Data Mining and Machine Learning (Machine Learning: Symbolische Ansätze)

Learning Rule Sets

- **Introduction**
	- **Learning Rule Sets**
- **Separate-and-Conquer Rule** Learning
	- **Covering algorithm**
- **Overfitting and Pruning**
- Multi-Class Problems

Learning Rule Sets

- many datasets cannot be solved with a single rule
	- not even the simple weather dataset
	- **they need a rule set for formulating a target theory**
- finding a computable generality relation for rule sets is not trivial
	- **E** adding a condition to a rule specializes the theory
	- **adding a new rule to a theory generalizes the theory**
- practical algorithms use different approaches
	- covering or separate-and-conquer algorithms
	- based on heuristic search

A Sample Database

Property of Interest ("class variable")

A Learned Rule Set

• The solution is

- a set of rules
- **that is complete and consistent on the training examples**
- \rightarrow it must be part of the version space
	- but it does not generalize to new examples!

The Need for a Bias

- rule sets can be generalized by
	- **generalizing an existing rule (as in (Batch-)Find-S)**
	- **T** introducing a new rule (this is new)
- **a** minimal generalization could be
	- **The introduce a new rule that covers only the new example**
- Thus:
	- The solution on the previous slide will be found as a result of the FindS algorithm
	- FindG (or Batch-FindG) are less likely to find such a bad solution because they prefer general theories
- But in principle this solution is part of the hypothesis space and also of the version space
	- ⇒*we need a search bias to prevent finding this solution!*

A Better Solution

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Recap: Subgroup Discovery

Abstract algorithm for learning a single rule:

- 1. Start with an empty theory *T* and training set *E*
- 2. Learn a single (*consistent*) rule *R* from *E* and add it to *T*

3. return *T*

- Problem:
	- **the basic assumption is that the found rules are complete, i.e., they** cover all positive examples
	- **What if they don't?**
- Simple solution:
	- If we have a rule that covers part of the positive examples:
	- **add some more rules that cover the remaining examples**

Key idea of Covering algorithms

Properties of Subgroup Discovery algorithms:

- Consistency can always be maximized
	- **a** rule that covers no negative examples can always be found
- Completeness can not necessarily be ensured
	- Many concepts can only be formulated with multiple rules

Learning strategy:

- Try to learn a rule that is as consistent as possible
- Fix completeness by repeating this step until each (positive) training example is covered by at least one rule

Relaxing Completeness and Consistency

- So far we have defined correctness on training data as consistency + completeness
	- $\blacksquare \rightarrow$ we aim for a rule that covers all positive and no negative examples
- This is not always a good idea (\rightarrow overfitting)

Example:

Training set with 200 examples, 100 positive and 100 negative

Rule Set A consists of 100 complex rules, each covering a single positive example and no negatives

 \rightarrow A is complete and consistent on the training set

- **Rule Set B** consists of a single rule, covering 99 positive and 1 negative example
	- \rightarrow B is incomplete and inconsistent on the training set
- Which one will generalize better to unseen examples?

Separate-and-Conquer Rule Learning

Learn a set of rules, one rule after the other using greedy covering

- 1. Start with an empty theory *T* and training set *E*
- 2. Learn a single (*consistent*) rule *R* from *E* and add it to *T*
- 3. If *T* is satisfactory (*complete*), return *T*
- 4. Else:
	- *Separate:* Remove examples explained by *R* from E
	- *Conquer:* goto 2.
- One of the oldest family of learning algorithms
- Different learners differ in how they find a single rule
- Completeness and consistency requirements are typically loosened

Separate-and-Conquer Rule Learning

Quelle für Grafiken: http://www.cl.uni-heidelberg.de/kurs/ws03/einfki/KI-2004-01-13.pdf

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Covering Strategy

- **EXP** Covering or Separate-and-Conquer rule learning learning algorithms learn one rule at a time
	- **and then removes the examples covered by this rule**
- **This corresponds to a path** in coverage space:
	- \blacksquare The empty theory R_0 (no rules) corresponds to (0,0)
	- **Adding one rule never** decreases *p* or *n* because adding a rule covers *more* examples (generalization)
	- **The universal theory R+** (all examples are positive) corresponds to (N,P)

Rule Selection with Precision

Precision tries to pick the steepest continuation of the curve

- **times to maximize the area under this curve** $(\rightarrow$ AUC: Area Under the ROC Curve)
- no particular angle of isometrics is preferred, i.e. no preference for a certain cost model Ω

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- Accuracy assumes the same costs in all subspaces
	- a local optimum in a sub-space is also a global optimum in the entire space

Which Heuristic is Best?

