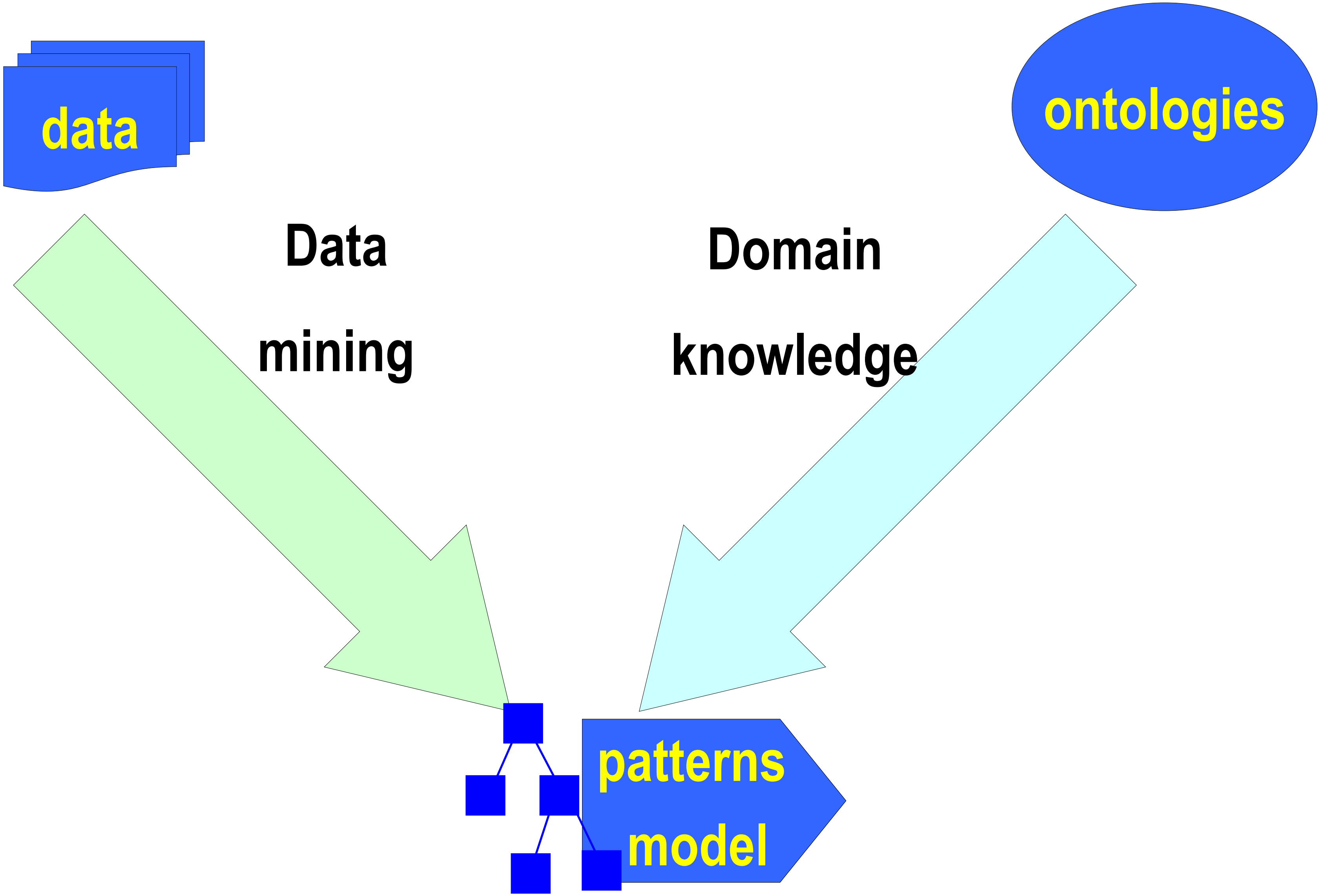
- Machine learning techniques
  - classification rule learning
  - subgroup discovery
  - relational data mining and ILP
  - equation discovery
  - inductive databases
- Data mining and decision support integration
- Data mining applications
  - medicine, health care
  - ecology, agriculture
  - knowledge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



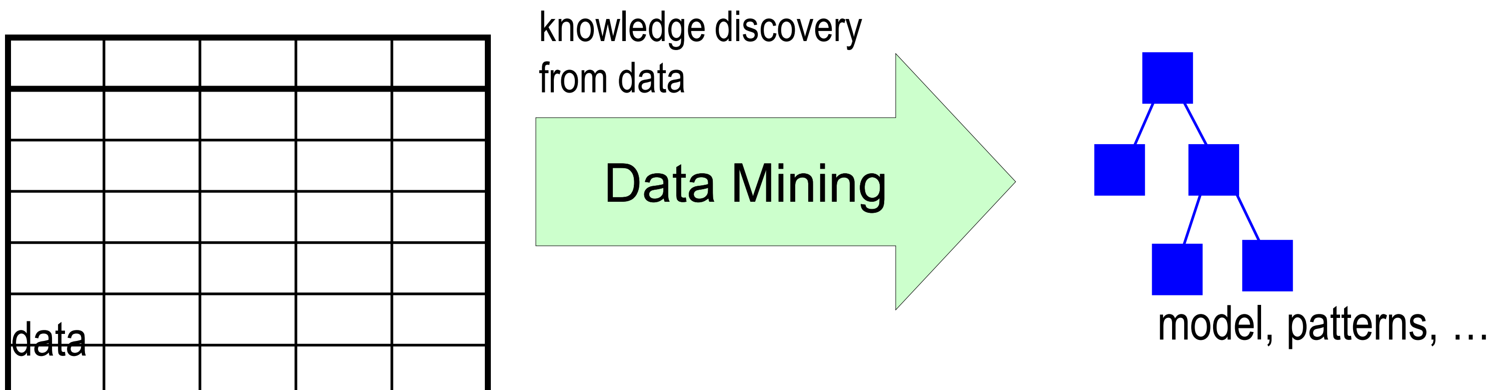
Relational data mining: domain knowledge = relational database



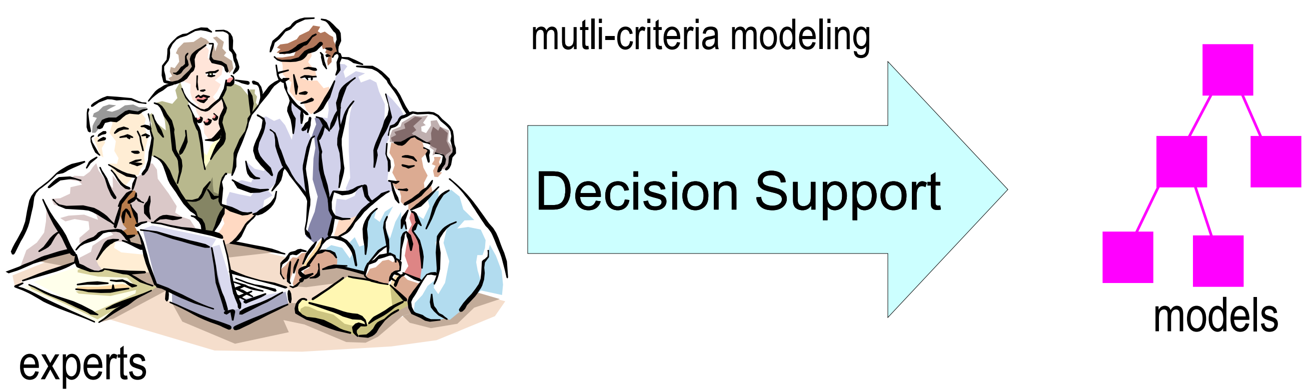
Semantic data mining: domain knowledge = ontologies



Basic DM and DS Tasks

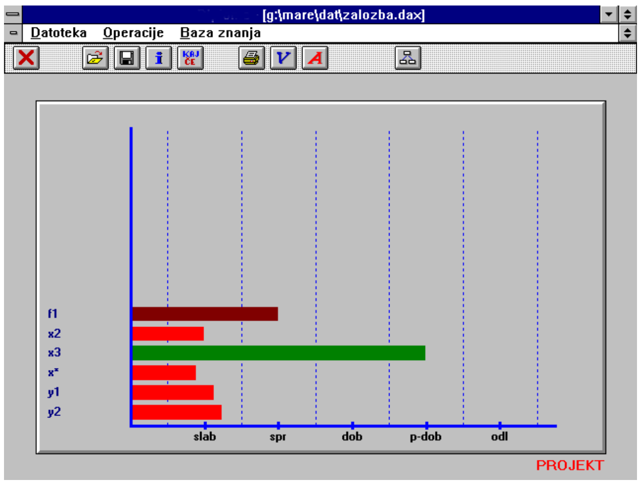


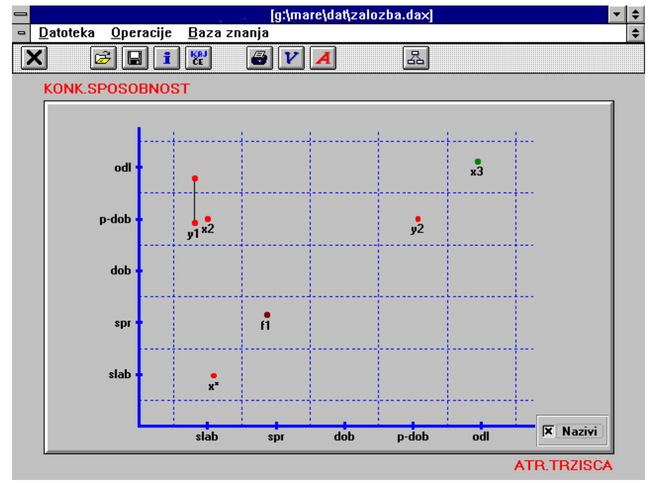
Input: transaction data table, relational database, text documents, Web pages
Goal: build a classification model, find interesting patterns in data, ...

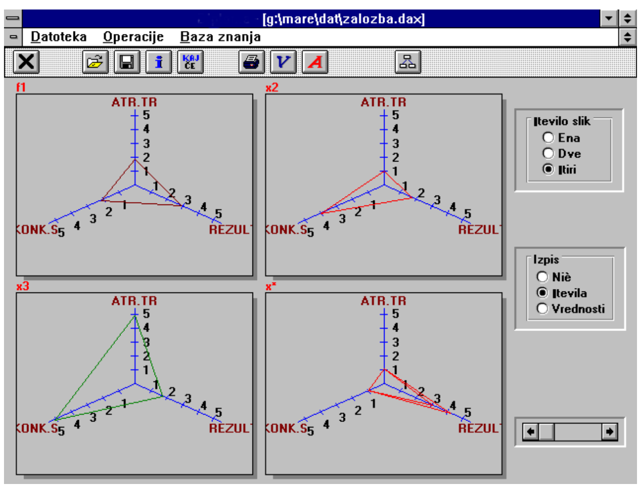


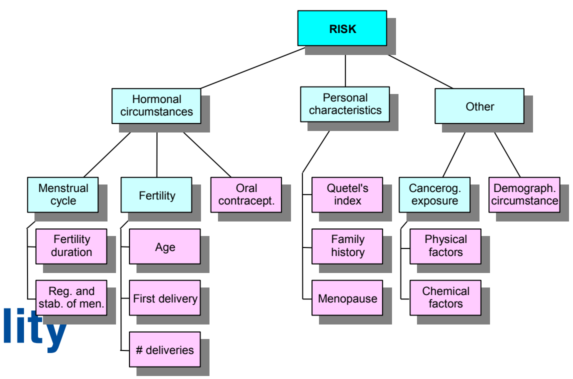
Input: expert knowledge about data and decision alternatives
Goal: construct decision support model – to support the evaluation and choice of best decision alternatives

Decision support tools: DEXi





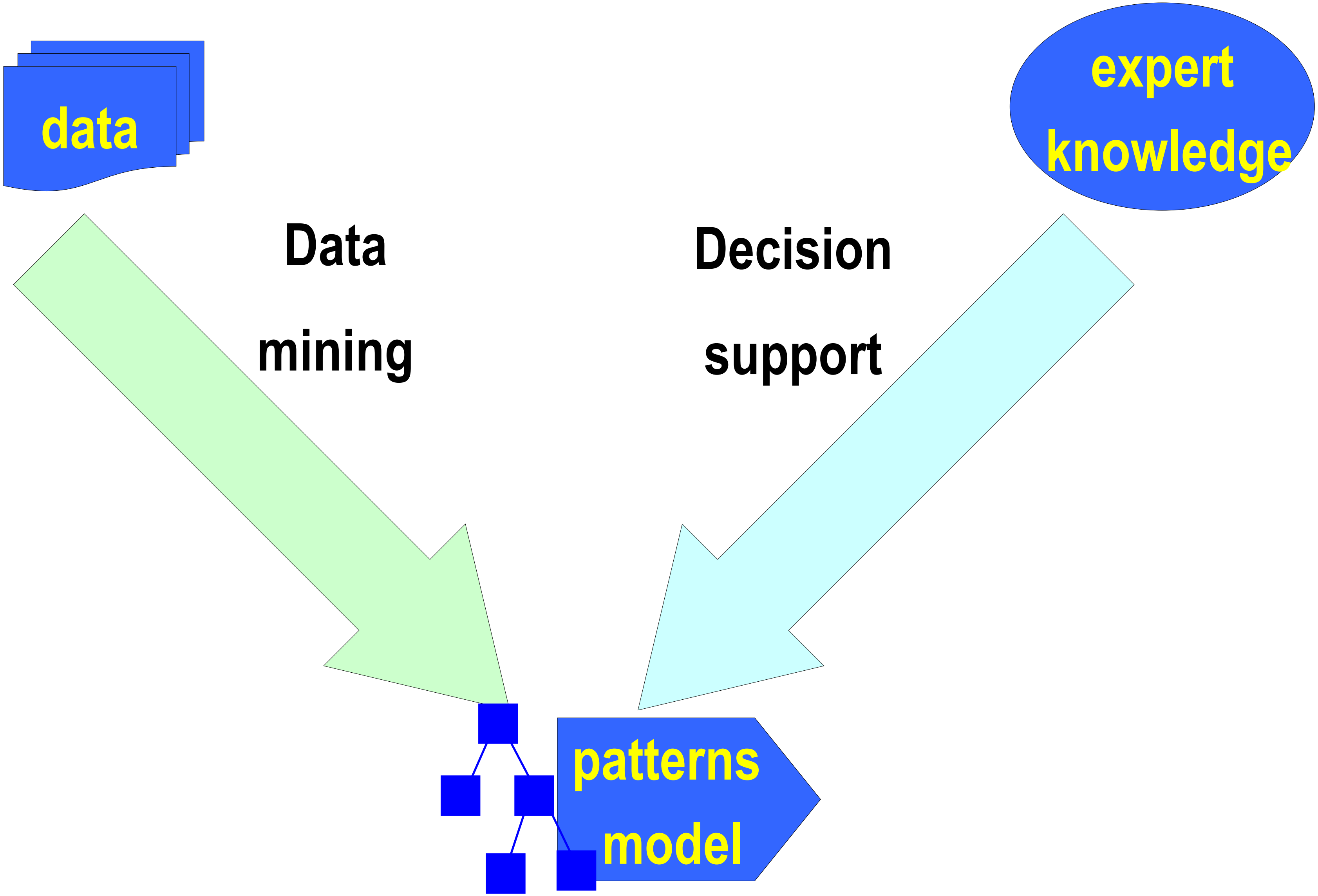




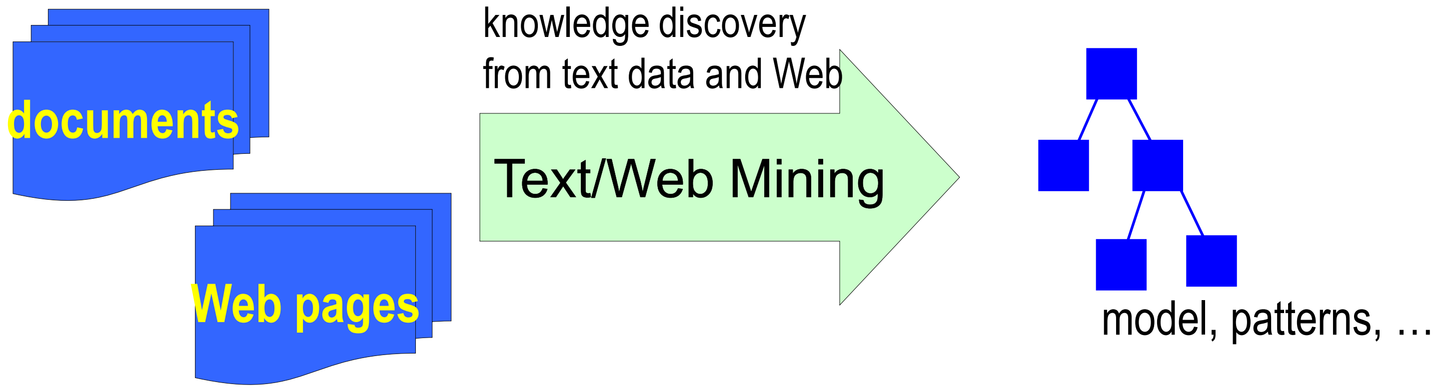
DEXi supports :

- *if-then* analysis
- analysis of stability
- Time analysis
- *how* explanation
- *why* explanation

DM and DS integration



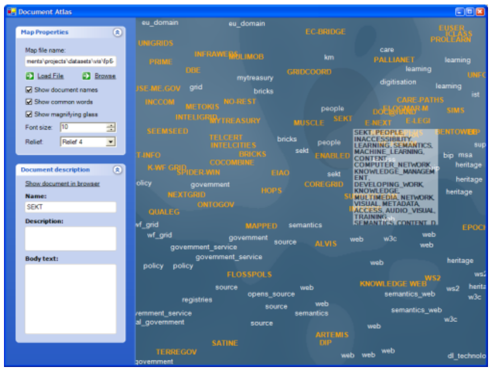
Basic Text and Web Mining Task



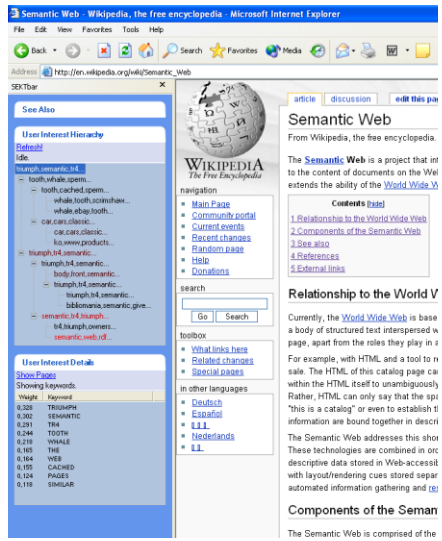
Input: text documents, Web pages
Goal: text categorization, user modeling, data visualization...

Text Mining Tools

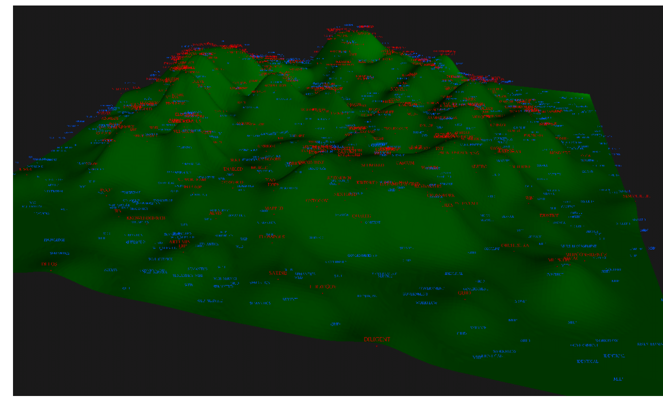
Document-Atlas

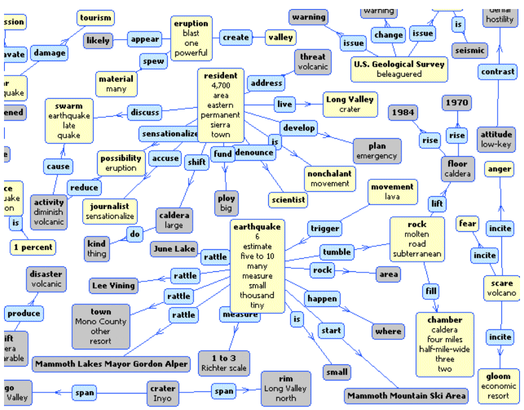


SEKTbar

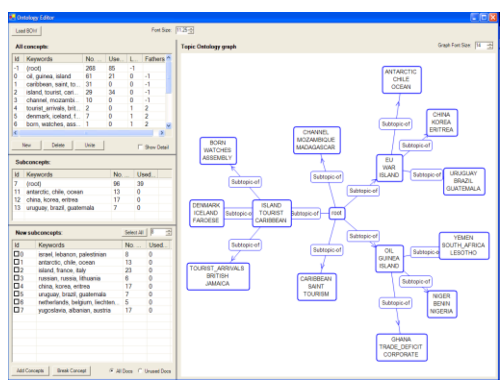


Content-Land

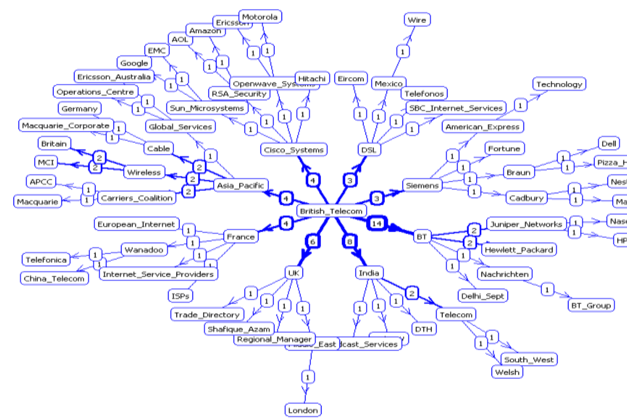




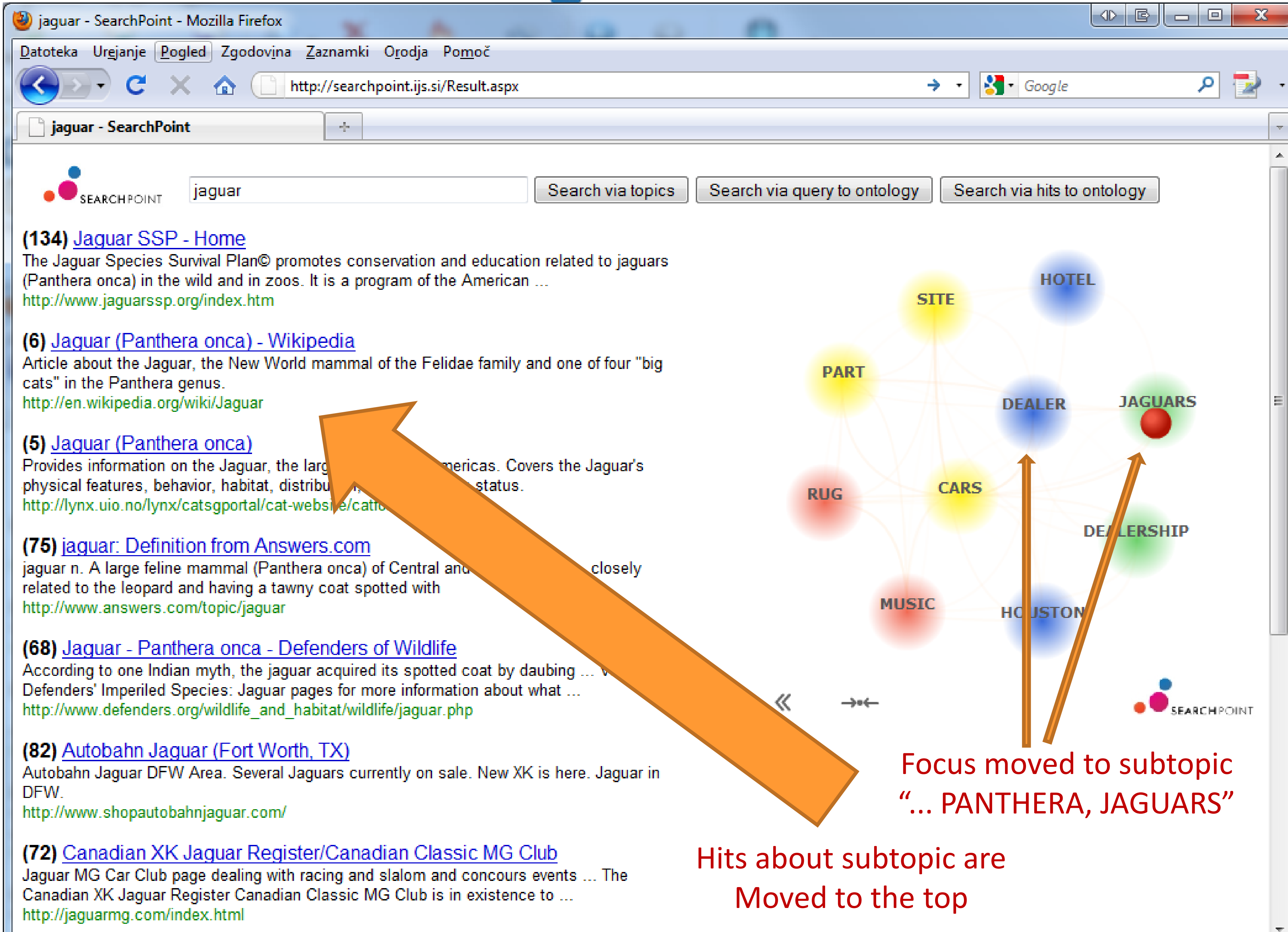
Semantic-Graphs



OntoGen



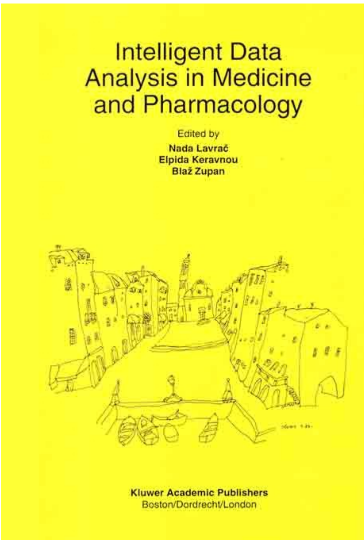
Contexter

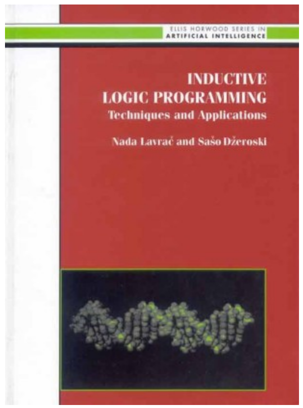


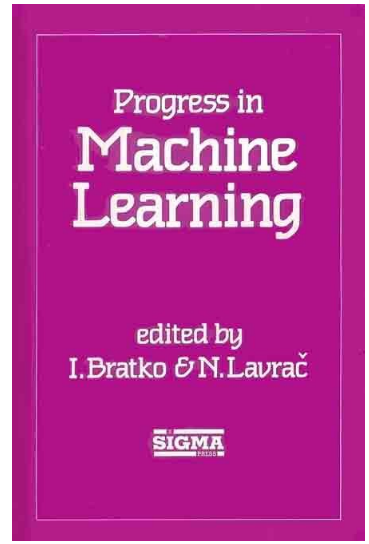
Focus moved to subtopic "... PANTHERA, JAGUARS"

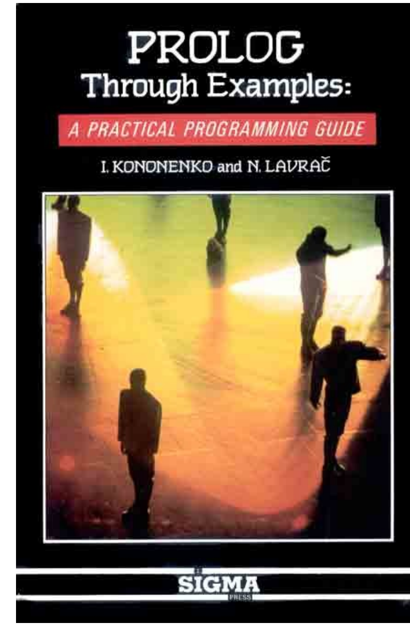
Hits about subtopic are Moved to the top

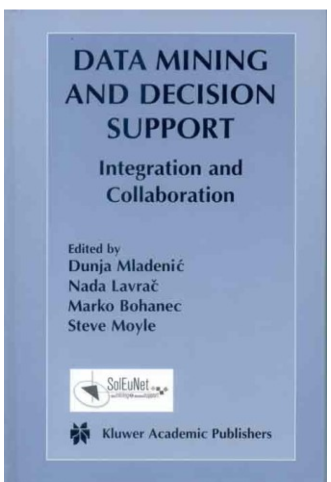
Selected Publications

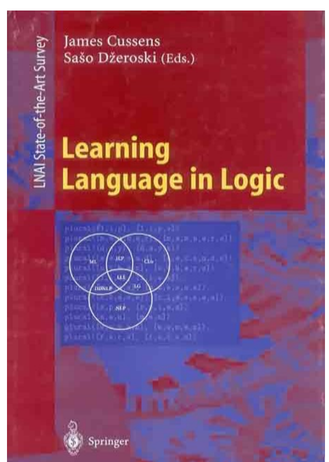


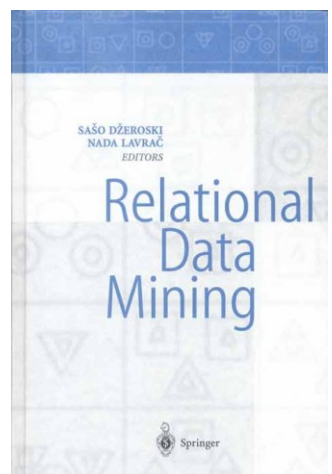


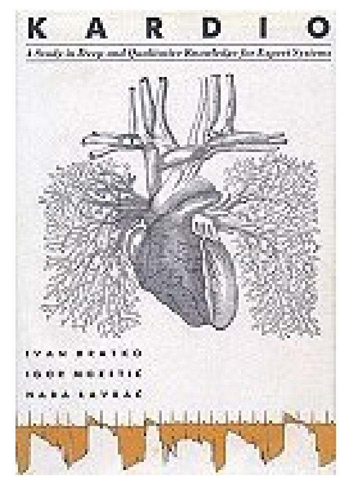


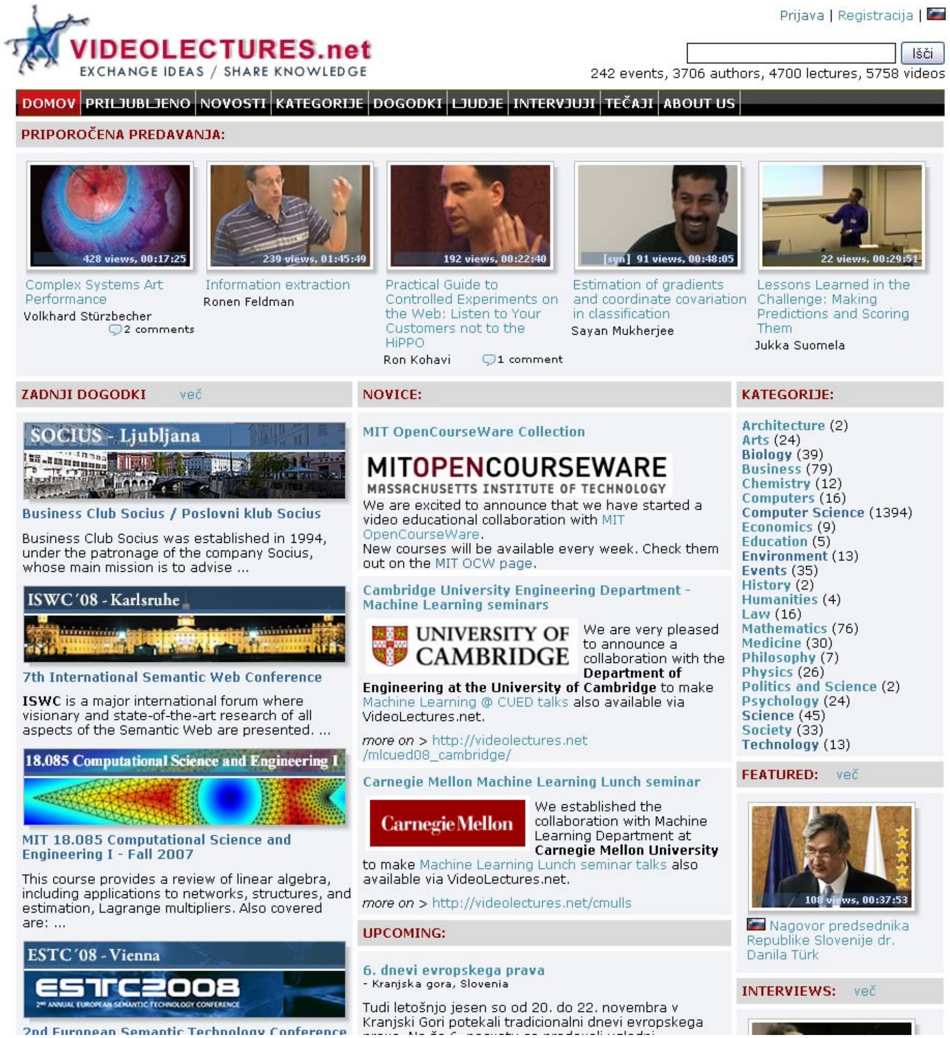












ideolectures.net portal

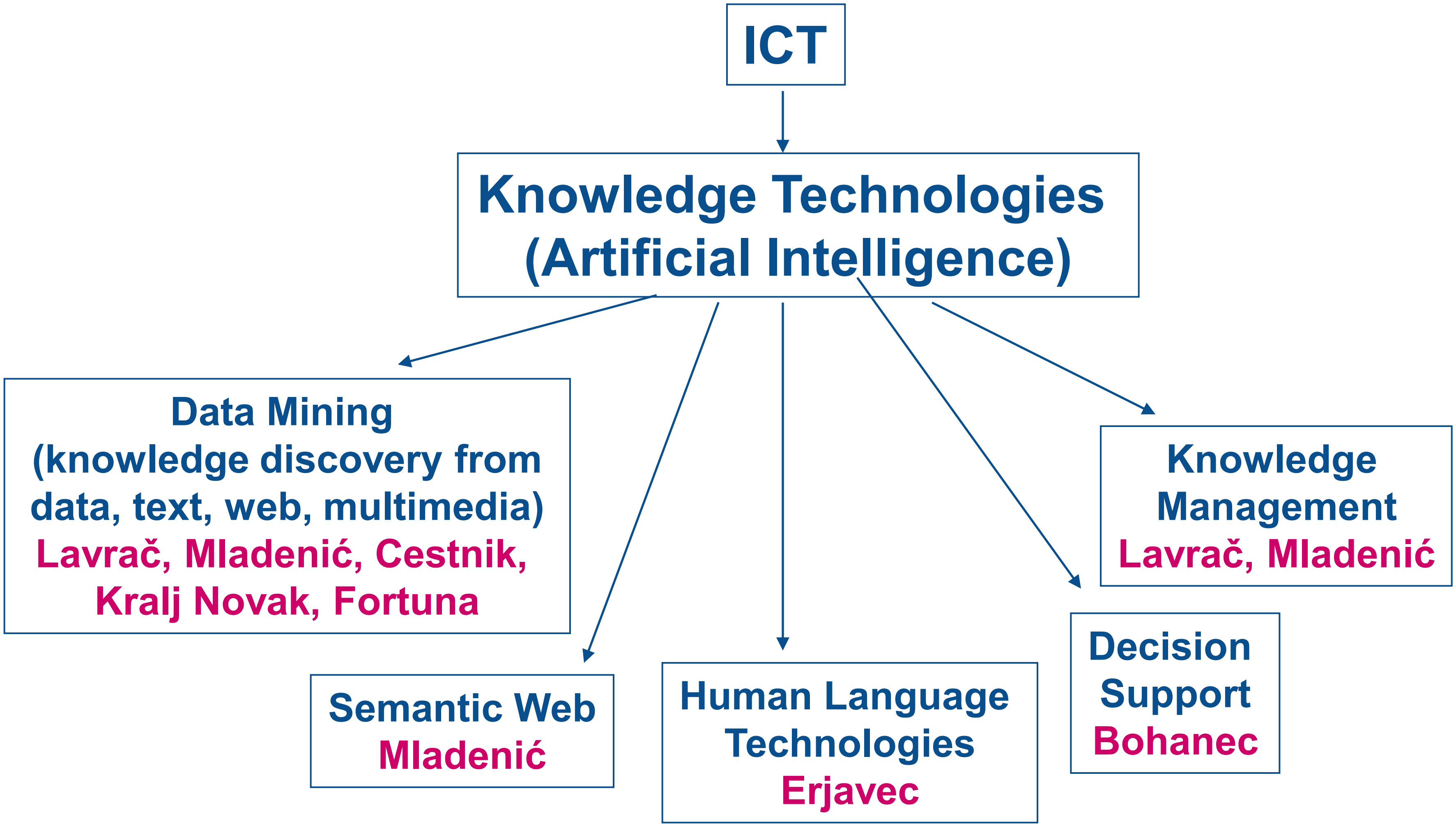
- 8782 videos
- 7014 lectures
- 5548 authors
- 352 events
- 6118 registed users

THE BEST IN E-CONTENT & CREATIVITY

World Summit Award

http//:videolectures.net

Knowledge Technologies: Main research areas & IPS lectures



Introductory seminar lecture

X. JSI & Knowledge Technologies

I. Introduction: First generation data mining

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

  (Mladenić et al. Ch. 1 and 11, Kononenko & Kukar Ch. 1)

XX. Selected data mining techniques: Advanced subgroup discovery techniques and applications

XXX. Recent advances: Cross-context link 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

What is DM

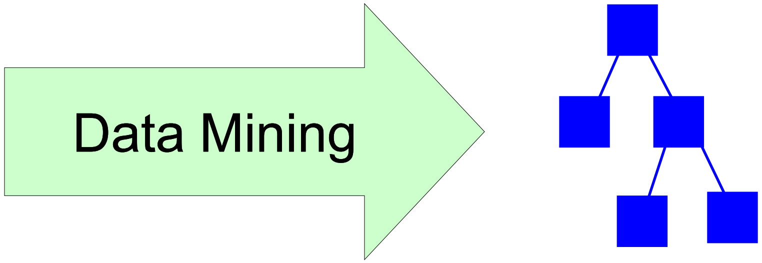
- Extraction of useful information from data: discovering relationships that have not previously been known
- The viewpoint in this course: Data Mining is the application of Machine Learning techniques to solve real-life data analysis problems

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

knowledge discovery
from data



model, patterns, …

Given: transaction data table, relational database, text documents, Web pages

Find: a classification model, a set of interesting patterns

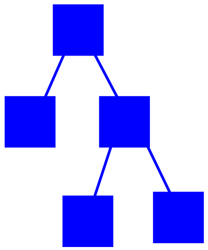
Data Mining in a Nutshell

Person	Age	Spect. presc.	Astigm.	Tear prod.	Lenses
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

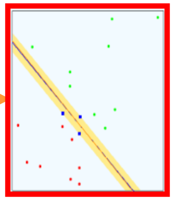


model, patterns, …

Given: transaction data table, relational database, text documents, Web pages

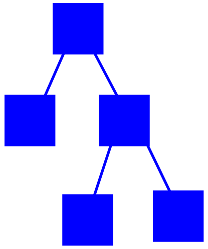
Find: a classification model, a set of interesting patterns

new unclassified instance



classified instance

black box classifier
no explanation



symbolic model
symbolic patterns

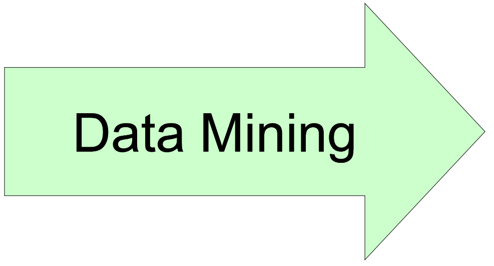
explanation

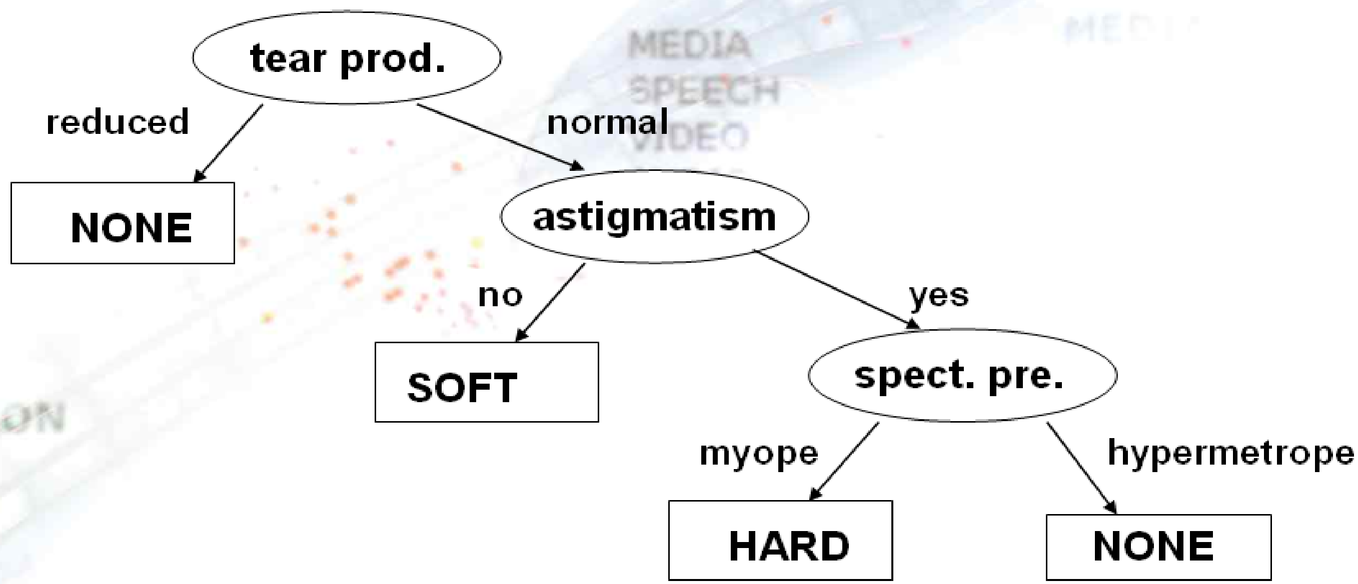
Simplified example: Learning a classification model from contact lens data

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

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-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





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

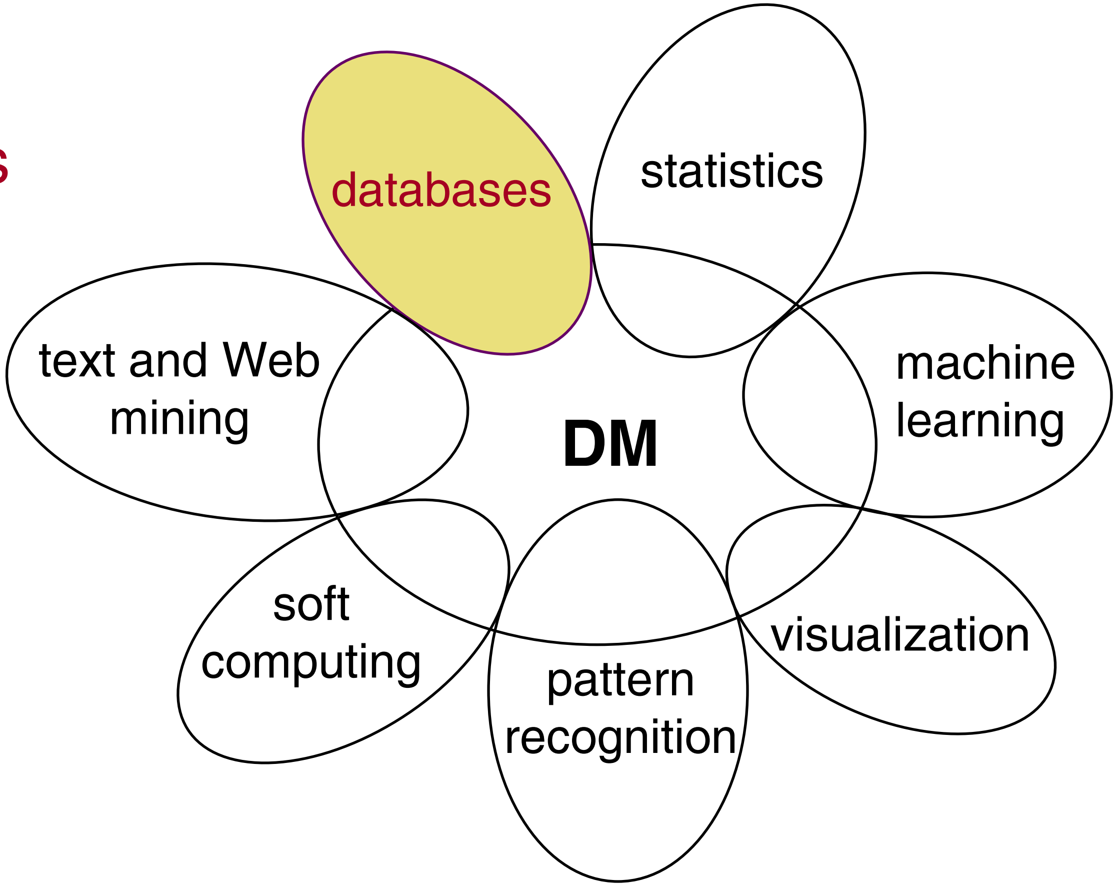
Person	Age	Spect. presc.	Astigm.	Tear prod.	~~Lenses~~
O1	17	myope	no	reduced	~~NONE~~
O2	23	myope	no	normal	~~SOFT~~
O3	22	myope	yes	reduced	~~NONE~~
O4	27	myope	yes	normal	~~HARD~~
O5	19	hypermetrope	no	reduced	~~NONE~~
O6-O13	...	...	...	...	~~...~~
O14	35	hypermetrope	no	normal	~~SOFT~~
O15	43	hypermetrope	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

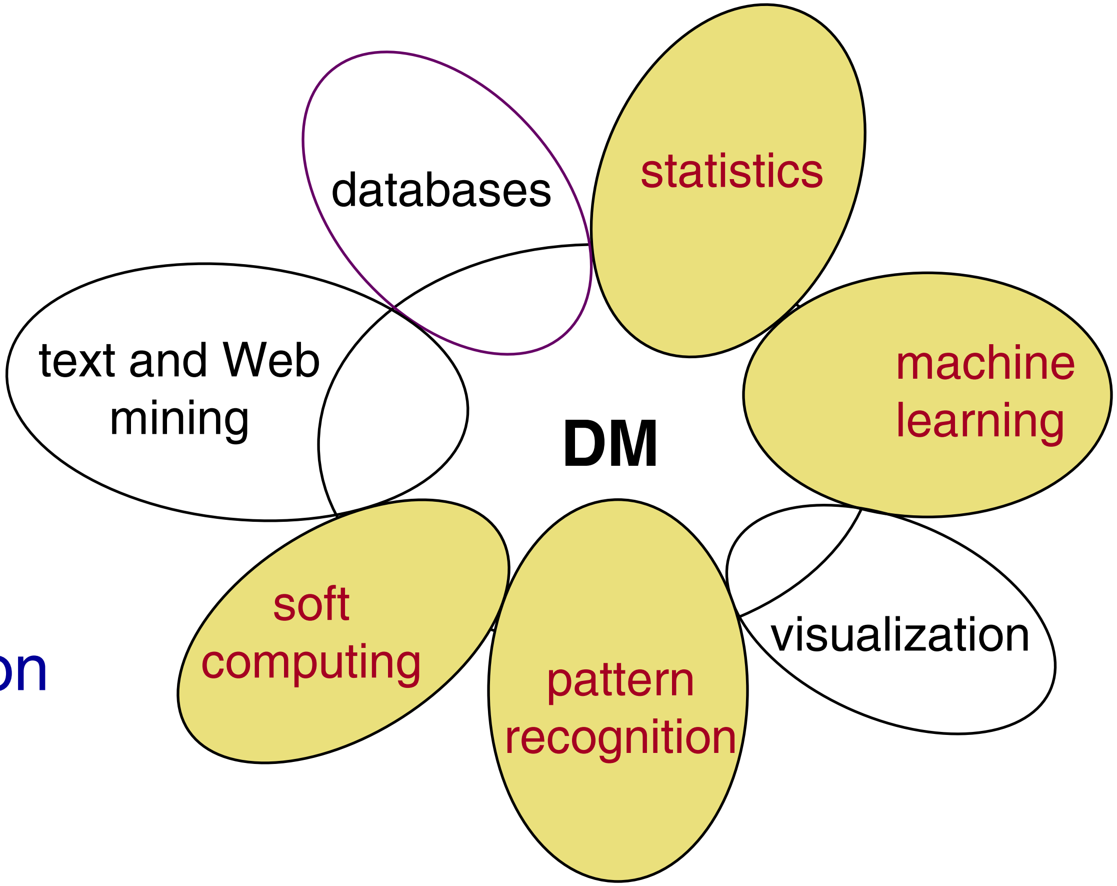
- efficient storage, access and manipulation of data



Related areas

Statistics,
machine learning,
pattern recognition
and soft computing*

- classification techniques and techniques for knowledge extraction from data

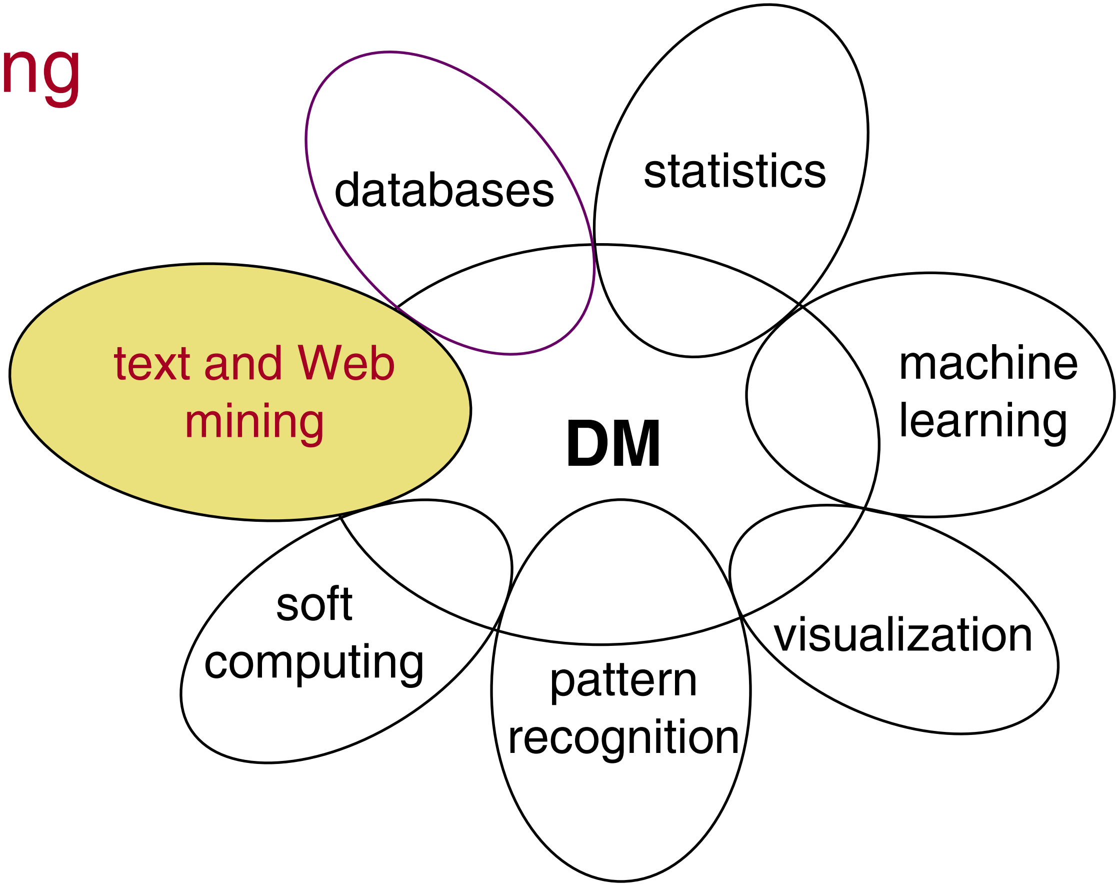


*neural networks, fuzzy logic, genetic algorithms, probabilistic reasoning

Related areas

Text and Web mining

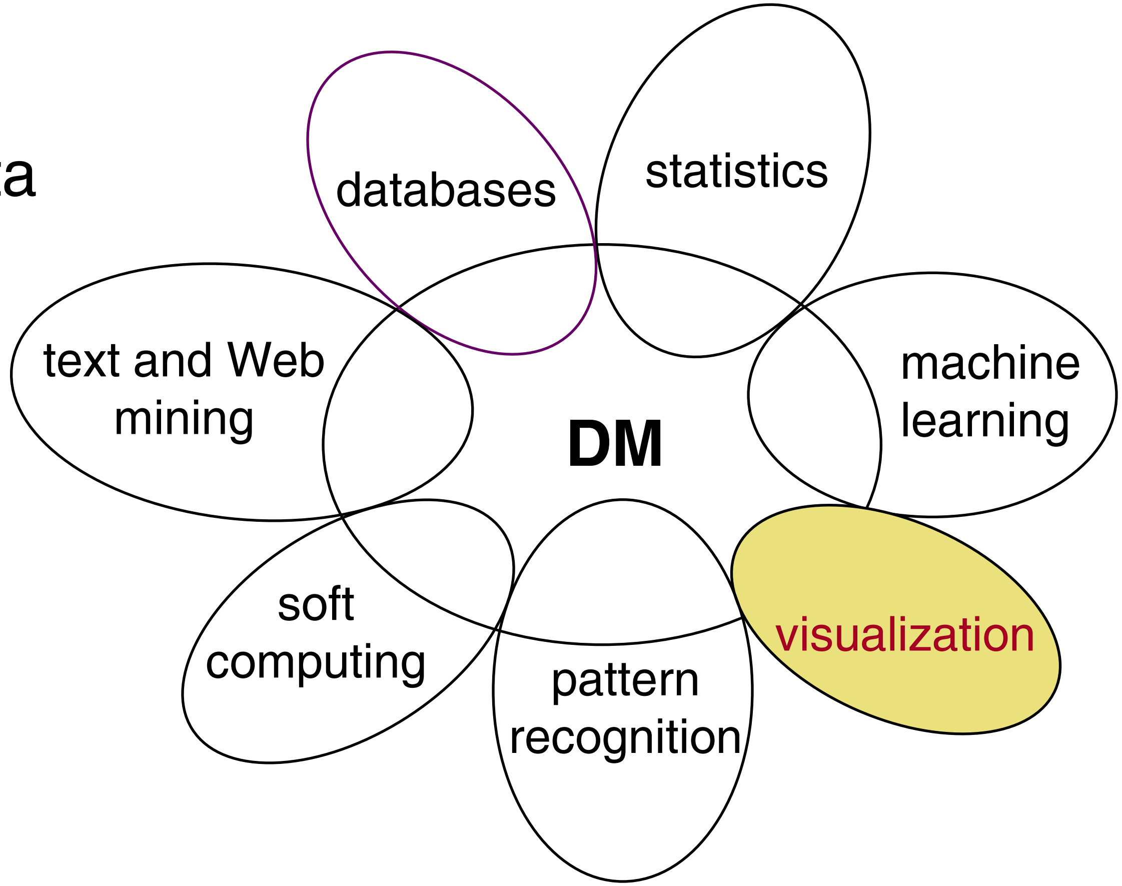
- Web page analysis
- text categorization
- acquisition, filtering and structuring of textual information
- natural language processing



Related areas

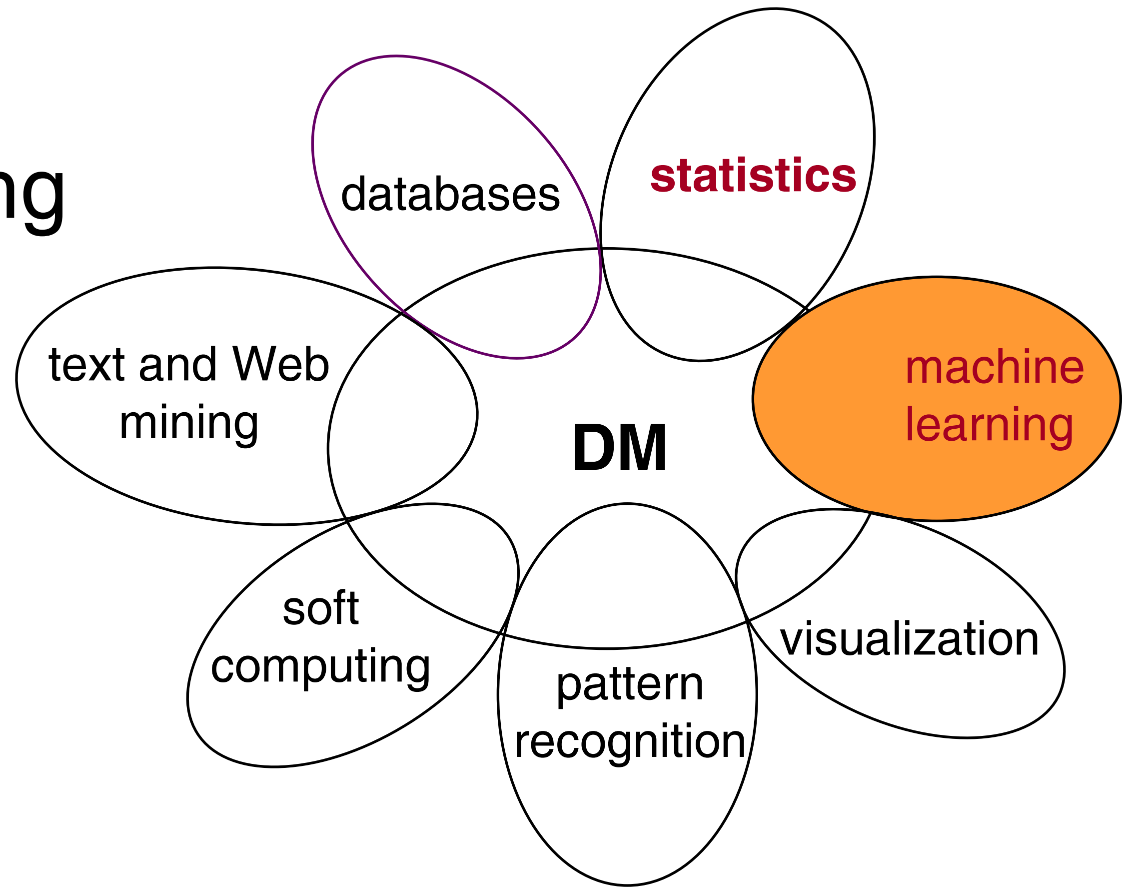
Visualization

- 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

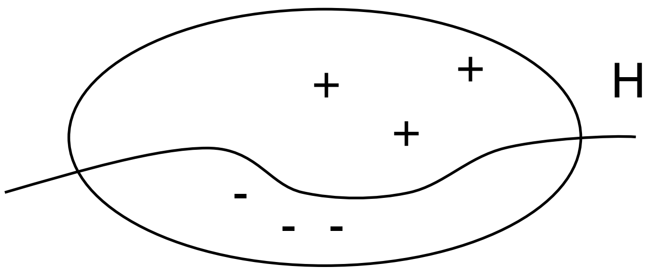
- All three areas have a long tradition of developing inductive techniques for data analysis.
  - reasoning from properties of a data sample to properties of a population
- **DM vs. Statistics:**
  - **Statistics**
    - Hypothesis testing when certain theoretical expectations about the data distribution, 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

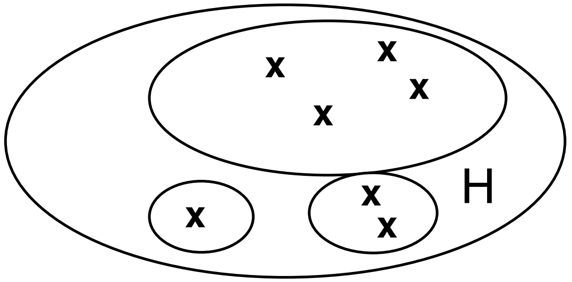
- Data Mining in a Nutshell
- Predictive and descriptive DM techniques
- Data Mining and the KDD process
- DM standards, tools and visualization

Types of DM tasks

- **Predictive DM:**
  - Classification (learning of rules, decision trees, ...)
  - Prediction and estimation (regression)
  - Predictive relational DM (ILP)

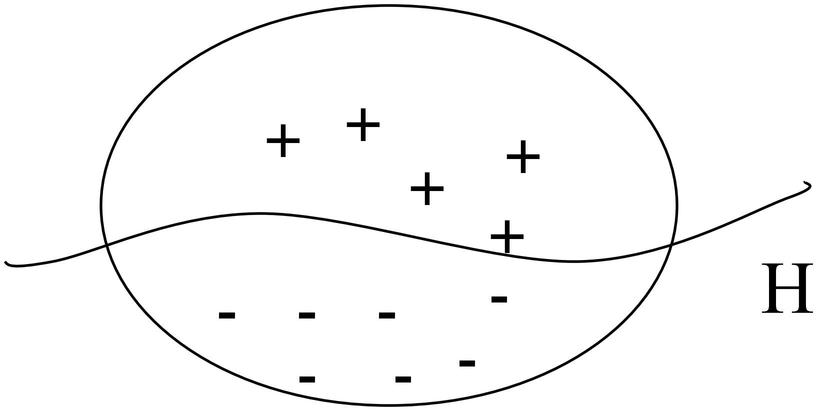


- **Descriptive DM:**
  - description and summarization
  - dependency analysis (association rule learning)
  - discovery of properties and constraints
  - segmentation (clustering)
  - subgroup discovery

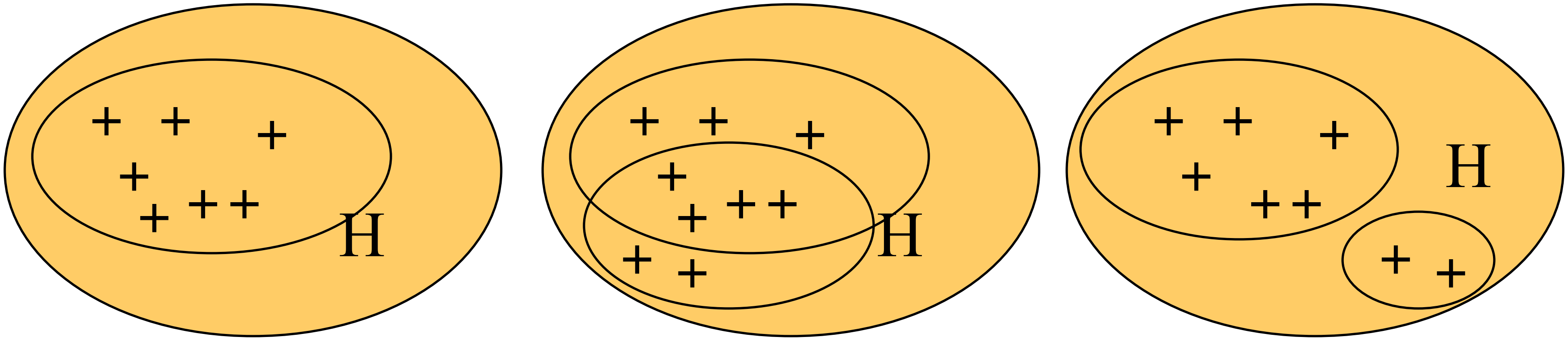


Predictive vs. descriptive DM

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:

$$(A_i = v_{i,k}) \ \& \ (A_j = v_{j,l}) \ \& \ \ldots \Rightarrow Class = C_n$$

Predictive DM - Classification

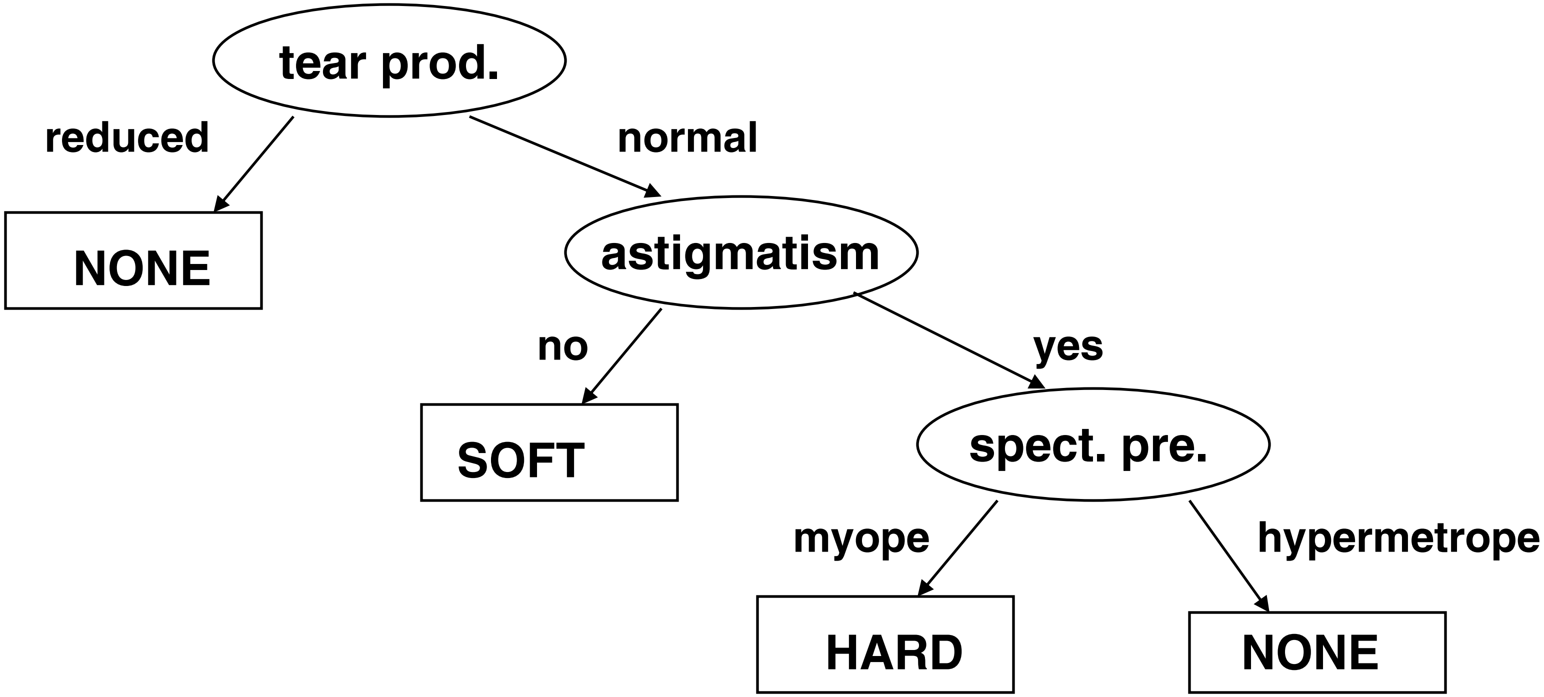
- data are objects, characterized with attributes - they belong to different classes (discrete labels)
- given objects described with attribute values, induce a model to predict different classes
- decision trees, if-then rules, discriminant analysis, ...

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-presbyo	hypermetrope	no	normal	YES
O15	pre-presbyo	hypermetrope	yes	reduced	NO
O16	pre-presbyo	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

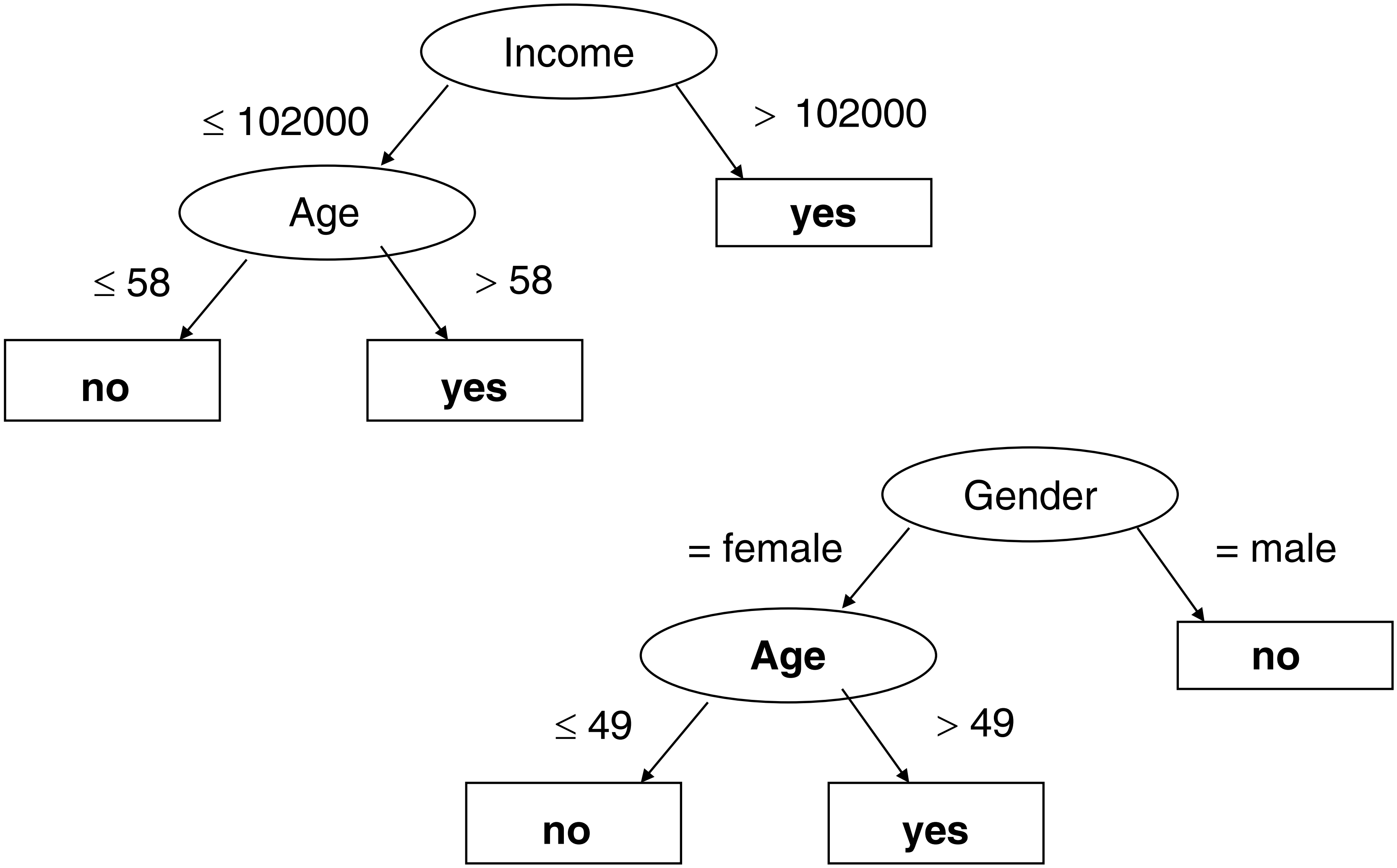
Target class: yes

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



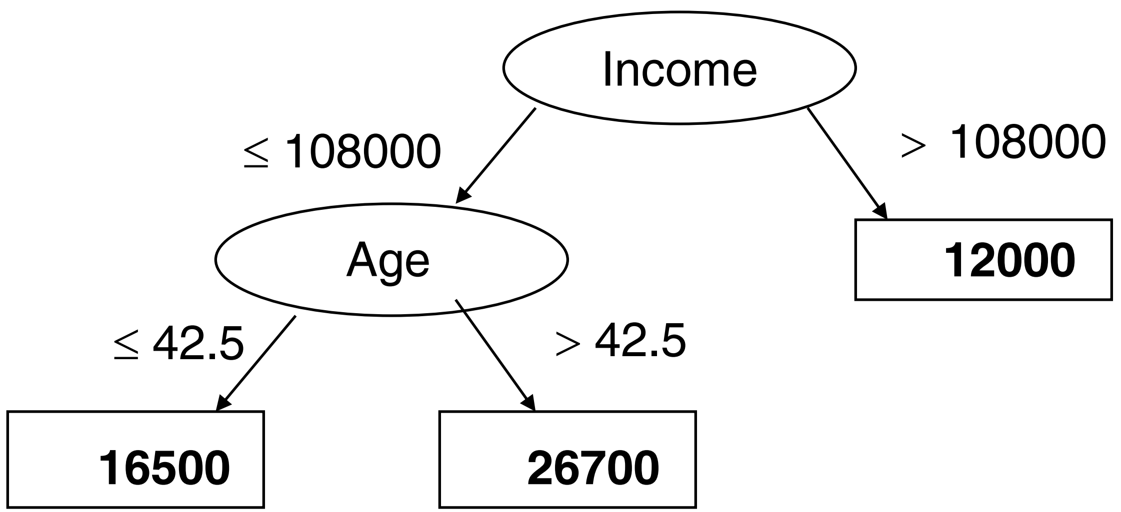
Predictive DM - Estimation

- 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

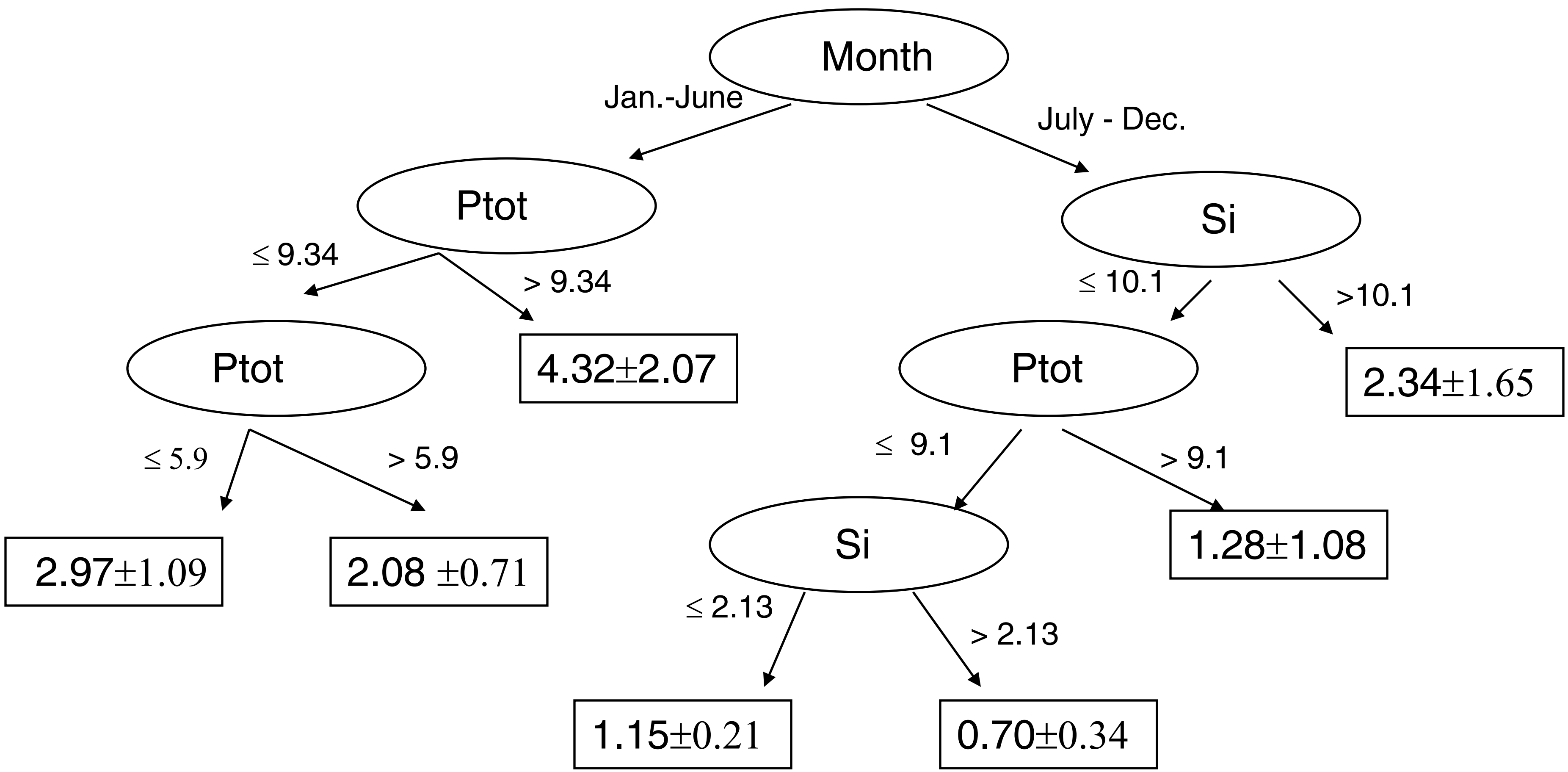
Customer	Gender	Age	Income	Spent	
c1	male	30	214000	18800	
c2	female	19	139000	15100	
c3	male	55	50000	12400	
c4	female	48	26000	8600	
c5	male	63	191000	28100	
O6-O13	...	...	...	...	
c14	female	61	95000	18100	
c15	male	56	44000	12000	
c16	male	36	102000	13800	
c17	female	57	215000	29300	
c18	male	33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

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

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

Relational Data Mining (Inductive Logic Programming) in a Nutshell

customer

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

order

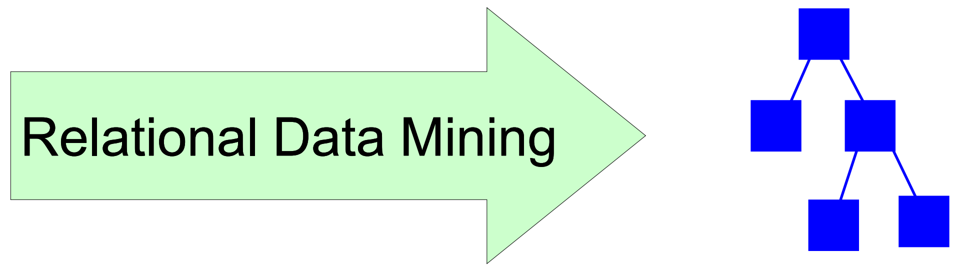
Customer ID	Order ID	Store ID	Delivery Mode	Paymt Mode
...	...	...	...	...
3478	2140267	12	regular	cash
3478	3446778	12	express	check
3478	4728386	17	regular	check
3479	3233444	17	express	credit
3479	3475886	12	regular	credit
...	...	...	...	...

store

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

Relational representation of customers, orders and stores.

knowledge discovery from data



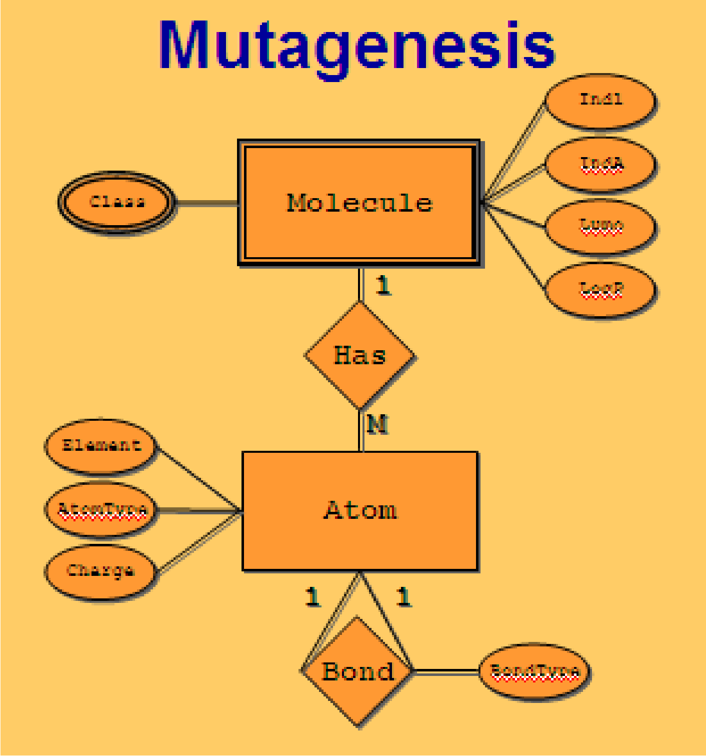
model, patterns, …

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



Relational Data Mining (ILP)

customer							
ID	Zip	Sex	SoSt	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.

customer							
ID	Zip	S ex	So St	In come	A ge	Cl ub	Re sp
...	...	...	...	...	...	...	...
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.

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

customer							
ID	Zip	Sex	SoSt	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.

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

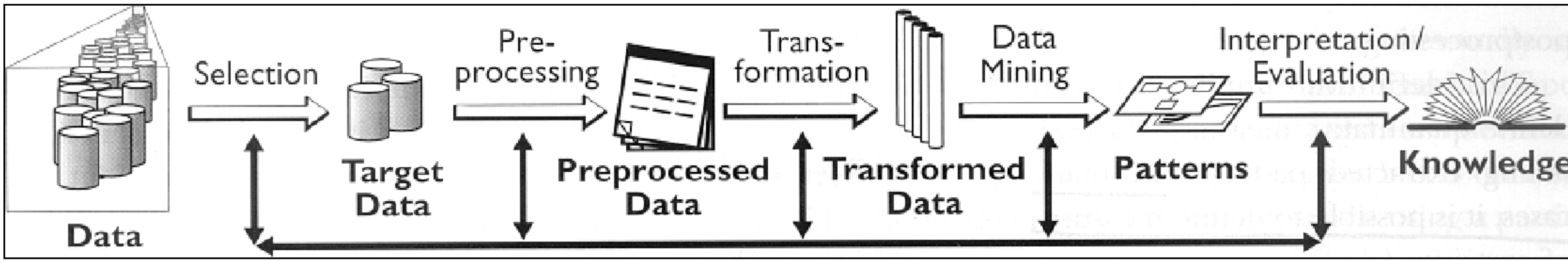
Data Mining and KDD

- 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

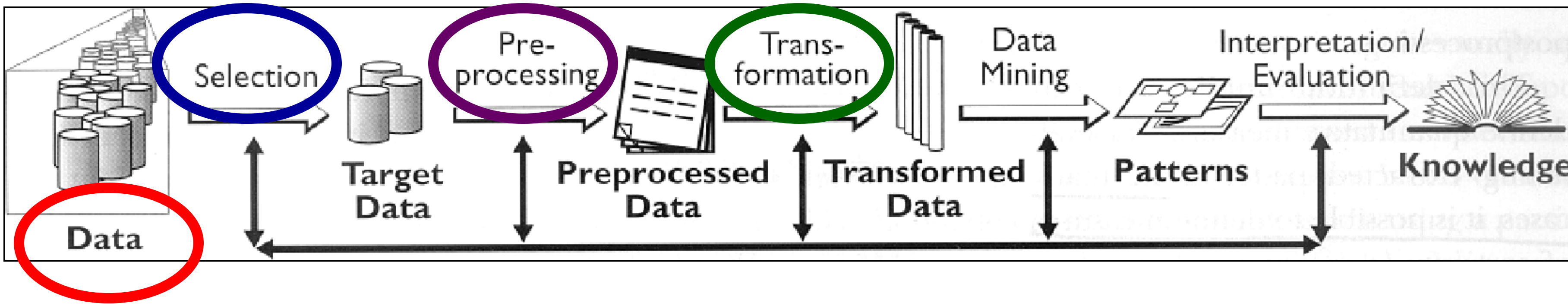
KDD Process

KDD process of discovering useful knowledge from data



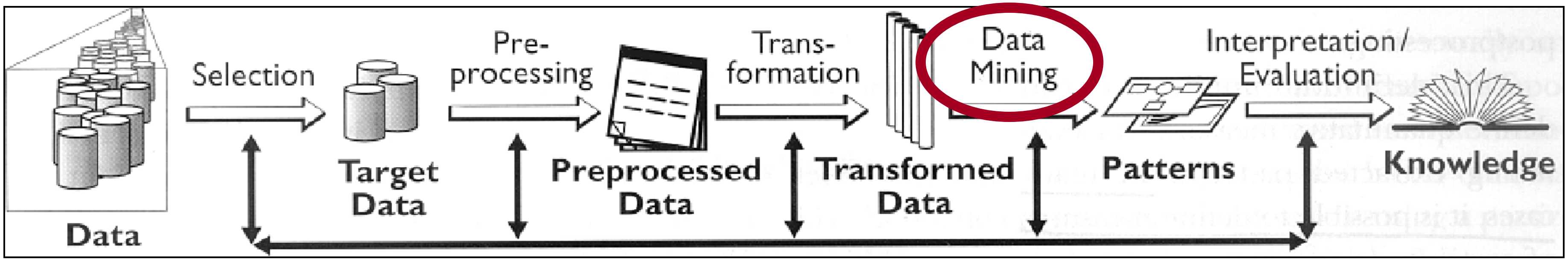
- KDD process involves several phases:
  - data preparation
  - data mining (machine learning, statistics)
  - evaluation and use of discovered patterns
- Data mining is the key step, but represents only 15%-25% of the entire KDD process

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.

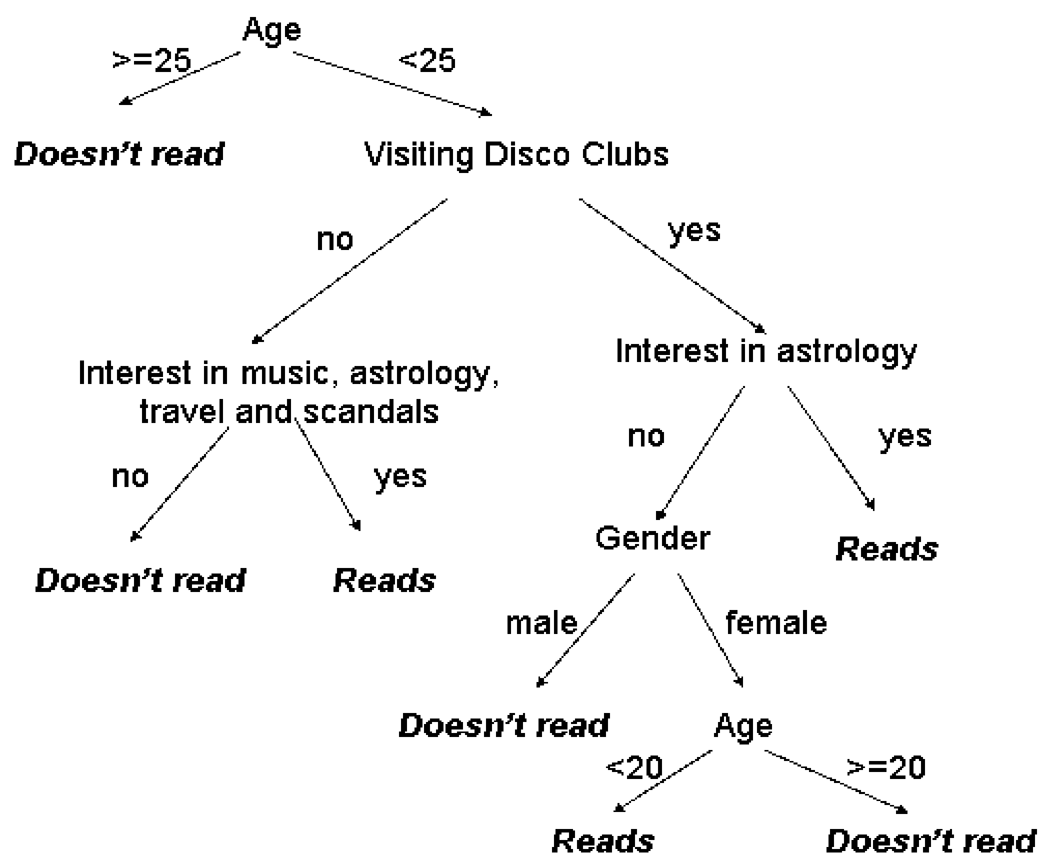
Simplified association rules

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.

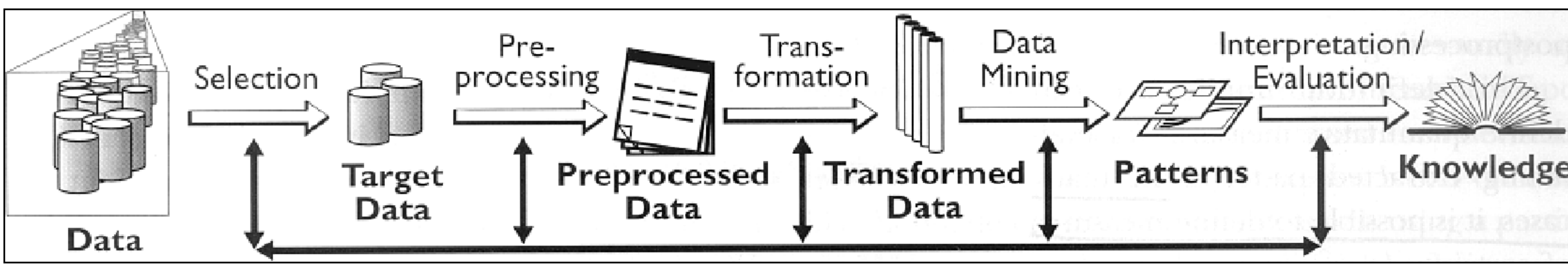


Part I. Introduction

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

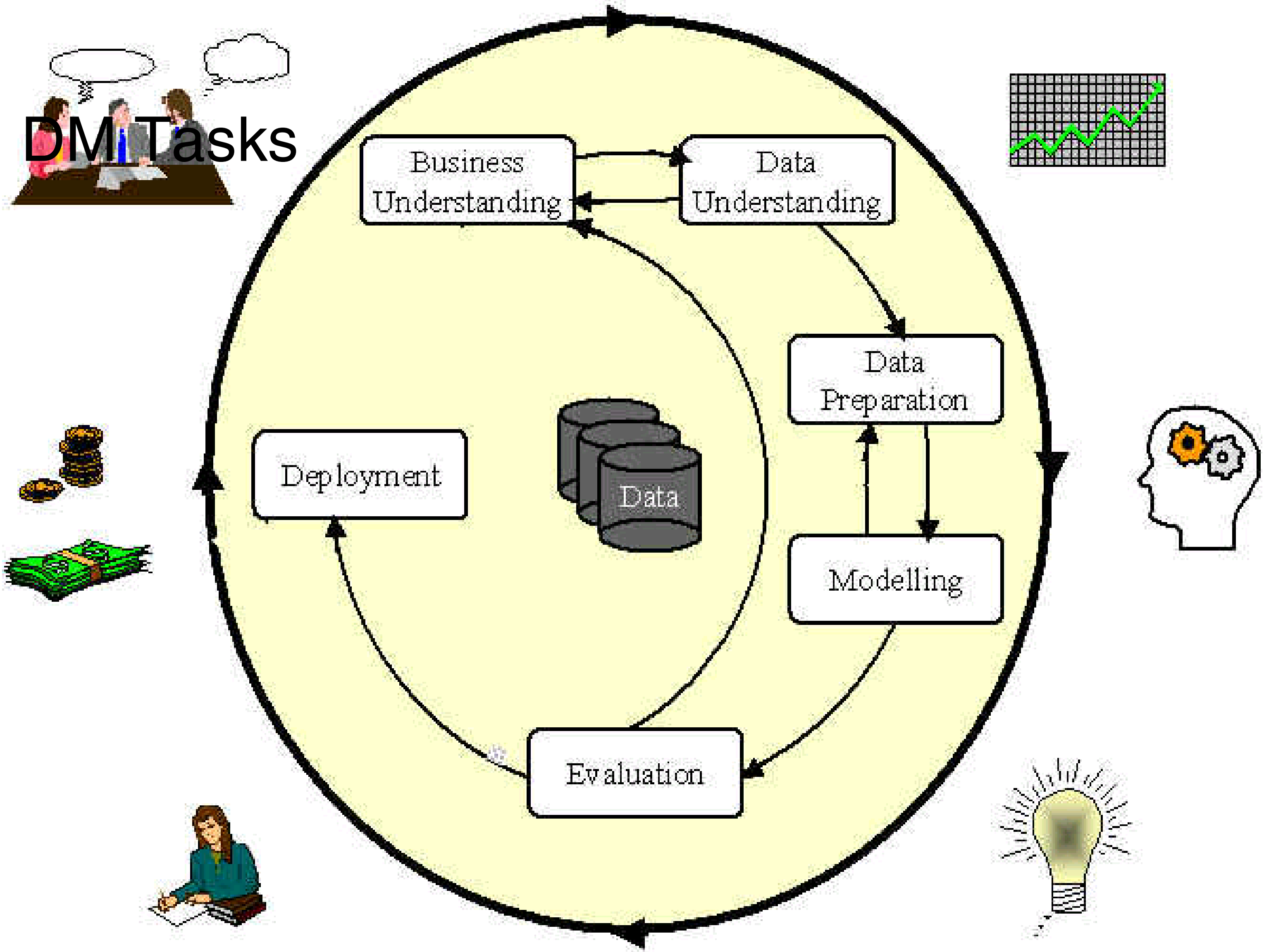
CRISP-DM

- 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):

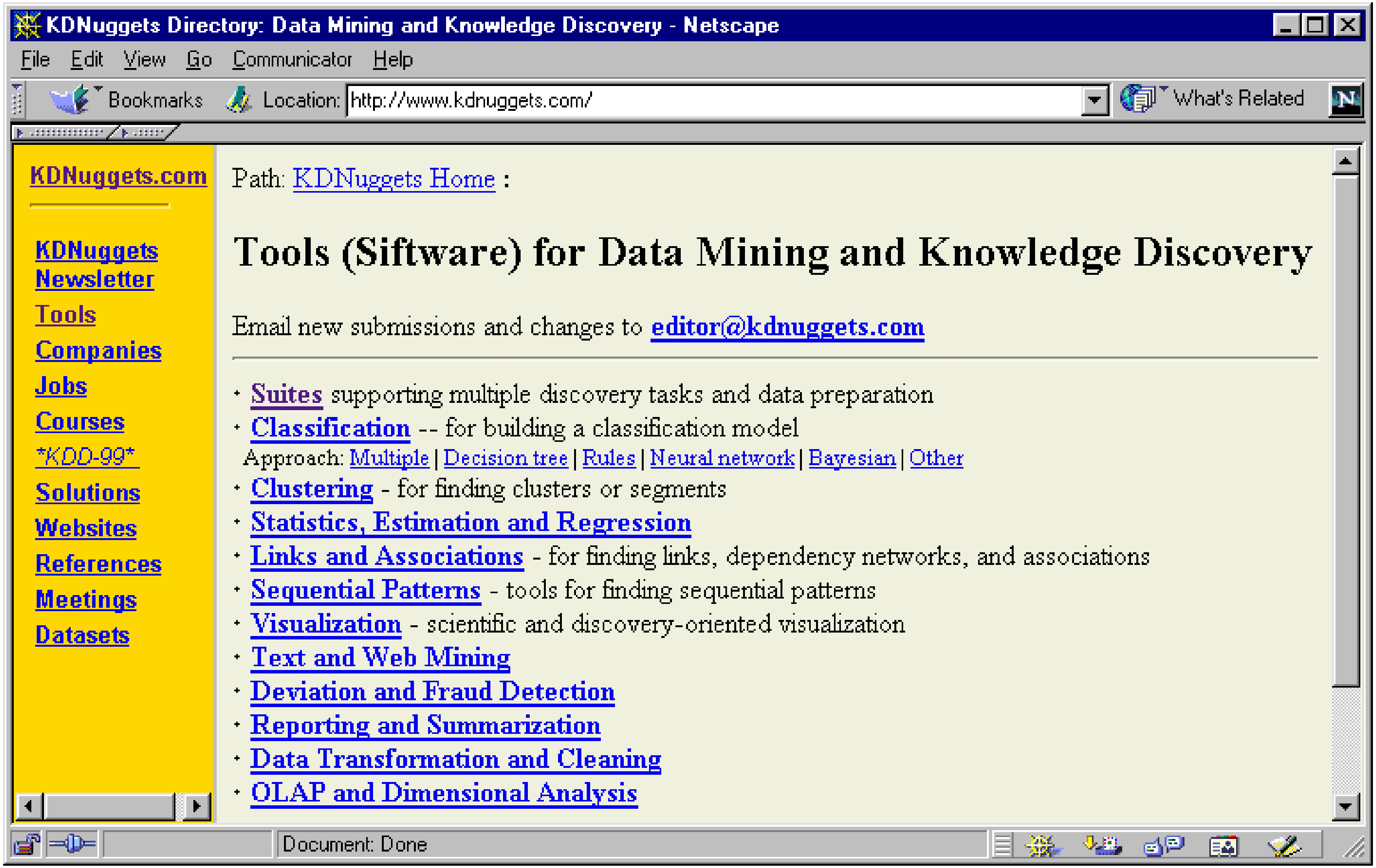


CRISP Data Mining Process

- DM Tasks

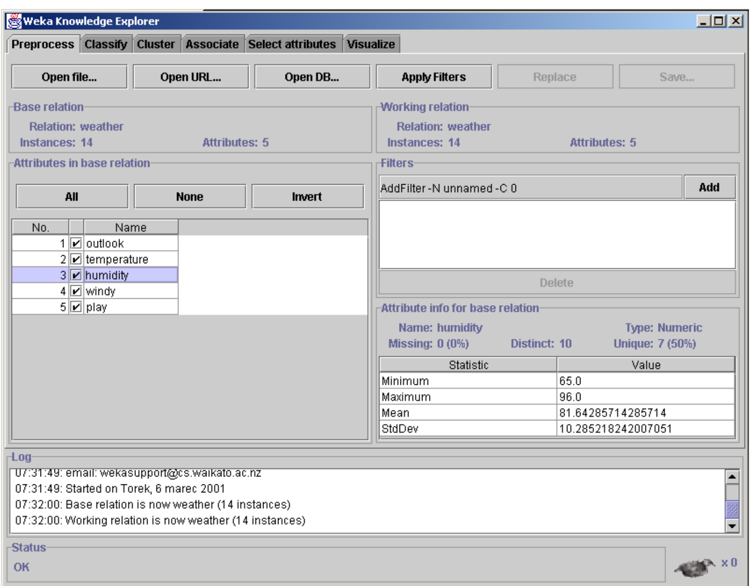


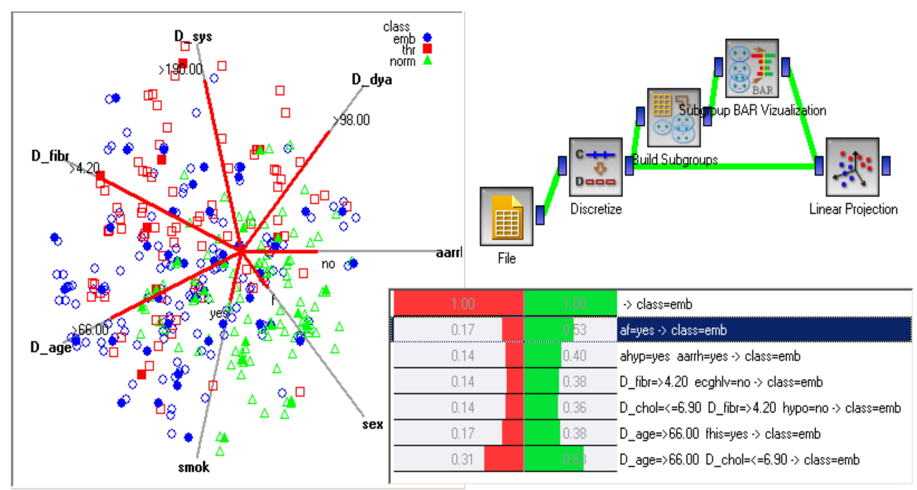
DM tools


KDNuggets Directory: Data Mining and Knowledge Discovery - Netscape
File Edit View Go Communicator Help
Bookmarks Location: http://www.kdnuggets.com/ What's Related
KDNuggets.com
KDNuggets Newsletter
Tools
Companies
Jobs
Courses
KDD-99
Solutions
Websites
References
Meetings
Datasets
Path: KDNuggets Home :
Tools (Siftware) for Data Mining and Knowledge Discovery
Email new submissions and changes to editor@kdnuggets.com
Suites supporting multiple discovery tasks and data preparation
Classification -- for building a classification model
Approach: Multiple | Decision tree | Rules | Neural network | Bayesian | Other
Clustering - for finding clusters or segments
Statistics, Estimation and Regression
Links and Associations - for finding links, dependency networks, and associations
Sequential Patterns - tools for finding sequential patterns
Visualization - scientific and discovery-oriented visualization
Text and Web Mining
Deviation and Fraud Detection
Reporting and Summarization
Data Transformation and Cleaning
OLAP and Dimensional Analysis
Document: Done