- There have been many proposals for different heuristics
	- **and many different justifications for these proposals**
	- some measures perform better on some datasets, others on other datasets
- Large-Scale Empirical Comparison:
	- 27 training datasets
		- on which parameters of the heuristics were tuned)
	- **30 independent datasets**
		- which were not seen during optimization
	- Goals:
		- **See which heuristics perform best**
		- determine good parameter values for parametrized functions

TECHNISCHE Best Parameter Settings UNIVERSITÄT **DARMSTADT** for m-estimate: $m = 22.5$ m-Estimate $\mathbf P$ for relative cost metric: $c = 0.342$ **Relative Linear Cost Metric** D θ $\overline{0}$ $\overline{0}$ N 0 Machine Learning and Data Mining | Learning Rule Sets 16 V3.0 | J. Fürnkranz $\left\langle \right\rangle$

Empirical Comparison of Different Heuristics

- Ripper is best, but uses pruning (the others don't)
- the optimized parameters for the m-estimate and the relative cost metric perform better than all other heuristics
	- **also on the 30 datasets on which they were not optimized**
- some heuristics clearly overfit (bad performance with large rules)
- WRA over-generalizes (bad performance with small rules)

LeGo Approach to Rule Learning

- General framework for aggregating local patterns to global models
	- **Example 1 Figure 1 Figu**

Overfitting

Overfitting

Given

- a fairly general model class
- **enough degrees of freedom**
- you can always find a model that explains the data
	- **e** even if the data contains error (noise in the data)
	- **I** in rule learning: each example is a rule
- Such concepts do not generalize well! \rightarrow Pruning

Overfitting - Illustration

Overfitting Avoidance

- A perfect fit to the data is not always a good idea
	- data could be imprecise
		- e.g., random noise
	- the hypothesis space may be inadequate
		- a perfect fit to the data might not even be possible
		- or it may be possible but with bad generalization properties (e.g., generating one rule for each training example)
- Thus it is often a good idea to avoid a perfect fit of the data
	- fitting polynomials so that
		- not all points are exactly on the curve
	- **E** learning concepts so that
		- not all positive examples have to be covered by the theory
		- some negative examples may be covered by the theory

Overfitting Avoidance

- learning concepts so that
	- not all positive examples have to be covered by the theory
	- **some negative examples may be covered by the theory**

Complexity of Concepts

- For simpler concepts there is less danger that they are able to overfit the data
	- for a polynomial of degree *n* one can choose *n*+1 parameters in order to fit the data points
- \rightarrow many learning algorithms focus on learning simple concepts
	- a short rule that covers many positive examples (but possibly also a few negatives) is often better than a long rule that covers only a few positive examples
- Pruning: Complex rules will be simplified
	- **Pre-Pruning:**
		- **during learning**
	- **Post-Pruning:**
		- **after learning**

Pre-Pruning

- keep a theory simple *while* it is learned
	- **-** decide when to stop adding conditions to a rule (*relax consistency* constraint)
	- **decide when to stop adding** rules to a theory (*relax completeness* constraint)
	- **E** efficient but not accurate

Pre-Pruning Heuristics

1. Thresholding a heuristic value

- **P** require a certain minimum value of the search heuristic
- e.g.: Precision > 0.8.
- 2. Foil's Minimum Description Length Criterion
	- the length of the theory plus the exceptions (misclassified examples) must be shorter than the length of the examples by themselves
	- lengths are measured in bits (information content)
- 3. CN2's Significance Test
	- tests whether the distribution of the examples covered by a rule deviates significantly from the distribution of the examples in the entire training set
	- **F** if not, discard the rule

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Minimum Coverage Filtering

filter rules that do not cover a minimum number of

positive examples (support) all examples (coverage)

Support/Confidence Filtering

- *basic idea:* filter rules that
	- **Cover not enough positive** examples (*p < suppmin*)
	- are not precise enough $(h_{prec} < conf_{min})$
- *effects:*
	- all but a region around $(0,P)$ is filtered

 \rightarrow we will return to support/confidence in the context of association rule learning algorithms!

 α

N

CN2's likelihood ratio statistics

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$$
h_{LRS} = 2(p \log \frac{p}{e_p} + n \log \frac{n}{e_n})
$$

$$
e_p = (p+n)\frac{P}{P+N}; \quad e_n = (p+n)\frac{N}{P+N}
$$

are the expected number of positive and negative example in the $p+n$ covered examples.

- *basic idea:* measure significant deviation from prior probability distribution
- *effects:*
	- non-linear isometrics
		- **Similar to m-estimate**
		- **but prefer rules near the** edges
	- **distributed** χ^2
	- significance levels 95% (dark) and 99% (light grey)

Correlation

- *basic idea:* measure correlation coefficient of predictions with target
- *effects:*
	- **non-linear isometrics**
	- **in comparison to WRA**
		- **prefers rules near the edges**
		- steepness of connection of intersections with edges increases
	- equivalent to χ^2
	- grey area $=$ cutoff of 0.3

$$
h_{Corr} = \frac{p\left(N-n\right) - \left(P-p\right)n}{\sqrt{PN\left(p+n\right)\left(P-p+N-n\right)}}
$$

MDL-Pruning in Foil

- based on the Minimum Description Length-Principle (MDL)
	- **Examplerhist is it more effective to transmit the rule or the covered examples?**
		- compute the information contents of the rule (in bits)
		- compute the information contents of the examples (in bits)
		- if the rule needs more bits than the examples it covers, on can directly transmit the examples \rightarrow no need to further refine the rule
	- Details \rightarrow (Quinlan, 1990)
- doesn't work all that well
	- **T** if rules have expections (i.e., are inconsistent), the negative examples must be encoded as well
		- they must be transmitted, otherwise the receiver could not reconstruct which examples do not conform to the rule
	- finding a minimal encoding (in the information-theoretic sense) is practically impossible

Foil's MDL-based Stopping Criterion

costs for transmitting how many examples we have (can be ignored)

basic idea:

compare the encoding length of the rule *l(r)* to the encoding length h_{MDL} of the example.

- we assume $l(r) = c$ constant
- *effects:*
	- **E** equivalent to filtering on support
	- because function only depends on *p*

PN

p

costs for transmitting which of the *P+N*

 $h_{MDL} = \log_2(P+N) + \log_2\left(P+N\right)$

Anomaly of Foil's Stopping criterion

- We have tacitly assumed *N > P*...
- h_{MDL} assumes its maximum at $p = (P+N)/2$
	- **thus, for** $P > N$ **, the maximum is not on top!**

there may be rules

- **of equal length**
- covering the same number of negative examples
- so that the rule covering fewer positive examples is acceptable
- but the rule covering more positive examples is not!

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How Foil Works

- \rightarrow Foil (almost) implements Support/Confidence Filtering (will be explained later \rightarrow association rules)
	- filtering of rules with no information gain
		- **a** after each refinement step, the region of acceptable rules is adjusted as in precision/ confidence filtering
	- filtering of rules that exceed rule length
		- after each refinement step, the region of acceptable rules adjusted as in support filtering

Pre-Pruning Systems

■ Foil:

- **Search heuristic: Foil Gain**
- **Pruning: MDL-Based**

CN2:

- **Search heuristic: Laplace**
- **Pruning: Likelihood Ratio**
- Fossil:
	- **Search heuristic: Correlation**
	- **Pruning: Threshold**