Public DM tools

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

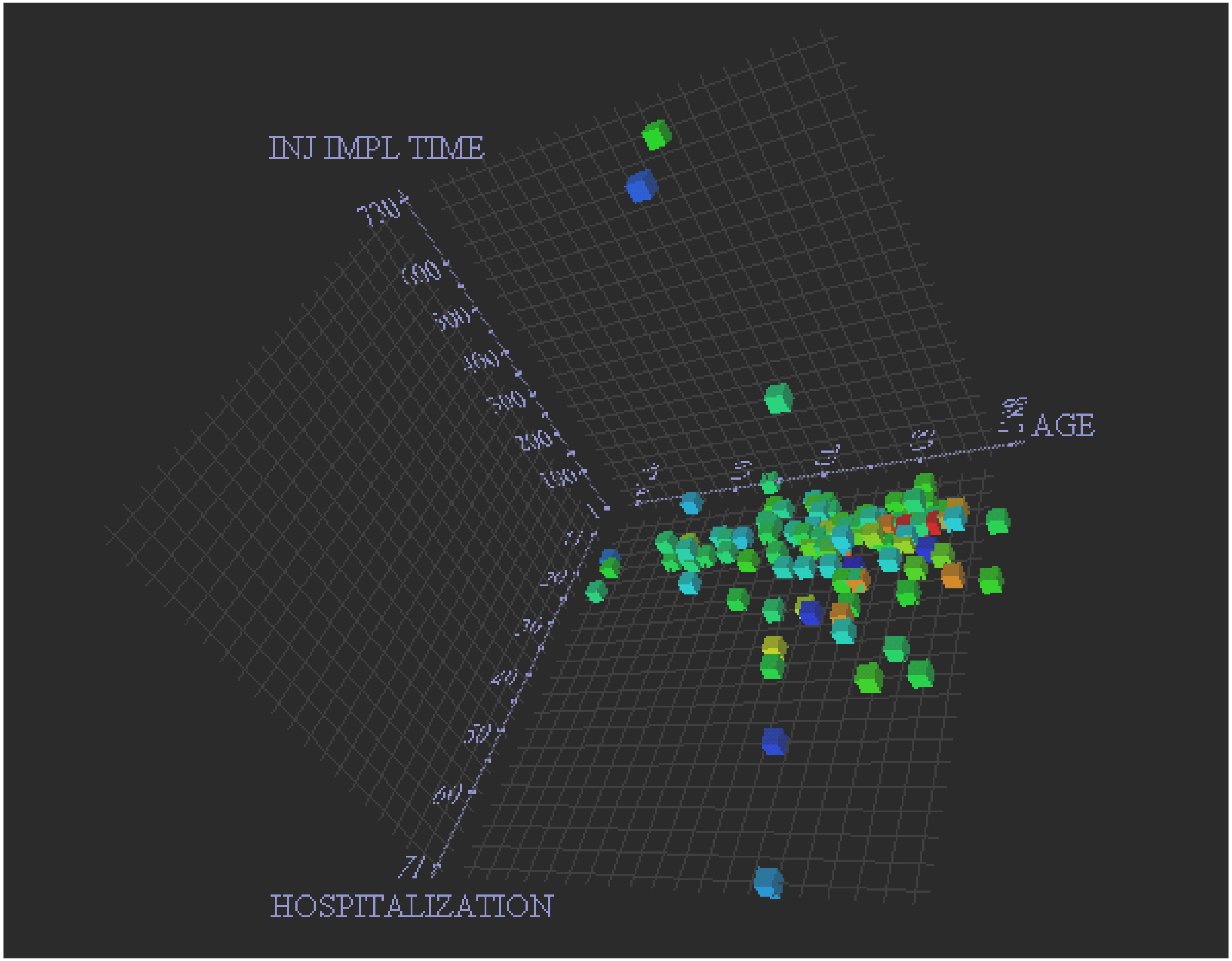




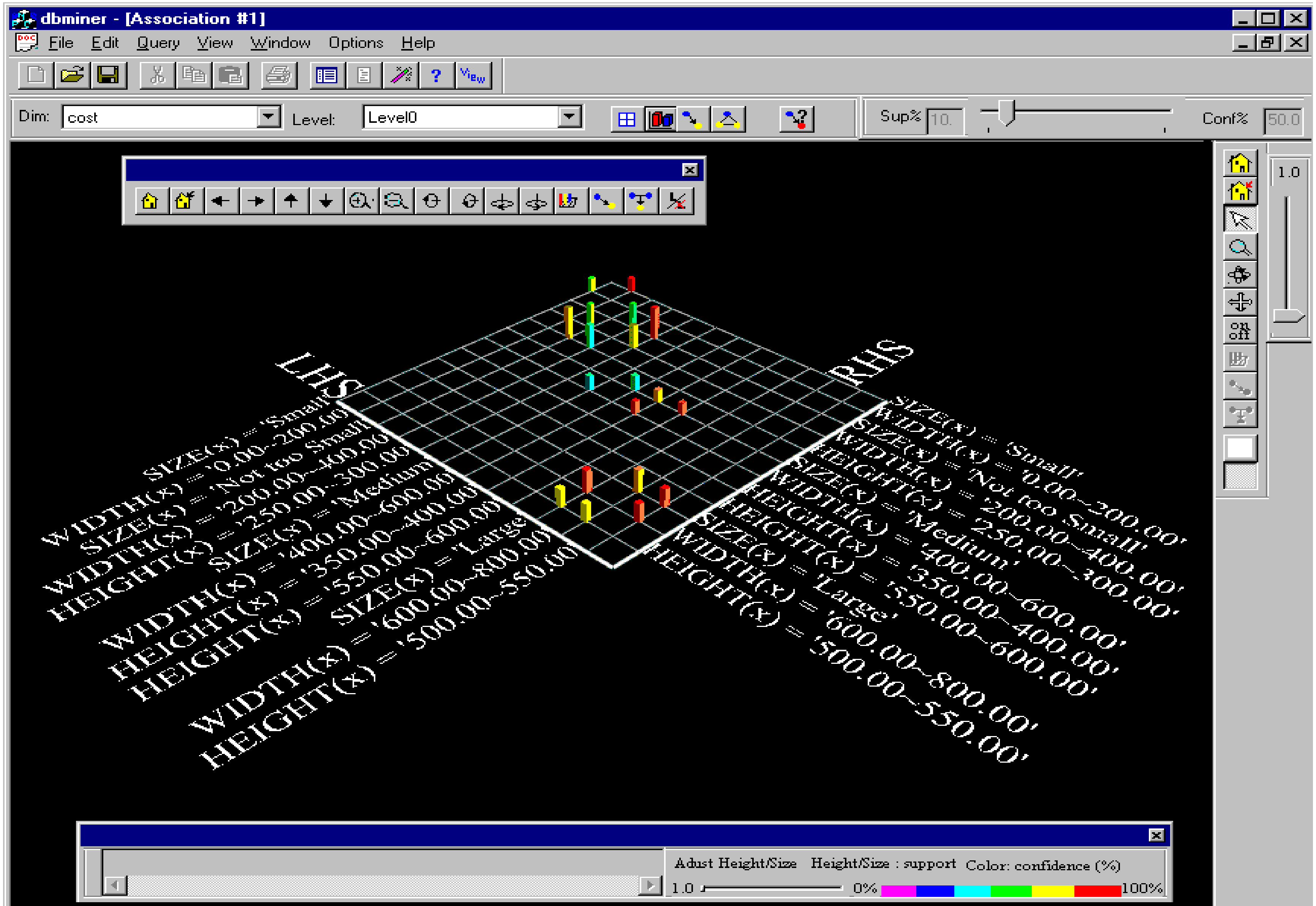
Visualization

- 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

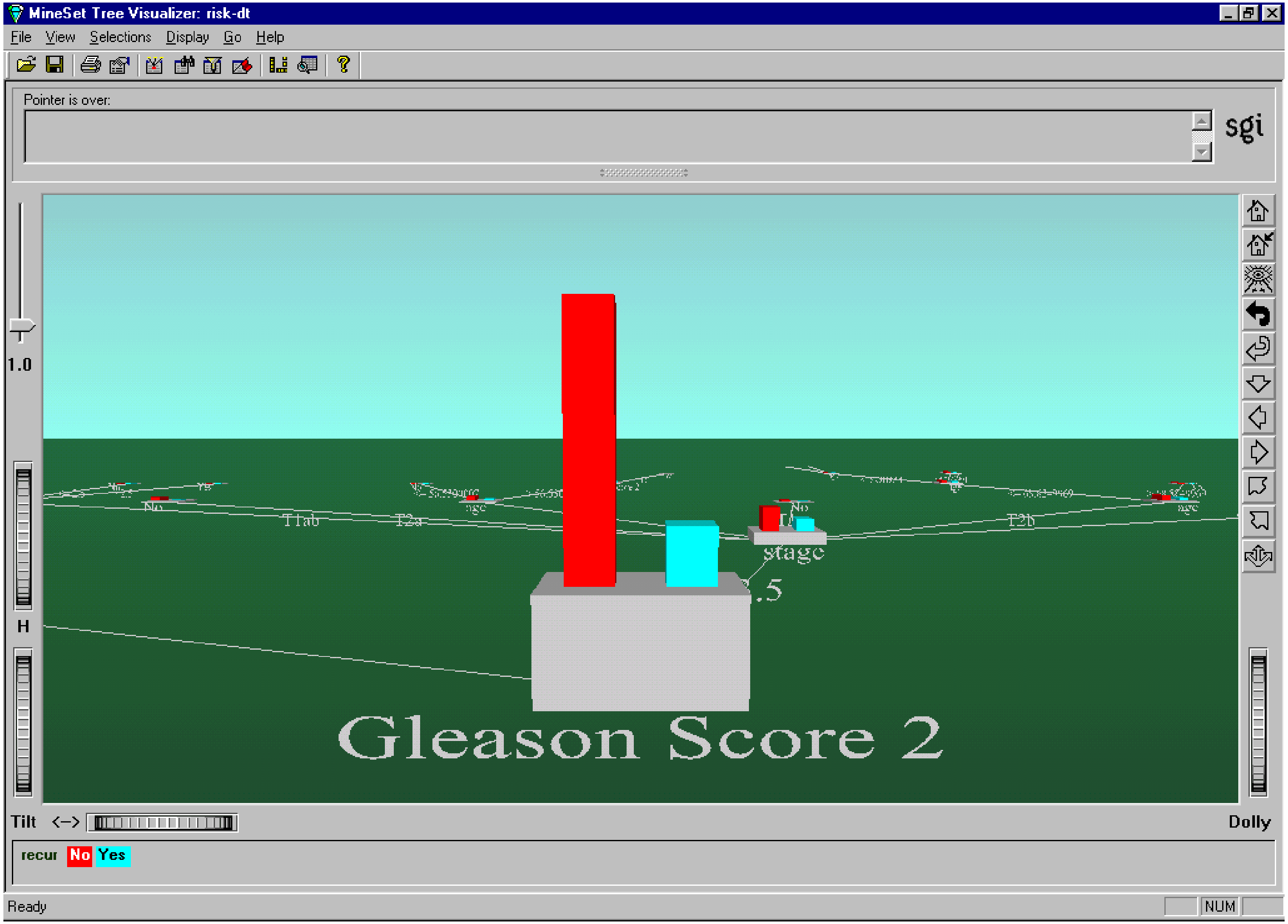
Data visualization: Scatter plot



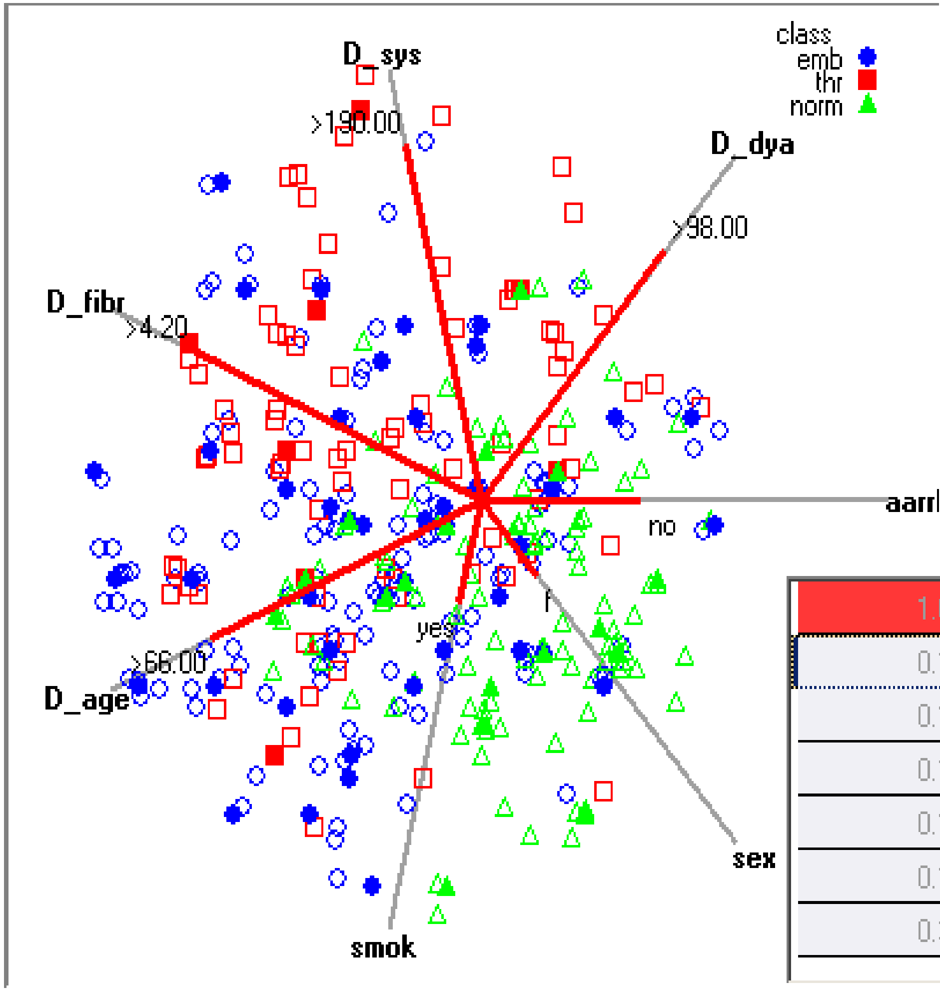
DB Miner: Association rule visualization

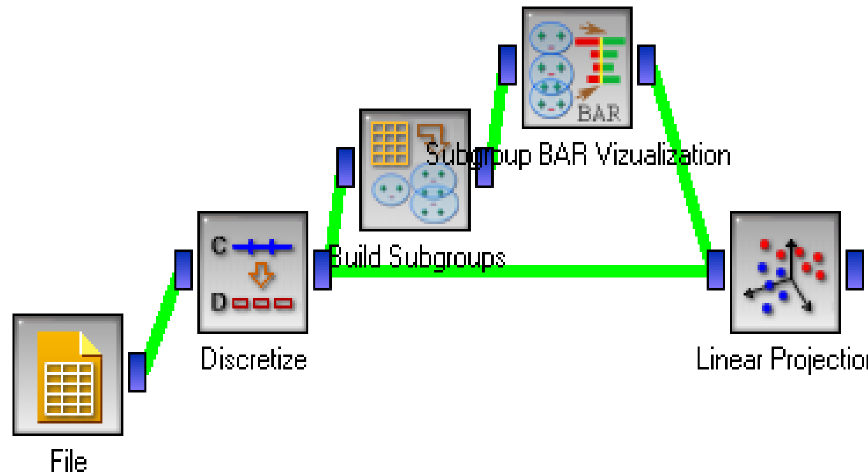


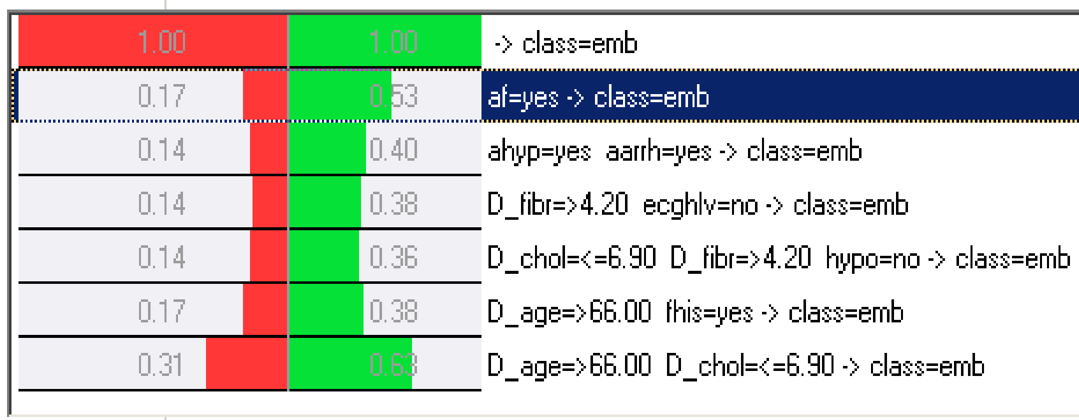
MineSet: Decision tree visualization



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

Introductory seminar lecture

X. JSI & Knowledge Technologies

I. Introduction: First generation data mining

- Data Mining in a nutshell
- Data Mining and KDD process
- DM standards, tools and visualization
- Classification of Data Mining techniques: Predictive and descriptive DM

  (Mladenić et al. Ch. 1 and 11, Kononenko & Kukar Ch. 1)

XX. Selected data mining techniques: Advanced subgroup discovery techniques and applications

XXX. Recent advances: Cross-context link discovery

XX. Talk outline

- Subgroup discovery in a nutshell
- Relational data mining and propositionalization in a nutshell
- Semantic data mining: Using ontologies in SD

Task reformulation: Binary Class Values

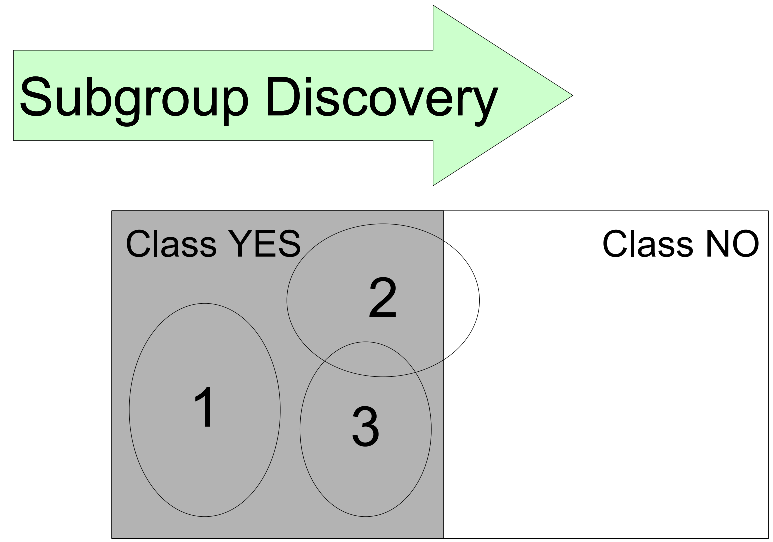
Person	Age	Spect. presc.	Astigm.	Tear prod.	Lenses
O1	17	myope	no	reduced	NO
O2	23	myope	no	normal	YES
O3	22	myope	yes	reduced	NO
O4	27	myope	yes	normal	YES
O5	19	hypermetrope	no	reduced	NO
O6-O13	...	...	...	...	...
O14	35	hypermetrope	no	normal	YES
O15	43	hypermetrope	yes	reduced	NO
O16	39	hypermetrope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

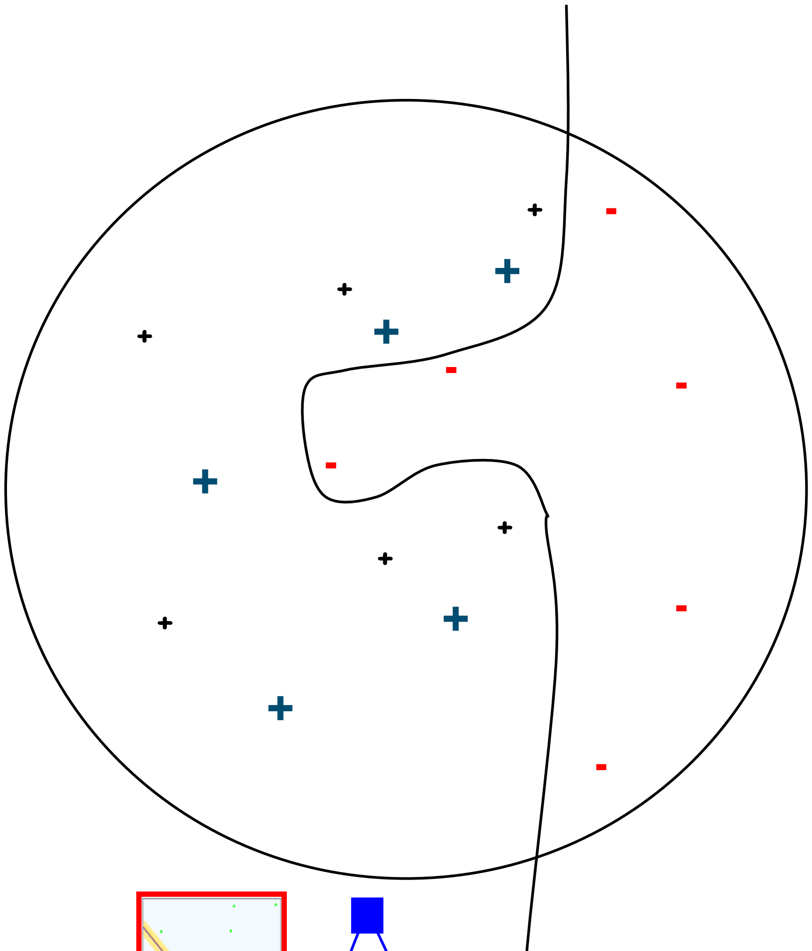


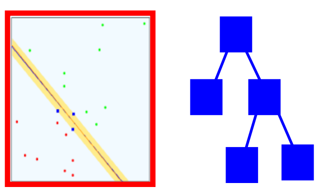
- A task in which individual interpretable patterns in the form of rules are induced from data, labeled by a predefined property of interest.
- SD algorithms learn several independent rules that describe groups of target class examples
  - subgroups must be large and significant

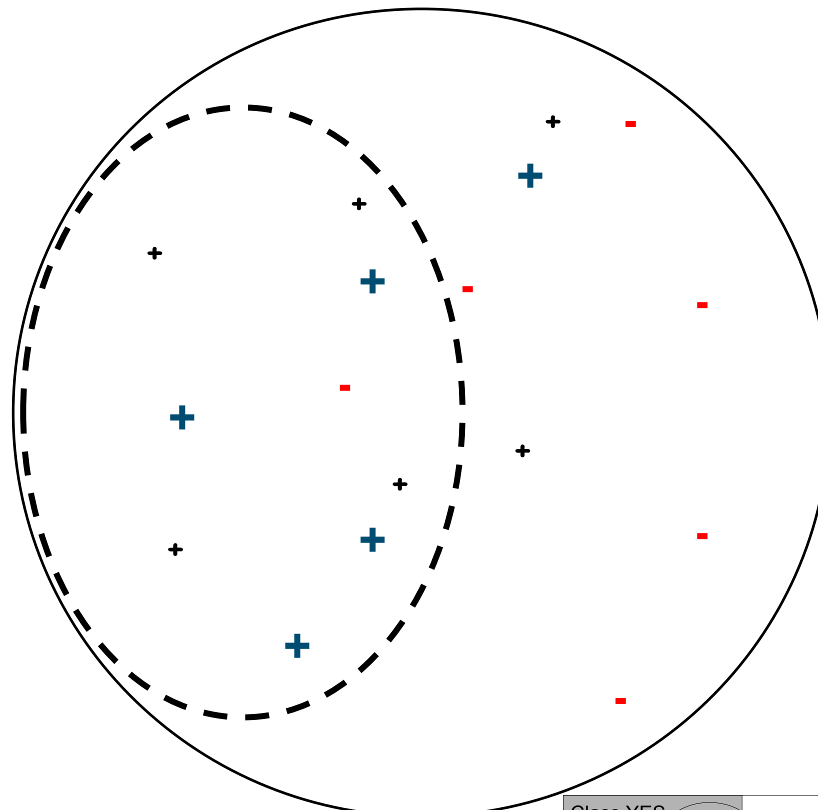
Classification versus Subgroup Discovery

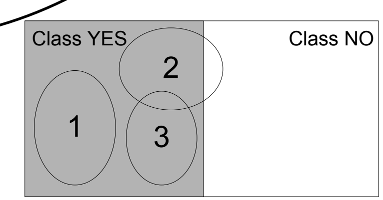
- **Classification (predictive induction) - constructing sets of classification rules**
  - aimed at learning a model for classification or prediction
  - rules are dependent
- **Subgroup discovery (descriptive induction) – constructing individual subgroup describing rules**
  - aimed at finding interesting 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 (Kloesgen, Wrobel 1997)

– **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 example: CHD Risk Group Detection

Input: Patient records described by **stage A** (anamnestic), stage **B** (an. & lab.), **and stage C** (an., lab. & ECG) attributes

Task: Find and characterize population subgroups with high CHD risk (large enough, distributionally unusual)

From **best induced descriptions**, five were selected by the expert as **most actionable** for CHD risk screening (by GPs):

CHD-risk ← male & pos. fam. history & age > 46

CHD-risk ← female & bodymassIndex > 25 & age > 63

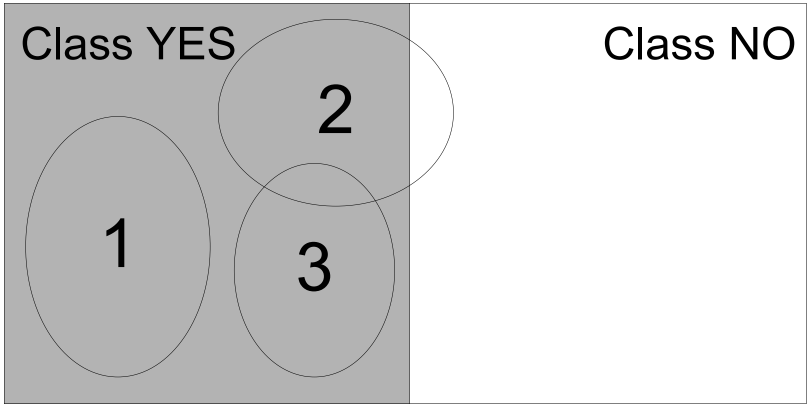
CHD-risk ← ...

CHD-risk ← ...

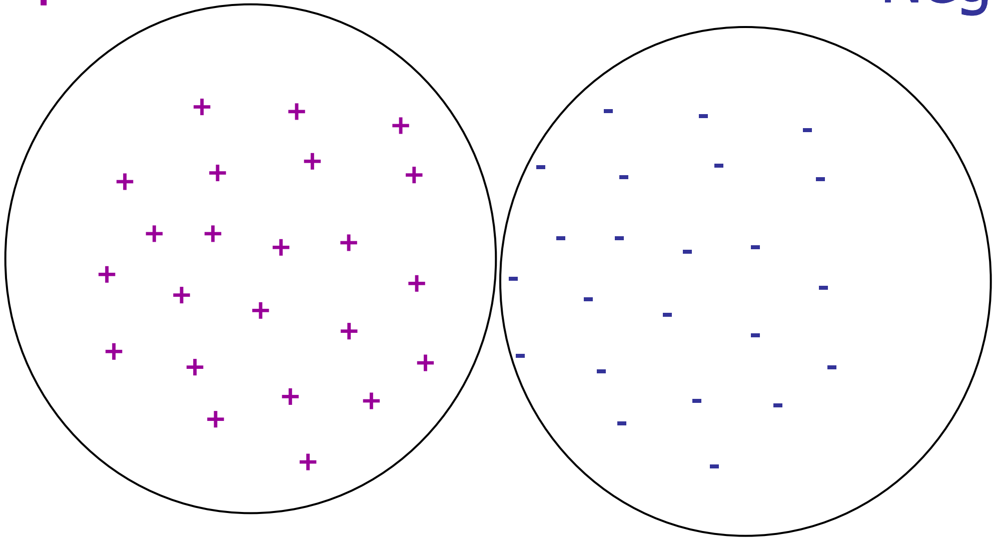
CHD-risk ← ...

Characteristics of SD Algorithms

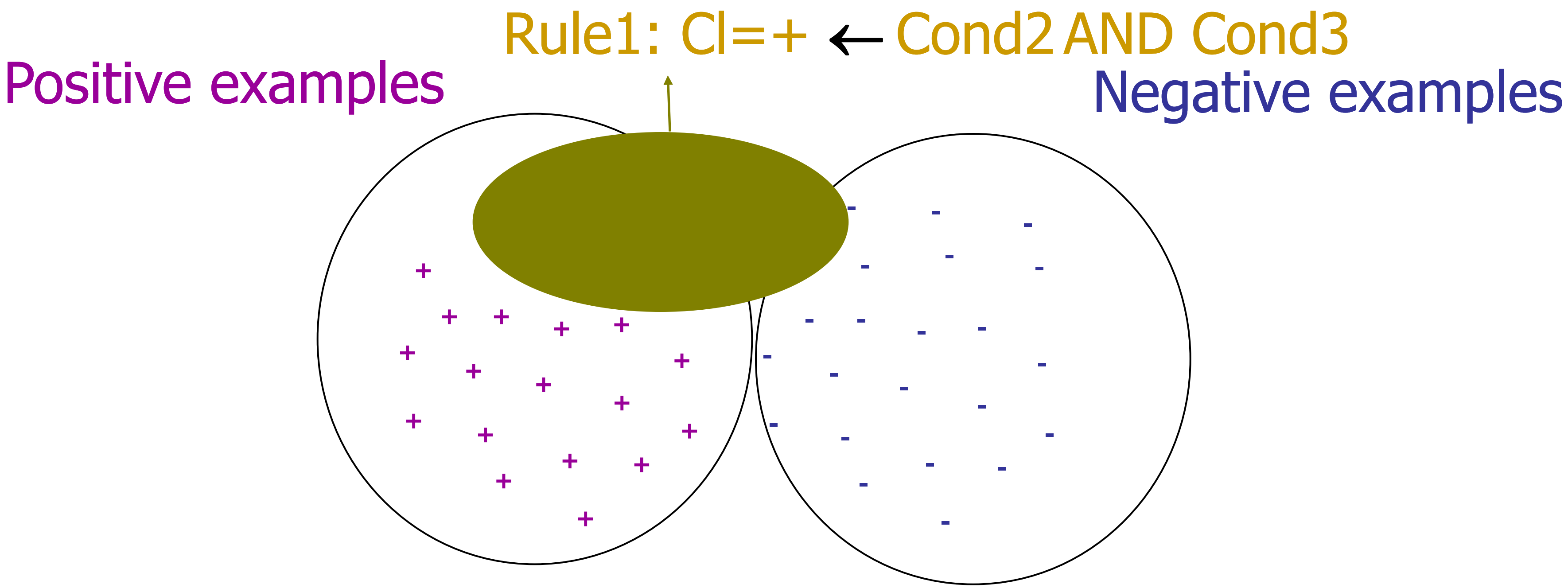
- SD algorithms do not look for a single complex rule to describe all examples of target class YES (all CHD-risk patients), but several rules that describe parts (subgroups) of YES.
- Standard rule learning approach: Using the covering algorithm for rule set construction



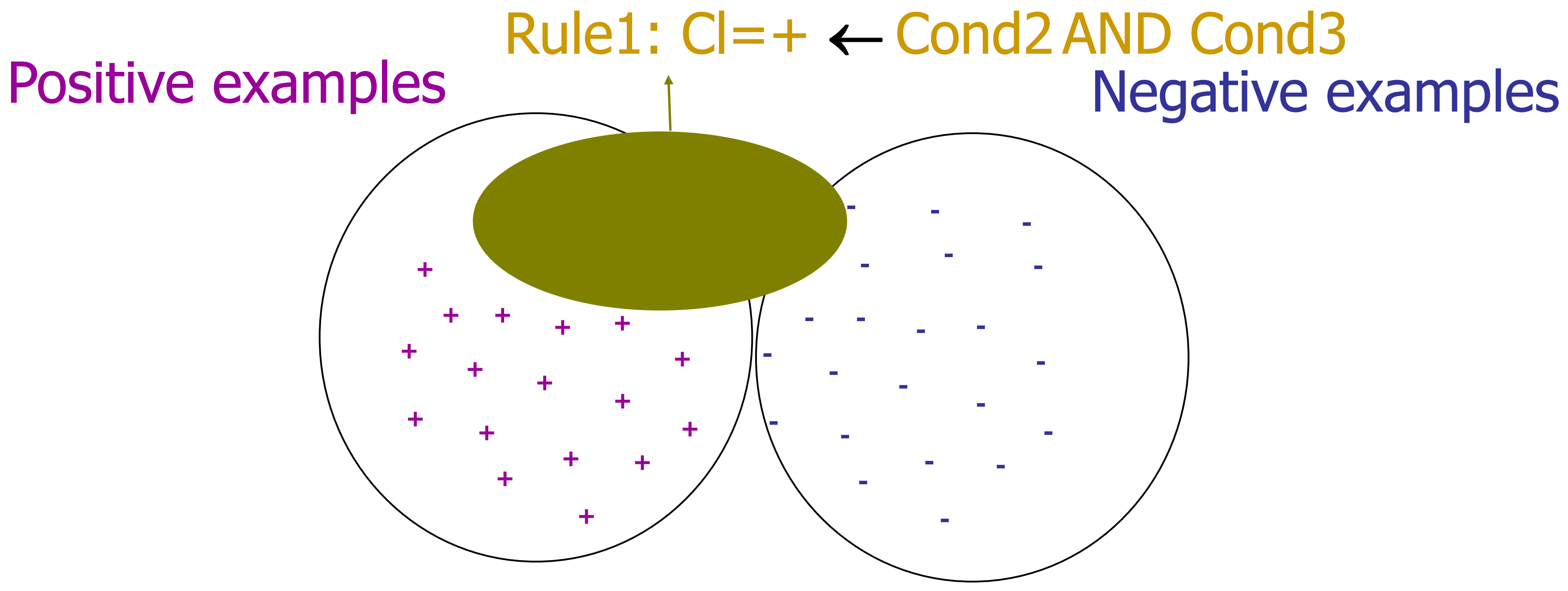
Covering algorithm



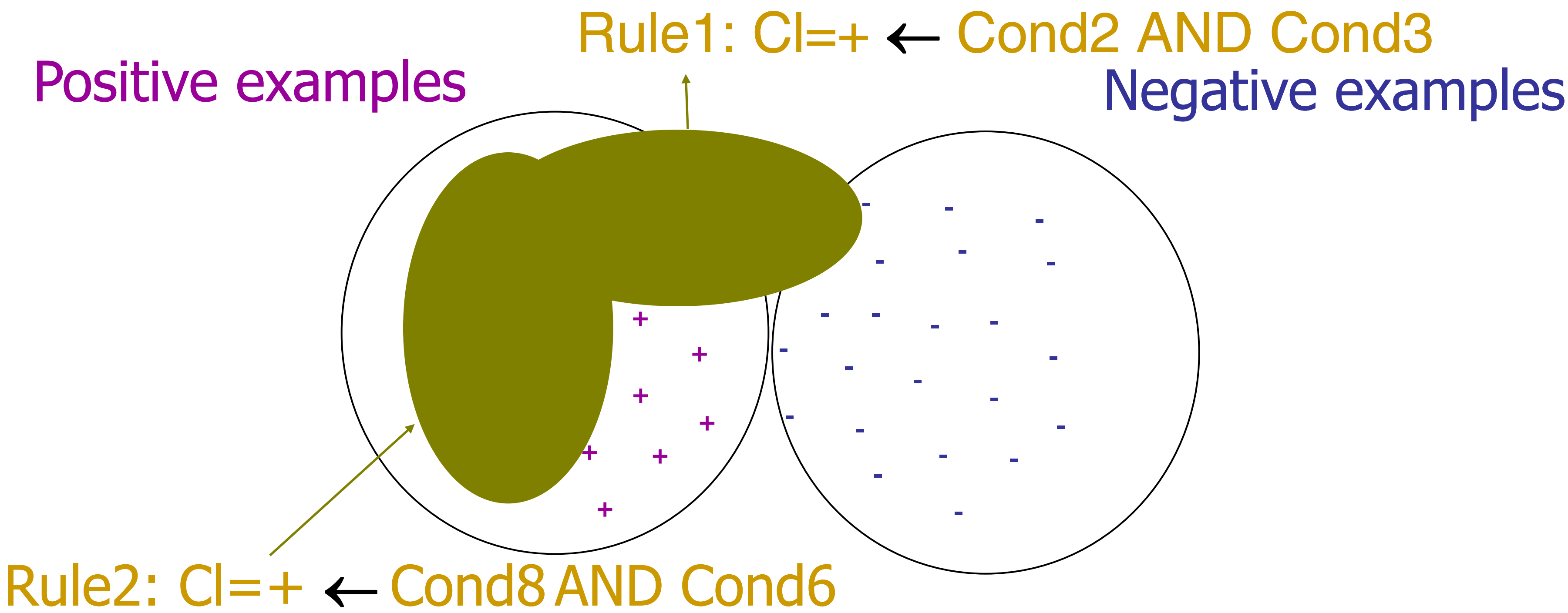
Covering algorithm



Covering algorithm

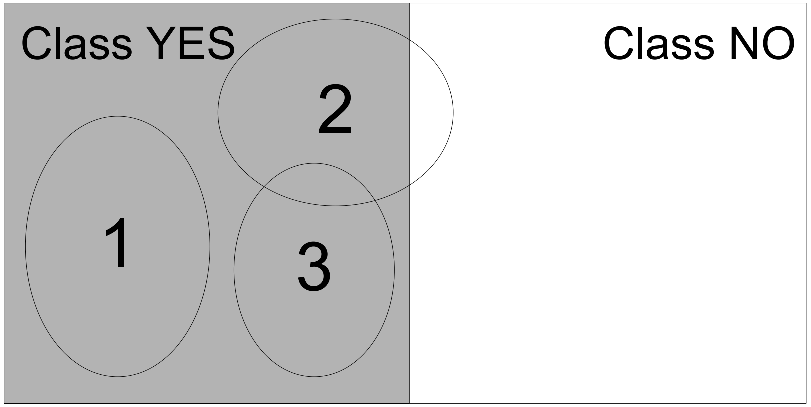


Covering algorithm

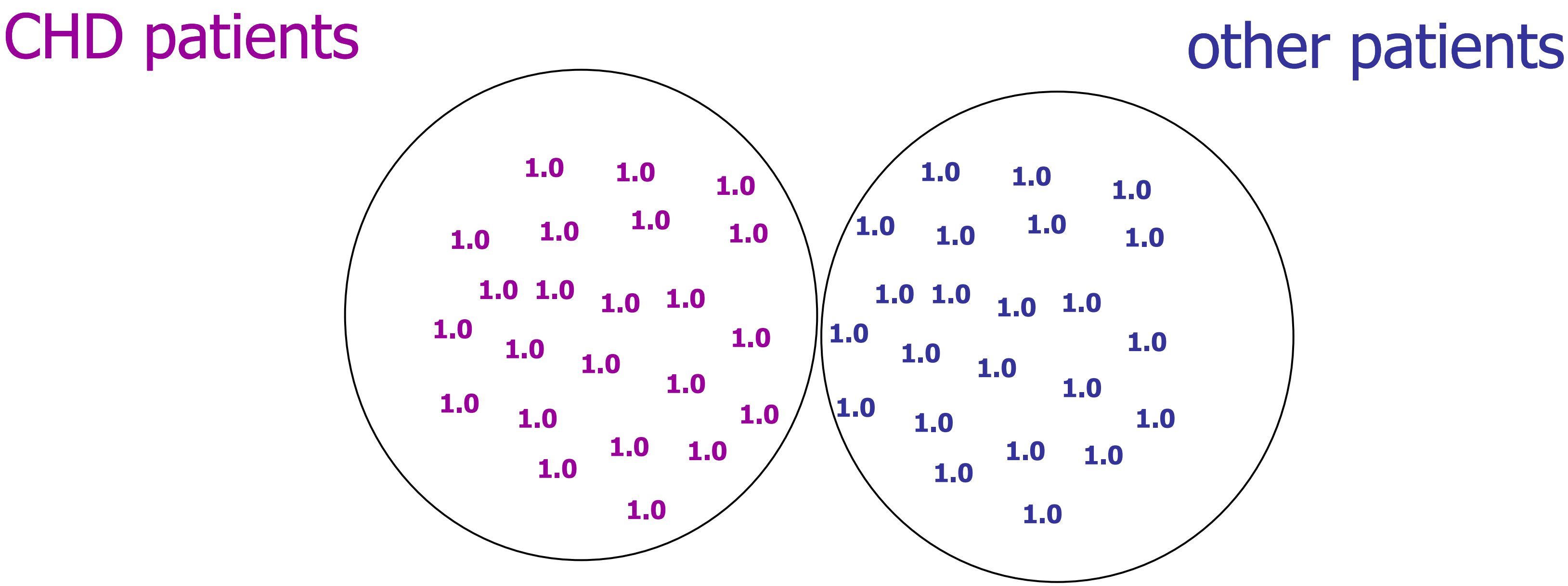


Characteristics of SD Algorithms

- SD algorithms do not look for a single complex rule to describe all examples of target class YES (all CHD-risk patients), but several rules that describe parts (subgroups) of YES.
- Advanced rule learning approach: using example weights in the weighted covering algorithm for repetitive subgroup construction and in the rule quality evaluation heuristics.

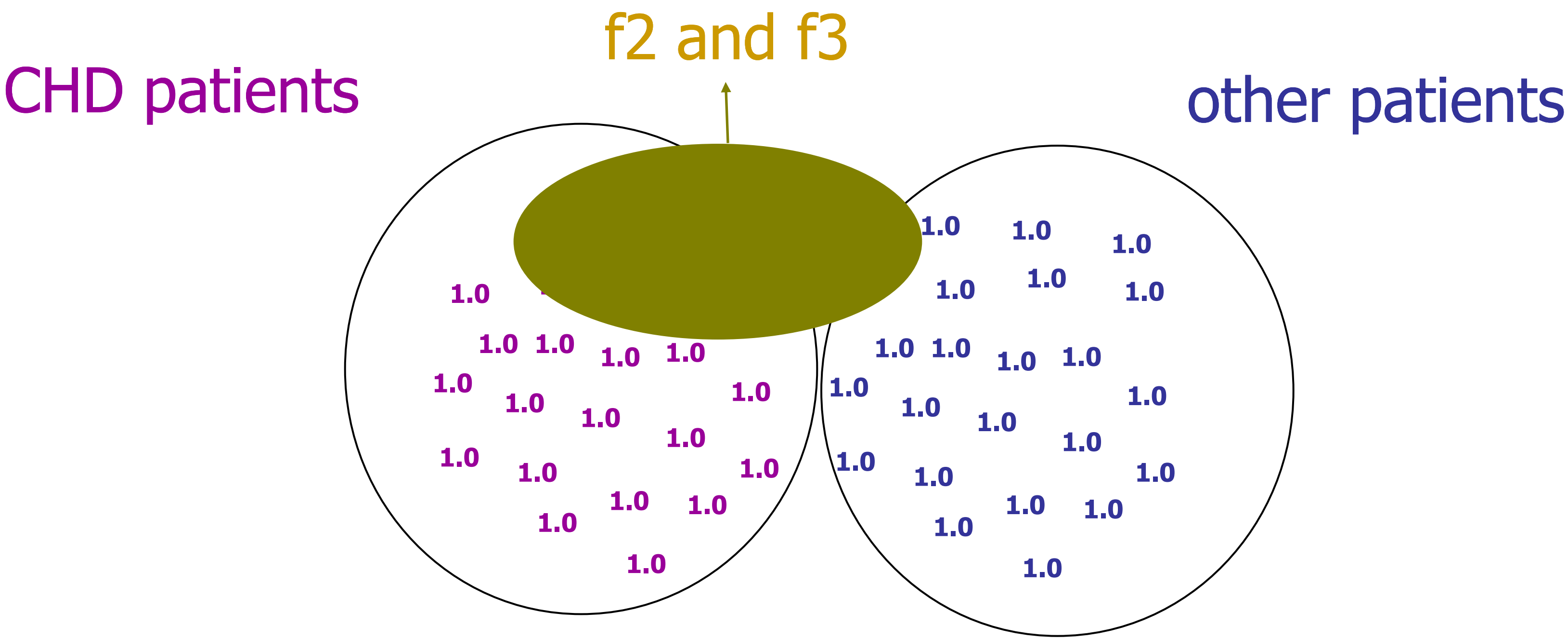


Weighted covering algorithm for rule set construction



- For learning a set of subgroup describing rules, SD implements an iterative weighted covering algorithm.
- Quality of a rule is measured by trading off coverage and precision.

Weighted covering algorithm for rule set construction

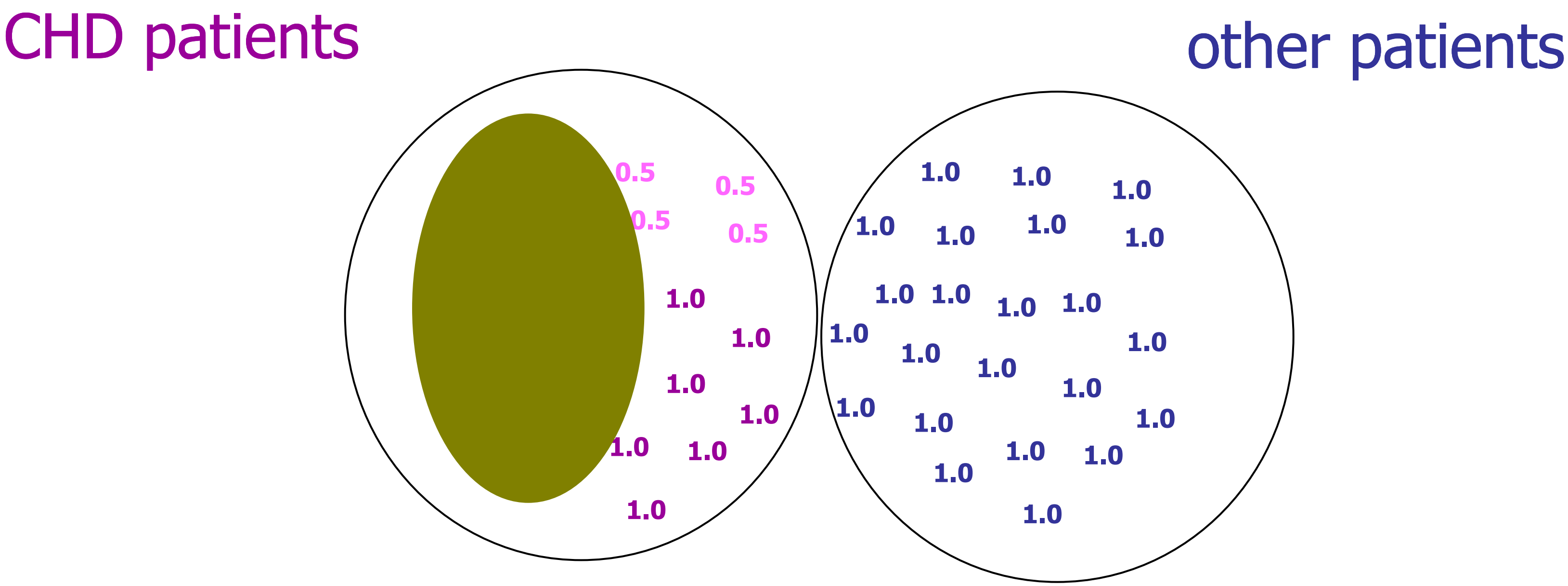


Rule quality measure in SD: $q(Cl \leftarrow Cond) = TP/(FP+g)$

Rule quality measure in CN2-SD: $WRAcc(Cl \leftarrow Cond) = p(Cond) \times [p(Cl \mid Cond) - p(Cl)]$ = coverage x (precision – default precision)

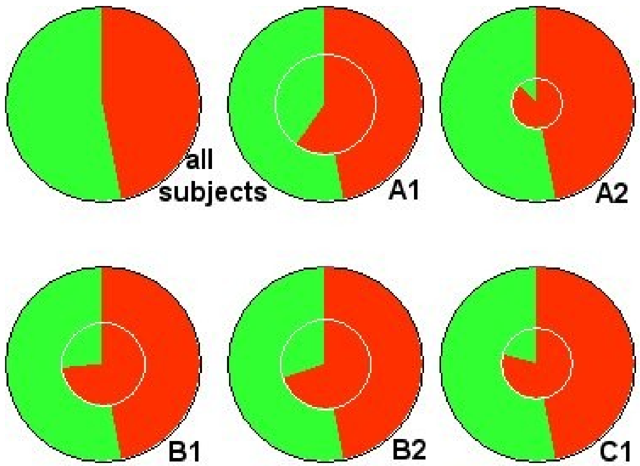
*__Coverage__ = sum of the covered weights, *__Precision__ = purity of the covered examples

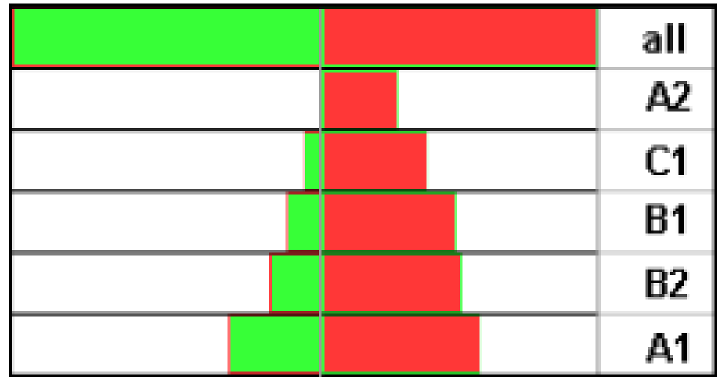
Weighted covering algorithm for rule set construction

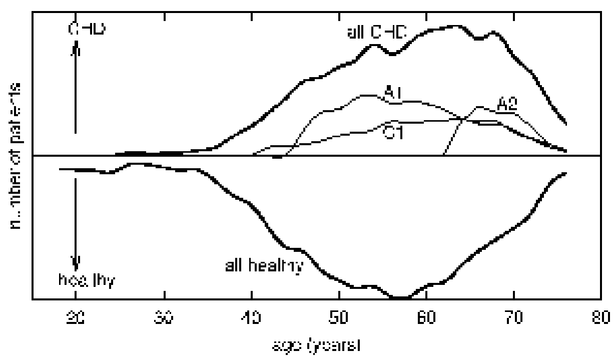


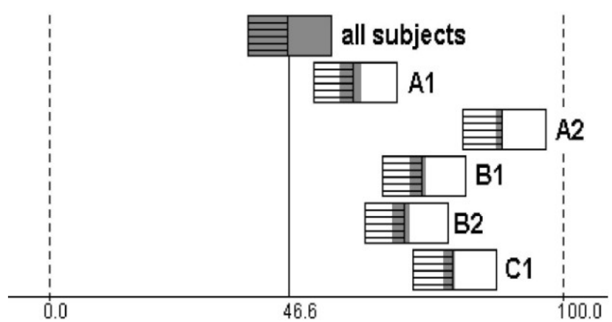
In contrast with classification rule learning algorithms (e.g. CN2), the covered positive examples are not deleted from the training set in the next rule learning iteration; they are re-weighted, and a next ‘best’ rule is learned.

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)

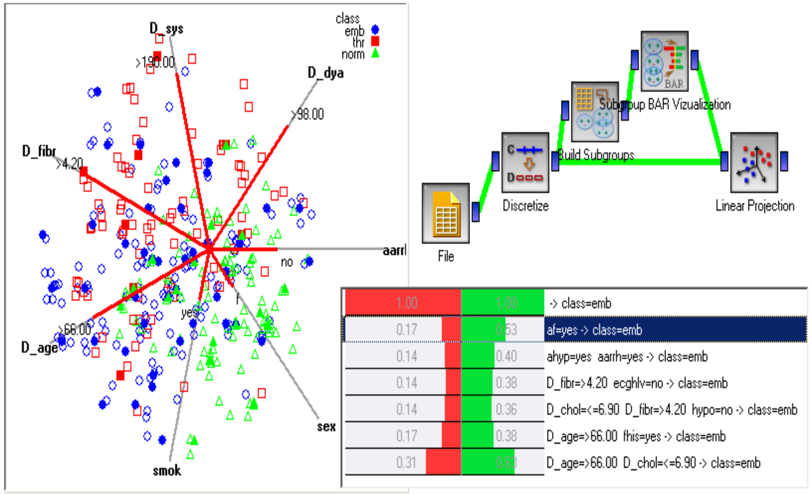
AND

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.

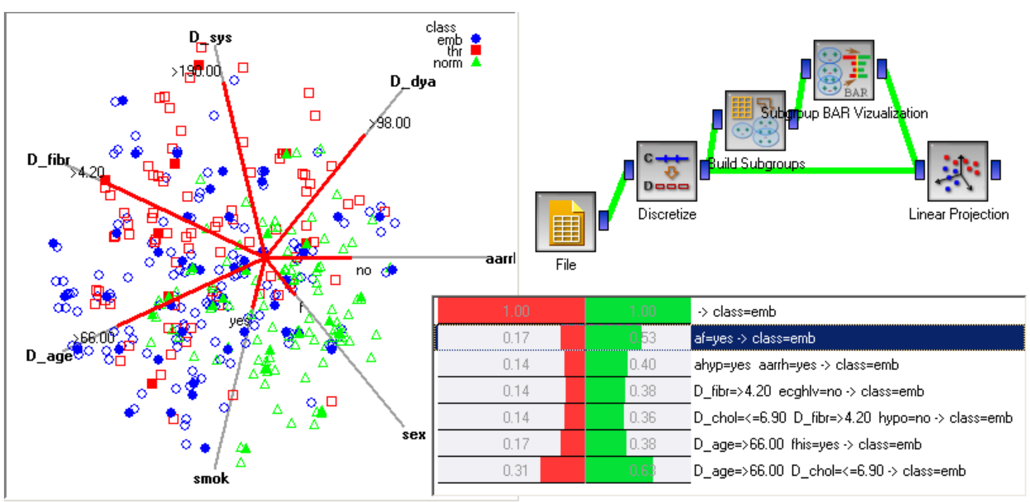
SD algorithms in the Orange DM Platform

- **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



XX. Talk outline

- Subgroup discovery in a nutshell
- Relational data mining and propositionalization in a nutshell
- Semantic data mining: Using ontologies in SD

Relational Data Mining (Inductive Logic Programming) in a nutshell

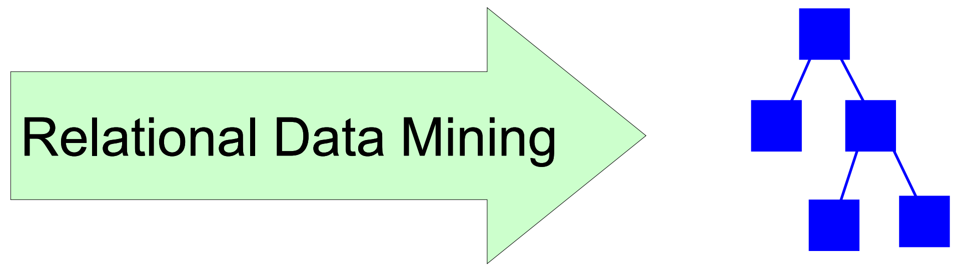
customer							
ID	Zip	Sex	SoSt	Income	Age	Club	Resp
...	...	...	...	...	...	...	...
3478	34677	m	si	60-70	32	me	nr
3479	43666	f	ma	80-90	45	nm	re
...	...	...	...	...	...	...	...

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.

knowledge discovery from data



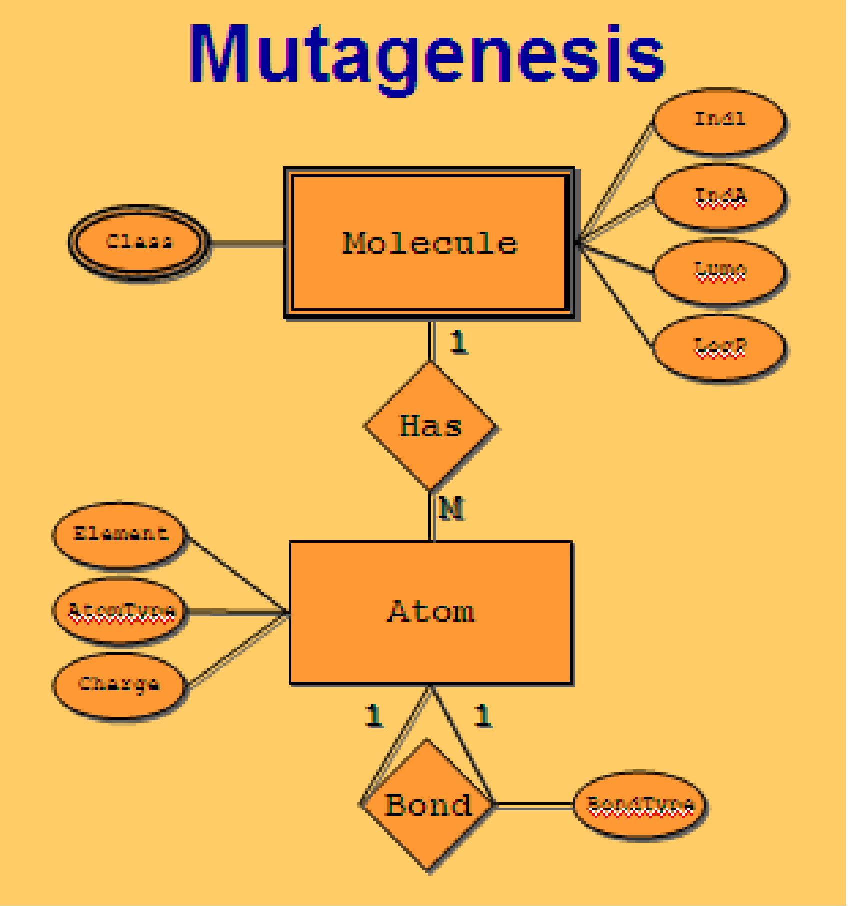
model, patterns, …

Given: a relational database, a set of tables. sets of logical facts, a graph, …

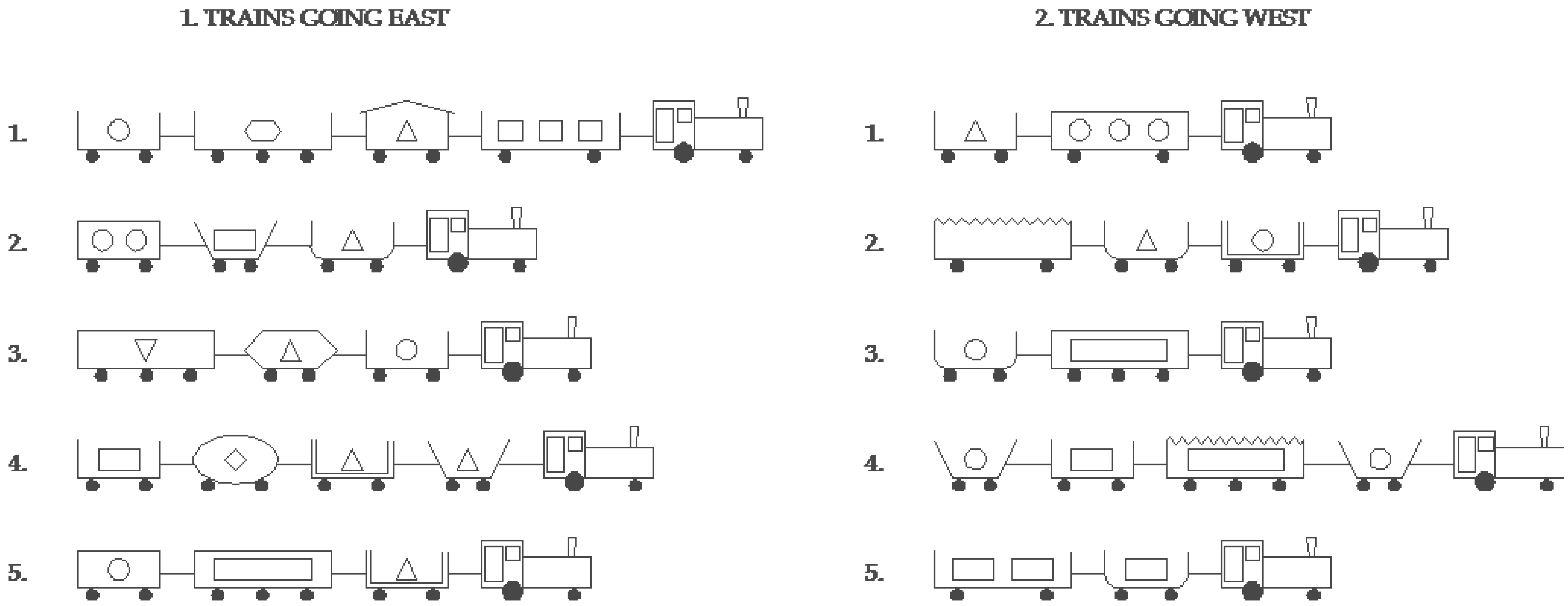
Find: a classification model, a set of interesting patterns

Relational Data Mining (ILP)

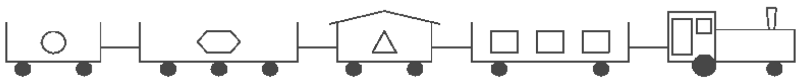
- Learning from multiple tables
  - patient records connected with other patient and demographic information
- Complex relational problems:
  - temporal data: time series in medicine, ...
  - structured data: representation of molecules and their properties in protein engineering, biochemistry, ...



Sample ILP problem: East-West trains



Relational data representation

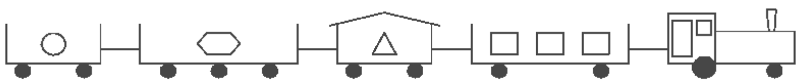


CAR	OBJECT	NUMBER
c1	circle	1
c2	hexagon	1
c3	triangle	1
c4	rectangle	3
...	...	

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
...	...	...			...

Relational data representation

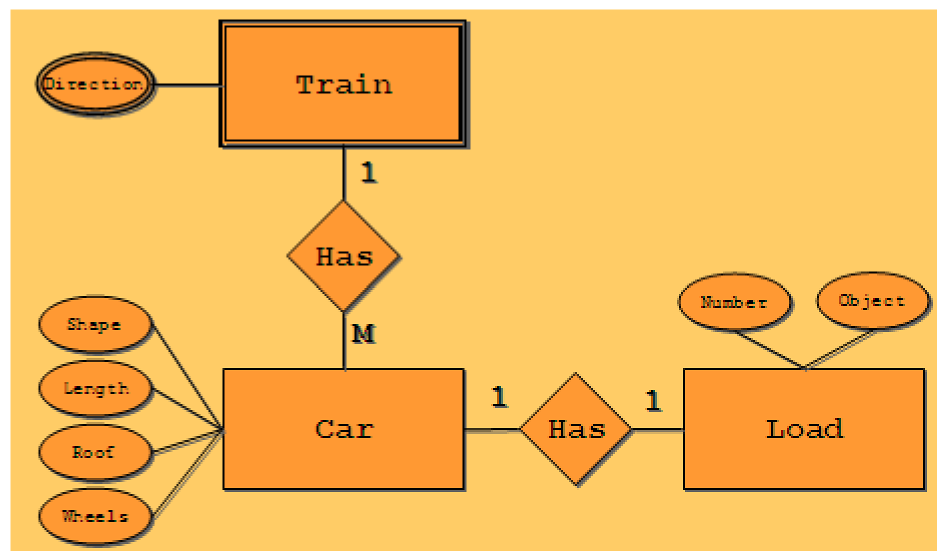


CAR	OBJECT	NUMBER
c1	circle	1
c2	hexagon	1
c3	triangle	1
c4	rectangle	3
...	...	

TRAIN_TABLE

TRAIN	EASTBOUND
	UE
	UE
	SE

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
...	...	...			...



Propositionalization in a nutshell

TRAIN_TABLE

…OUND
…UE
…UE
…SE

CAR	OBJECT	NUMBER
c1	circle	1
c2	hexagon	1
c3	triangle	1
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
...	...	...			...

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) :- ....

Propositional learning:

t(T) ← f1(T), f4(T)

Relational interpretation:

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

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

TRAIN_TABLE

UND
UE
UE
SE

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 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 Data Mining through Propositionalization

customer							
ID	Zip	Sex	SoSt	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.

Step 1

Propositionalization

	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

Relational Data Mining through Propositionalization

customer

ID	Zip	Sex	SoSt	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.

Step 1

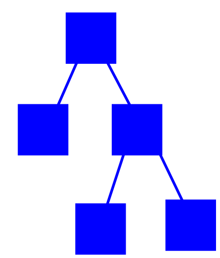
Propositionalization

	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

	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

Step 2

Data Mining



model, patterns, …

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

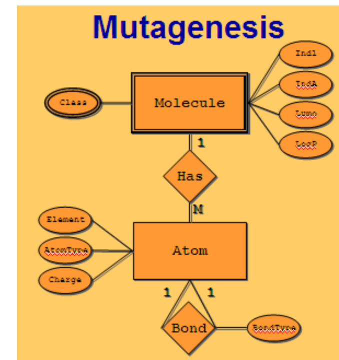
- service for propositionalization through efficient first-order feature construction (Železny and Lavrač, MLJ 2006)

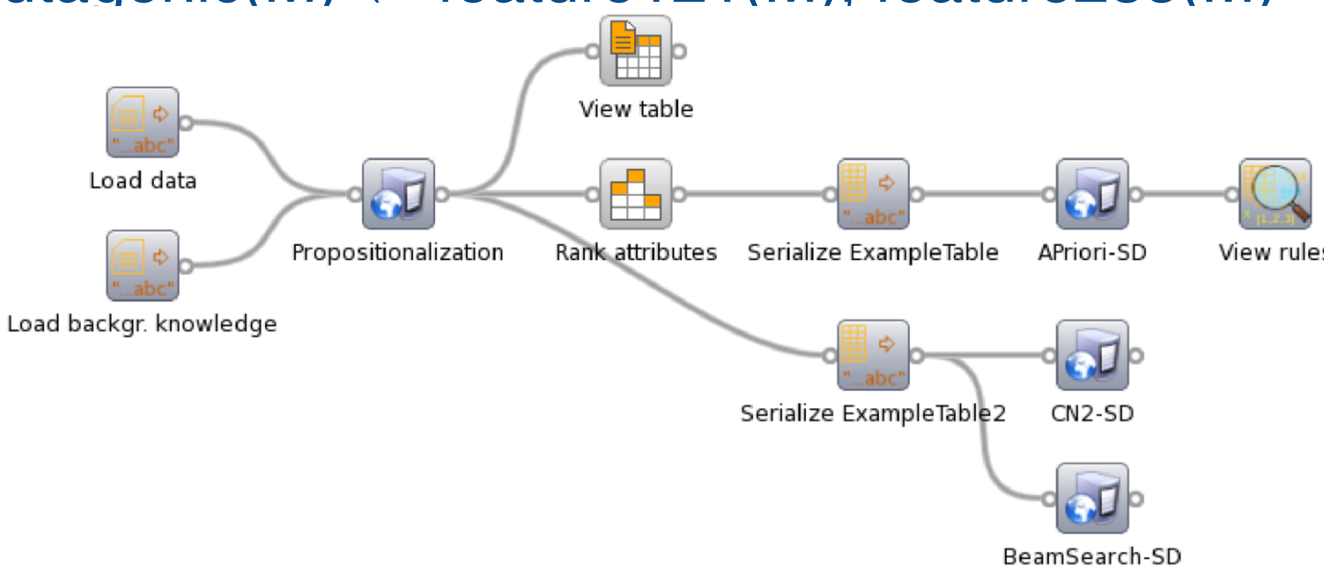
  f121(M):- hasAtom(M,A), atomType(A,21)

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

- subgroup discovery using CN2-SD

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





Talk outline

- Subgroup discovery in a nutshell
- Relational data mining and propositionalization in a nutshell
- Semantic data mining: Using ontologies in SD

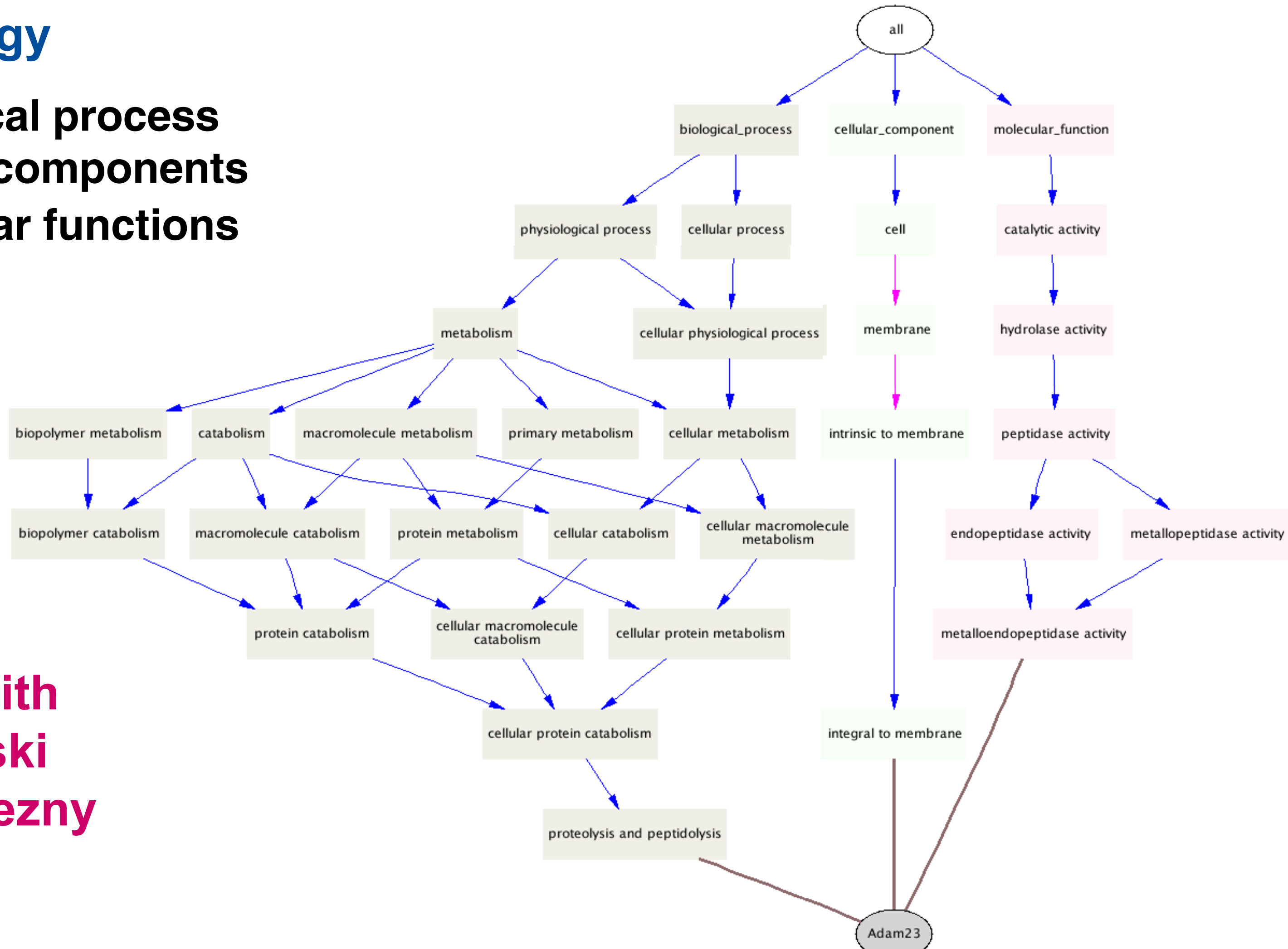
Semantic Data Mining in Orange4WS

- 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

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

Gene Ontology

12093 biological process
1812 cellular components
7459 molecular functions

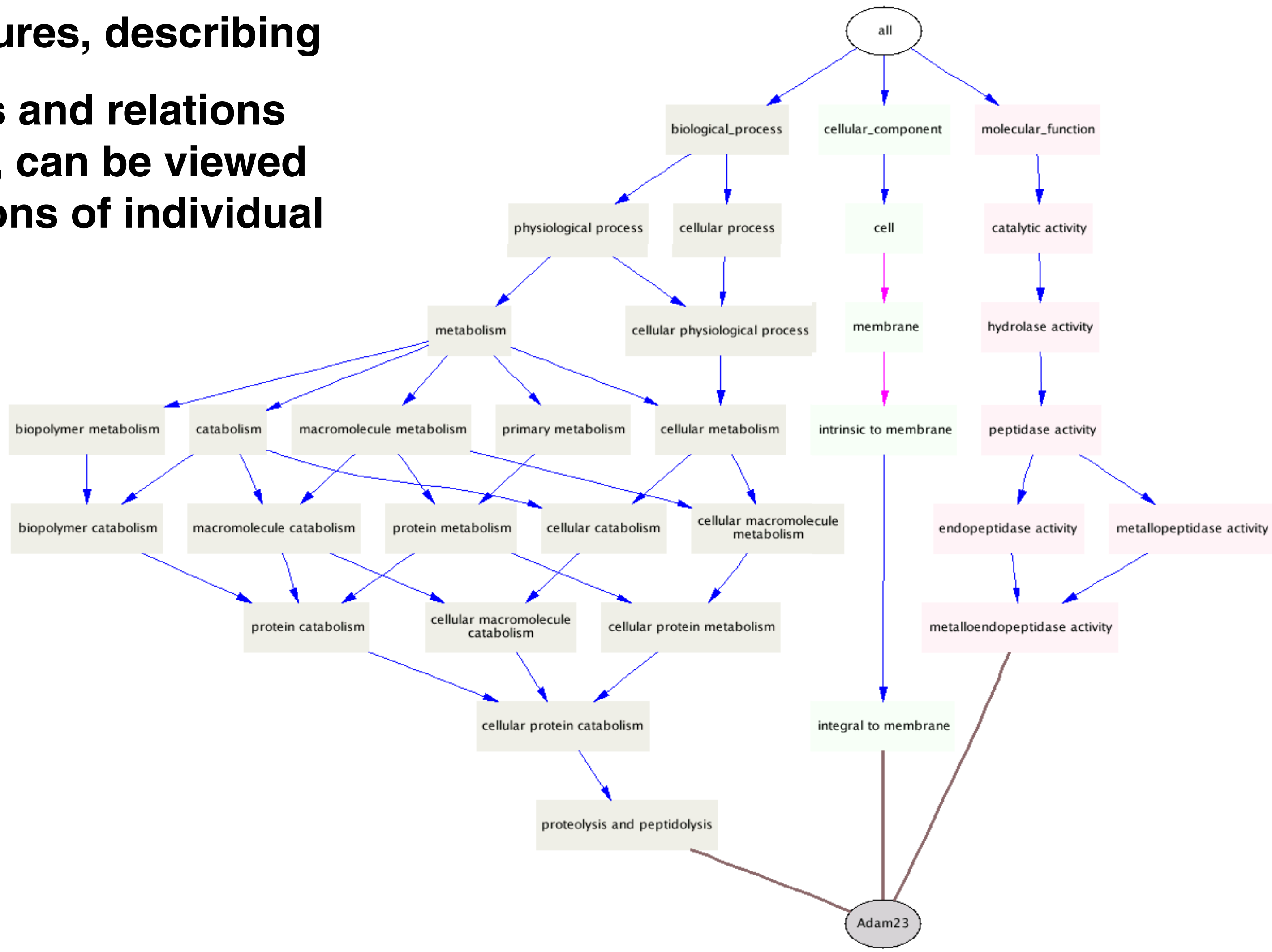


Joint work with Igor Trajkovski and Filip Zelezny

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

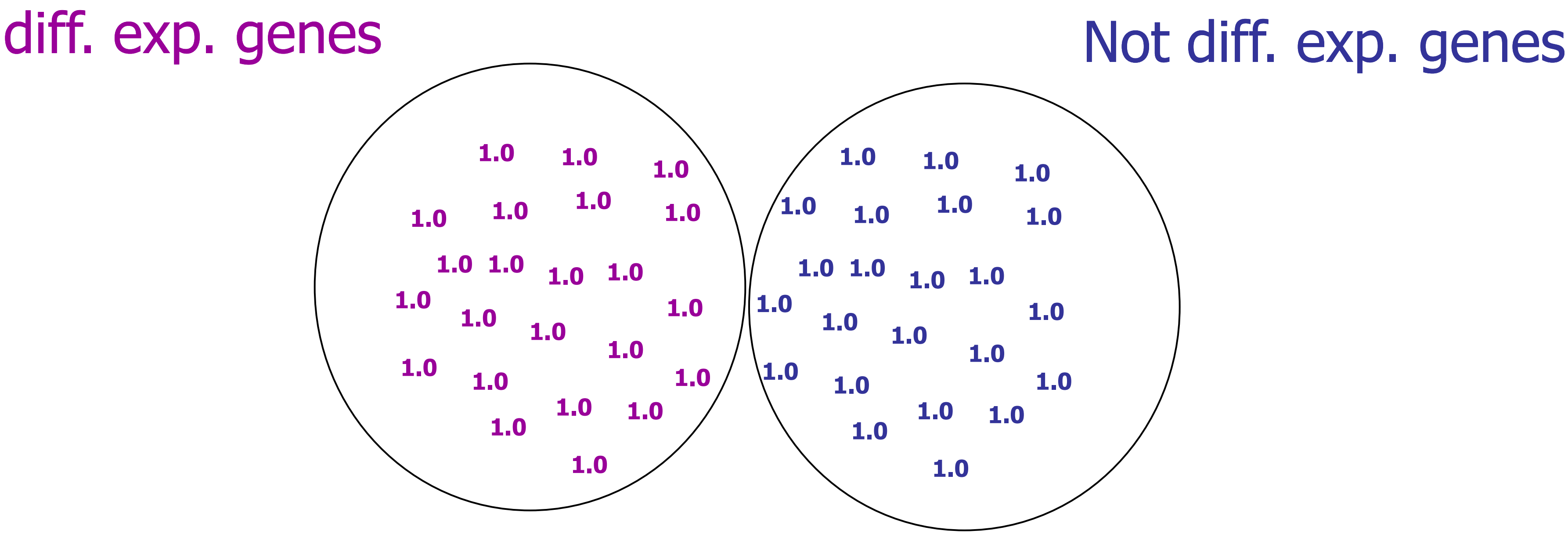
Propositional learning: subgroup discovery

	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

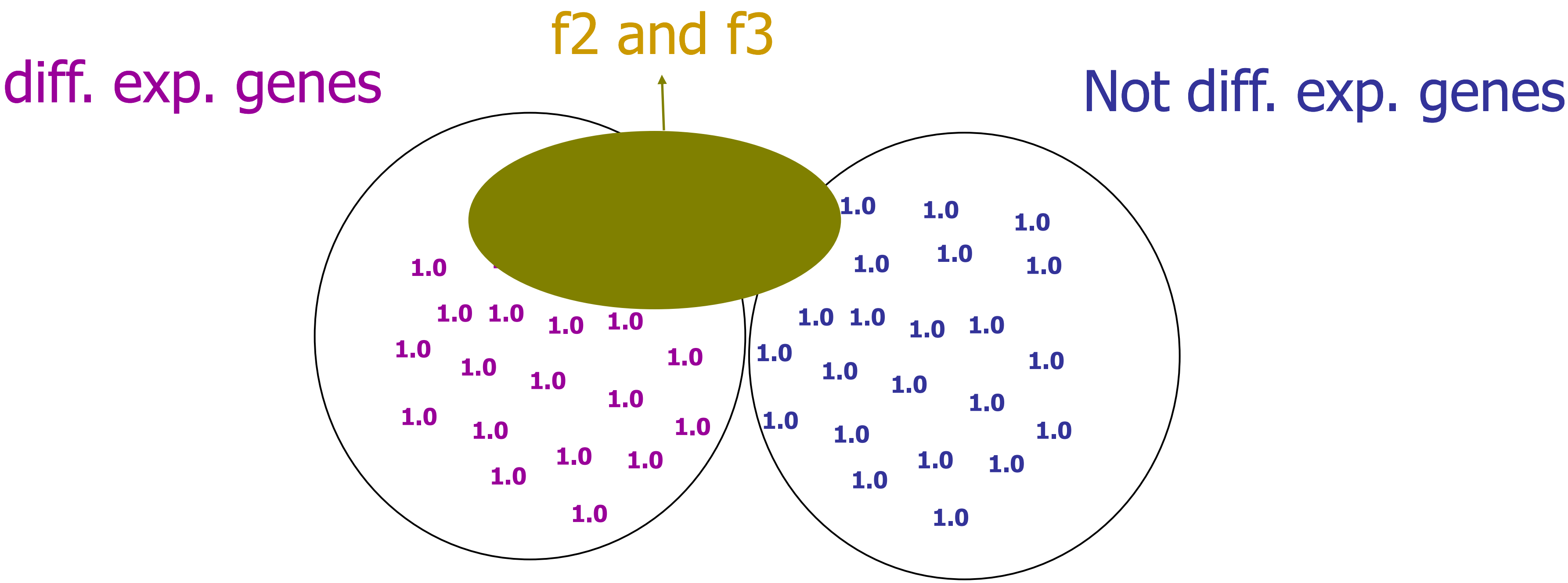
f2 and f3

[4,0]

Subgroup Discovery



Subgroup Discovery



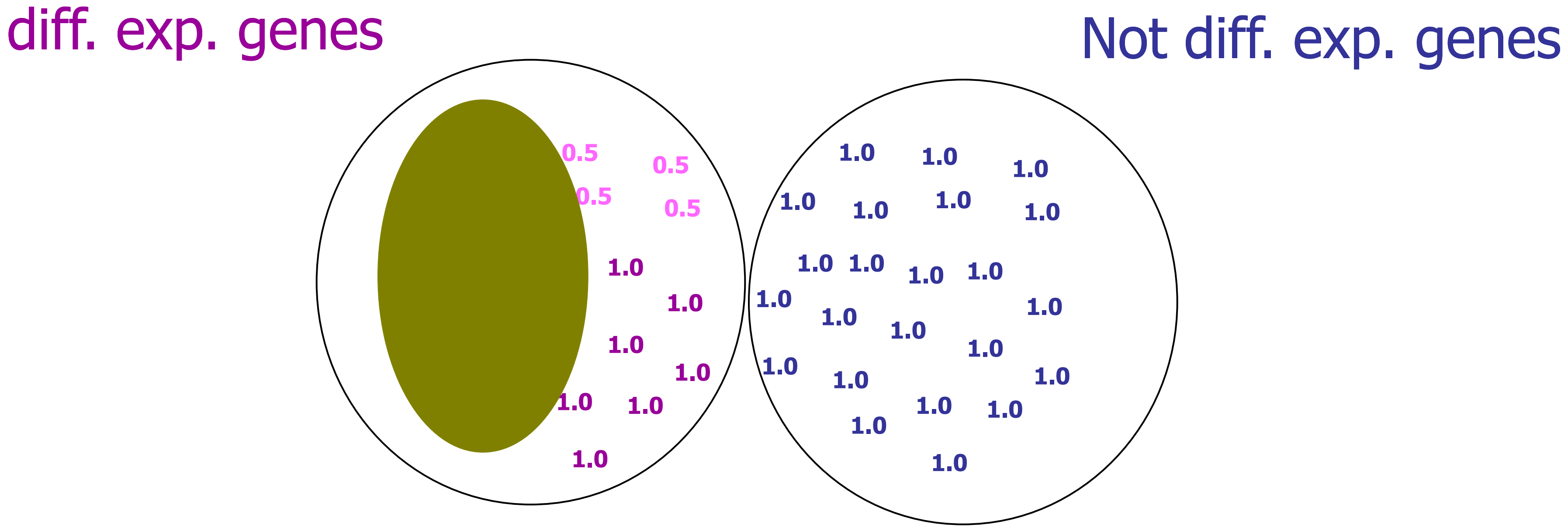
In RSD (using propositional learner CN2-SD):

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
- In past 2-3 years, 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

Introductory seminar lecture

X. JSI & Knowledge Technologies

I. Introduction

– Data Mining and KDD process
– DM standards, tools and visualization
– Classification of Data Mining techniques: Predictive and descriptive DM

(Mladenić et al. Ch. 1 and 11, Kononenko & Kukar Ch. 1)

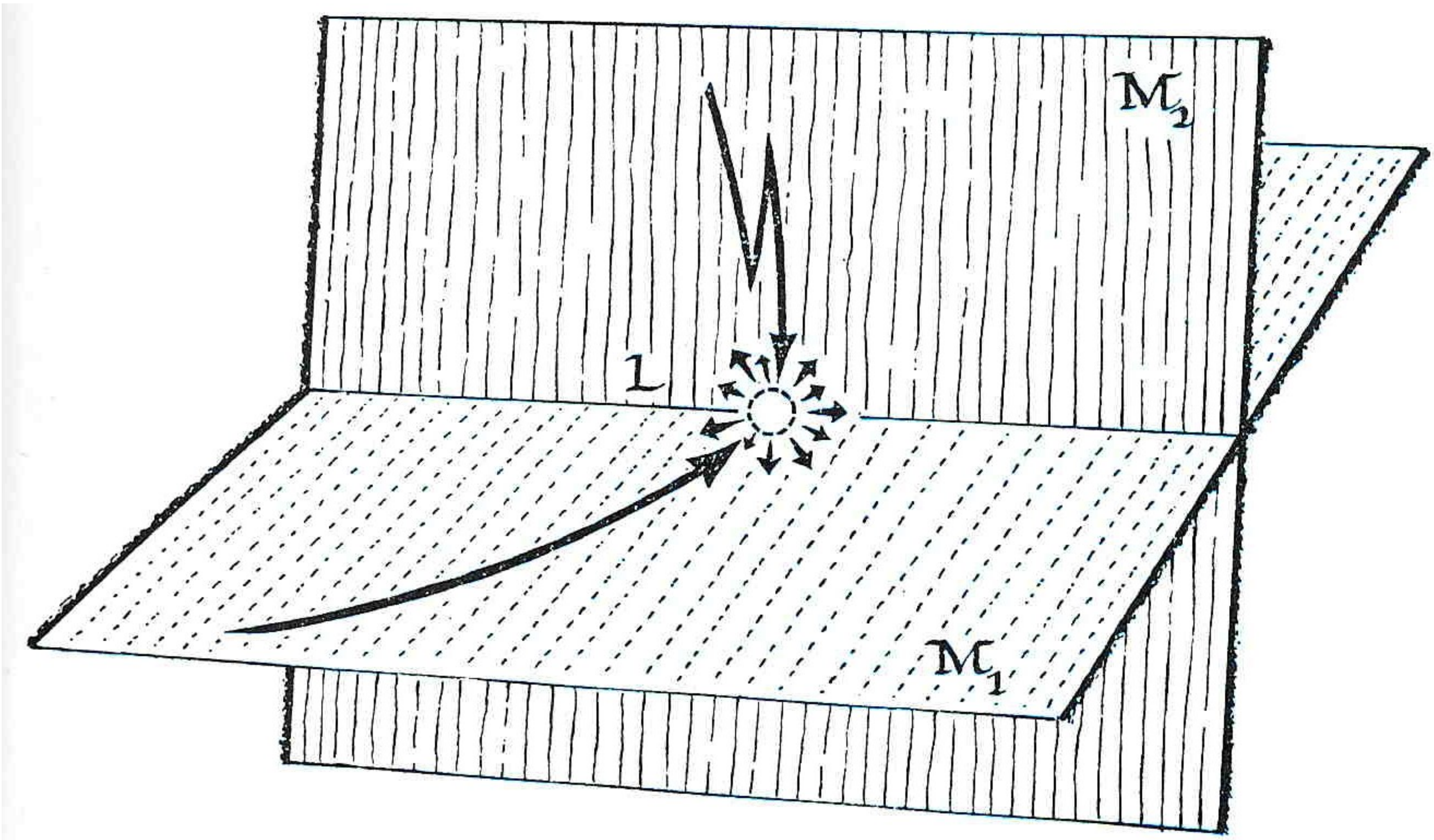
XX. Selected data mining techniques: Advanced subgroup discovery techniques and applications

XXX. Recent advances: Cross-context link discovery

The BISON project

- EU project: Bisociation networks for creative information discovery (www.bisonet.eu), 2008-2010
- Exploring the idea of bisociation (Arthur Koestler, The act of creation, 1964):
  - The mixture - in one human mind – of **two different contexts** or **different categories of objects,** that are normally considered **separate categories** by the processes of the mind.
  - The **thinking process** that is the functional basis of **analogical or metaphoric thinking** as compared to logical or associative thinking.
- Main challenge: Support humans to find **new interesting associations accross domains**

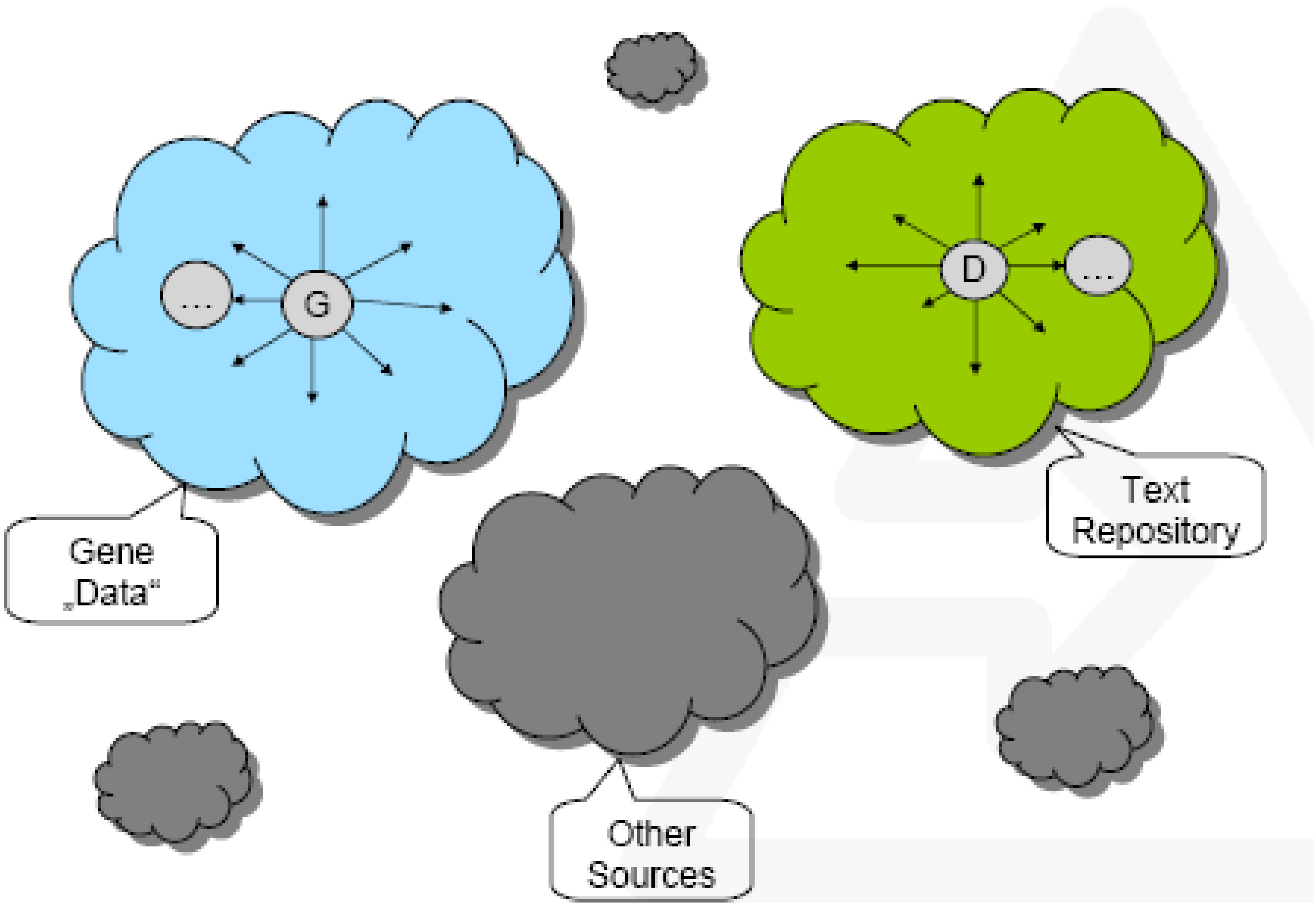
Bisociation (A. Koestler 1964)



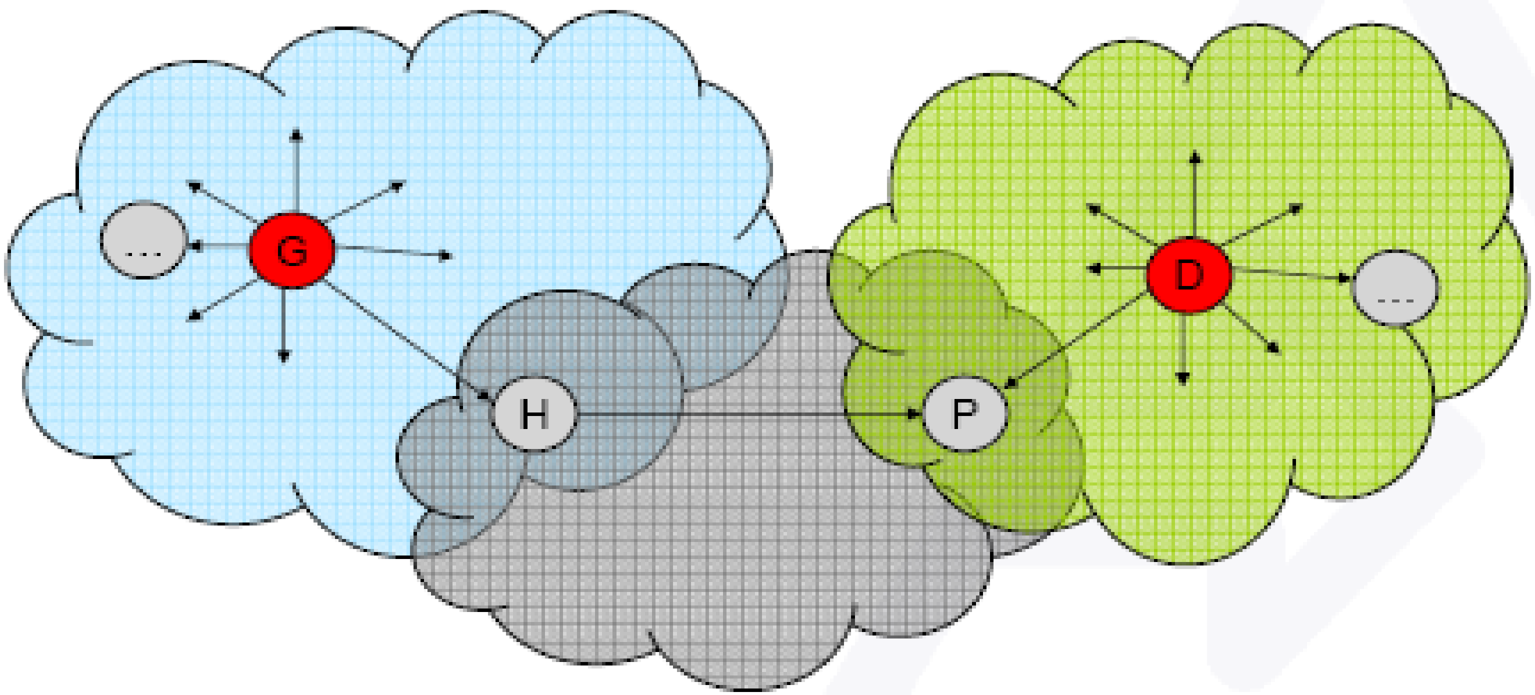
The BISON project

- BISON challenge: Support humans to find **new, interesting links accross domains,** named **bisociations**
  - across different contexts
  - across different types of data and knowledge sources
- Open problems:
  - Fusion of heterogeneous data/knowledge sources into a joint representation format - a large information network named BisoNet (consisting of nodes and relatioships between nodes)
  - Finding unexpected, previously unknown links between BisoNet nodes belonging to different contexts

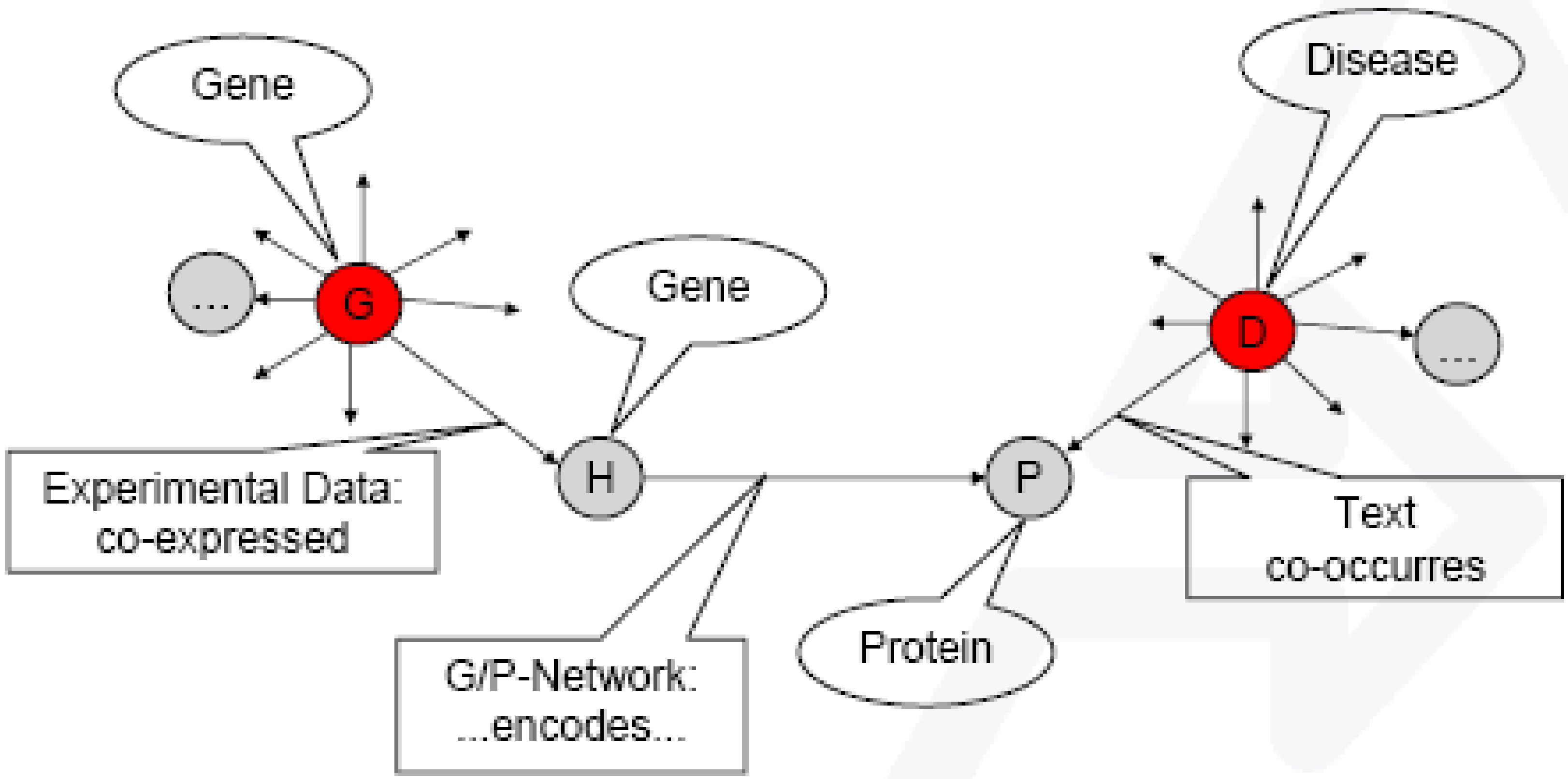
Heterogeneous data sources (BISON, M. Berthold, 2008)



Bridging concepts (BISON, M. Berthold, 2008)



Chains of associations across domains (BISON, M. Berthold, 2008)



Semantic Data Mining for DNA Microarray Data Analysis

- Semantic data mining integrates public gene annotation data through relational features
- It is implemented in the SEGS algorithm (Trajkovski, Železny, Lavrač and Tolar, JBI 2008), available in Orange4WS
- It can be combined with additional biomedical resources (BioMine), providing additional means for creative knowledge discovery from publicly available data sources

Biomine graph exploration (Toivonnen et al., Uni. Helsinki)

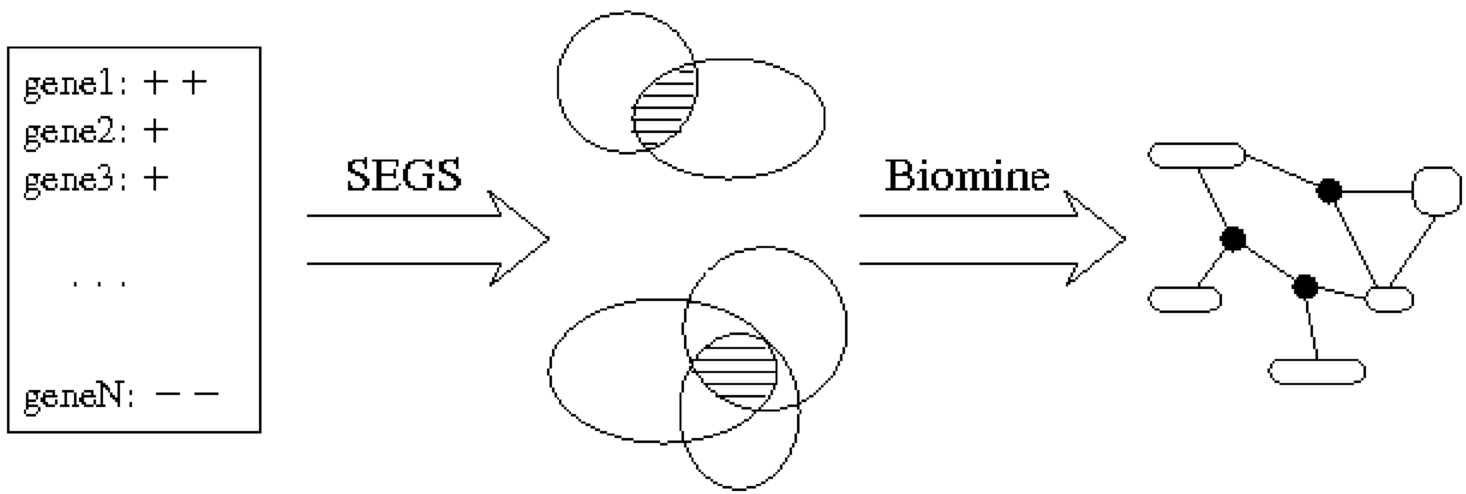
- **BioMine graph** contains information from public databases, including annotated sequences, proteins, orthology groups, genes and gene expressions, gene and protein interactions, PubMed articles, and different ontologies.
  - **nodes (~1 mio)** correspond to different concepts (such as gene, protein, domain, phenotype, biological process, tissue)
  - **semantically labeled edges (~7 mio)** connect related concepts
- **BioMine query engine** answers queries to potentially discover new links between entities by sophisticated graph exploration algorithms