Post Pruning

Post-Pruning: Example

Post-Pruning: Example

Reduced Error Pruning

- basic idea
	- optimize the accuracy of a rule set on a separate pruning set
	- 1. split training data into a growing and a pruning set
	- 2. learn a complete and consistent rule set covering all positive examples and no negative examples
	- 3. as long as the error on the pruning set does not increase
		- delete condition or rule that results in the largest reduction of error on the pruning set
	- 4. return the remaining rules
- REP is accurate but not efficient
	- \blacksquare O(n^4)

Incremental Reduced Error Pruning

Incremental Reduced Error Pruning

Prune each rule right after it is learned:

- 1. split training data into a growing and a pruning set
- 2. learn a consistent rule covering only positive examples
- 3. delete conditions as long as the error on the pruning set does not increase
- 4. if the rule is better than the default rule
	- add the rule to the rule set
	- goto 1.
- More accurate, much more efficient
	- because it does not learn overly complex intermediate concept
	- REP: $O(n^4)$ *)* I-REP: $O(n \log^2 n)$
- Subsequently used in RIPPER rule learner (Cohen, 1995)
	- JRip in Weka

Multi-Class Classification

Property of Interest ("class variable")

Multi-class problems

- GOAL: discriminate *c* classes from each other
- PROBLEM: many learning algorithms are only suitable for binary (2-class) problems
- SOLUTION: *"Class binarization":*

Transform an *c*-class problem into a series of 2 class problems

Class Binarization for Rule Learning

None

- **-** class of a rule is defined by the majority of covered examples
- decision lists, CN2 (Clark & Niblett 1989)

One-against-all / unordered

- foreach class c: label its examples positive, all others negative
- CN2 (Clark & Boswell 1991), Ripper -a unordered
- Another variant in Ripper sorts the classes first and learns first against rest - remove first - repeat
- Pairwise Classification / one-vs-one
	- Learn one rule-set for each *pair* of classes
- **Error Correcting Output Codes (Dietterich & Bakiri, 1995)**
	- generalized by (Allwein, Schapire, & Singer, JMLR 2000)
		- \rightarrow Ensemble Methods

One-against-all binarization

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Treat each class as a separate concept:

- **c** binary problems, one for each class
- **label examples of one class positive, all others negative**

Prediction

- It can happen that multiple rules fire for a example
	- no problem for concept learning (all rules say +)
	- **but problematic for multi-class learning**
		- because each rule may predict a different class
	- **Typical solution:**
		- use rule with the highest (Laplace) precision for prediction
	- **nable in the complex approaches are possible: e.g., voting**
- It can happen that no rule fires on a example
	- no problem for concept learning (the example is then -)
	- **but problematic for multi-class learning**
		- **E** because it remains unclear which class to select
	- **Typical solution: predict the largest class**
	- more complex approaches:
		- e.g., rule stretching: find the most similar rule to an example
			- \rightarrow similarity-based learning methods

Pairwise Classification

- *c*(*c*-1)/2 problems
- **E** each class against each other class

- $\mathbf v$ smaller training sets
- $\mathbf v$ simpler decision boundaries
- $\mathbf{\cdot}$ larger margins

Prediction

Voting:

- **as in a sports tournament:**
	- **each class is a player**
	- each player plays each other player, i.e., for each pair of classes we get a prediction which class "wins"
	- the winner receives a point
	- the class with the most points is predicted
		- **tie breaks, e.g., in favor of larger classes**
- Weighted voting:
	- the vote of each theory is proportional to its own estimate of its correctness
	- e.g., proportional to proportion of examples of the predicted class covered by the rule that makes the prediction

Accuracy

- **error rates on 20** datasets with 4 or more classes
	- **10 significantly better** $(p > 0.99,$ McNemar)
	- **2** significantly better $(p > 0.95)$
	- 8 equal
	- never (significantly) worse

Advantages of the Pairwise Approach

Accuracy

- **better than one-against-all** (also in independent studies)
- improvement appr. on par with 10 boosting iterations
- **Example Size Reduction**
	- **Subtasks might fit into memory** where entire task does not