The SEGS + BioMine Methodology

Microarray

Gene sets

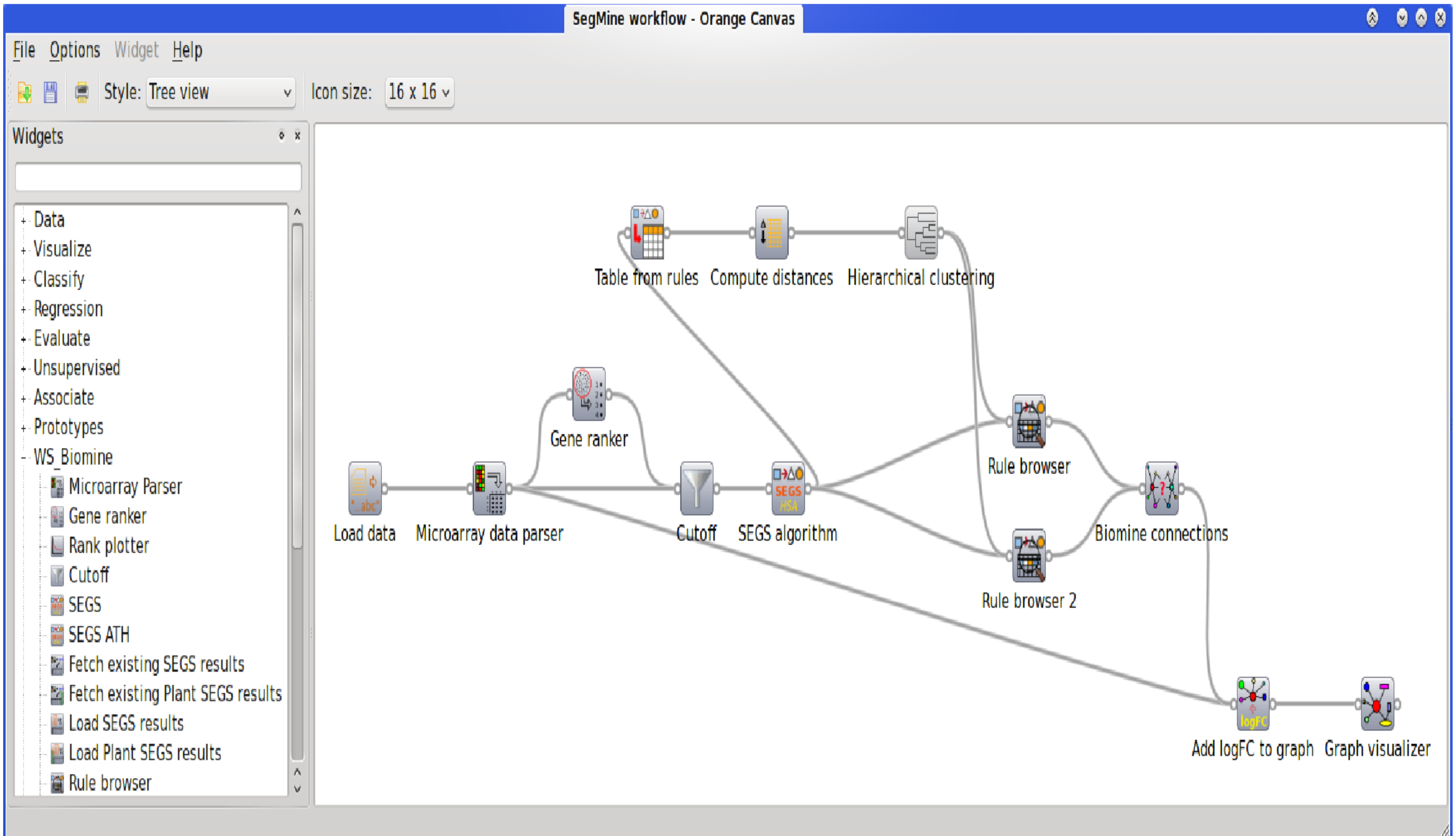
Exploratory
link discovery



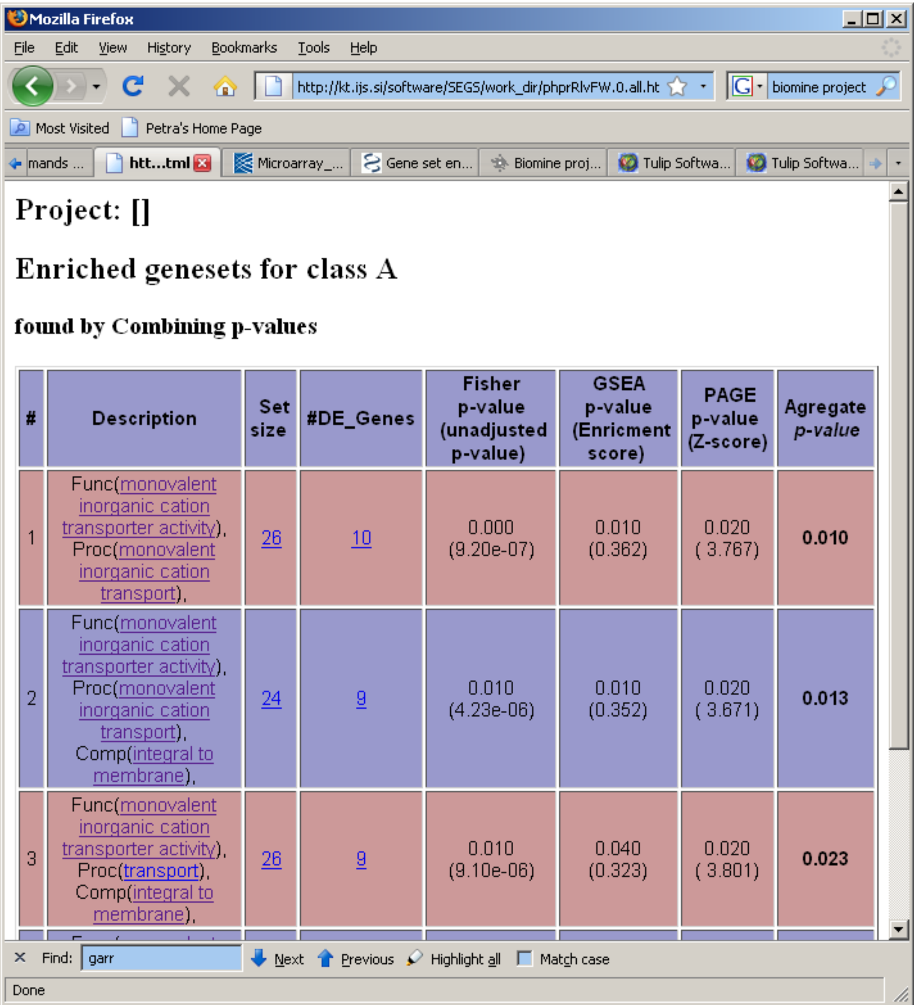
e.g. slow-vs-fast
cell growth

Work by
Lavrač et al. 2009, 2010
Podpečan et al. 2010

Semantic Data Mining in Orange4WS: SEGS + BioMine workflow implementation



SEGS output: BioMine query:

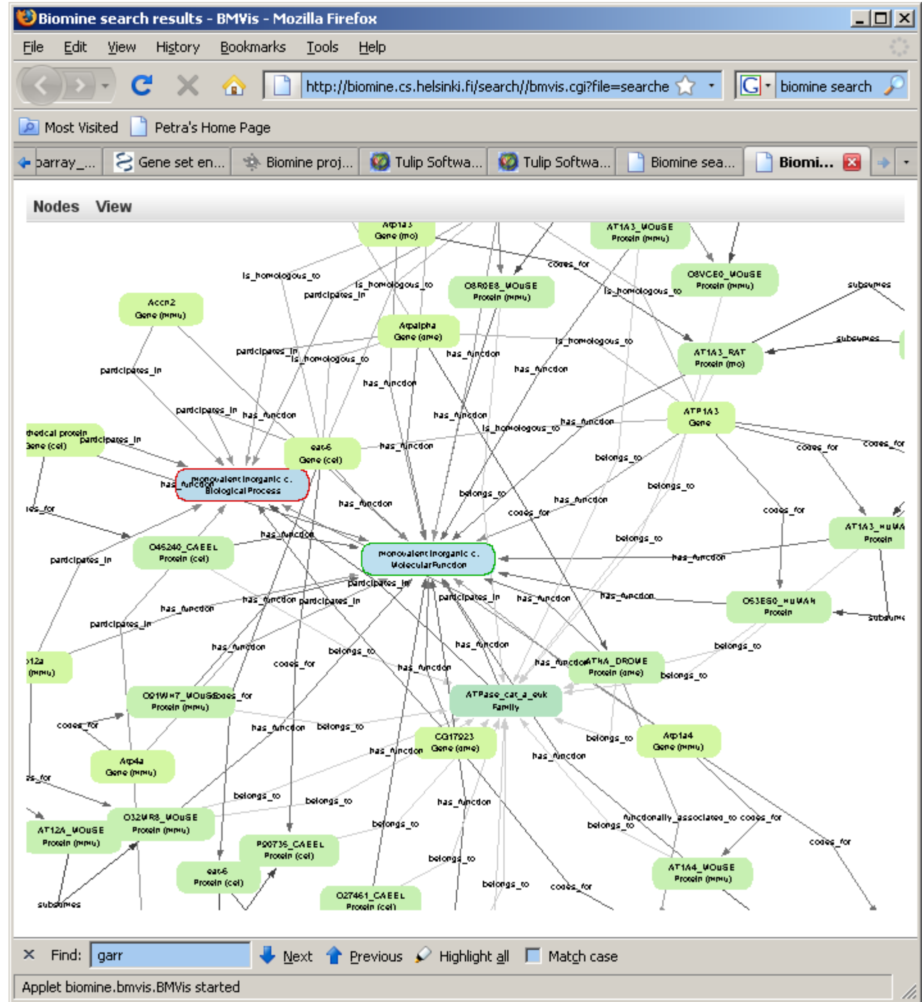


Project: []

Enriched genesets for class A

found by Combining p-values

#	Description	Set size	#DE_Genes	Fisher p-value (unadjusted p-value)	GSEA p-value (Enricment score)	PAGE p-value (Z-score)	Agregate *p-value*
1	Func(monovalent inorganic cation transporter activity), Proc(monovalent inorganic cation transport),	26	10	0.000 (9.20e-07)	0.010 (0.362)	0.020 (3.767)	**0.010**
2	Func(monovalent inorganic cation transporter activity), Proc(monovalent inorganic cation transport), Comp(integral to membrane),	24	9	0.010 (4.23e-06)	0.010 (0.352)	0.020 (3.671)	**0.013**
3	Func(monovalent inorganic cation transporter activity), Proc(transport), Comp(integral to membrane),	26	9	0.010 (9.10e-06)	0.040 (0.323)	0.020 (3.801)	**0.023**



Summary of SEGS + BioMine

- Semantic Data Mining algorithm SEGS discovers interesting gene group descriptions as conjunctions of concepts from three ontologies: GO, KEGG and Entrez
- Biomine finds cross-context links (paths) between concepts discovered by SEGS, using other ontologies, PubMed and other biomedical resources
- Initial results in stem cell microarray data analysis (EMBC 2009) indicate that the SEGS+Biomine methodology may lead to new insights – in vitro experiments are in progress at NIB to verify and validate the preliminary insights
- A general purpose Semantic Data Mining algorithm g-SEGS is also available in Orange4WS

Introductory seminar lecture: Summary

- **JSI & Knowledge Technologies**
- **Introduction to Data mining and KDD**
  - Data Mining and KDD process
  - DM standards, tools and visualization
  - Classification of Data Mining techniques: Predictive and descriptive DM
- **Selected data mining techniques: Advanced subgroup discovery techniques and applications**
- **Recent advances: Cross-context link discovery**

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

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

- 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 $p(C_j | v_i)$)

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

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

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

Naïve Bayesian classifier

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

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

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

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)

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

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

* log p denotes binary logarithm

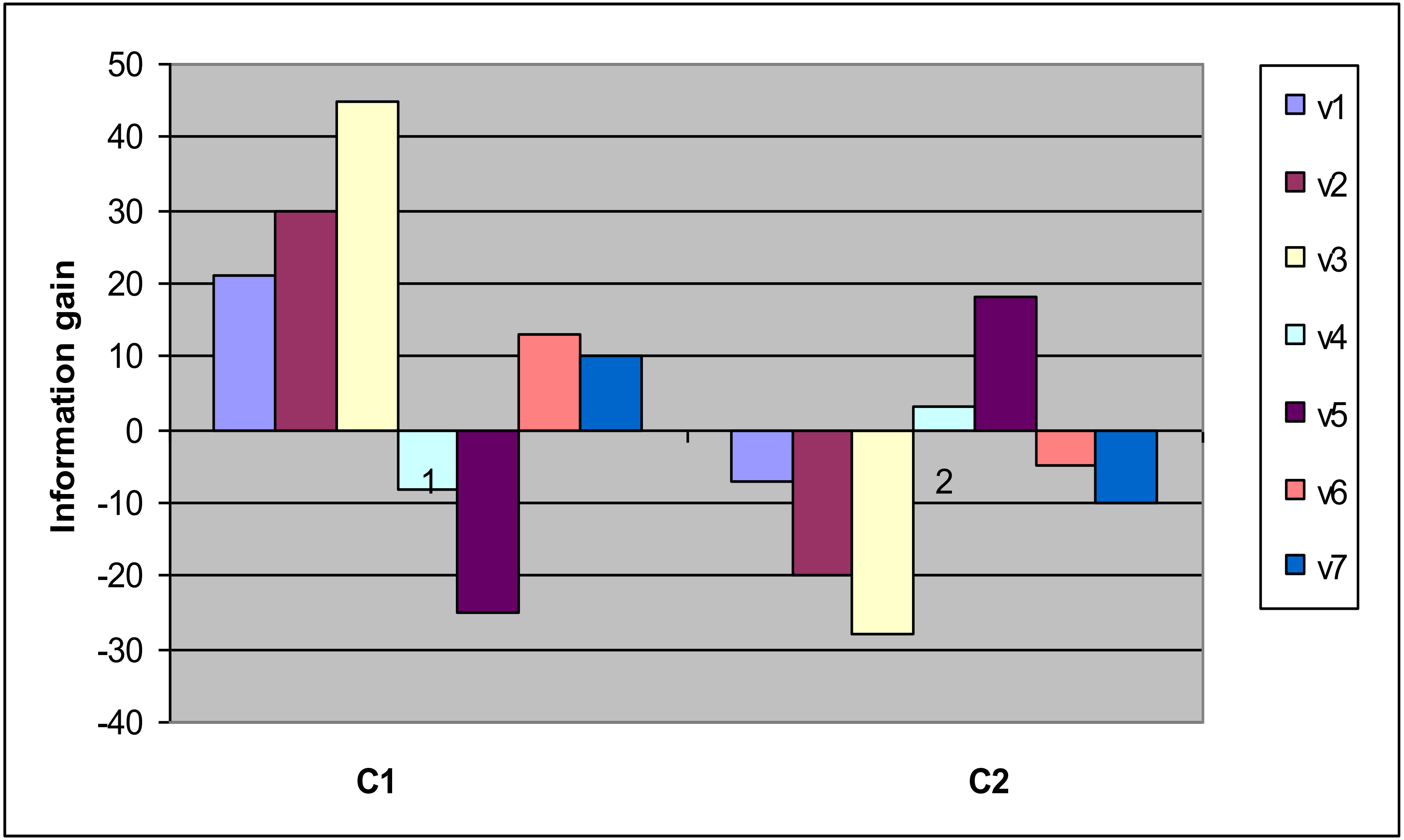
Example of explanation of semi-naïve Bayesian classifier

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		

Visualization of information gains for/against C_i



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, …

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%

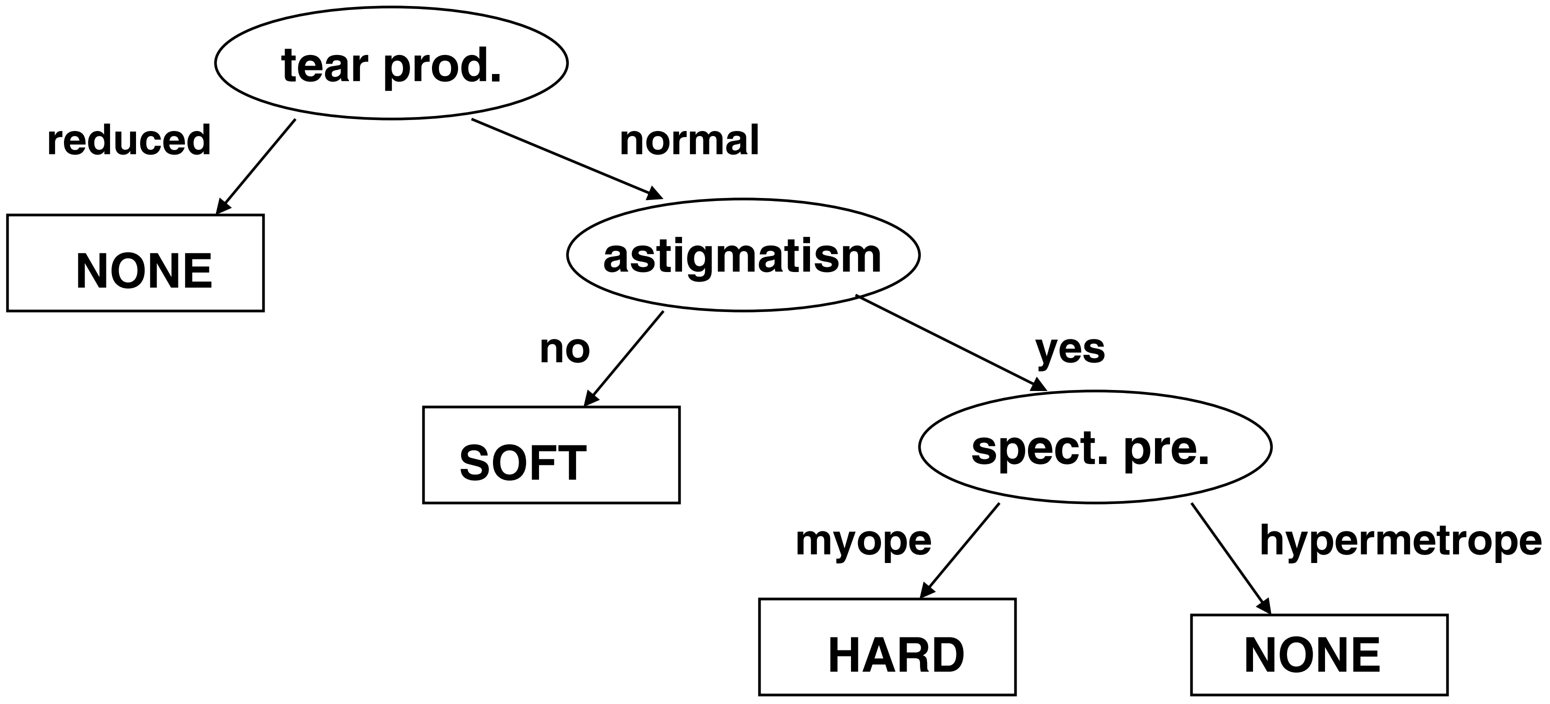
Part II. Predictive DM techniques

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

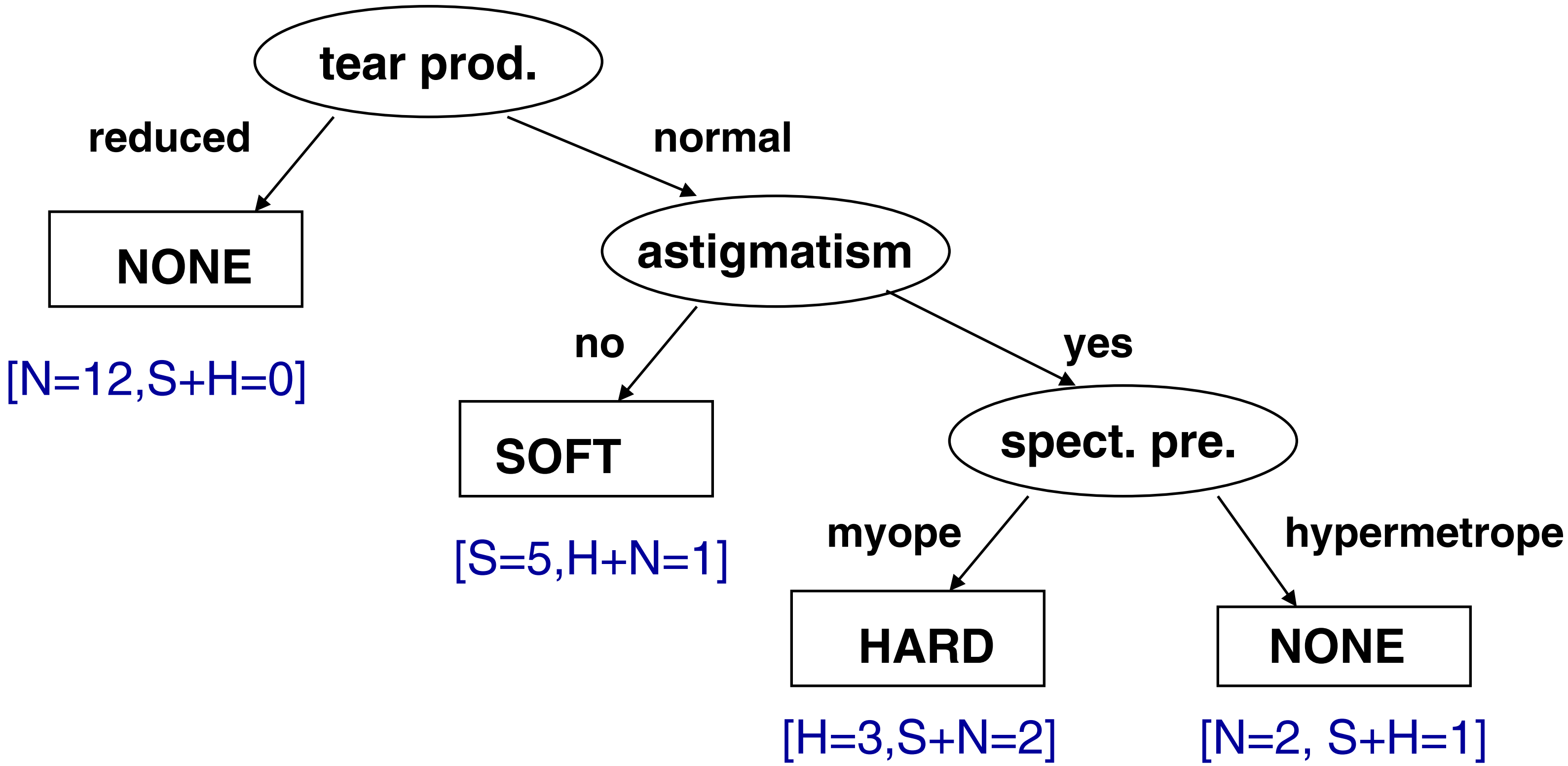
Illustrative example: Contact lenses data

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-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

Decision tree for contact lenses recommendation



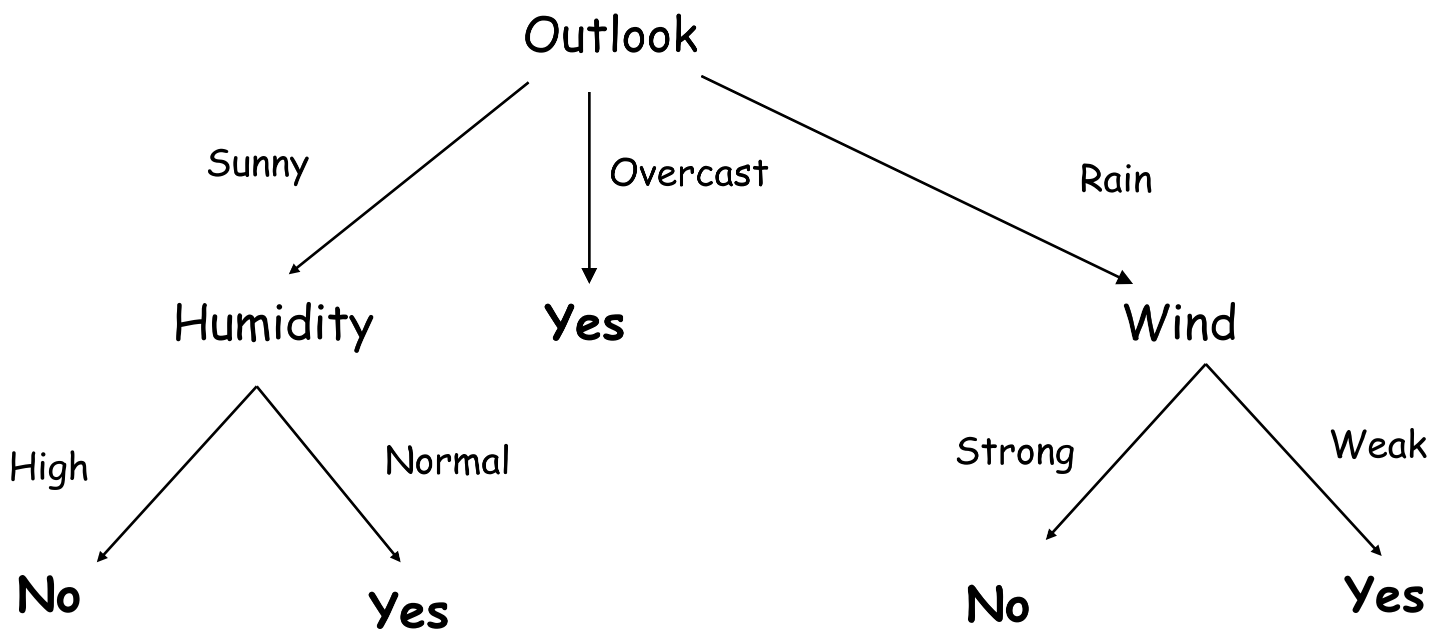
Decision tree for contact lenses recommendation



PlayTennis: Training examples

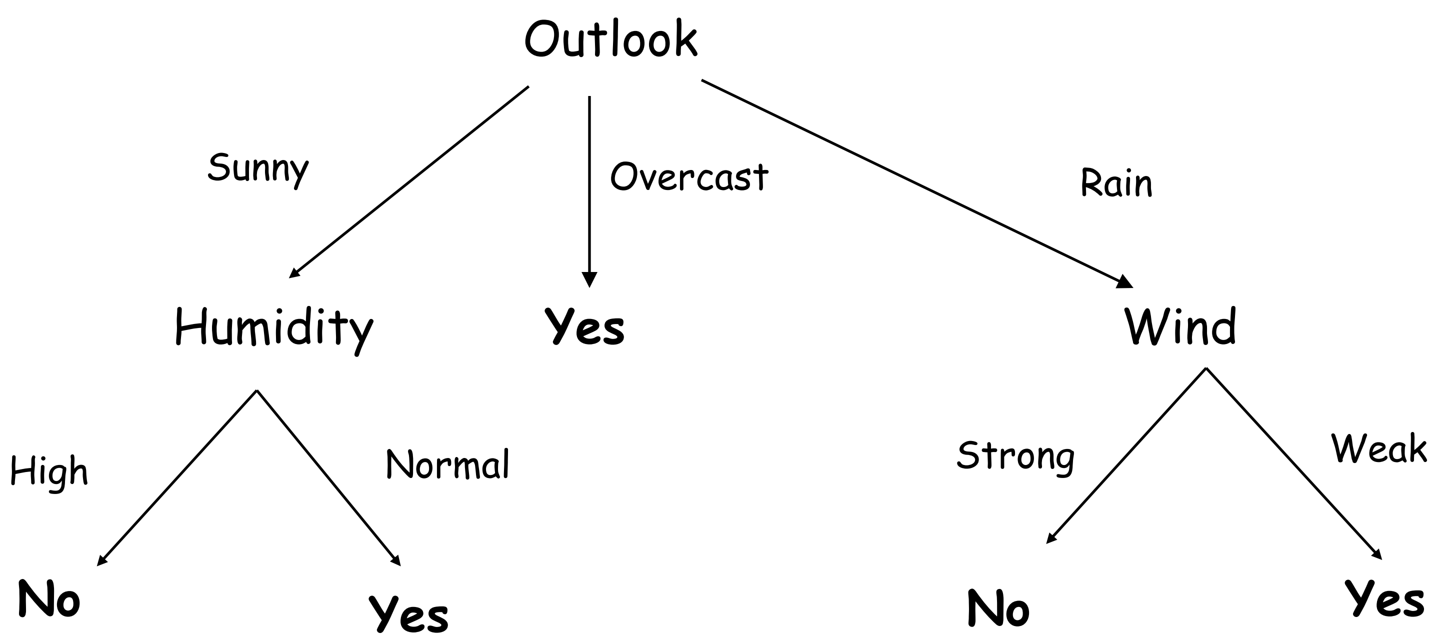
Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	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

Decision tree representation for PlayTennis



- 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 PlayTennis



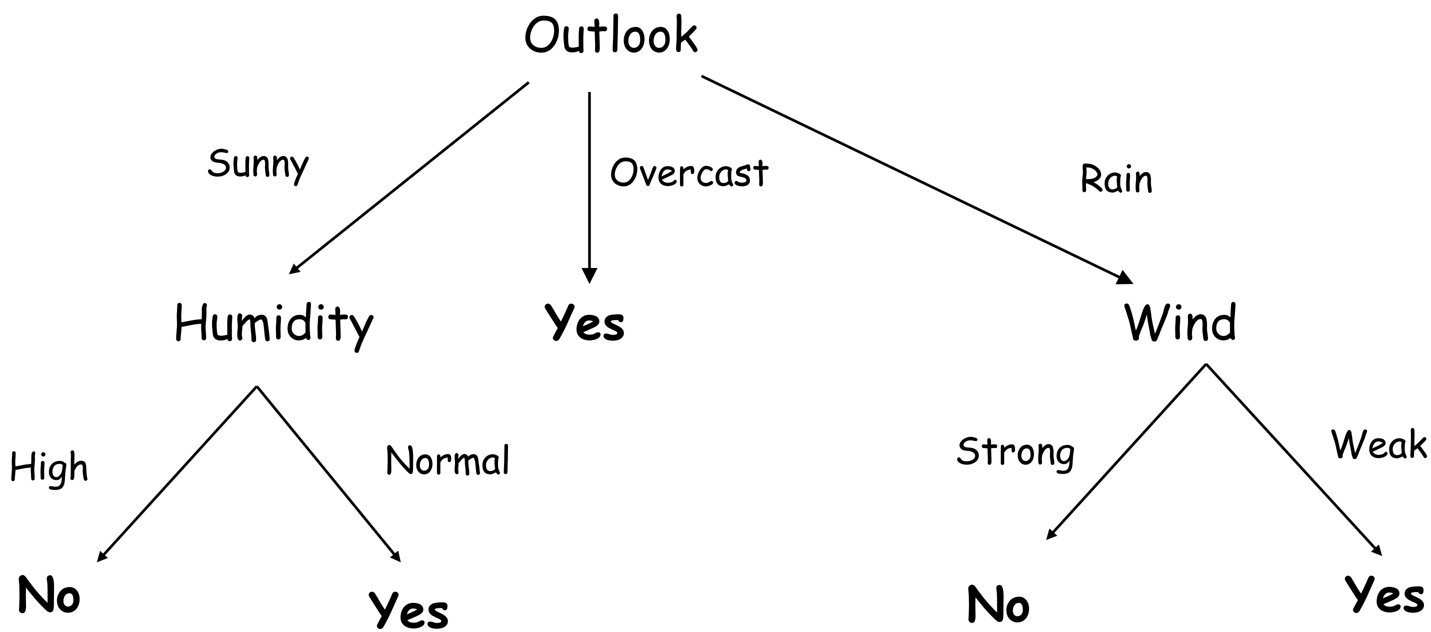
Decision trees represent a disjunction of conjunctions of constraints on the attribute values of instances

$$(\text{Outlook=Sunny} \wedge \text{Humidity=Normal}) \vee (\text{Outlook=Overcast}) \vee (\text{Outlook=Rain} \wedge \text{Wind=Weak})$$

PlayTennis: Other representations

- Logical expression for PlayTennis=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** PlayTennis=Yes
  - **IF** Outlook=Overcast **THEN** PlayTennis=Yes
  - **IF** Outlook=Rain $\wedge$ Wind=Weak **THEN** PlayTennis=Yes
  - **IF** Outlook=Sunny $\wedge$ Humidity=High **THEN** PlayTennis=No
  - **IF** Outlook=Rain $\wedge$ Wind=Strong **THEN** PlayTennis=No

PlayTennis: Using a decision tree for classification



Is Saturday morning OK for playing tennis?

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

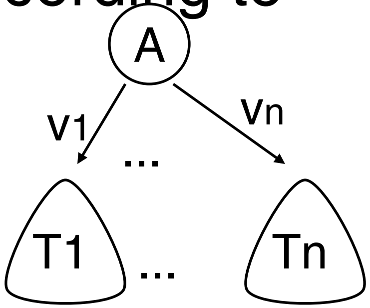
PlayTennis = No, because Outlook=Sunny $\wedge$ Humidity=High

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

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

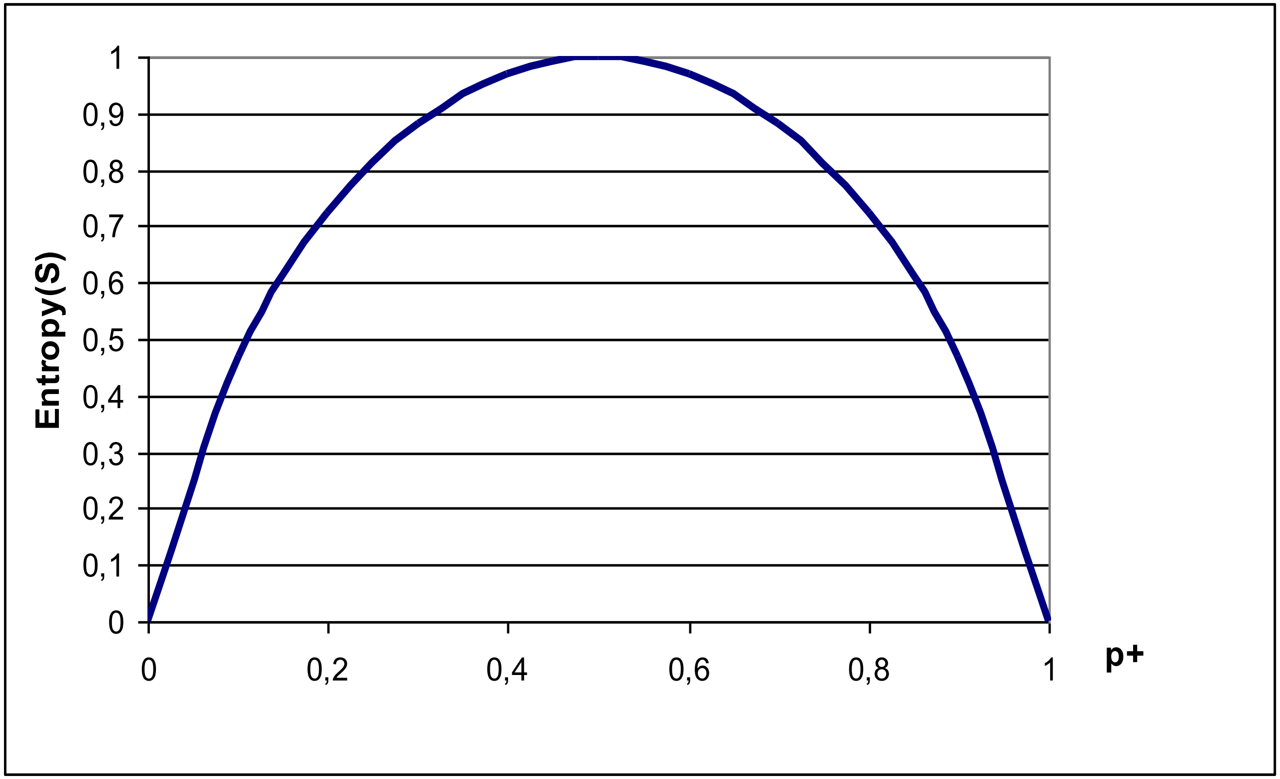
$\mathbf{p_c}$ - prior probability of class $\mathbf{C_c}$
(relative frequency of $\mathbf{C_c}$ in **S**)

- 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 $\mathbf{p_+}$ 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:

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

PlayTennis: 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

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

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

$= 0.940$

PlayTennis: 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**

Outlook? $\xrightarrow{\text{Sunny}}$ {D1,D2,D8,D9,D11} [2+, 3-] E=0.970

Outlook? $\xrightarrow{\text{Overcast}}$ {D3,D7,D12,D13} [4+, 0-] E=0

Outlook? $\xrightarrow{\text{Rain}}$ {D4,D5,D6,D10,D14} [3+, 2-] E=0.970

Humidity? $\xrightarrow{\text{High}}$ [3+, 4-] E=0.985

Humidity? $\xrightarrow{\text{Normal}}$ [6+, 1-] E=0.592

Wind? $\xrightarrow{\text{Weak}}$ [6+, 2-] E=0.811

Wind? $\xrightarrow{\text{Strong}}$ [3+, 3-] E=1.00

Information gain search heuristic

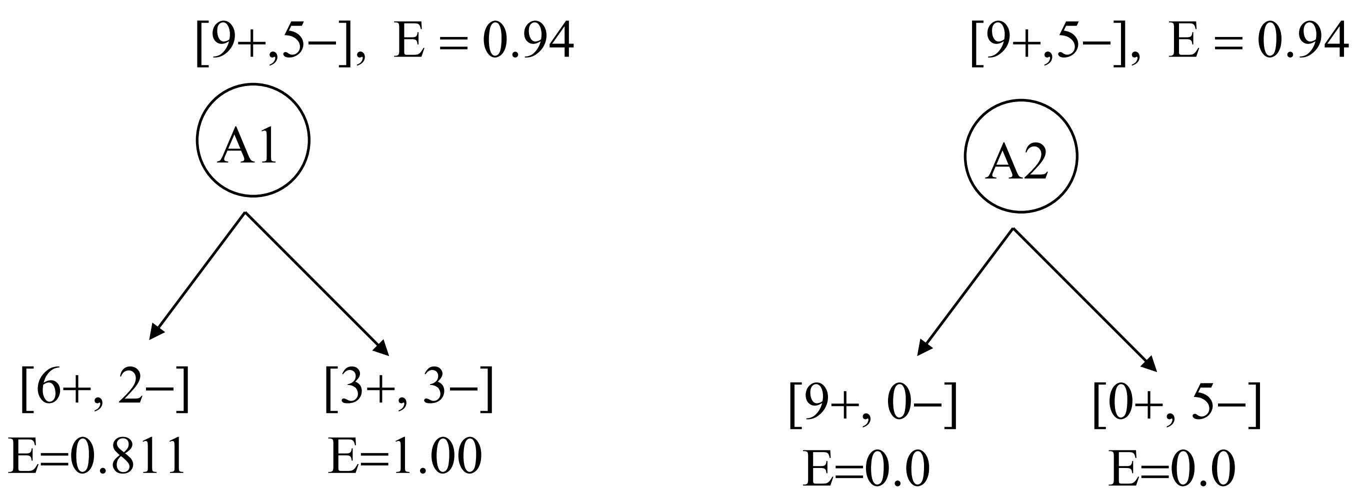
- **Information gain** measure is aimed to minimize the number of tests needed for the classification of a new object
- **Gain(S,A)** – expected reduction in entropy of S due to sorting on A

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

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

Information gain search heuristic

- Which attribute is more informative, A1 or A2 ?

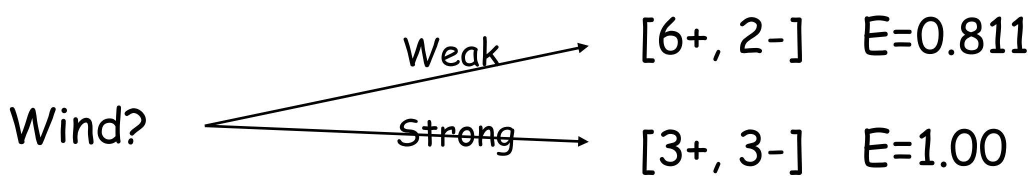


- Gain(S,A1) = 0.94 – (8/14 x 0.811 + 6/14 x 1.00) = 0.048
- Gain(S,A2) = 0.94 – 0 = 0.94 A2 has max Gain

PlayTennis: Information gain

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

- Values(Wind) = {Weak, Strong}

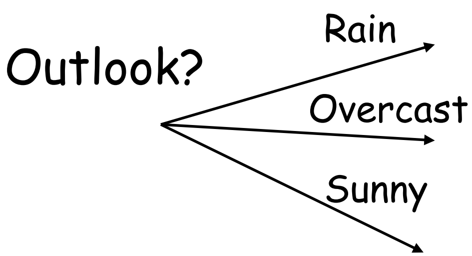


  - S = [9+,5-], E(S) = 0.940
  - S_{weak} = [6+,2-], $E(S_{weak})$ = 0.811
  - S_{strong} = [3+,3-], $E(S_{strong})$ = 1.0
  - **Gain(S,Wind) =** E(S) - (8/14)$E(S_{weak})$ - (6/14)$E(S_{strong})$ = 0.940 - (8/14)x0.811 - (6/14)x1.0=**0.048**

PlayTennis: 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

PlayTennis: Information gain



{D4,D5,D6,D10,D14} [3+, 2-] E > 0 **???**

{D3,D7,D12,D13} [4+, 0-] E = 0 **OK - assign class Yes**

{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

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

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

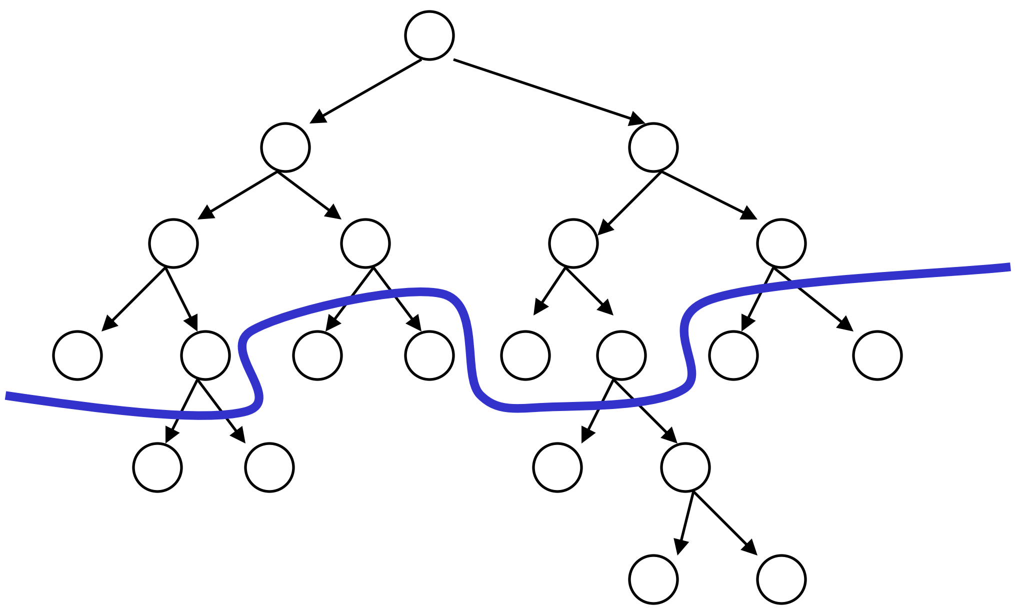
[2+,0-] (2) = 2+1 / 2+2 = 3/4

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

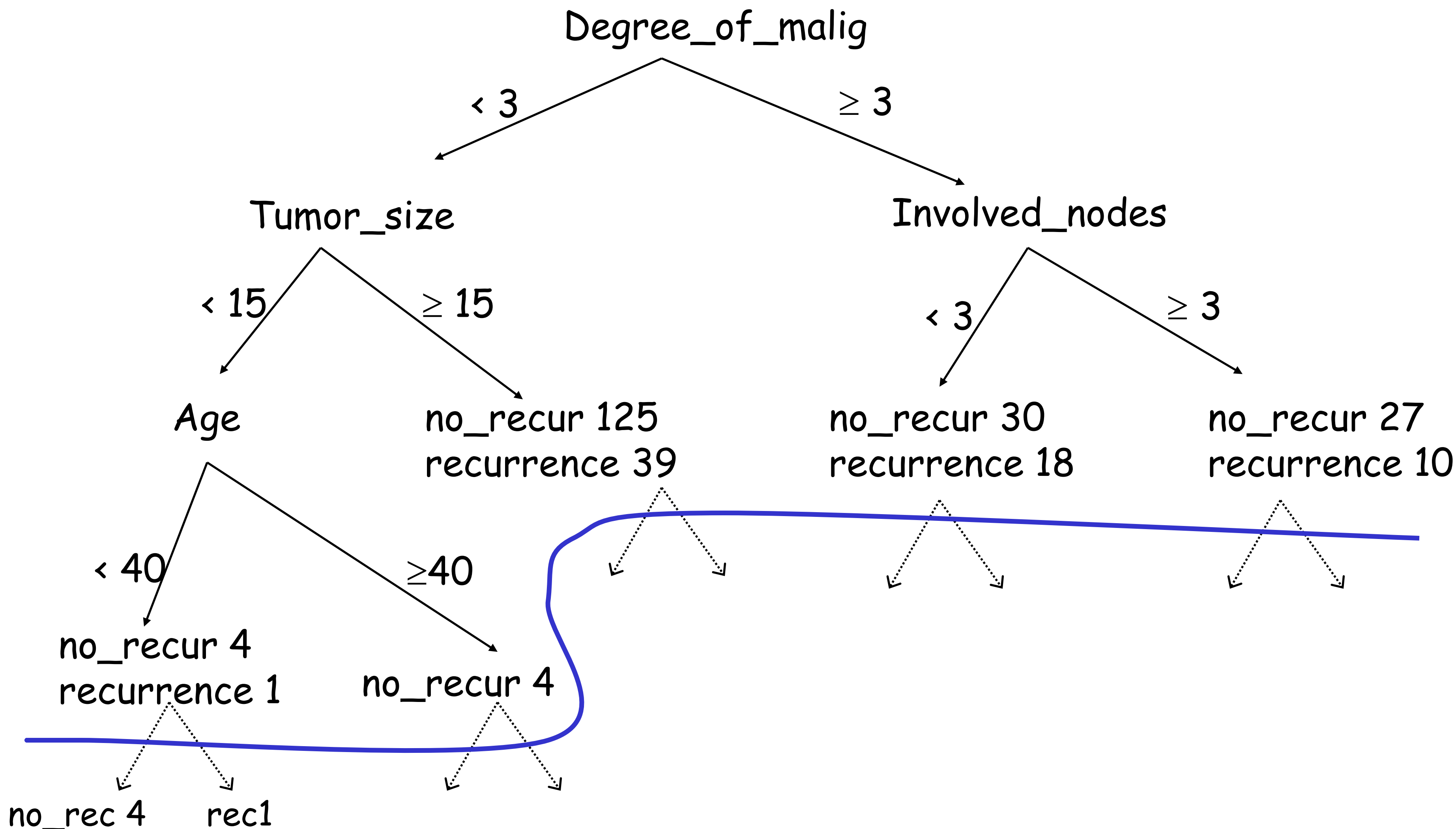
Sources of imperfection

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

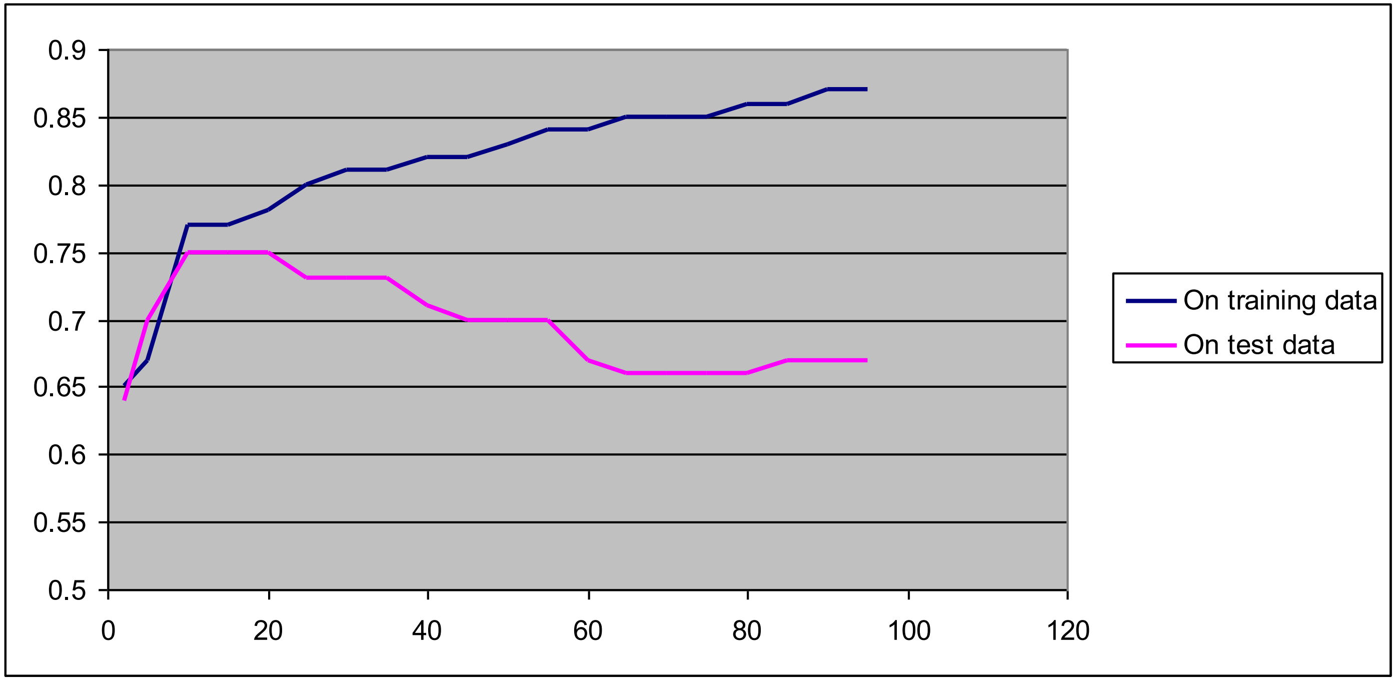


Accuracy and error

- 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

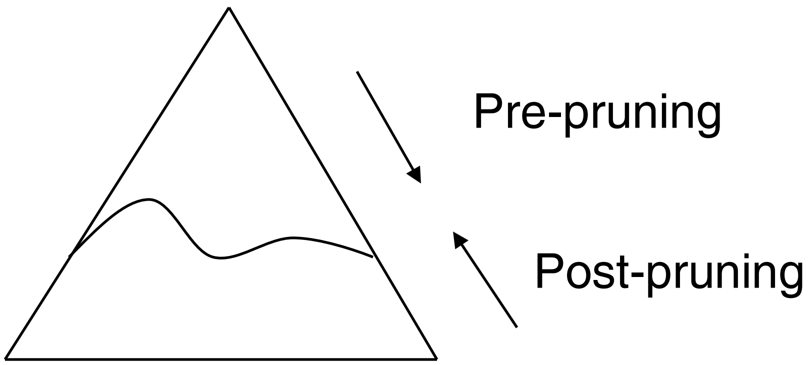
- Typical relation between tree size and accuracy



- 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))

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)

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

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

Part II. Predictive DM techniques

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

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-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

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

Rule set representation

- Rule base is a disjunctive set of conjunctive rules
- Standard form of rules:

  IF Condition THEN Class

  Class IF Conditions

  Class $\leftarrow$ Conditions

IF Outlook=Sunny $\wedge$ Humidity=Normal **THEN** PlayTennis=Yes
IF Outlook=Overcast **THEN** PlayTennis=Yes
IF Outlook=Rain $\wedge$ Wind=Weak **THEN** PlayTennis=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	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: Classification rules

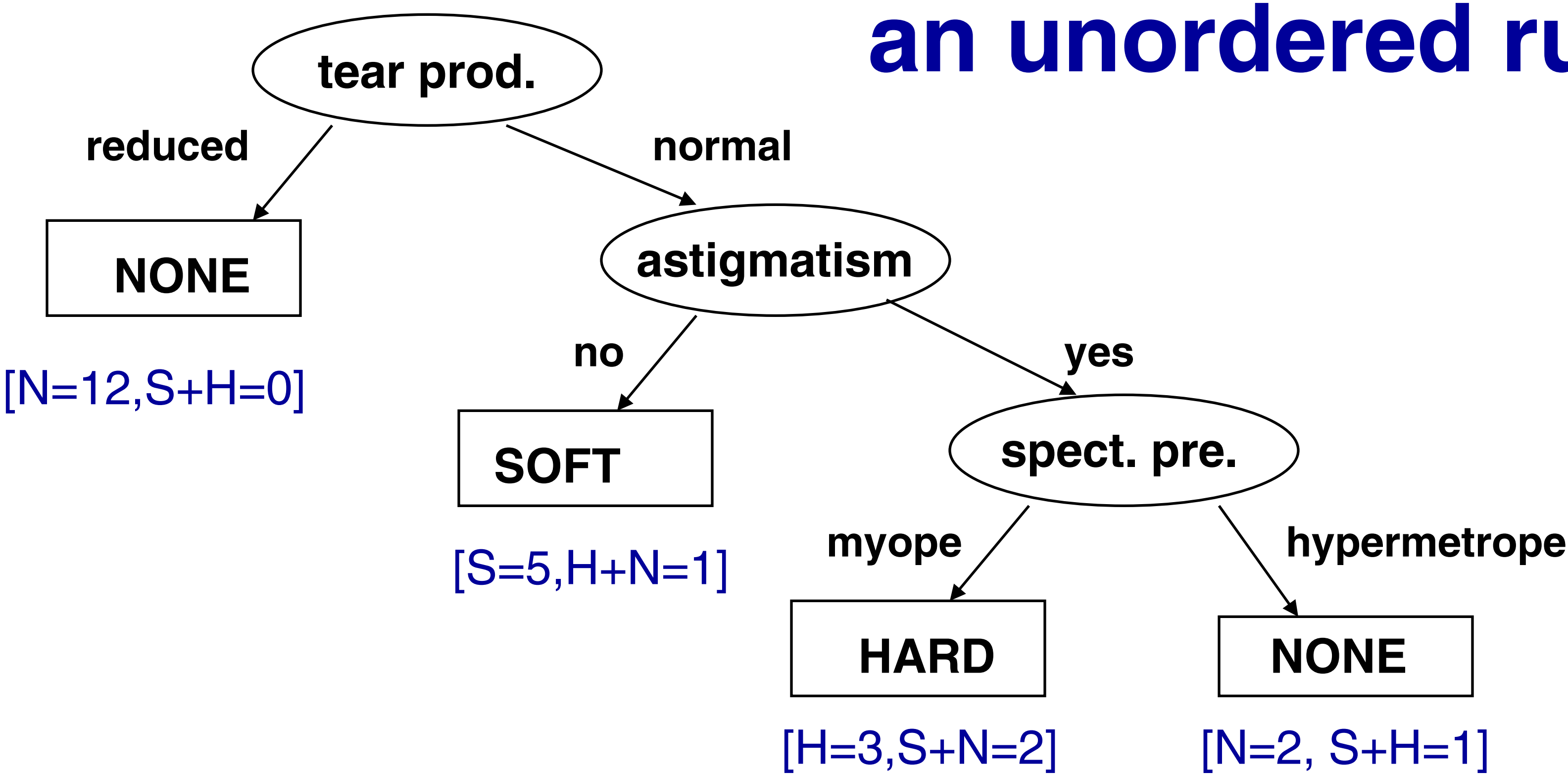
Type of task: prediction and classification
Hypothesis language: rules X ➔ C, if X then C
X conjunction of attribute values, C class

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

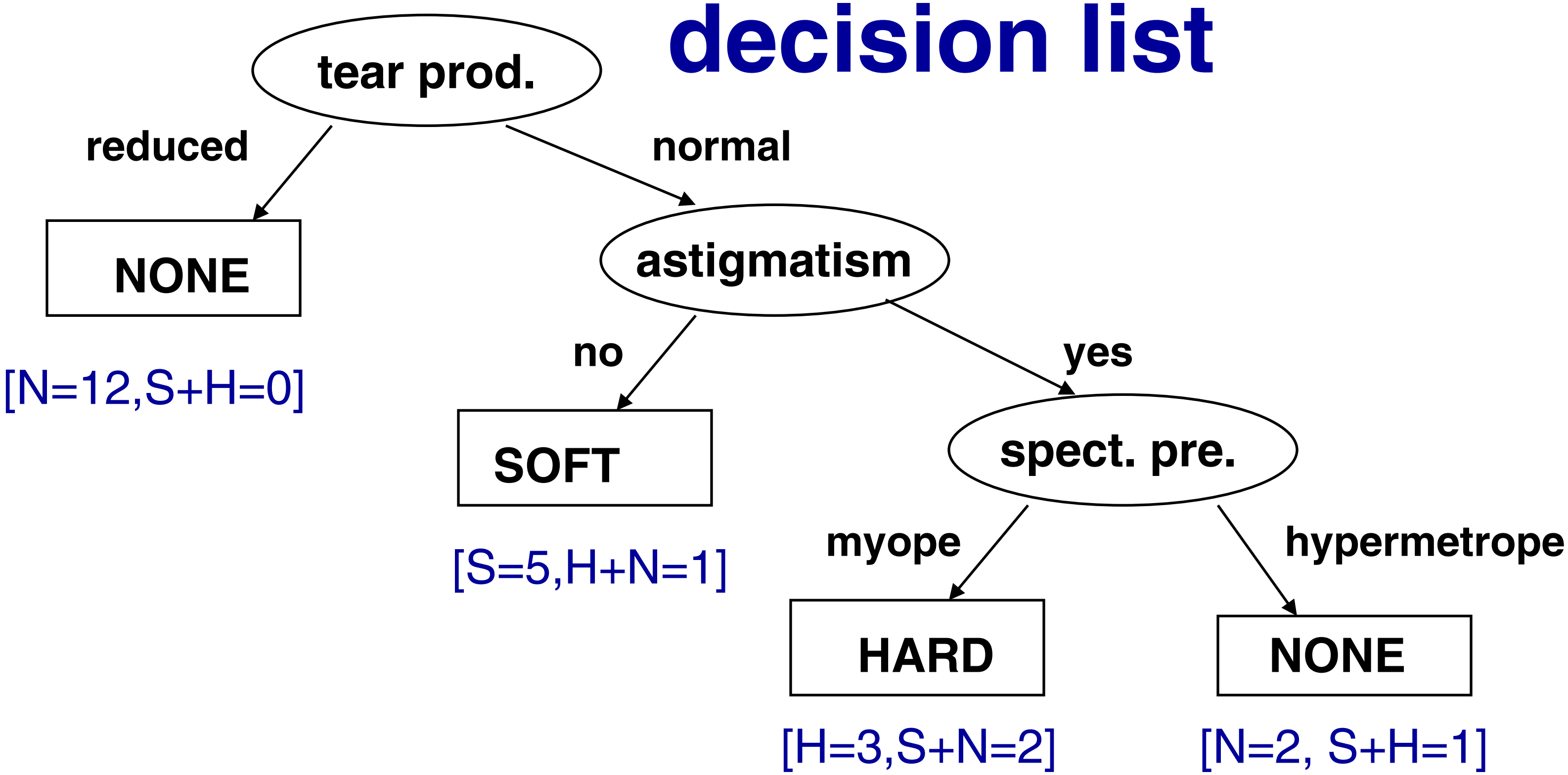
Contact lenses: convert decision tree to an unordered rule set



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

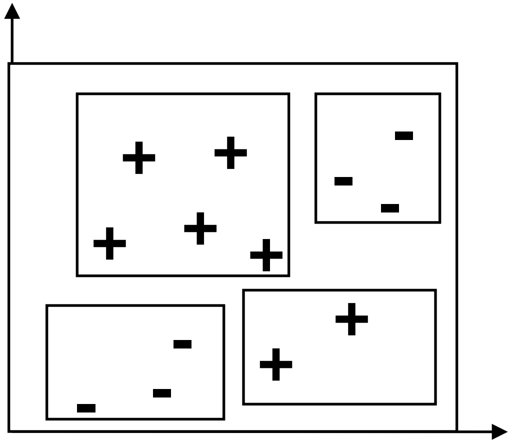
Converting decision tree to rules, and rule post-pruning (Quinlan 1993)

- 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-presbyo	hypermetrope	no	normal	YES
O15	pre-presbyo	hypermetrope	yes	reduced	NO
O16	pre-presbyo	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)

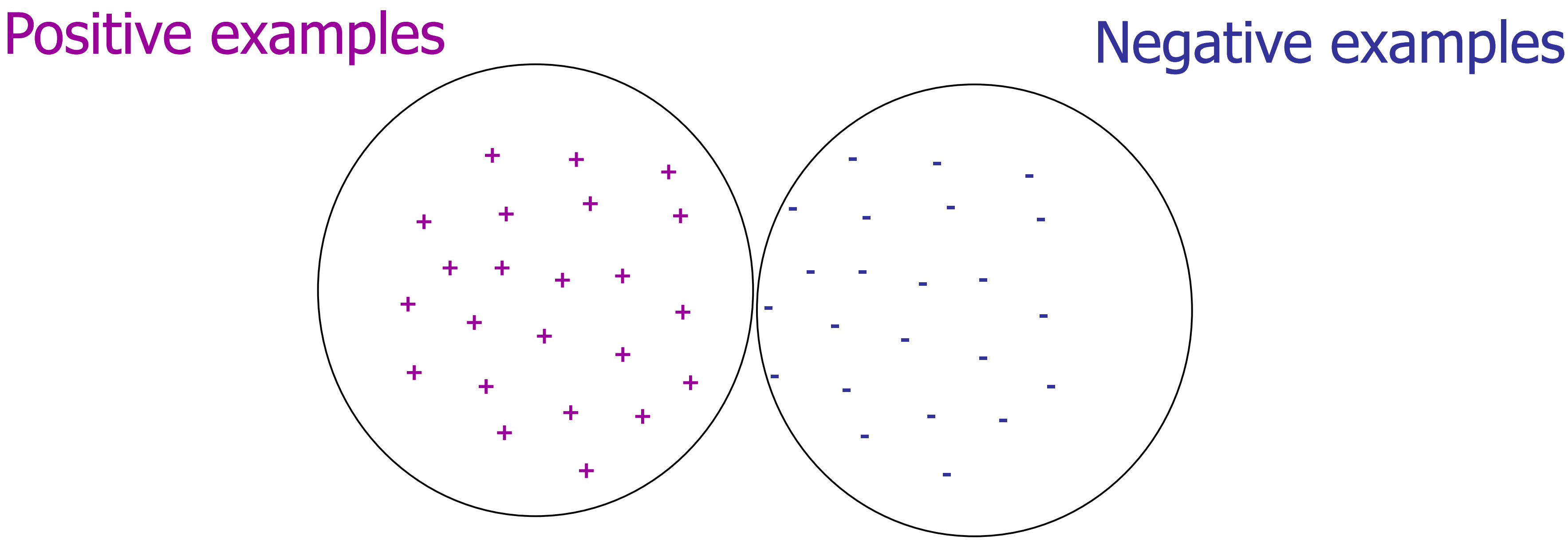


Given examples of N classes C_1, …, C_N

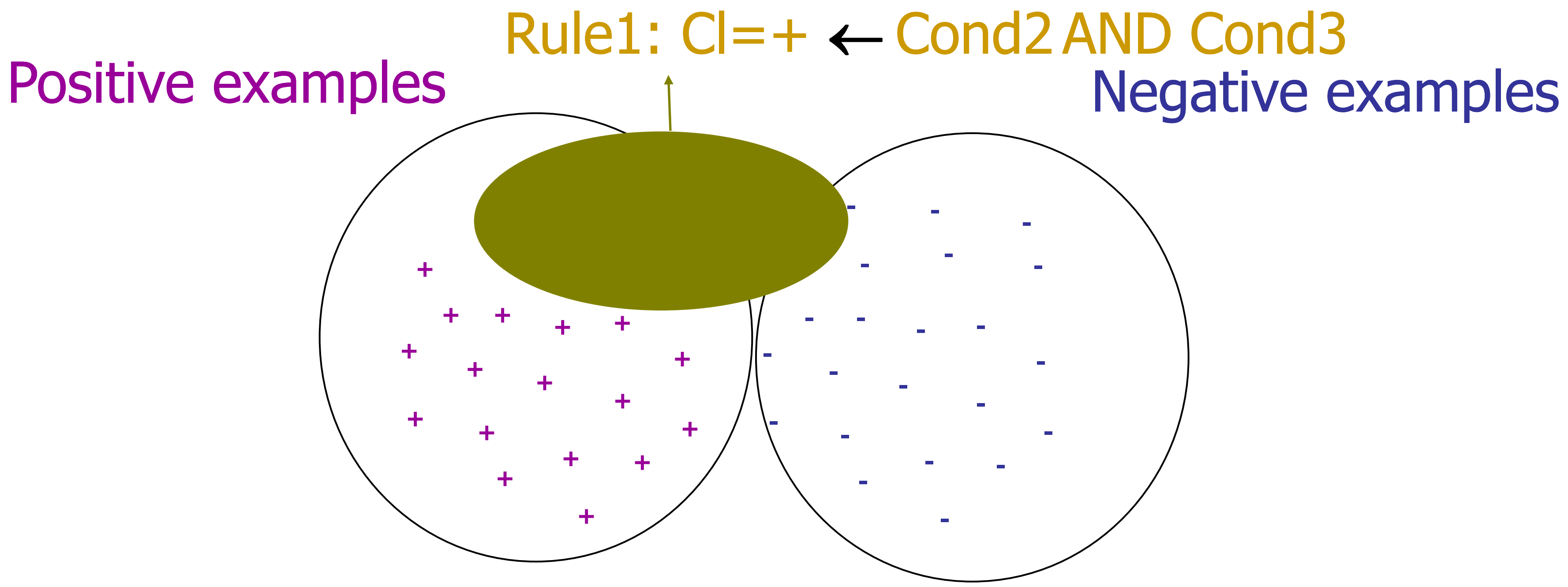
for each class Ci **do**

- 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

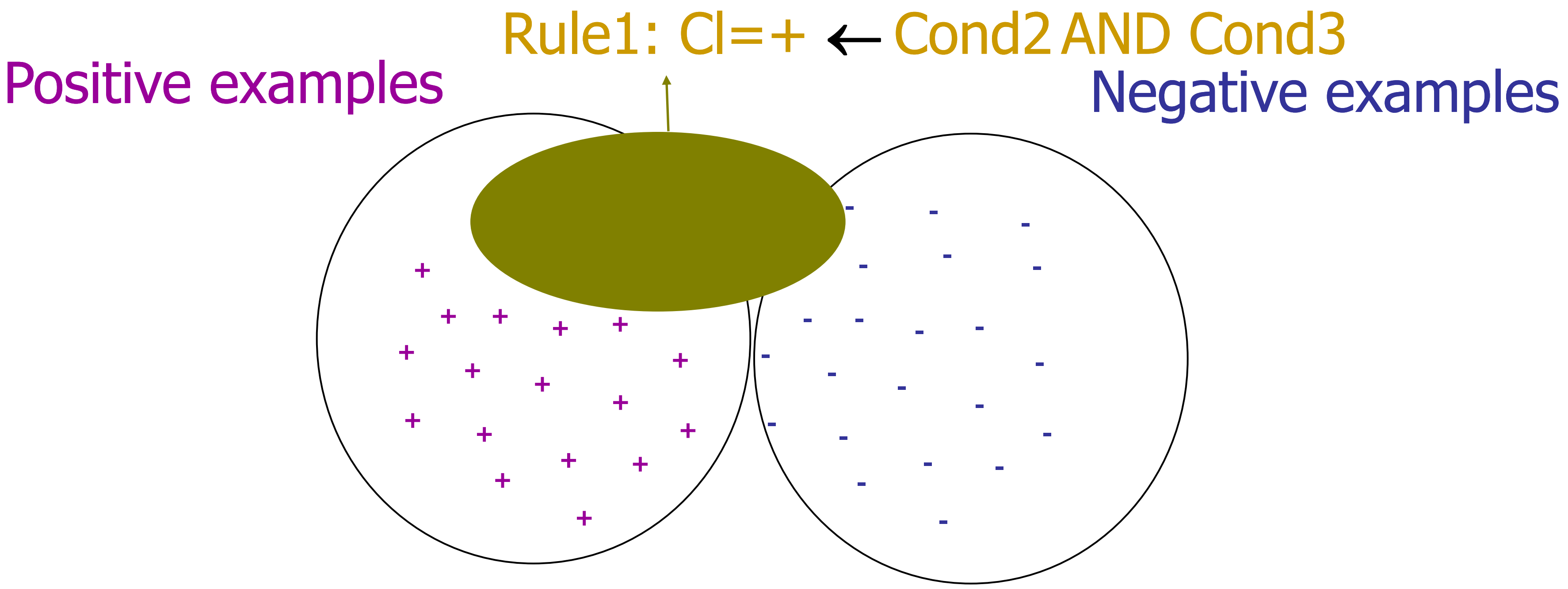
Covering algorithm



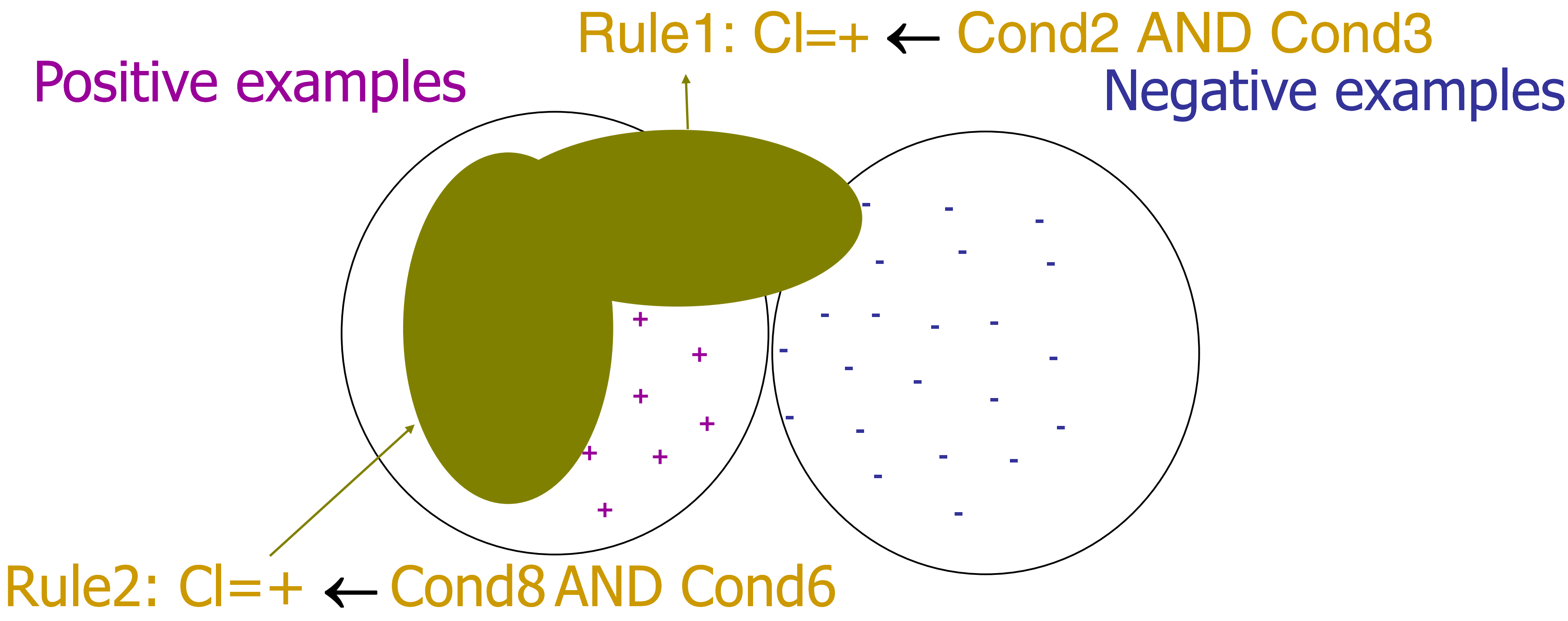
Covering algorithm



Covering algorithm



Covering algorithm



PlayTennis: 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: PlayTennis example

PlayTennis = yes [9+,5-] (14)

PlayTennis = yes $\leftarrow$ Wind=weak [6+,2-] (8)
$\leftarrow$ Wind=strong [3+,3-] (6)
$\leftarrow$ Humidity=normal [6+,1-] (7)
$\leftarrow$ …

PlayTennis = yes $\leftarrow$ Humidity=normal
Outlook=sunny [2+,0-] (2)
$\leftarrow$ …

Estimating **rule accuracy (rule precision)** with the **probability** that a covered example is positive

A(Class $\leftarrow$ 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

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

[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 $\leftarrow$ Cond from the RuleBase.
- Specializarion R' of rule R = Cl $\leftarrow$ Cond

  has the form R' = Cl $\leftarrow$ 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

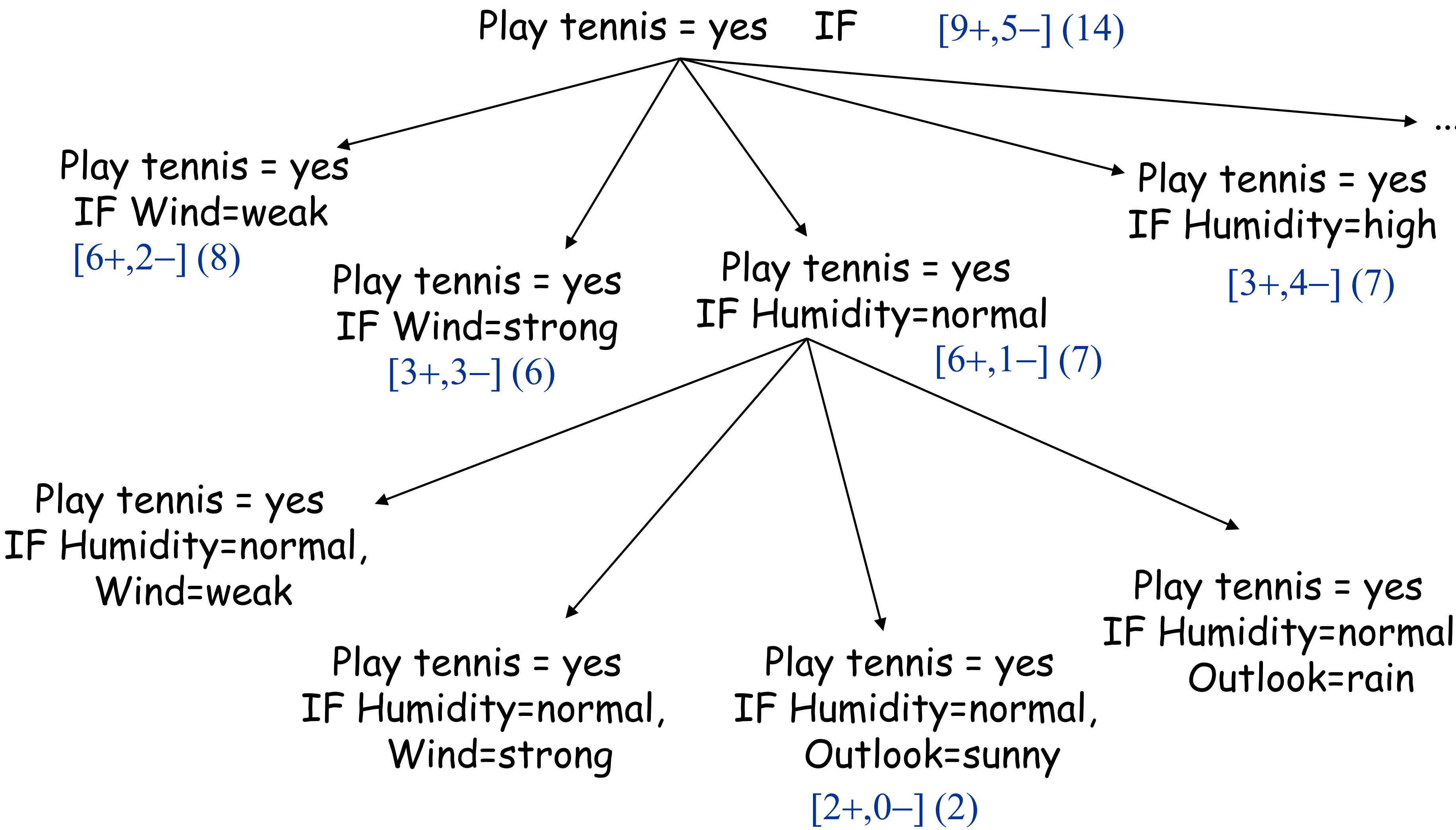
- learn-one-rule by greedy general-to-specific search, at each step selecting the `best' descendant, no backtracking
  - e.g., the best descendant of the initial rule

    PlayTennis = yes ←
  - is rule PlayTennis = 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: PlayTennis example

- Play tennis = yes IF
  - Play tennis = yes IF Wind=weak
  - Play tennis = yes IF Wind=strong
  - Play tennis = yes IF Humidity=normal
    - Play tennis = yes IF Humidity=normal, Wind=weak
    - Play tennis = yes IF Humidity=normal, Wind=strong
    - Play tennis = yes IF Humidity=normal, Outlook=sunny
    - Play tennis = yes IF Humidity=normal, Outlook=rain
  - Play tennis = yes IF Humidity=high
  - ...

Learn-one-rule as heuristic search: PlayTennis example



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**
  - RAcc(Cl ←Cond) = p(Cl | Cond) – p(Cl)

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

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))

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})

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

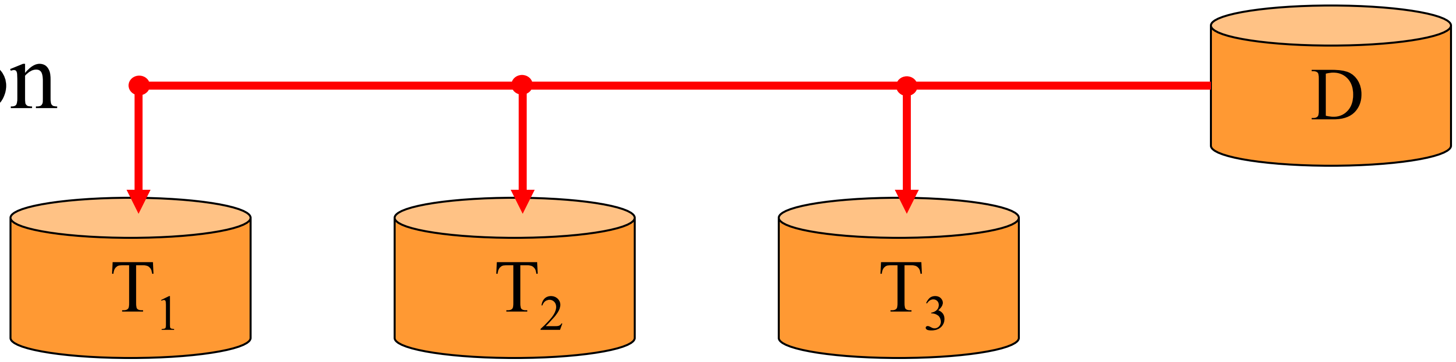
Evaluating hypotheses

- **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

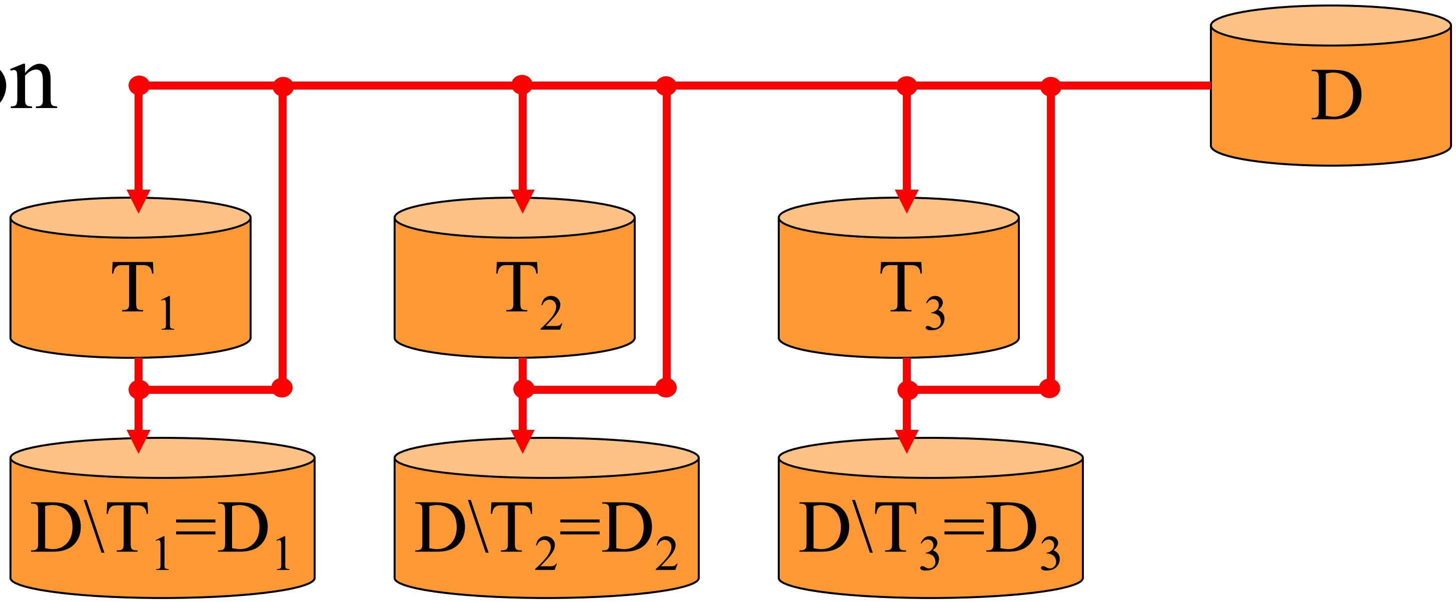
n-fold cross validation

- 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 = $D \backslash T_i$
  - 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

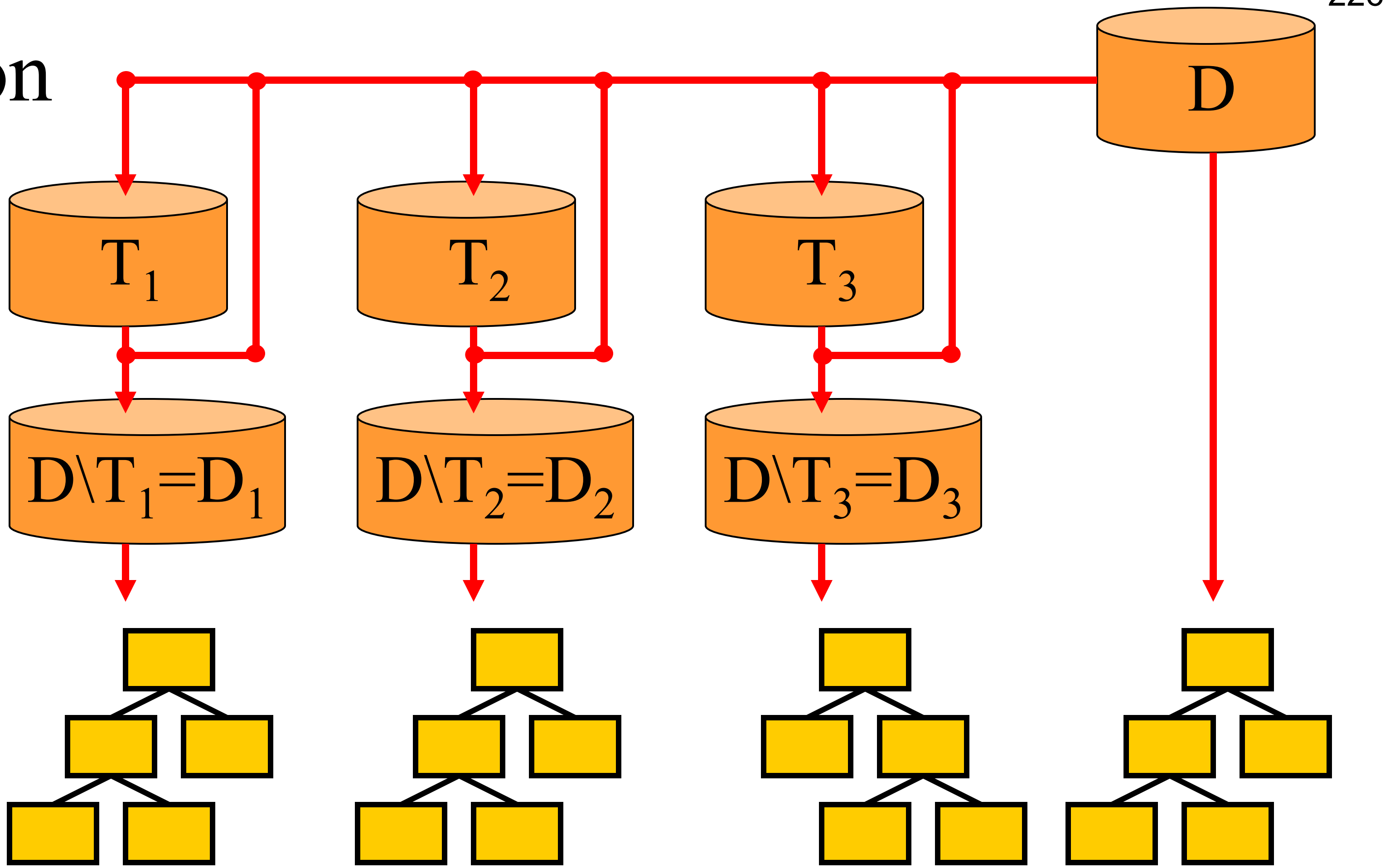
- Partition



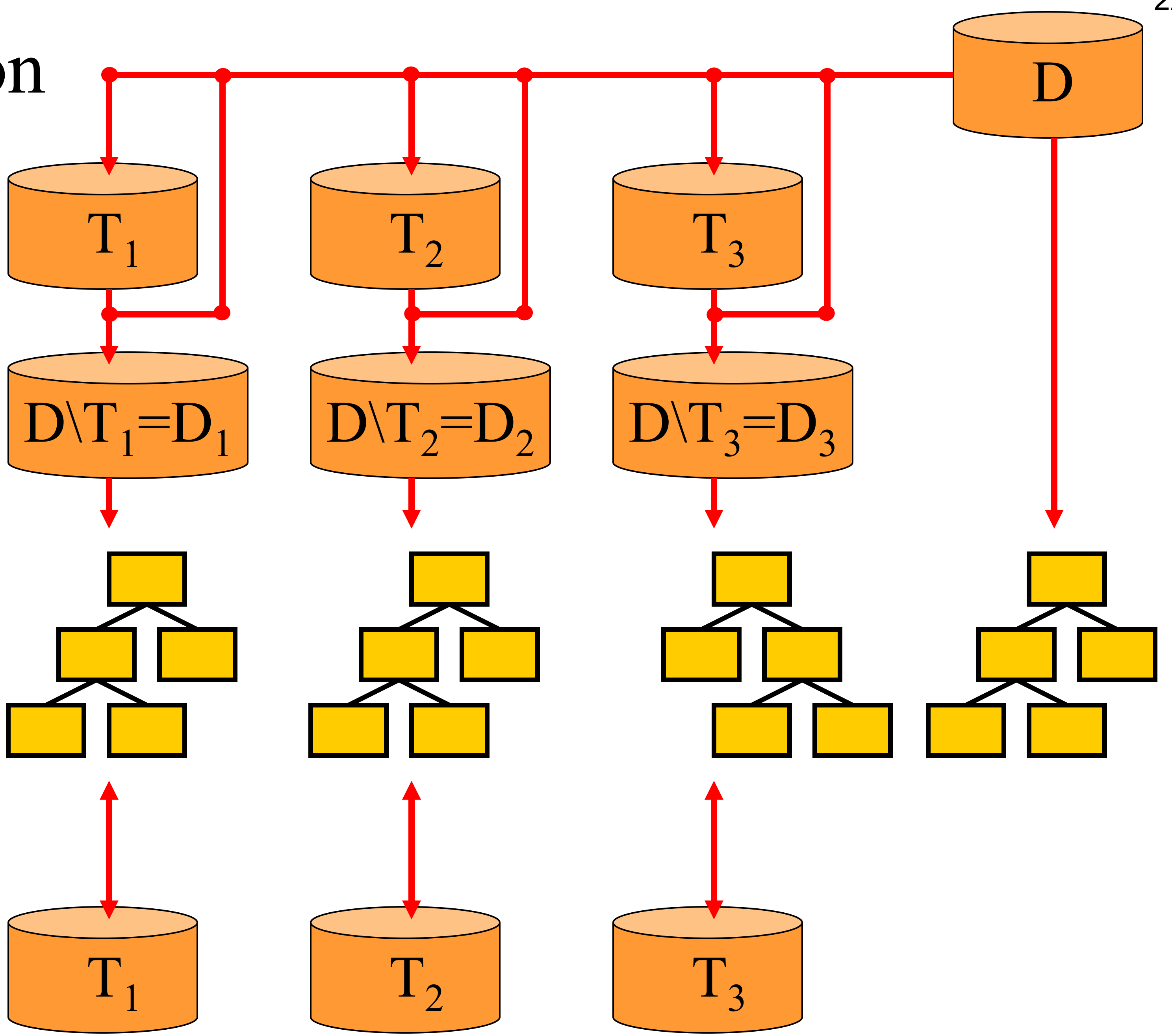
- Partition
- Train



- Partition
- Train



- Partition
- Train
- Test



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

	Predicted positive	Predicted negative	
Positive examples	**True positives**	**False negatives**	
Negative examples	**False positives**	**True negatives**	

- 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

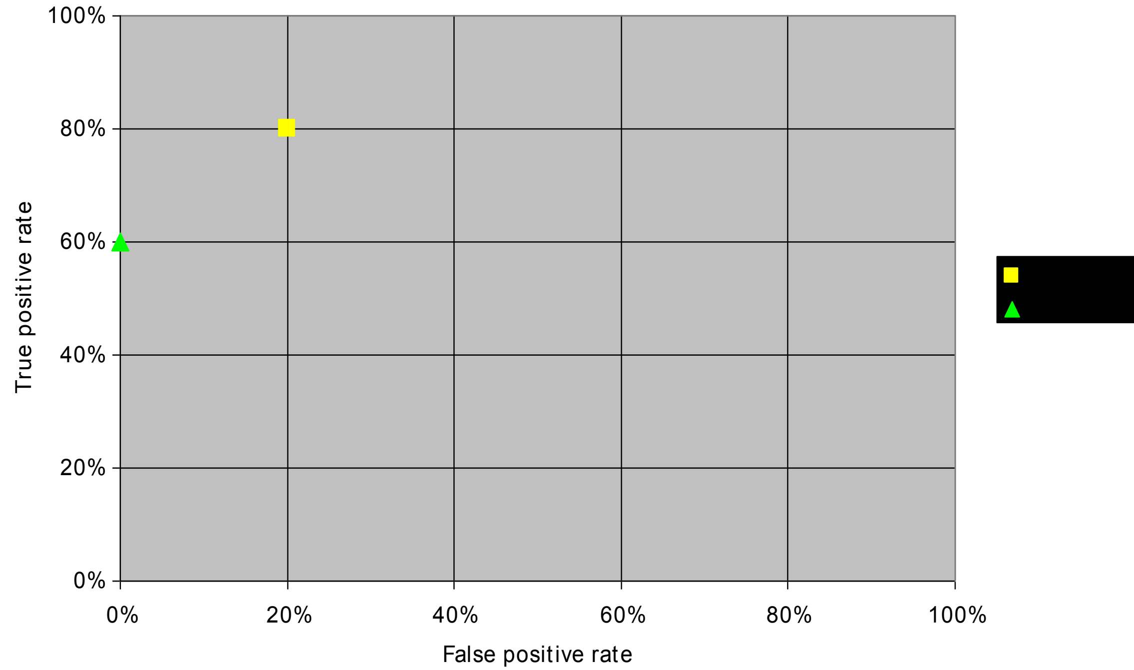
- ***True positive rate*** = #true pos. / #pos.
  - $TPr_1 = 40/50 = 80\%$
  - $TPr_2 = 30/50 = 60\%$
- ***False positive rate*** = #false pos. / #neg.
  - $FPr_1 = 10/50 = 20\%$
  - $FPr_2 = 0/50 = 0\%$
- ***ROC space*** has
  - FPr on X axis
  - TPr on Y axis

Classifier 1

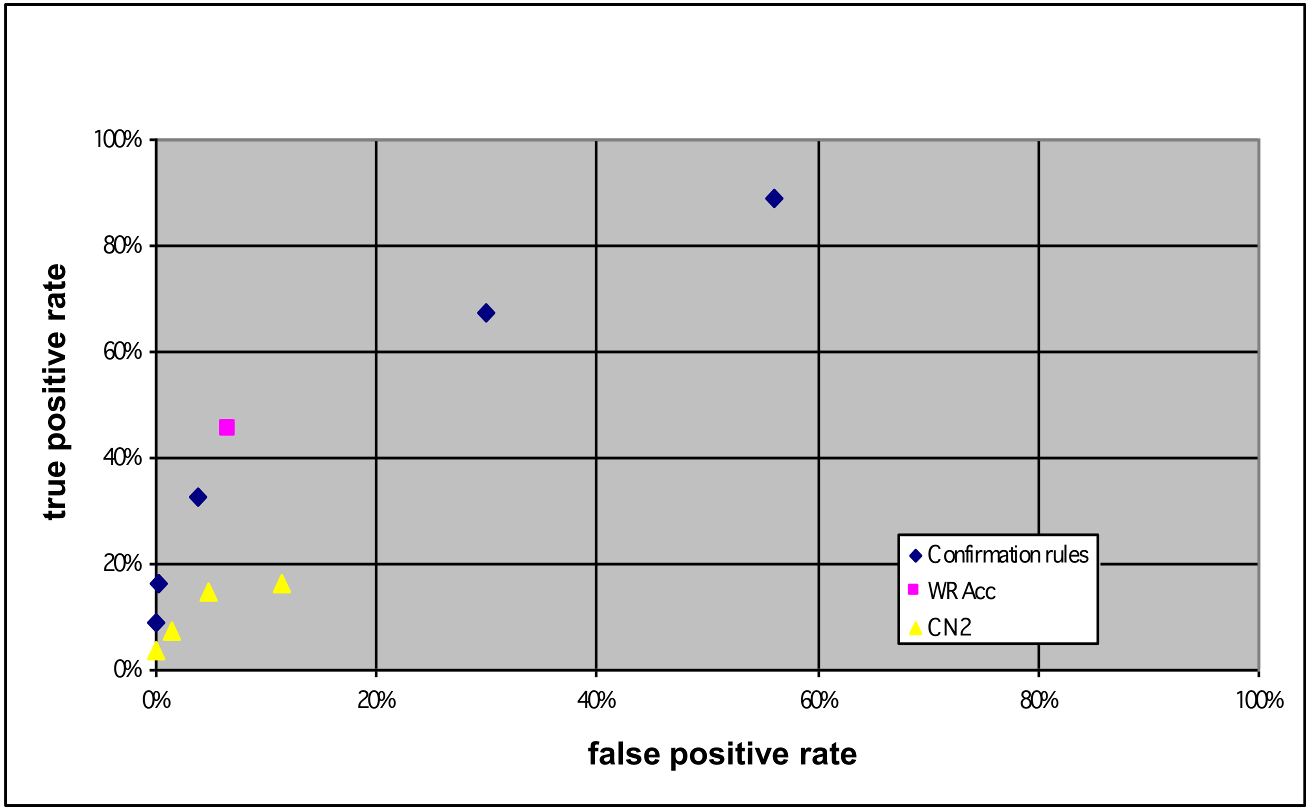
	Predicted positive	Predicted negative	
Positive examples	**40**	**10**	50
Negative examples	**10**	**40**	50
	50	50	100

Classifier 2

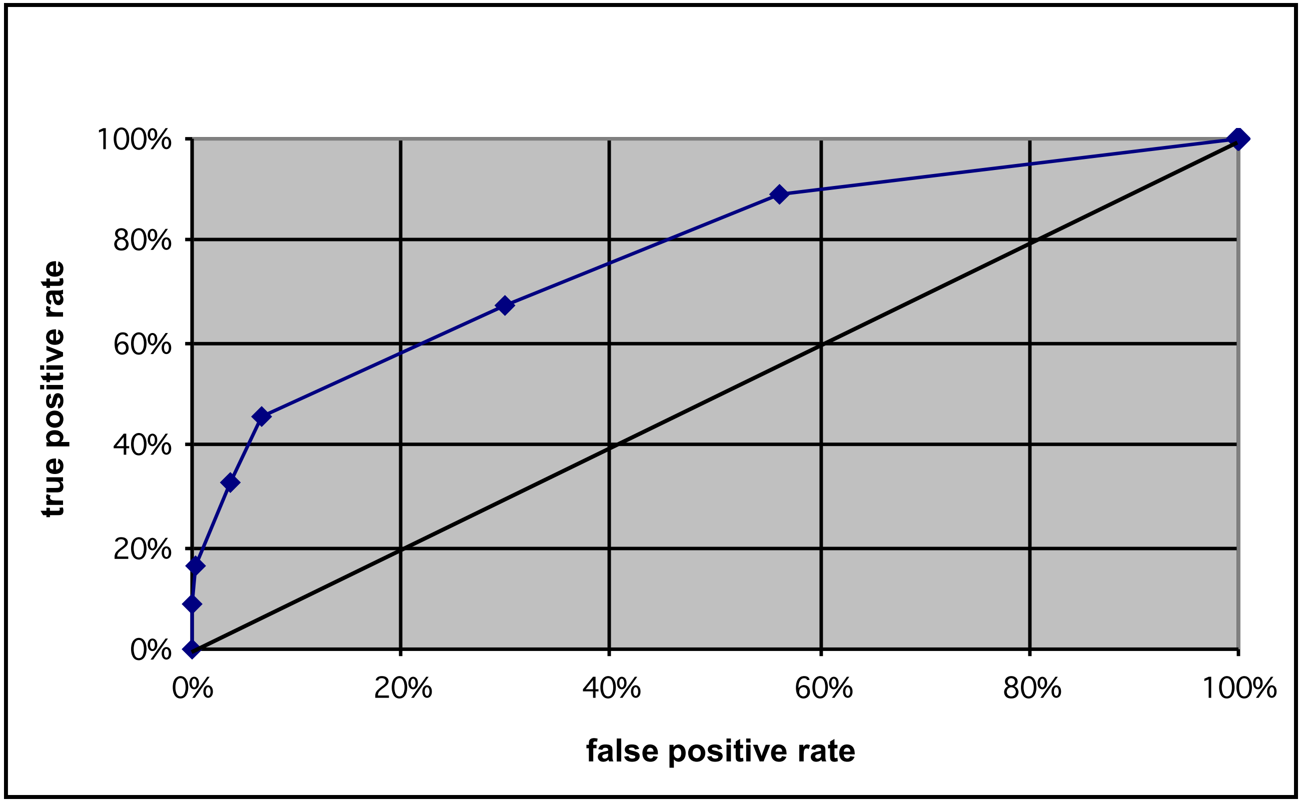
	Predicted positive	Predicted negative	
Positive examples	**30**	**20**	50
Negative examples	**0**	**50**	50
	30	70	100



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

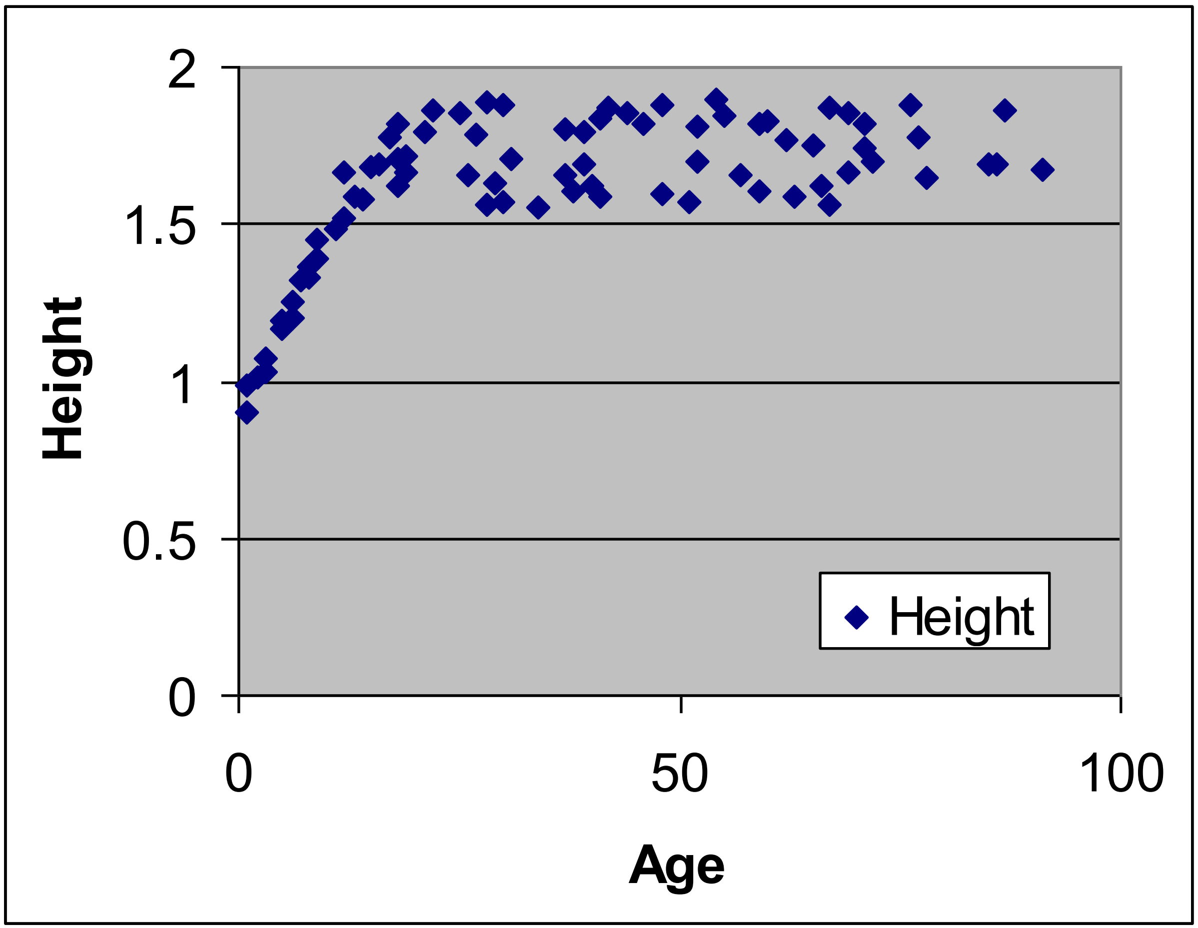
Part III. Numeric prediction

- 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



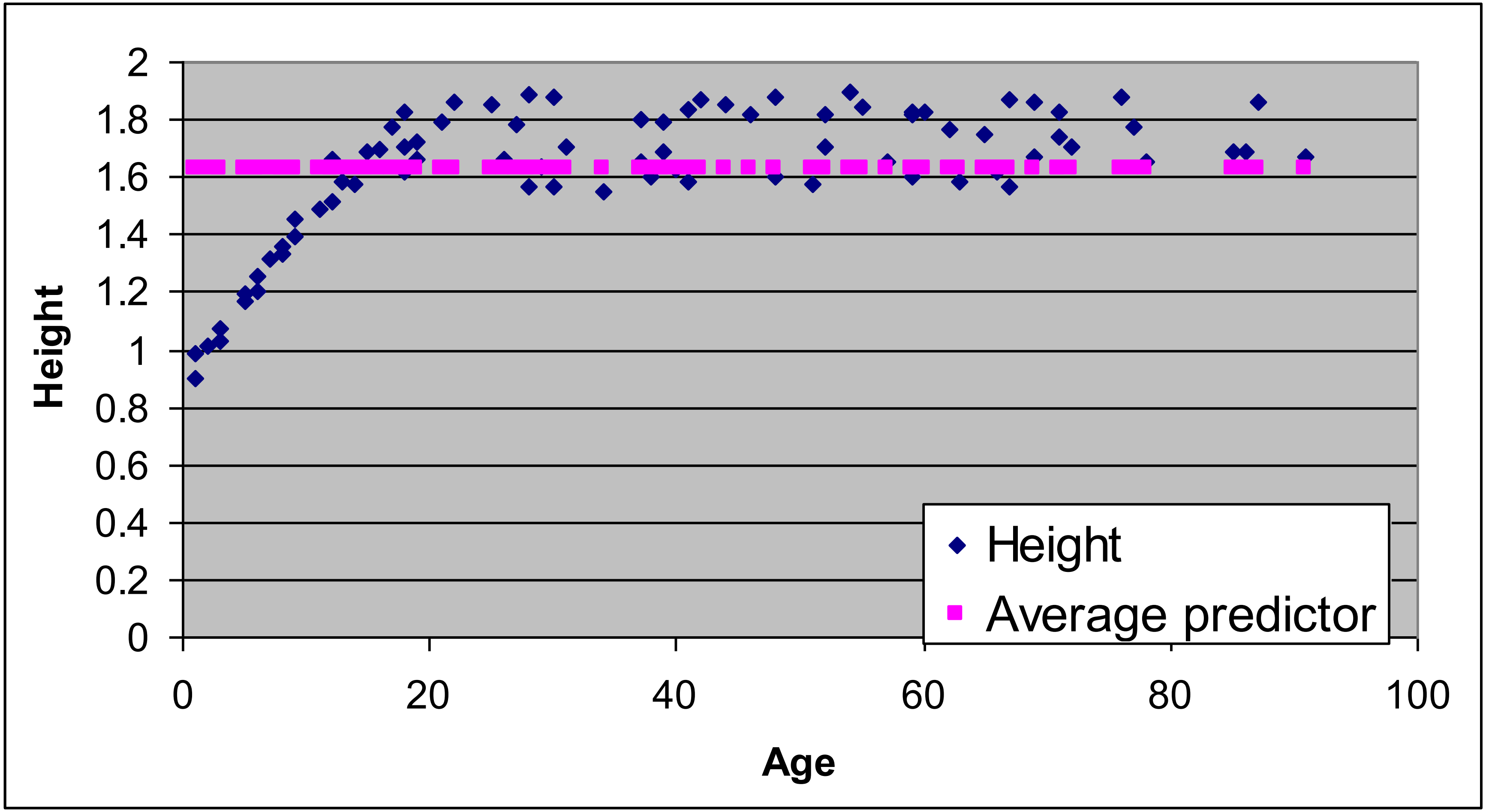
Age	Height
3	1.03
5	1.19
6	1.26
9	1.39
15	1.69
19	1.67
22	1.86
25	1.85
41	1.59
48	1.60
54	1.90
71	1.82
...	...