■ Stability

- **Simpler boundaries/concepts** with possibly larger margins
- **Understandability**
	- **Similar to pairwise ranking as** recommended by Pyle (1999)
- Parallelizable
	- each task is independent of all other tasks
- **Modularity**
	- train binary classifiers once
	- **Can be used with different** combiners
- Ranking ability
	- provides a ranking of classes for free
- **Complexity?**
	- **we have to learn a quadratic** number of theories...
	- but with fewer examples

Training Complexity of PC

Lemma: The total number of training examples for all binary **Lemma:** The total number of training examples for all binary classifiers in a pairwise classification ensemble is (*c–*1)∙*n* classifiers in a pairwise classification ensemble is (*c–*1)∙*n*

Proof:

• each of the *n* training examples occurs in all binary tasks where its class is paired with one of the other *c−*1 classes

Theorem: For learning algorithms with at least linear complexity, **Theorem:** For learning algorithms with at least linear complexity, pairwise classification is more efficient than one-against-all. pairwise classification is more efficient than one-against-all.

Proof Sketch:

- one-against-all binarization needs a total of *c*∙*n* examples
- fewer training examples are distributed over more classifiers
- more small training sets are faster to train than few large training sets
- for complexity $f(n) = n^{\circ}$ ($o > 1$): $o > 1 \rightarrow \sum n_i^{\circ} < (\sum n_i)^{\circ}$

Preference Data

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Class Information encodes Preferences

General Label Preference Learning Problem

Label Ranking

- Preference learning scenario in which
	- **Contexts are characterized by features**
	- no information about the items is given except a unique name (a label)

GIVEN: GIVEN:

- a set of *labels*: a set of *labels*:
- a set of *contexts*: a set of *contexts*:
- for each training context *ek*: for each training context *ek*:
	- a set of *preferences* a set of *preferences*

$$
L = {\lambda_i | i = 1 \dots c}
$$

$$
E = {e_k | k = 1 \dots n}
$$

$$
\boldsymbol{P}_k = \left\{ \lambda_i \boldsymbol{\succ}_k \lambda_j \right\} \boldsymbol{\subseteq} \boldsymbol{L} \boldsymbol{X} \boldsymbol{L}
$$

FIND: FIND:

a label ranking function that orders the labels for any given context context

Pairwise Preference Learning

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Regression

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Rule-Based Regression

- Regression trees are quite successful
- Work on directly learning regression rules was not yet able to match that performance
	- **Main Problem: How to define a good heuristic?**
- **Transformation approach:**
	- **Reduce regression to classification**
	- **use the idea of** ε **-insensitive loss functions** proposed for SVMS:
	- all examples in an ε -environment of the value predicted in the rule head are considered to be positive, all others negative
	- **T** rules can then be learned using regular heuristics for classification rules

$$
\begin{vmatrix} negative\\ |y - y_r| > t, \end{vmatrix}
$$

$$
|y_r| = 0 - \left|\frac{\text{positive}}{|y - y_r|} \le t_r\right|
$$

 \mathbf{v} $-$

$$
\begin{array}{c}\n\text{negative} \\
|y - y_{r}| > t_{r}\n\end{array}
$$

Application Example: Venus Express Power Consumption

Goal

- Learn a model of the energy consumption of the heating system of the Venus express
- Approach
	- Information about the consumption is available in hindsight
		- **Can be used to train a model**
	- Best results obtained with ensembles of regression trees
		- **local differences cannot be modeled**
		- **but trends can be captured well**
- Partner
	- **ESA / ESOC**
	- University of Cordoba

Summary

- Rules can be learned via top-down hill-climbing
	- **add one condition at a time until the rule covers no more negative exs.**
- **Heuristics are needed for guiding the search**
	- can be visualize through isometrics in coverage space
- Rule Sets can be learned one rule at a time
	- **using the covering or separate-and conquer strategy**
- Overfitting is a serious problem for all machine learning algorithms too close a fit to the training data may result in bad generalizations
- Pruning can be used to fight overfitting
	- **Pre-pruning and post-pruning can be efficiently integrated**
- Multi-class problems can be addressed by multiple rule sets
	- **-** one-against-all classification or pairwise classification