Test set

Age	Height
2	0.85
10	1.4
35	1.7
70	1.6

Baseline numeric predictor

- Average of the target variable



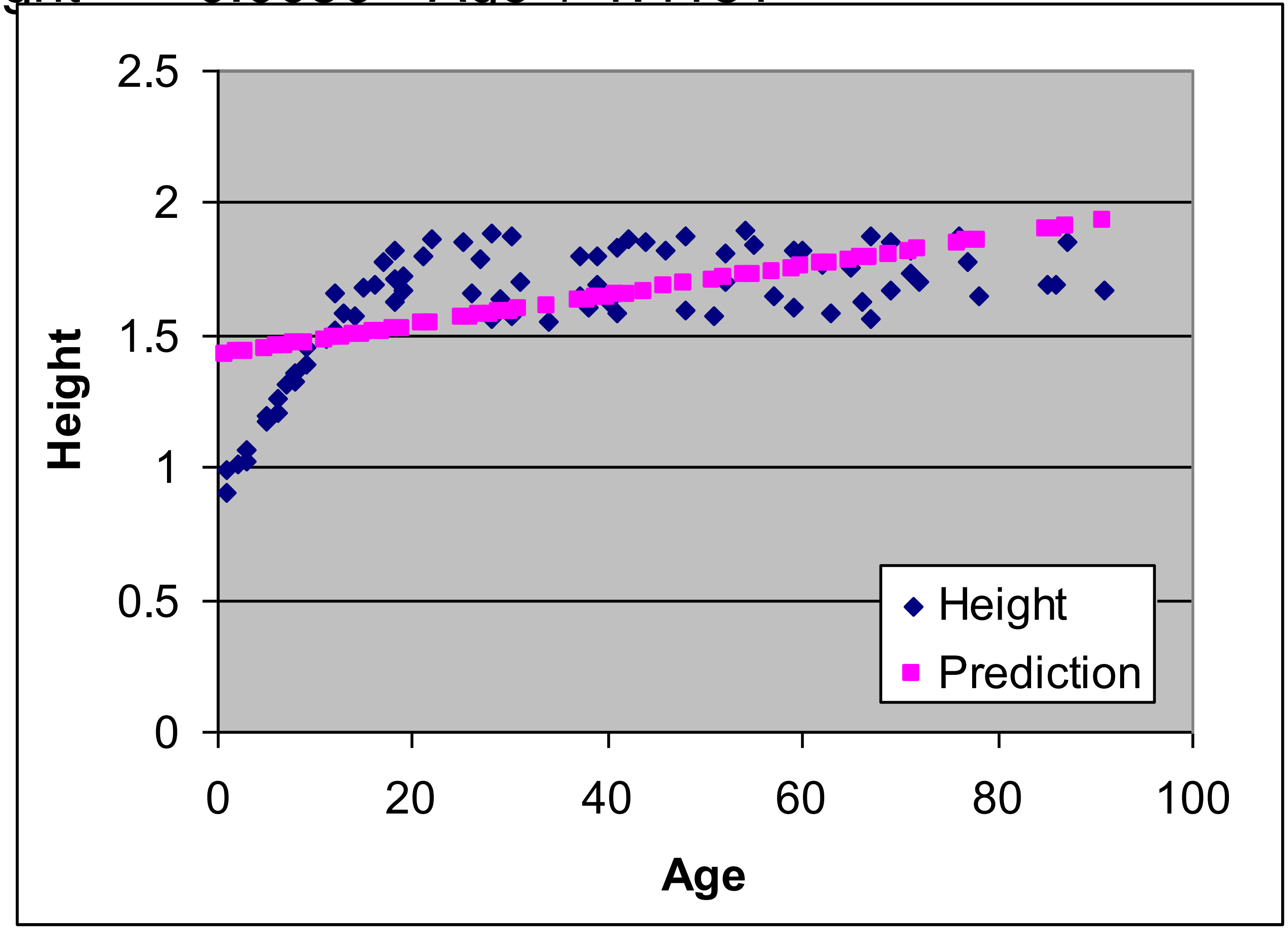
Baseline predictor: prediction

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

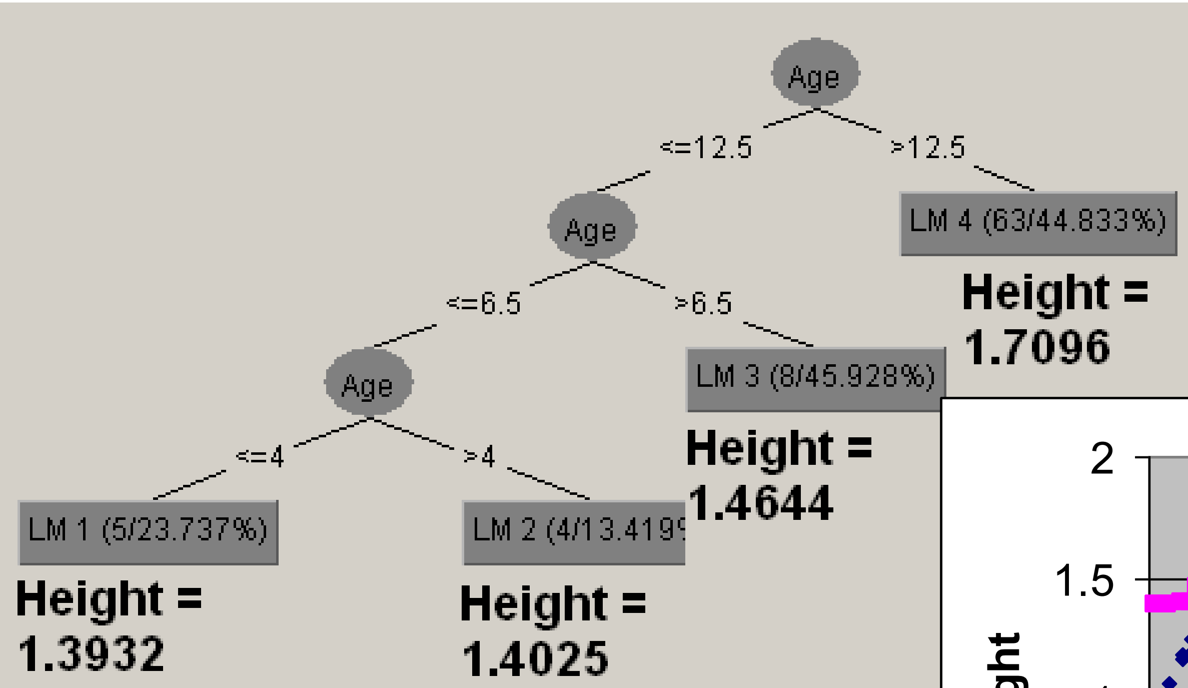


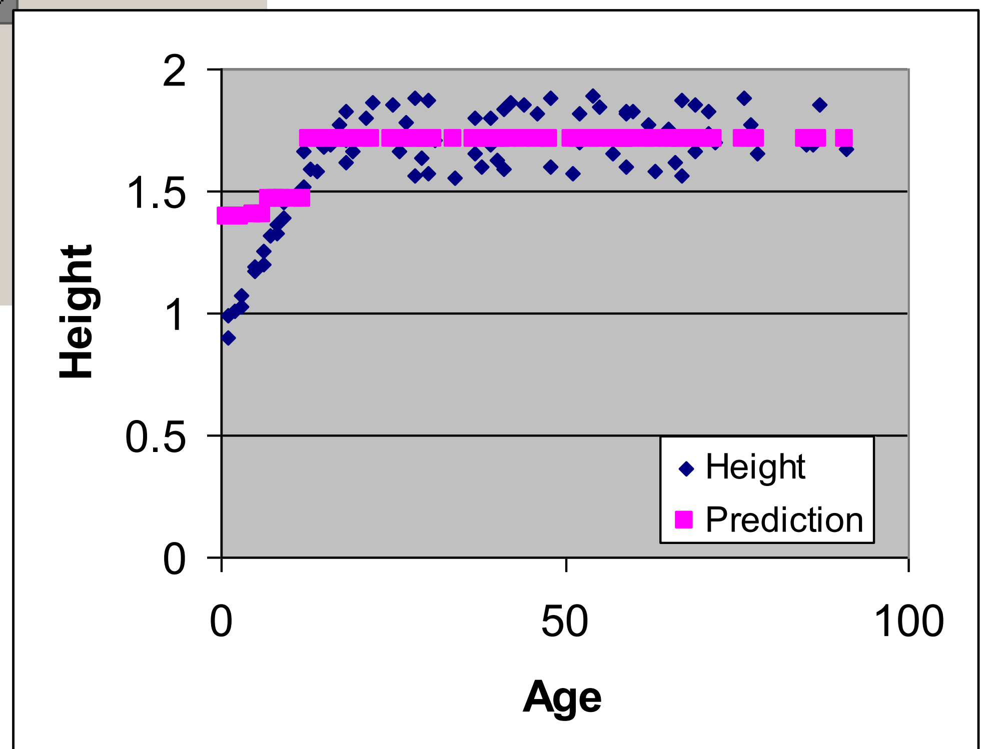
Linear Regression: prediction

Height = 0.0056 * Age + 1.4181

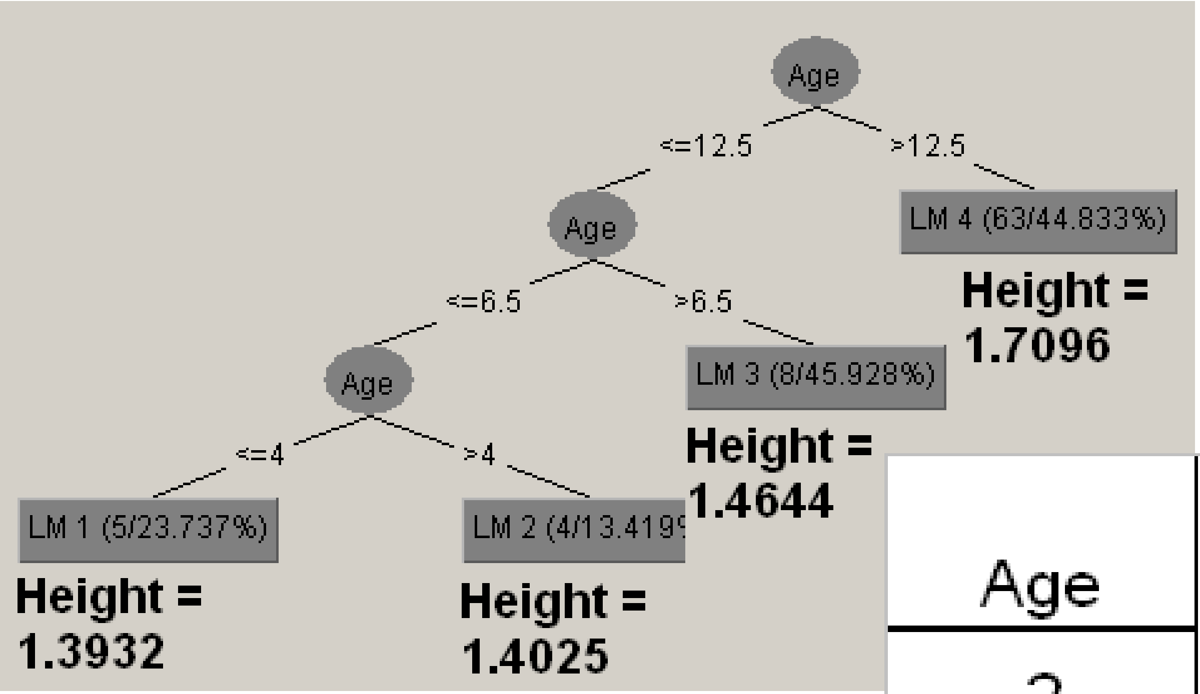
Age	Height	Linear regression
2	0.85	
10	1.4	
35	1.7	
70	1.6	

Regression tree



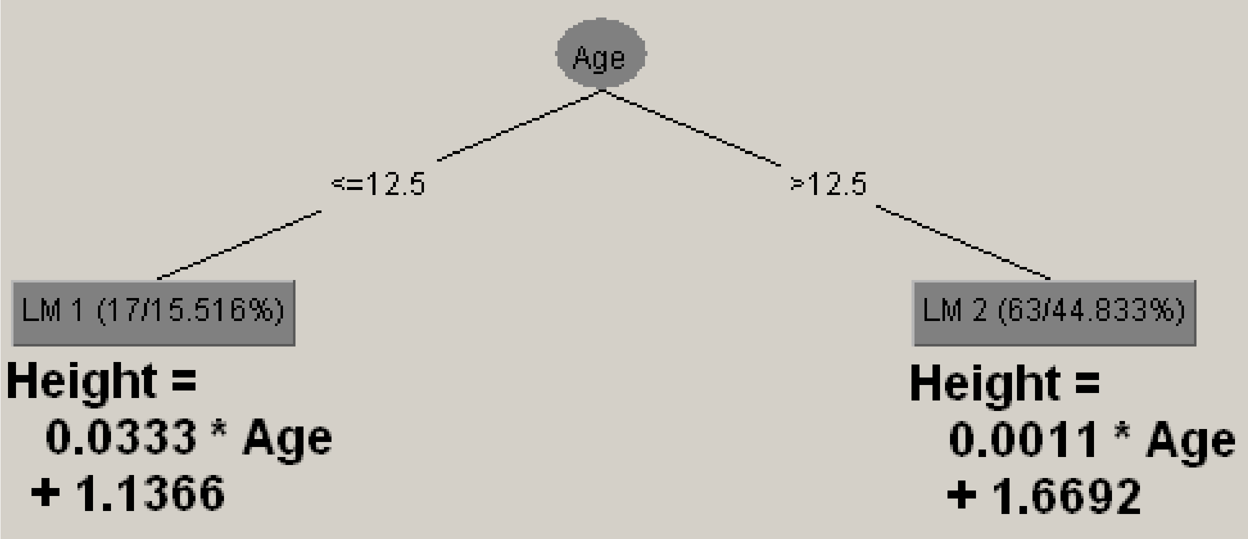


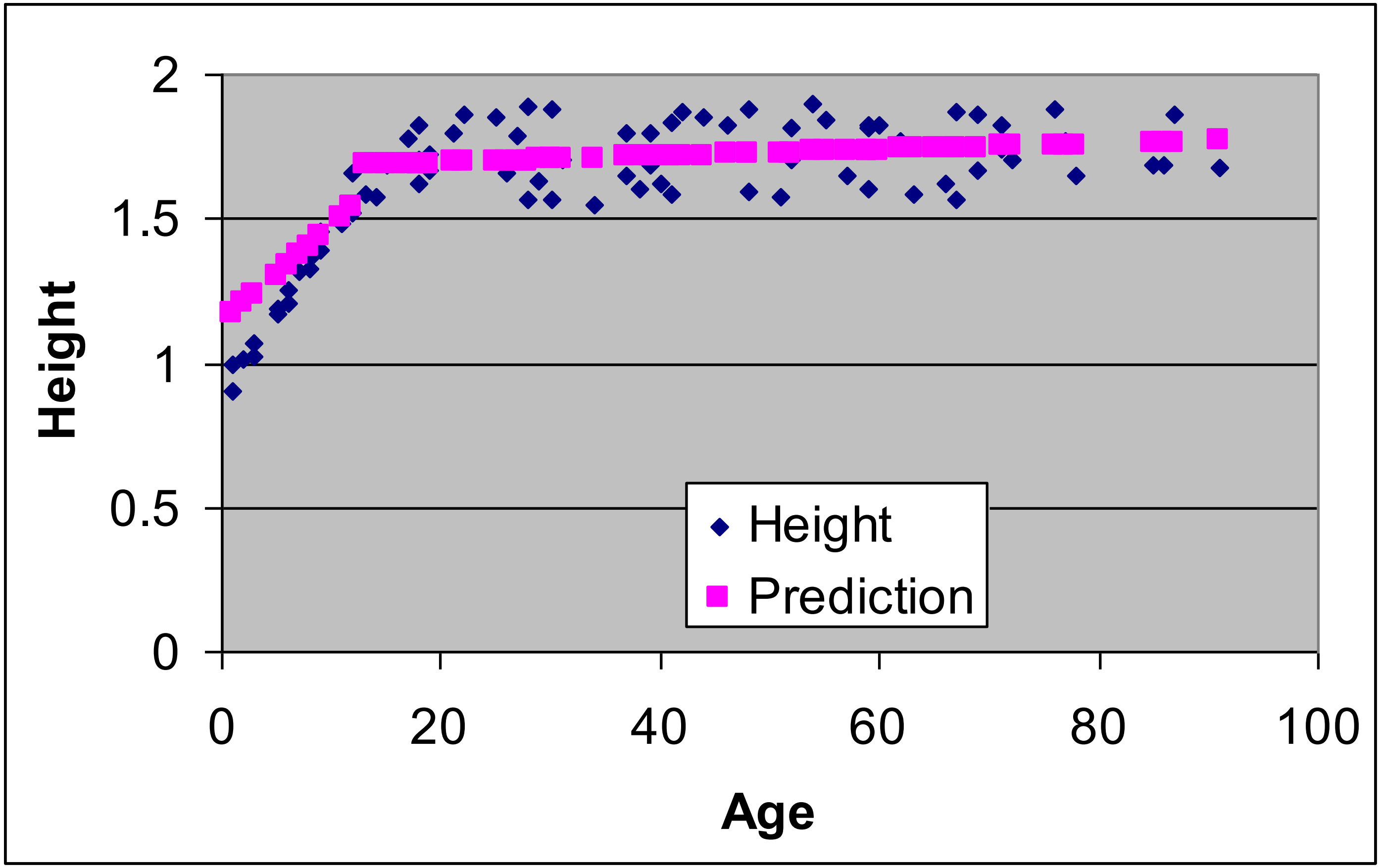
Regression tree: prediction



Age	Height	Regression tree
2	0.85	
10	1.4	
35	1.7	
70	1.6	

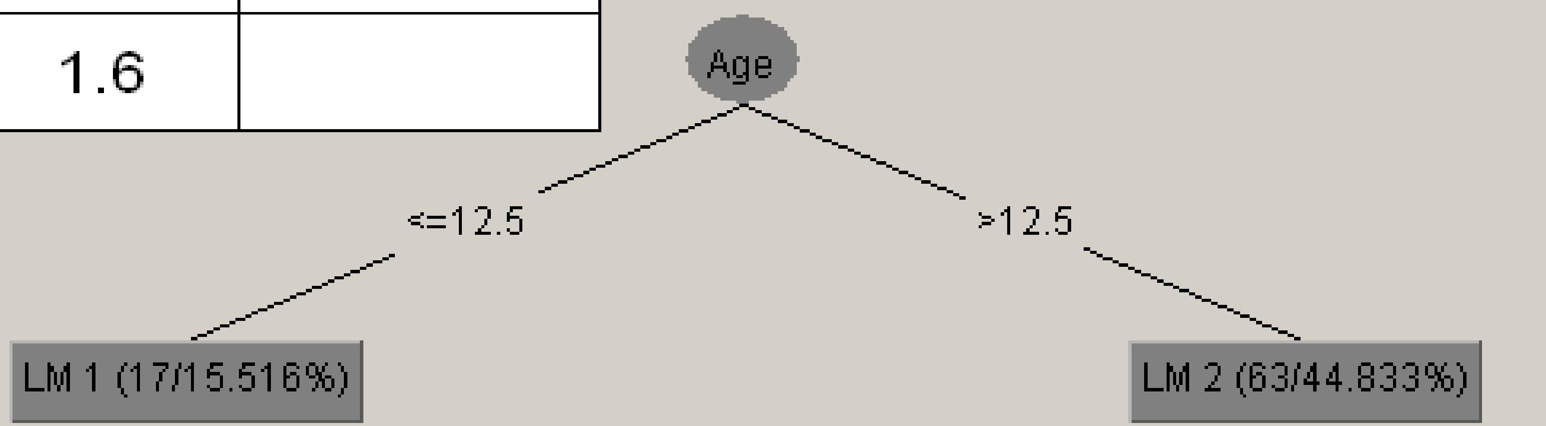
Model tree


Age
<=12.5
>12.5
LM 1 (17/15.516%)
LM 2 (63/44.833%)
Height = 0.0333 * Age + 1.1366
Height = 0.0011 * Age + 1.6692


2
1.5
1
0.5
0
Height
0
20
40
60
80
100
Age
Height
Prediction

Model tree: prediction

Age	Height	Model tree
2	0.85	
10	1.4	
35	1.7	
70	1.6	

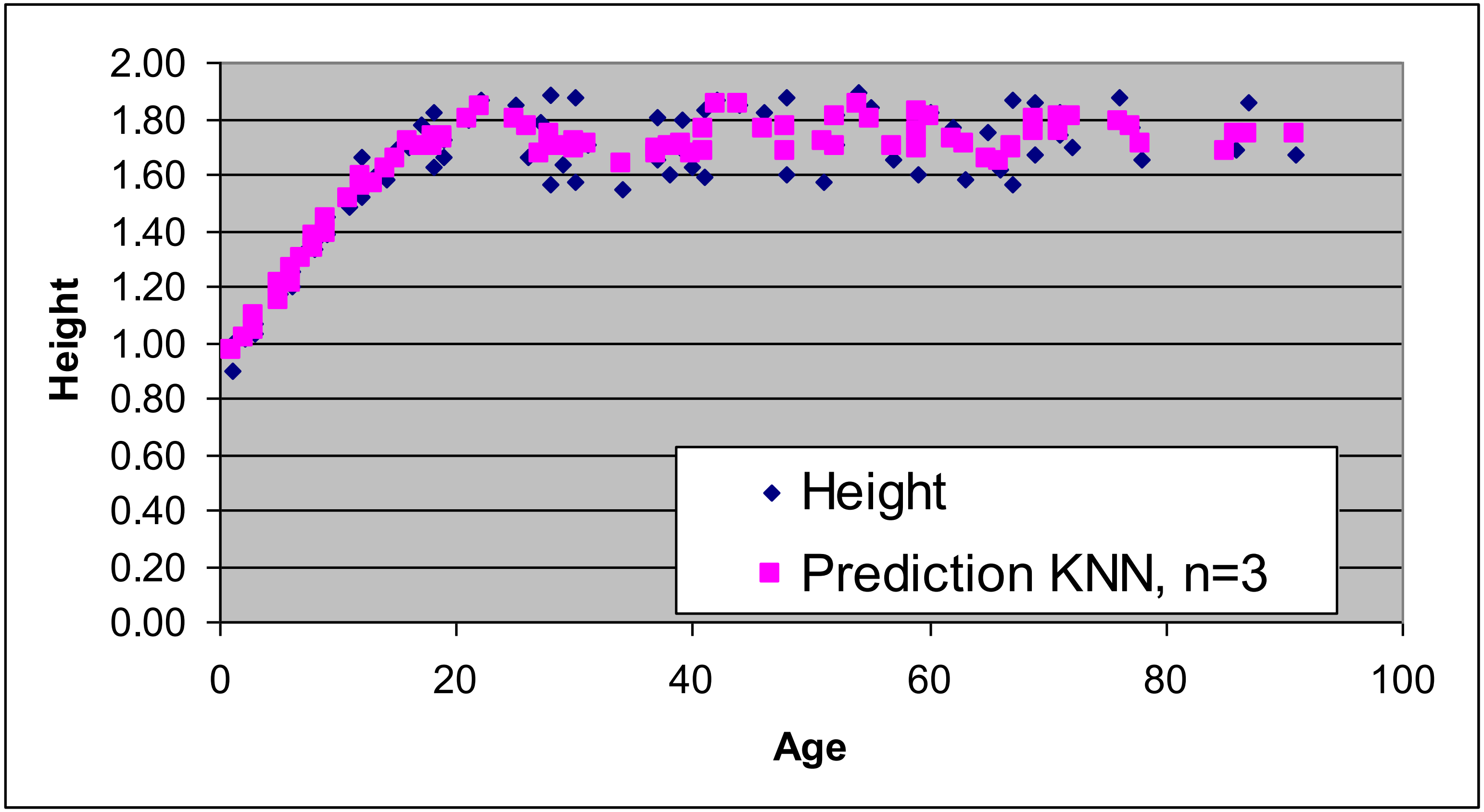


Height =
0.0333 * Age
+ 1.1366

Height =
0.0011 * Age
+ 1.6692

kNN – K nearest neighbors

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



kNN prediction

Age	Height
1	0.90
1	0.99
2	1.01
3	1.03
3	1.07
5	1.19
5	1.17

Age	Height	kNN
2	0.85	
10	1.4	
35	1.7	
70	1.6	

kNN prediction

Age	Height
8	1.36
8	1.33
9	1.45
9	1.39
11	1.49
12	1.66
12	1.52
13	1.59
14	1.58

Age	Height	kNN
2	0.85	
10	1.4	
35	1.7	
70	1.6	

kNN prediction

Age	Height
30	1.57
30	1.88
31	1.71
34	1.55
37	1.65
37	1.80
38	1.60
39	1.69
39	1.80

Age	Height	kNN
2	0.85	
10	1.4	
35	1.7	
70	1.6	

kNN prediction

Age	Height
67	1.56
67	1.87
69	1.67
69	1.86
71	1.74
71	1.82
72	1.70
76	1.88

Age	Height	kNN
2	0.85	
10	1.4	
35	1.7	
70	1.6	

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 $S_A=\frac{\sum_i(a_i-\bar{a})^2}{n-1}$

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**
- **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

Part IV. Descriptive DM techniques

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

Subgroup Discovery

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

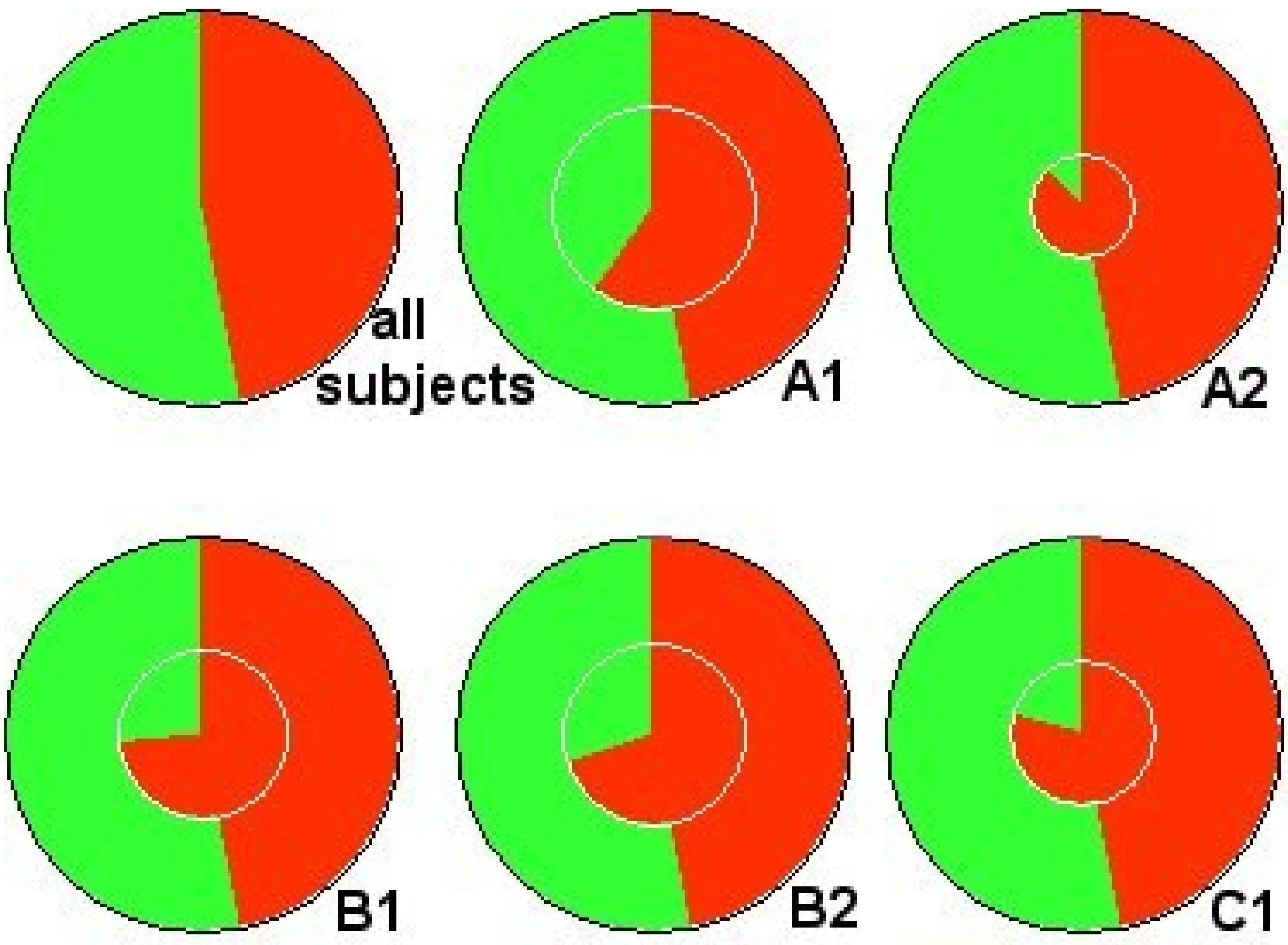
Subgroup Discovery: Medical Case Study

- **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

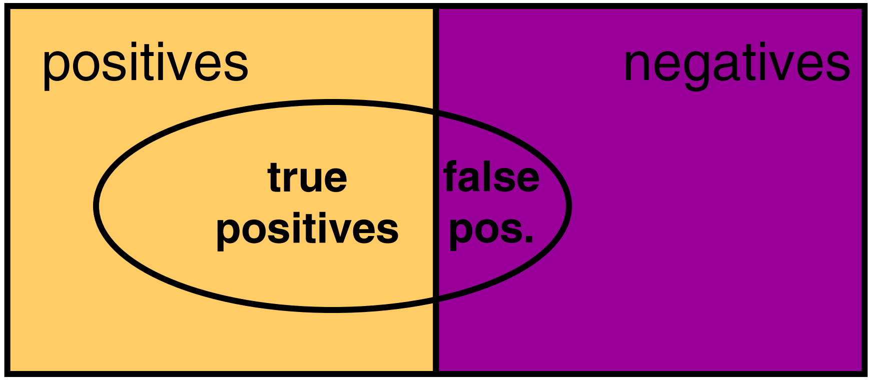


Subgroups of patients with CHD risk

[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 $\leftarrow$ Cond) =

    = p(Class|Cond) = $(n_c+1)/(n_{rule}+k)$
  - CN2-SD: Weighted Relative Accuracy

    WRAcc(Class $\leftarrow$ Cond) =

    p(Cond) (p(Class|Cond) - p(Class))
- Weighted covering approach (example weights)
- Significance testing (likelihood ratio statistics)
- Output: Unordered rule sets (probabilistic classification)

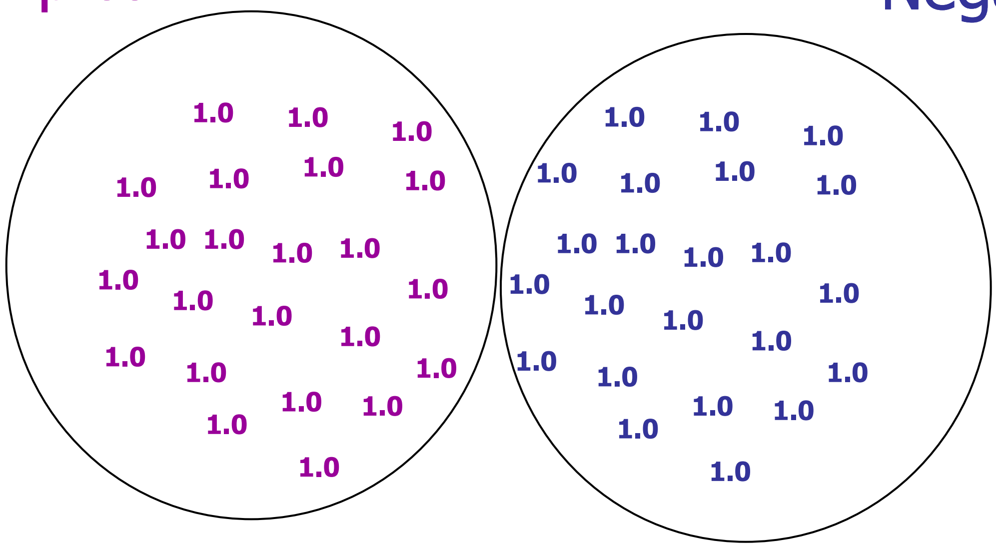
CN2-SD: Weighted Covering

- 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

Positive examples

Negative examples

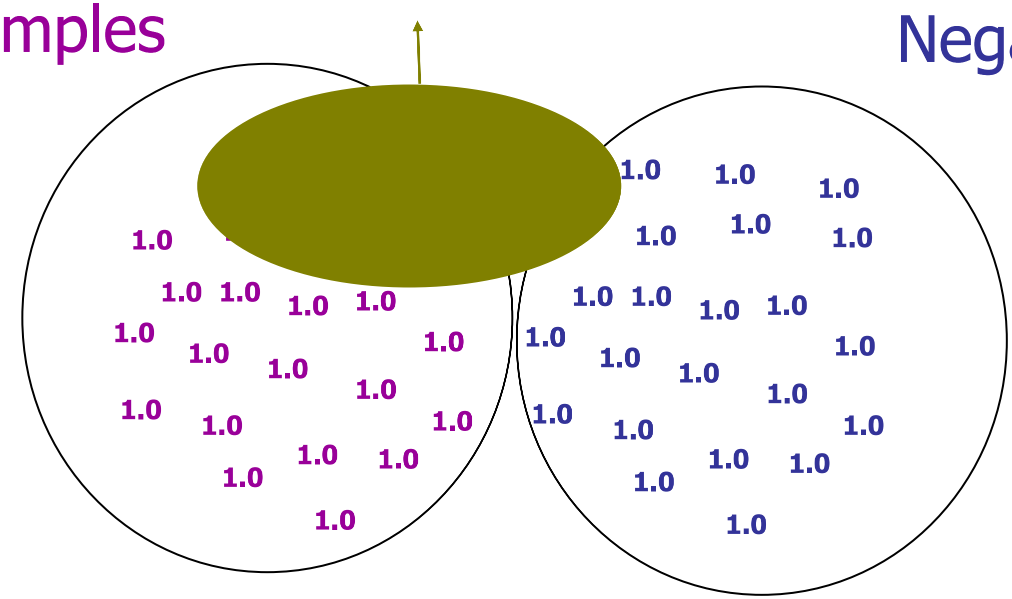


Subgroup Discovery

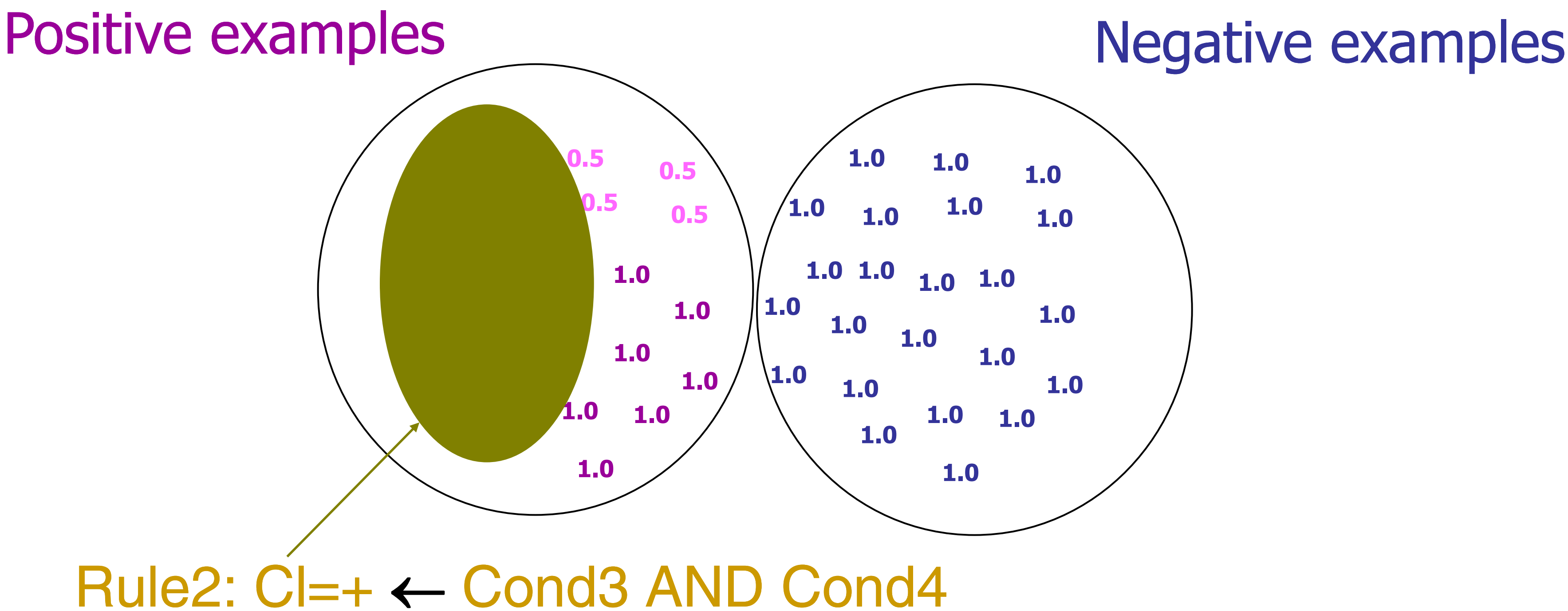
Rule1: Cl=+ ← Cond6 AND Cond2

Positive examples

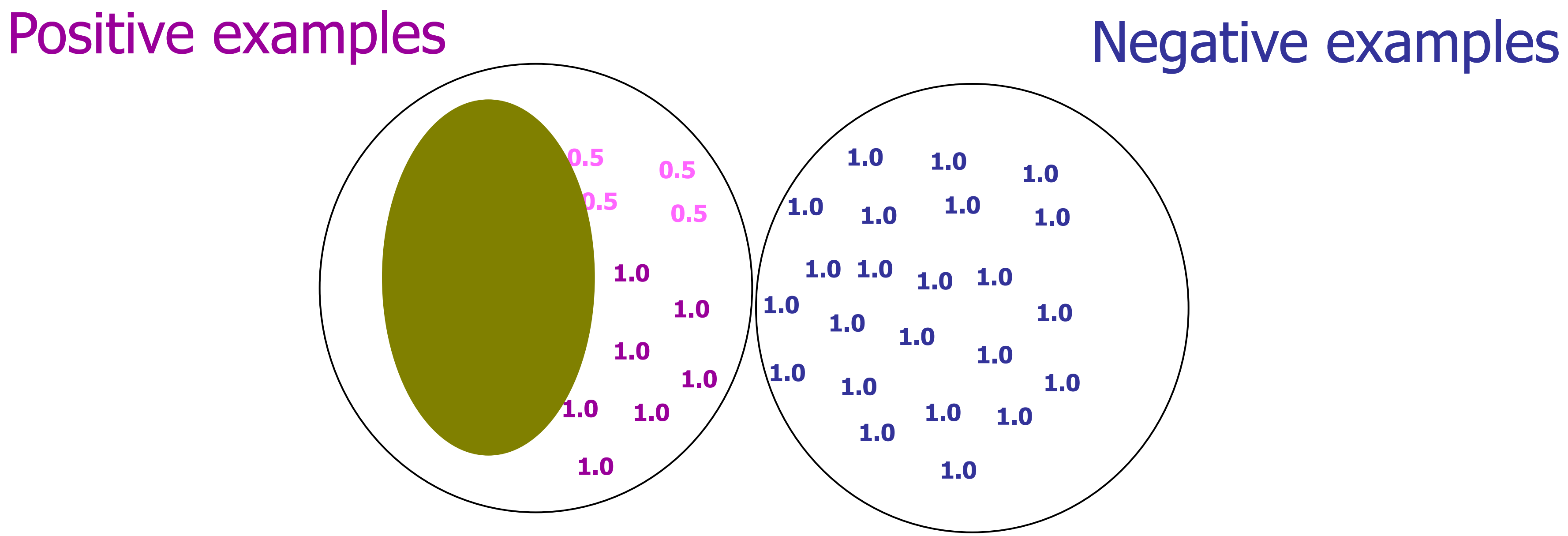
Negative examples



Subgroup Discovery



Subgroup Discovery



CN2-SD: Weighted WRAcc Search Heuristic

- **Weighted relative accuracy (WRAcc) search heuristics, with added example weights**

  $WRAcc(Cl \leftarrow Cond) = p(Cond)\ (p(Cl|Cond) - p(Cl))$

  increased coverage, decreased # of rules, approx. equal accuracy (PKDD-2000)

- In WRAcc computation, probabilities are estimated with relative frequencies, adapt:

  $$WRAcc(Cl \leftarrow Cond) = p(Cond)\ (p(Cl|Cond) - p(Cl)) =$$
  $$n'(Cond)/N'\ (\ n'(Cl.Cond)/n'(Cond) - n'(Cl)/N'\ )$$

  – 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

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 $\Rightarrow$ 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 $\Rightarrow$ 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 $\Rightarrow$ 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

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

- 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):

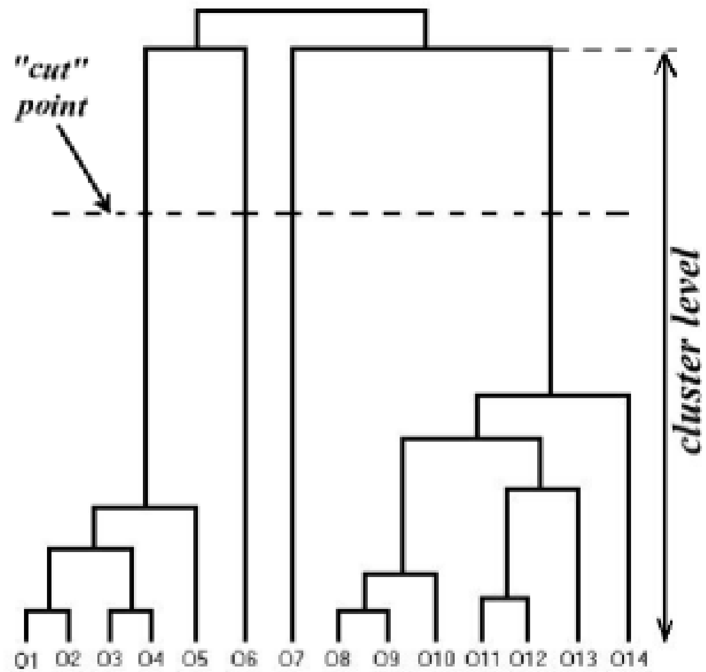
Each instance is a cluster;

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;**

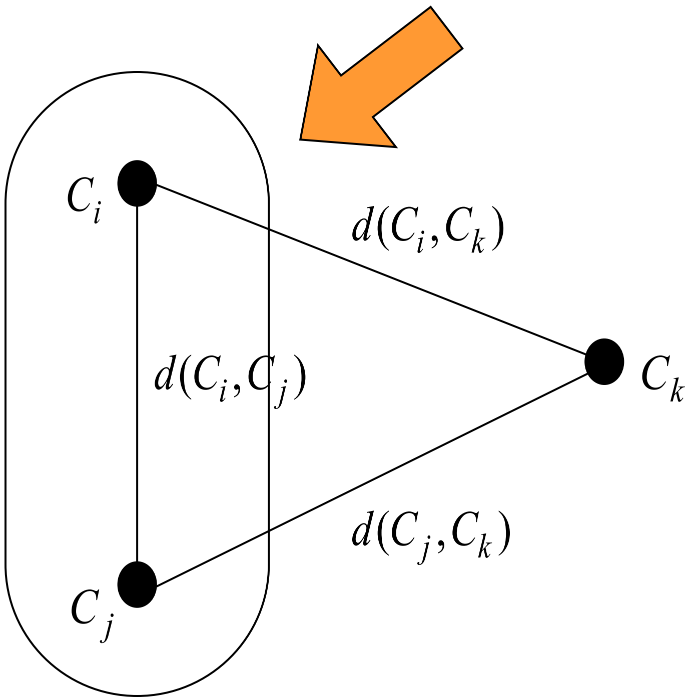
until one cluster left;

- Dendogram:



Hierarchical clustering

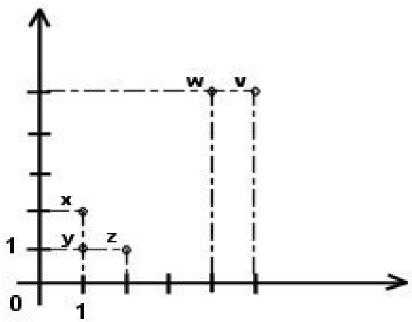
- Fusing the nearest pair of clusters



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

- Computing the dissimilarities from the “new” cluster

Hierarchical clustering: example



a) sample problem

	x	y	z	w	v
x	0	1	1	5	5.66
y		0	1.41	4.24	5
z			0	4.47	5
w				0	1
v					0

b) dissimilarity matrix

	(x,y)	z	w	v
(x,y)	0	1.41	5	5.66
z		0	4.47	5
w			0	1
v				0

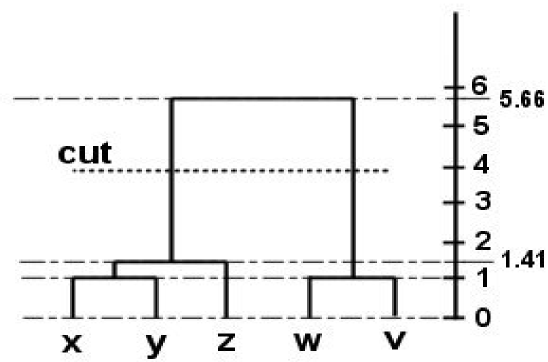
c) dissimilarity matrix after 'fusing' elements **x** and **y**

	(x,y)	z	(w,v)
(x,y)	0	1.41	5.66
z		0	5
(w,v)			0

d) dissimilarity matrix after 'fusing' elements **w** and **v**

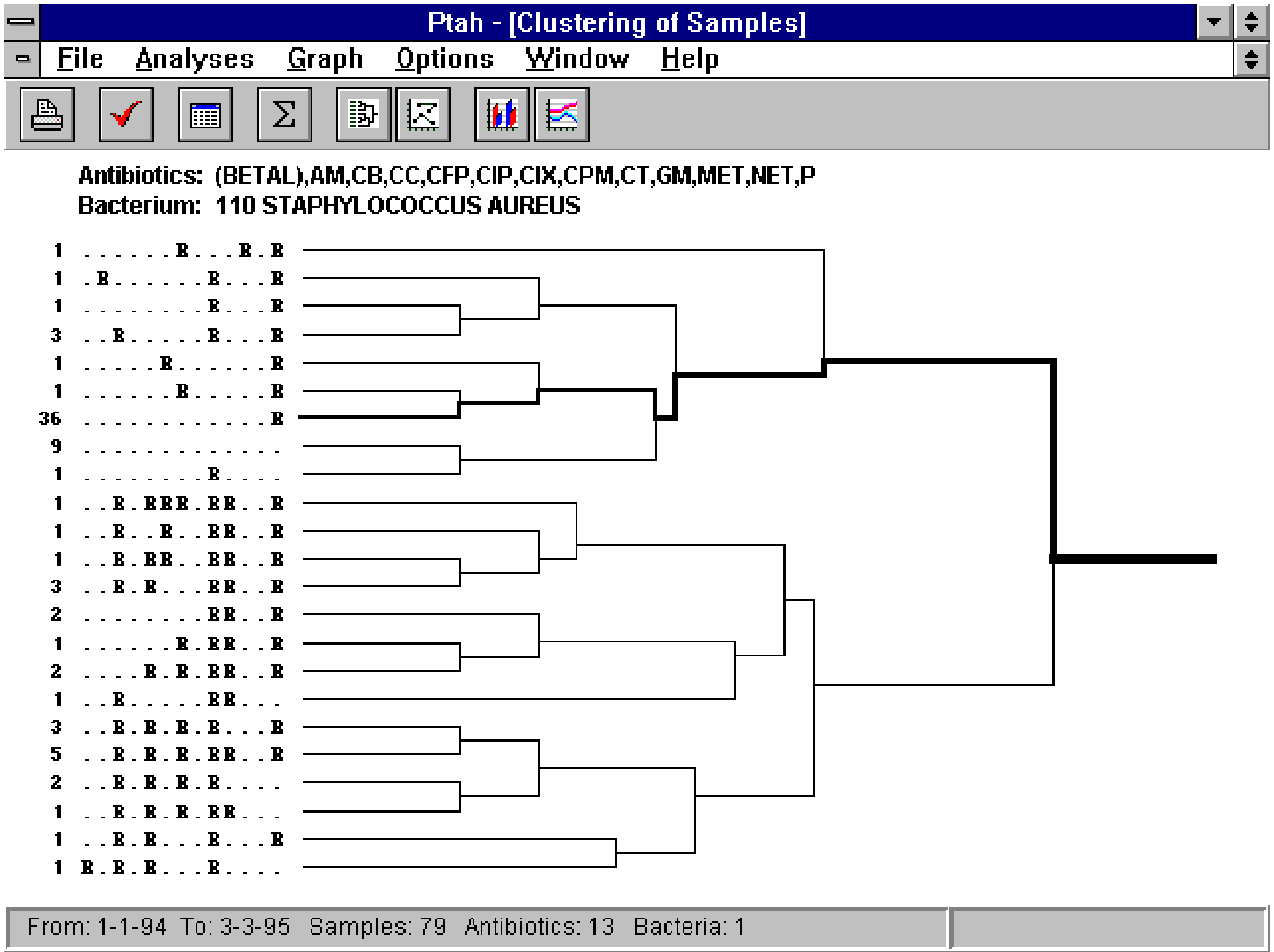
	(x,y,z)	(w,v)
(x,y,z)	0	5.66
(w,v)		0

e) dissimilarity matrix after 'fusing' cluster **(x,y)** and element **z**



f) dendrogram

Results of clustering



A dendogram of resistance vectors

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

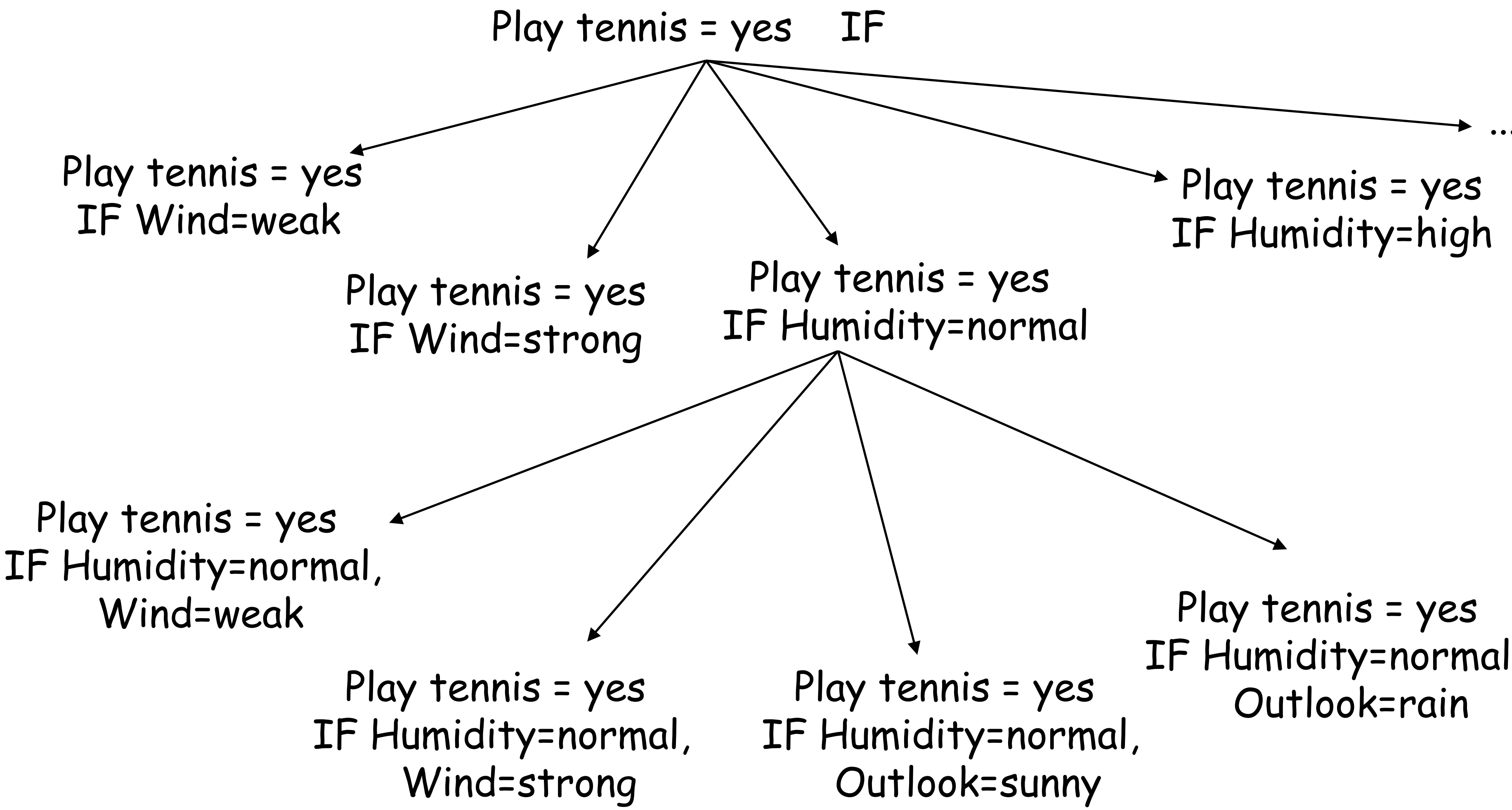
Part V: Relational Data Mining

- Learning as search
- What is RDM?
- Propositionalization techniques
- Inductive Logic Programming

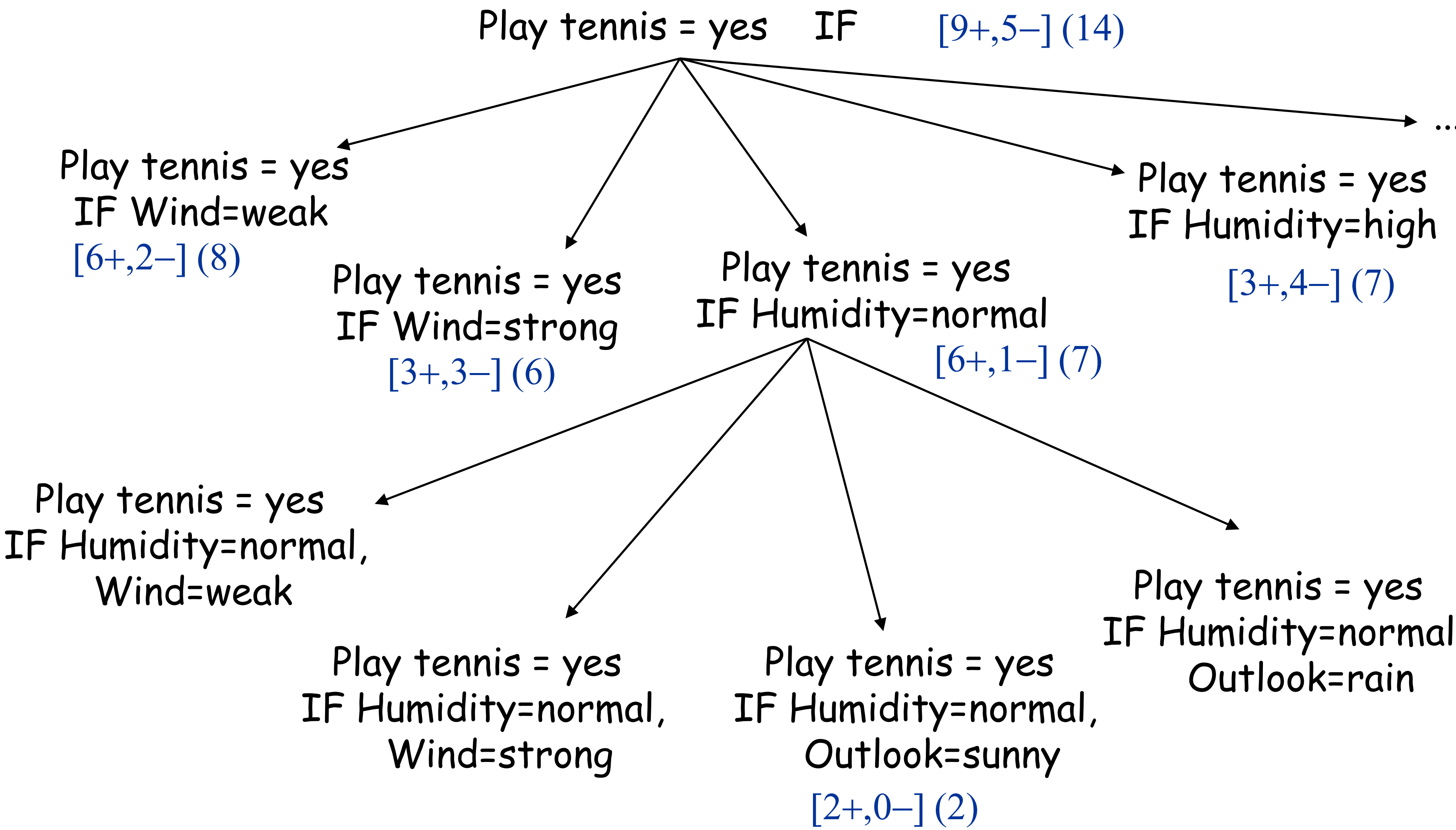
Learning as search

- **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: PlayTennis example

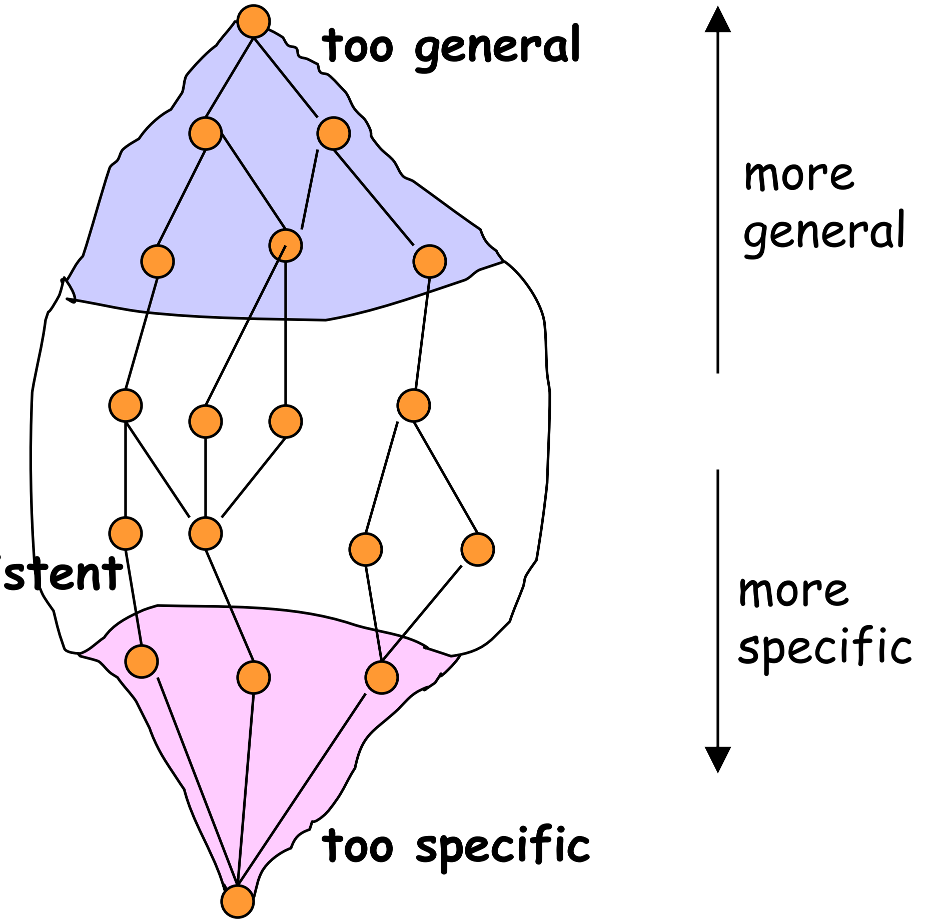


Learn-one-rule as heuristic search: PlayTennis example



Learning as search (Mitchell's version space model)

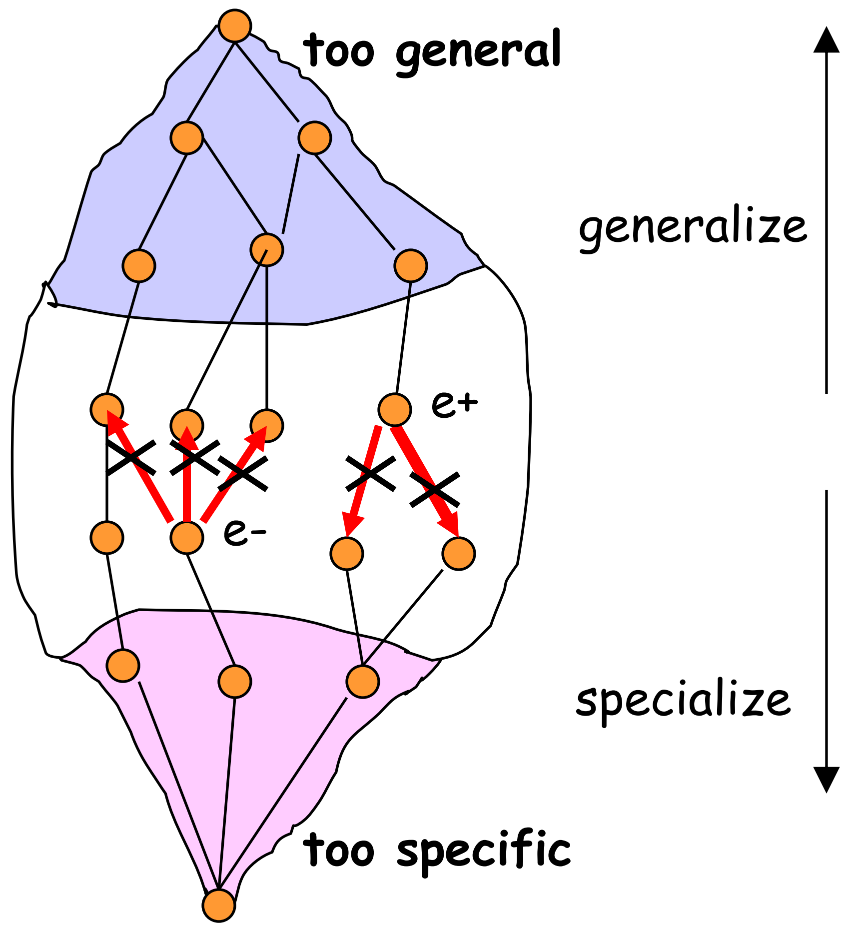
- Hypothesis language **L_H** defines the state space
- How to structure the hypothesis space **L_H**?
- How to move from one hypothesis to another?



- 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

    PlayTennis = yes $\leftarrow$
  - is rule PlayTennis = yes $\leftarrow$ 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

Part V:
Relational Data Mining

- Learning as search
- What is RDM?
- Propositionalization techniques
- Inductive Logic Programming

Predictive relational DM

- Data stored in relational databases
- Single relation - propositional DM
  - example is a tuple of values of a fixed number of attributes (one attribute is a class)
  - example set is a table (simple field values)
- Multiple relations - relational DM (ILP)
  - example is a tuple or a set of tuples (logical fact or set of logical facts)
  - example set is a set of tables (simple or complex structured objects as field values)

Data for propositional DM

Sample single relation data table

ID	Name	First Name	Street	City	Zip	Sex	Social Status	In- come	Age	Club Status	Res- ponse
...	...	...	...	...	...	...	...	...	...	...	...
3478	Smith	John	38, Lake Dr	Sam pleton	34677	male	single	i60 70k	32	mem ber	no_ res ponse
3479	Doe	Jane	45, Sea Ct	Inven- tion	43666	female	mar- ried	i80- 90k	45	non- mem- ber	res- ponse
...	...	...	...	...	...	...	...	...	...	...	...

Basic customer table.

ID	Zip	S ex	So St	In come	A ge	Cl ub	Re sp
...	...	...	...	...	...	...	...
3478	34677	m	si	60-70	32	me	nr
3479	43666	f	ma	80-90	45	nm	re
...	...	...	...	...	...	...	...

Customer table for analysis.

ID	Zip	S ex	So St	In come	A ge	Cl ub	Re sp	Delivery Mode	Paymt Mode	Store Size	Store Type	Store Locatn
...	...	...	...	...	...	...	...	...	...	...	...	...
3478	34677	m	si	60-70	32	me	nr	regular	cash	small	franchise	city
3479	43666	f	ma	80-90	45	nm	re	express	credit	large	indep	rural
...	...	...	...	...	...	...	...	...	...	...	...	...

Customer table including order and store information.

Multi-relational data made propositional

- Sample relation table

ID	Zip	Sex	So St	Income	Age	Club	Resp	Delivery Mode	Paymt Mode	Store Size	Store Type	Store Locatn
...	...	...	...	...	...	...	...	...	...	...	...	...
3478	34677	m	si	60-70	32	me	nr	regular	cash	small	franchise	city
3478	34677	m	si	60-70	32	me	nr	express	check	small	franchise	city
3478	34677	m	si	60-70	32	me	nr	regular	check	large	indep	rural
3479	43666	f	ma	80-90	45	nm	re	express	credit	large	indep	rural
3479	43666	f	ma	80-90	45	nm	re	regular	credit	small	franchise	city
...	...	...	...	...	...	...	...	...	...	...	...	...

Customer table with multiple orders.

- Making data using summary

ID	Zip	Sex	So St	Income	Age	Club	Resp	No. of Orders	No. of Stores
...	...	...	...	...	...	...	...	...	...
3478	34677	m	si	60-70	32	me	nr	3	2
3479	43666	f	ma	80-90	45	nm	re	2	2
...	...	...	...	...	...	...	...	...	...

Customer table using summary attributes.

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, ...

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

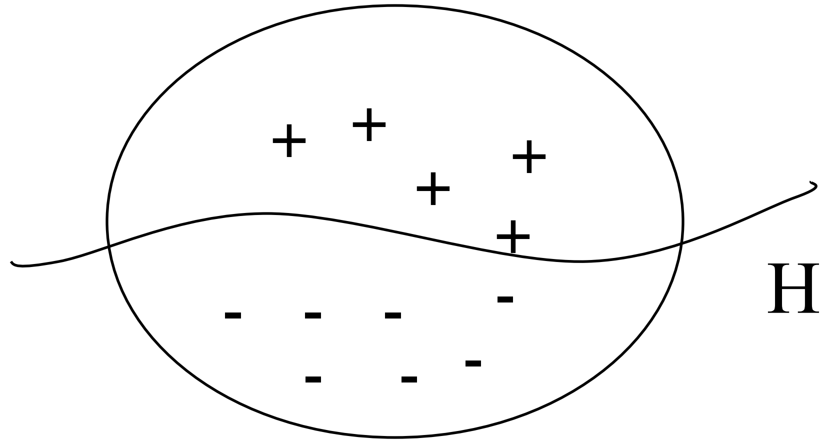
order				
Customer ID	Order ID	Store ID	Delivery Mode	Paymt Mode
...	...	...	...	...
3478	2140267	12	regular	cash
3478	3446778	12	express	check
3478	4728386	17	regular	check
3479	3233444	17	express	credit
3479	3475886	12	regular	credit
...	...	...	...	...

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

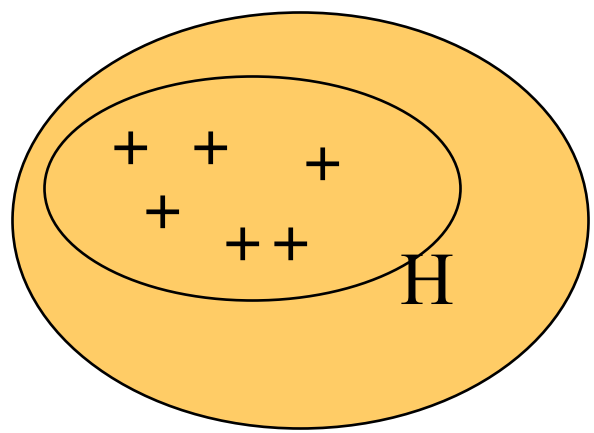
Relational representation of customers, orders and stores.

Basic Relational Data Mining tasks

Predictive RDM



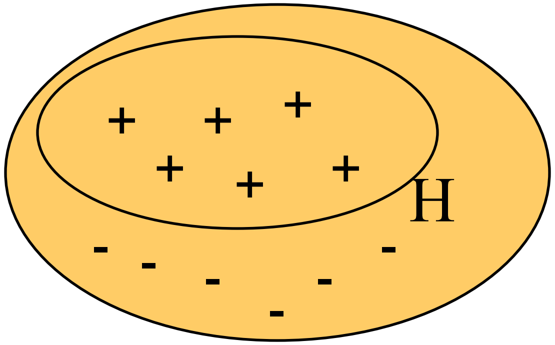
Descriptive RDM



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

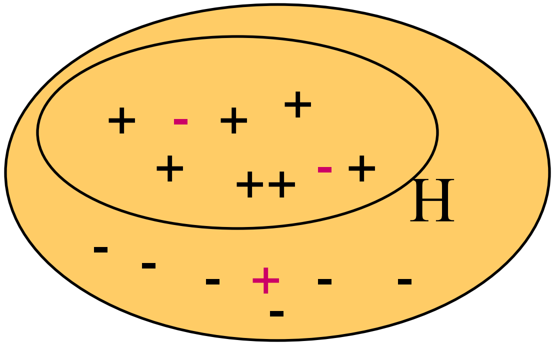


- In logic, **find** H such that
  - $\forall e \in E^+ : B \wedge H \models e$ (H is complete)
  - $\forall e \in E^- : B \wedge H \not\models e$ (H is consistent)

- 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:**

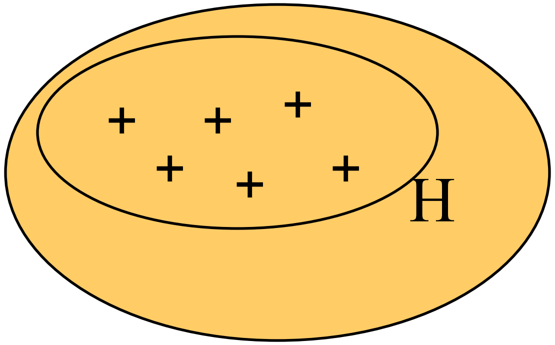
  A hypothesis $H \in L_H$, such that (given B) H is optimal w.r.t. some quality criterion, e.g., max. predictive accuracy A(H)

(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



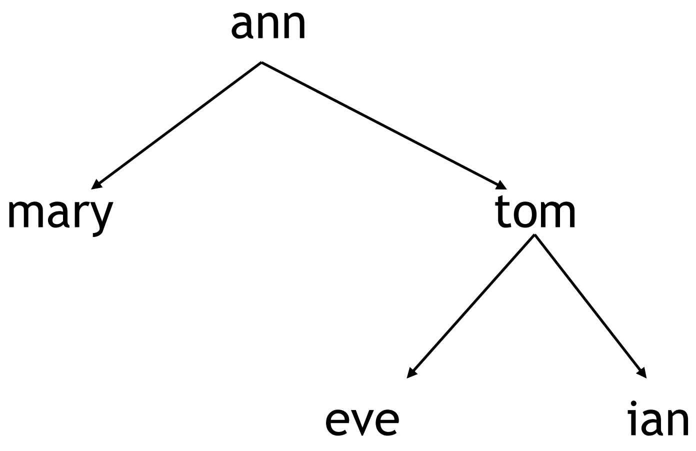
- In logic, **find** H such that $\forall c \in H$, c is true in some preferred model of $B \cup E$ (e.g., least Herbrand model $M(B \cup E)$)

- **In ILP, E are ground facts, B are (sets of) general clauses**

Sample problem
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 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).
```

Sample 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`

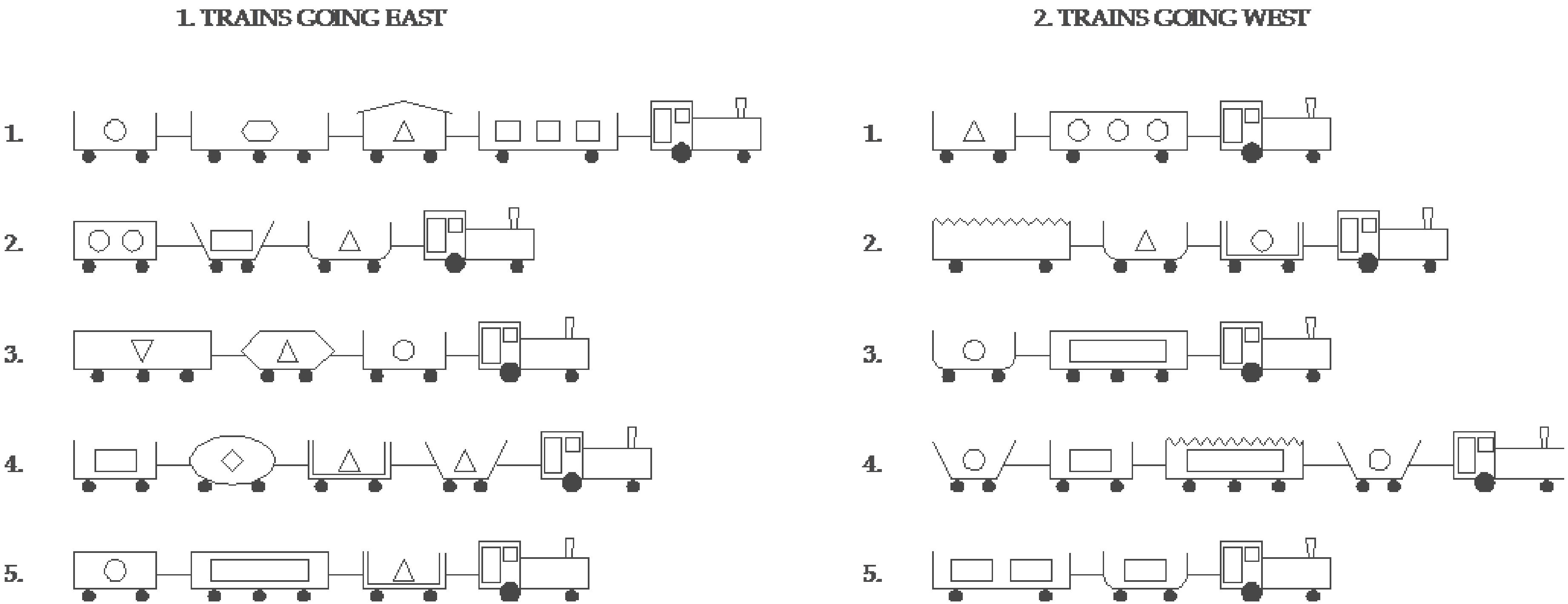
- **Predictive ILP**

```
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 problem: East-West trains



RDM knowledge representation (database)

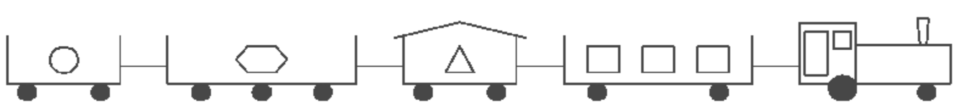
LOAD_TABLE

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

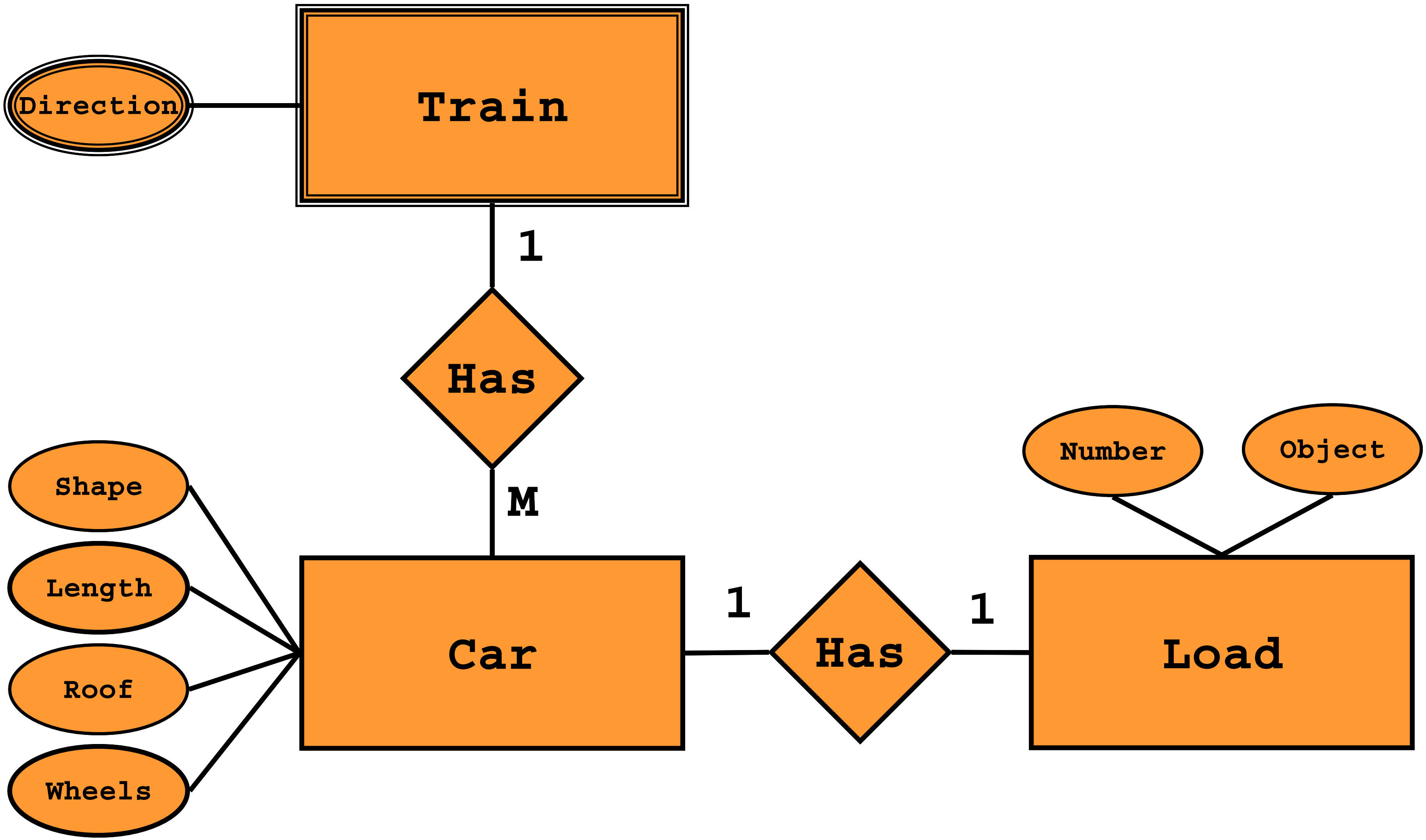
TRAIN_TABLE

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
					...

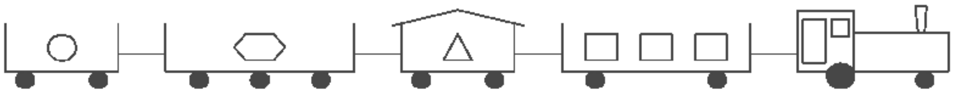


ER diagram for East-West trains



ILP representation: Dat

- Example:
  eastbound(t1).



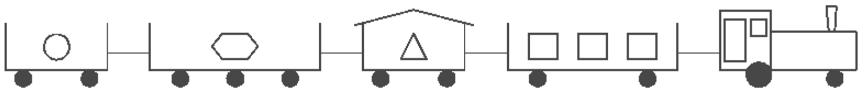
- Background theory:

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):

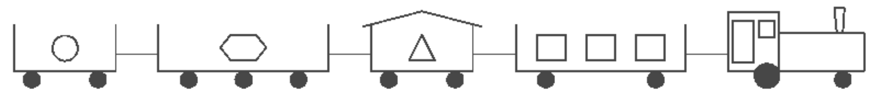
eastbound(T) :- car(T,C),short(C),not none(C).

ILP representation: Datalog



- Example:
  eastbound(t1):-
  car(t1,c1),rectangle(c1),short(c1),none(c1),two_wheels(c1),
  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 represer



- 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).

First-order representations

- **Propositional** representations:
  - datacase is ***fixed-size vector of values***
  - features are those given in the dataset
- **First-order** representations:
  - datacase is ***flexible-size, structured object***
    - sequence, set, graph
    - hierarchical: e.g. set of sequences
  - features need to be **selected** from potentially infinite set

Complexity of RDM problems

- Simplest case: single table with primary key
  - example corresponds to tuple of constants
  - ***attribute-value*** or ***propositional*** learning
- Next: single table without primary key
  - example corresponds to set of tuples of constants
  - ***multiple-instance*** problem
- Complexity resides in many-to-one foreign keys
  - lists, sets, multisets
  - ***non-determinate*** variables

Part V:
Relational Data Mining

- Learning as search
- What is RDM?
- Propositionalization techniques
- Inductive Logic Programming

Rule learning: The standard view

- **Hypothesis construction**: find a set of *n* rules
  - usually simplified by *n* separate rule constructions
    - exception: HYPER
- **Rule construction**: find a pair (Head, Body)
  - e.g. select head (class) and construct body by searching the VersionSpace
    - exceptions: CN2, APRIORI
- **Body construction**: find a set of *m* literals
  - usually simplified by adding one literal at a time
    - problem (ILP): literals introducing new variables

Rule learning revisited

- **Hypothesis construction**: find a set of *n* rules
- **Rule construction**: find a pair (Head, Body)
- **Body construction**: find a set of *m* features
  - Features can be either defined by background knowledge or constructed through constructive induction
  - In propositional learning features may increase expressiveness through negation
  - Every ILP system does constructive induction
- **Feature construction**: find a set of *k* literals
  - finding interesting features is discovery task rather than classification task e.g. interesting subgroups, frequent itemsets
  - excellent results achieved also by feature construction through predictive propositional learning and ILP (Srinivasan)

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)

Standard 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
$\oplus$	sue	eve	true	true	false	false	true	false	false
$\oplus$	ann	pat	true	false	false	false	true	false	false
$\ominus$	tom	ann	false	true	false	false	true	false	false
$\ominus$	eve	ann	true	true	false	false	false	false	false

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

Representation issues (1)

- In the database and Datalog ground fact representations individual examples are not easily separable
- Term and Datalog ground clause representations enable the separation of individuals
- Term representation collects all information about an individual in one structured term

Representation issues (2)

- Term representation provides strong language bias
- Term representation can be flattened to be described by ground facts, using
  - structural predicates (e.g. car(t1,c1), load(c1,l1)) to introduce substructures
  - utility predicates, to define properties of invididuals (e.g. long(t1)) or their parts (e.g., long(c1), circle(l1)).
- This observation can be used as a language bias to construct new features

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

- 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).
```

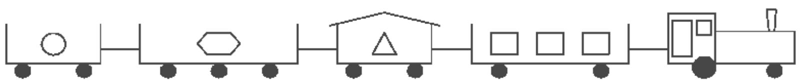
- Equivalent representation:

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

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

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

Propositionalization in a nutshell



CAR	OBJECT	NUMBER
c1	circle	1
c2	hexagon	1
c3	triangle	1
c4	rectangle	3
...	...	

TRAIN_TABLE

...OUND
...UE
...UE
...SE

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**)

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
…	…	…			…

Proposed in ILP systems LINUS (1991), 1BC (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) :- ....

Propositional learning:

t(T) ← f1(T), f4(T)

Relational interpretation:

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

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

TRAIN_TABLE

	OUND
	UE
	UE
	SE

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 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
...	...	...			...

LINUS revisited

- 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

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)).

Part V:
Relational Data Mining

- Learning as search
- What is RDM?
- Propositionalization techniques
- Inductive Logic Programming

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 ($C \models D$) iff
      covers(D) $\subseteq$ covers(C)
    - Example: $p(X,Y) \leftarrow r(Y,X)$ is more general than
      $p(X,Y) \leftarrow r(Y,X), q(X)$
  - 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 θ-subsumes c_2 ($c_1 \geq_\theta c_2$)
    if and only if $\exists\theta: c_1\theta \subseteq c_2$
  - Hypothesis $H_1 \geq \theta\, \mathrm{H}_2$
    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**

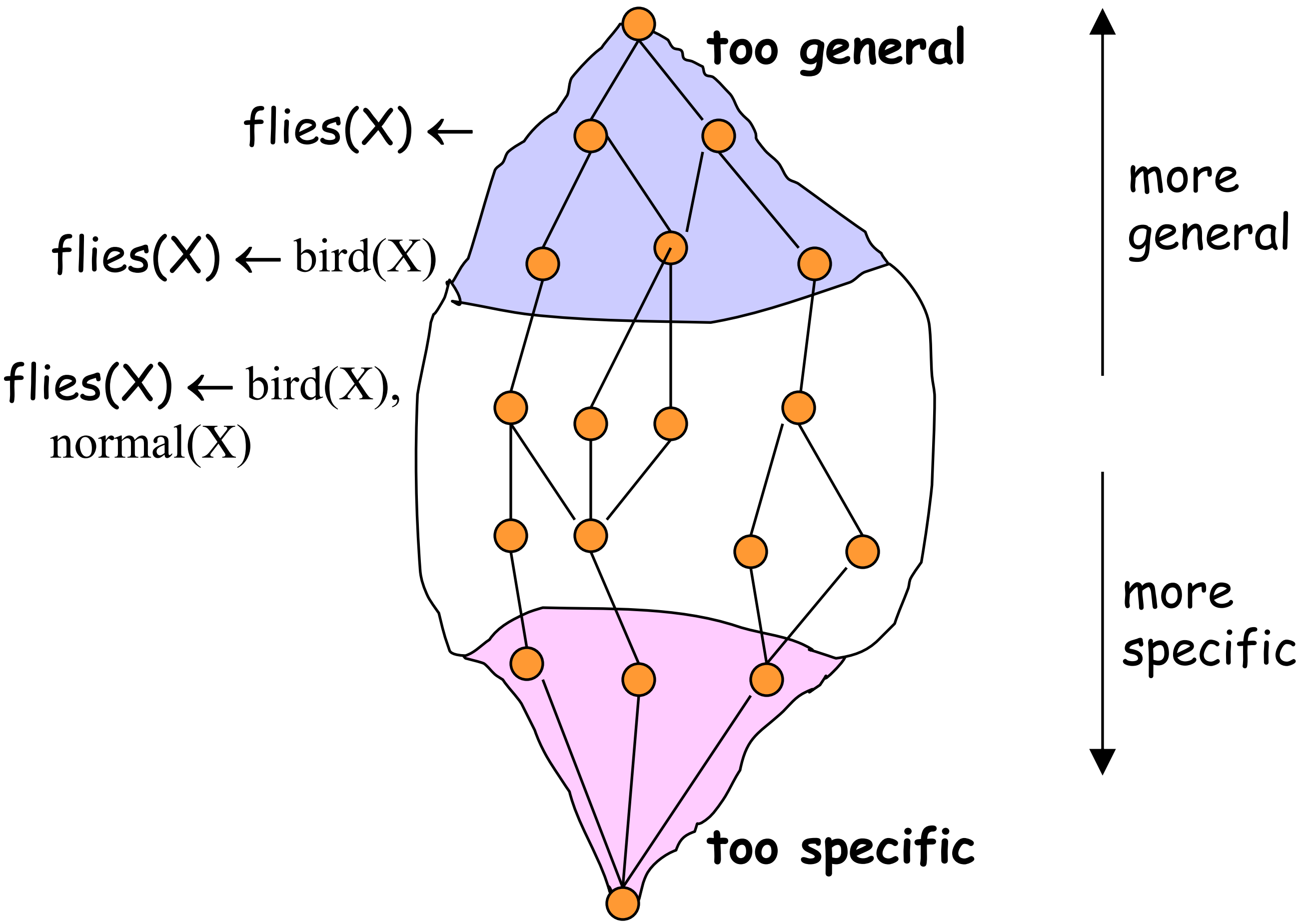
  c1 = daughter(X,Y) ← parent(Y,X)
  c2 = daughter(mary,ann) ← female(mary),
  parent(ann,mary),
  parent(ann,tom).

c1 θ-subsumes c_2 under θ = {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

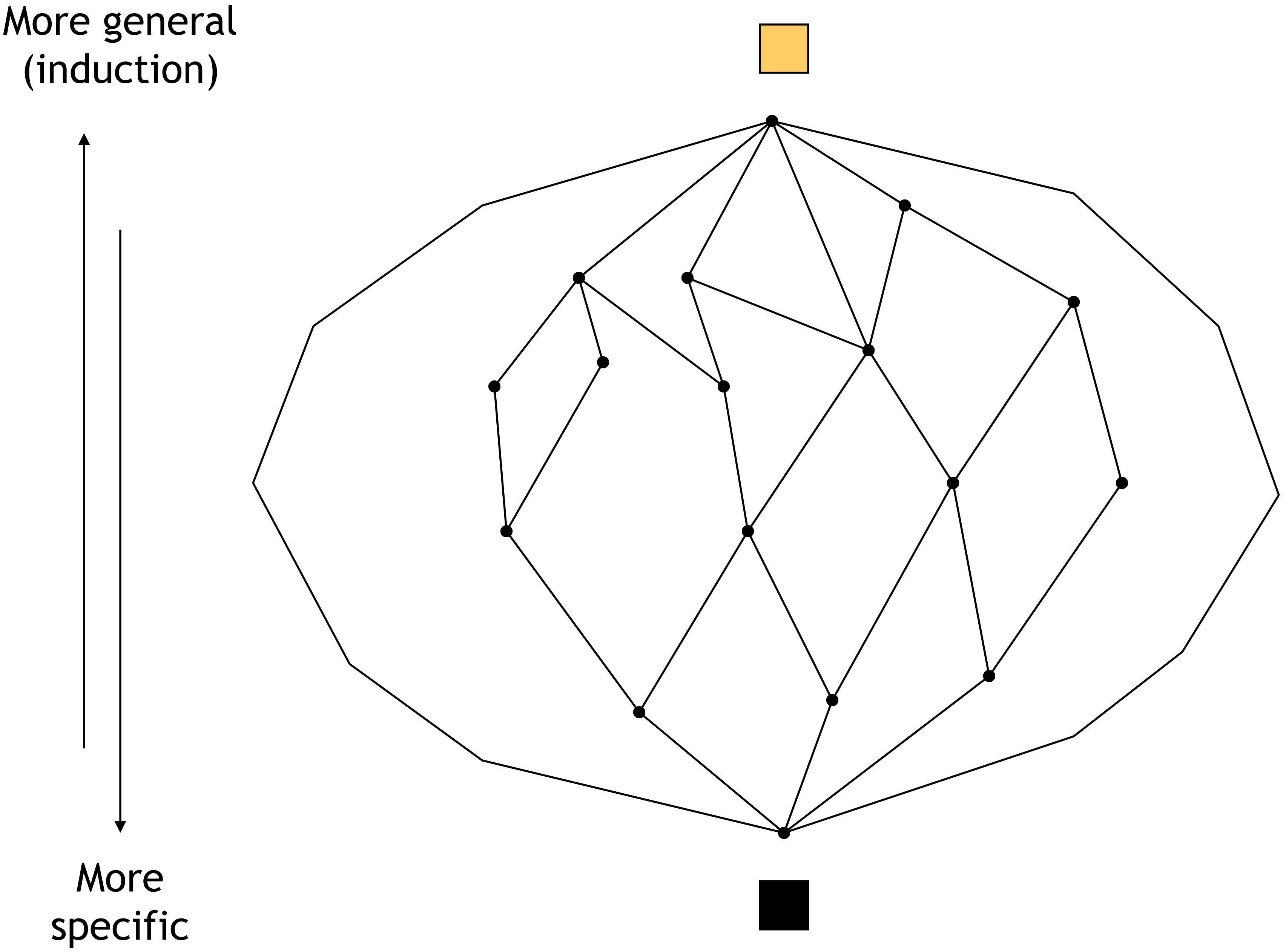


Two strategies for learning

- 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

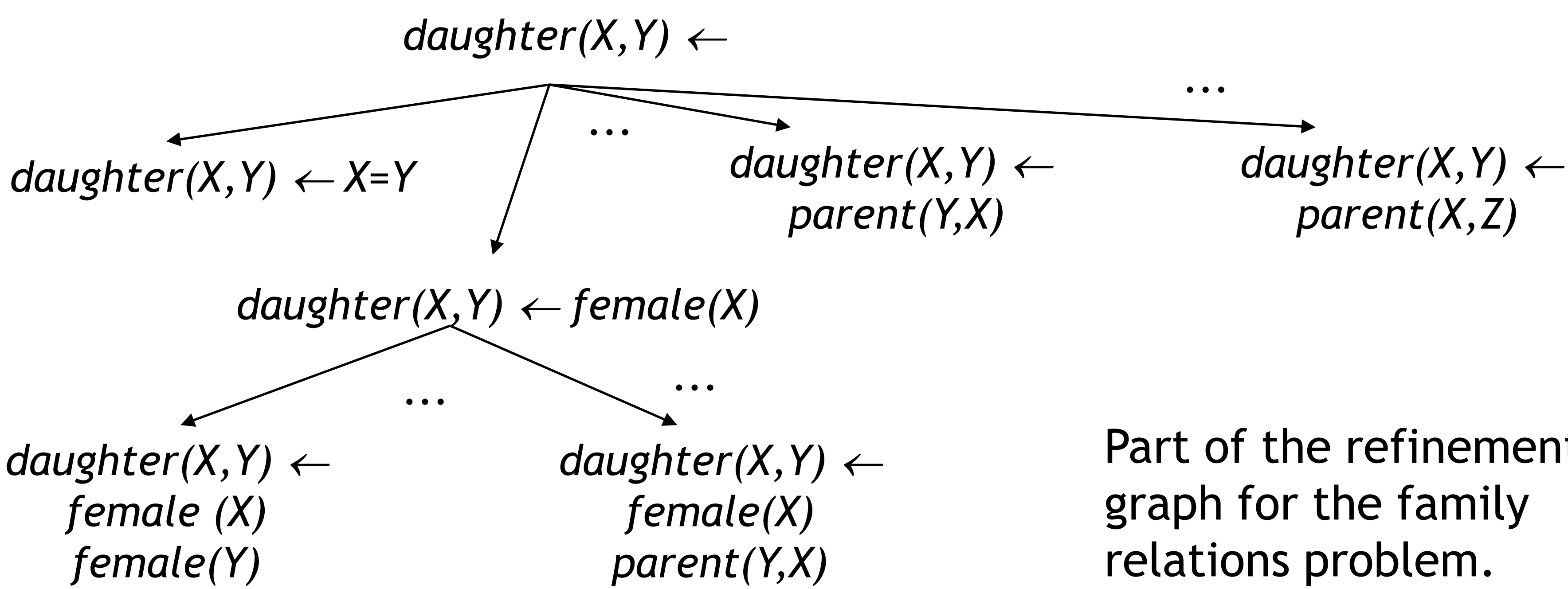
ILP as search of program clauses

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


More general
(induction)
More
specific

Generality ordering of clauses

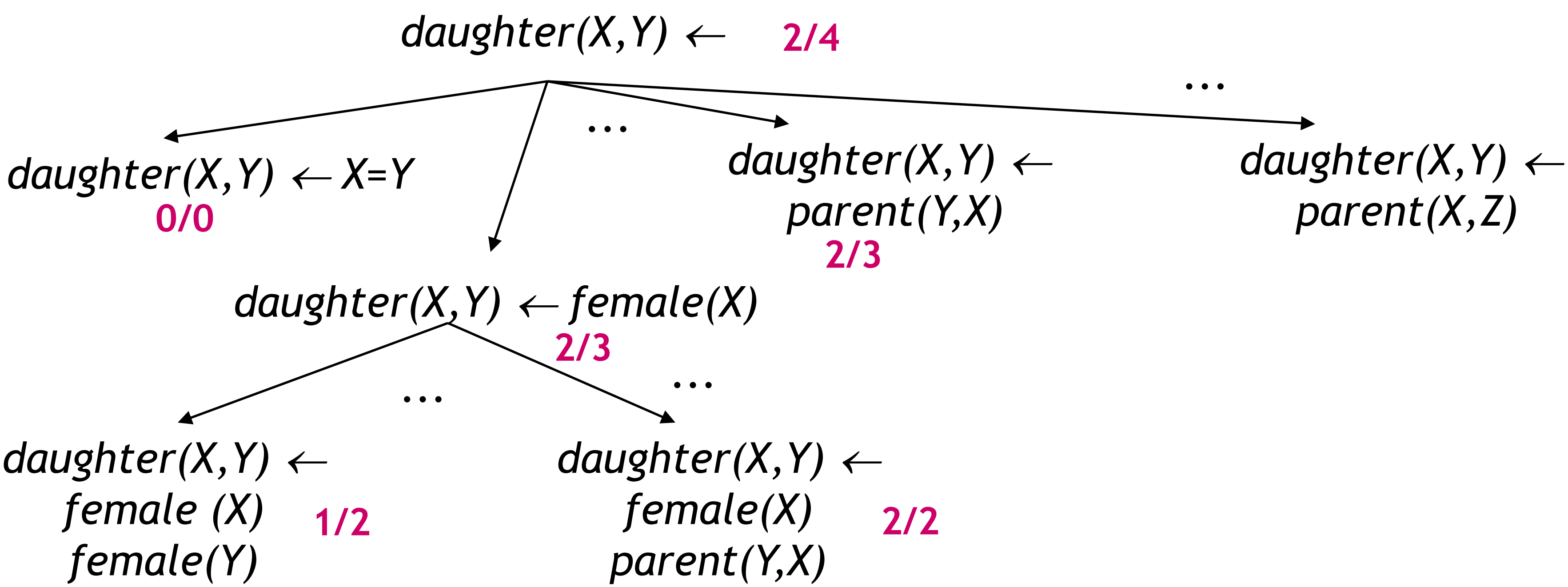
Training examples		Background knowledge	
daughter(mary,ann).	⊕	parent(ann,mary).	female(ann.).
daughter(eve,tom).	⊕	parent(ann,tom).	female(mary).
daughter(tom,ann).	⊖	parent(tom,eve).	female(eve).
daughter(eve,ann).	⊖	parent(tom,ian).	



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