Inductive Rule Learning

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	- **Version Spaces**
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Rule-based Classifiers

- A classifier basically is a function that computes the output (the *class*) from the input (the *attribute values*)
- Rule learning tries to represent this function in the form of (a set of) IF-THEN rules

IF (att i = val iI) AND (att j = val jJ) THEN class k

- Coverage
	- A rule is said to *cover* an example if the example satisfies the conditions of the rule.
- Correctness
	- *completeness*: Each example should be covered by (at least) one rule
	- **Consistency**: For each example, the predicted class should be identical to the true class.

A sample task

● Task:

■ Find a rule set that correctly predicts the dependent variable from the observed variables

A Simple Solution

A Better Solution

- Rule sets are at least as expressive as decision trees
	- **a** decision tree can be viewed as a set of non-overlapping rules
	- typically learned via *divide-and-conquer* algorithms (recursive partitioning)
- Many concepts have a shorter description as a rule set
	- exceptions: if one or more attributes are relevant for the classification of *all* examples (e.g., parity)

Generality Relation

- Rule r1 is *more general* than r2
	- **if it covers all examples that are covered by r1.**
- Rule r1 is *more specific* than r2
	- **if r2 is more general than r1.**
- Rule r1 is equivalent to r2
	- \blacksquare if it is more specific and more general than r2.
- Examples: IF size $>$ 5 THEN + IF size > 3 THEN +

```
IF outlook = sunny AND windy = false THEN +IF outlook = sunny THEN +
```
IF animal $=$ mammal THFN $+$ IF feeds children = milk THEN $+$

Structured Hypothesis Space

■ The availability of a generality relation allows to structure the hypothesis space:

Testing for Generality

- In general, we cannot check the generality of theories
	- We do not have all examples of the domain available (and it would be too expensive to generate them)
- For single rules, we can approximate generality via a *syntactic generality check*:
	- **Rule r1 is** *more general* **than r2 if the set of conditions of r1** forms a *subset* of the set of conditions of r2.
	- Why is this only an approximation?
- For the general case, computable generality relations will rarely be available
	- E.g., rule sets
- Structured hypothesis spaces and version spaces are also a theoretical model for learning

Algorithm Find-S

Note: when the first positive examples is encountered, step II.b) reduces to converting the example into a rule

Properties of Find-S

● completeness:

- **h** covers all positive examples
- consistency:
	- **h** will not cover any negative training examples
	- **but only if the hypothesis space contains a target concept** (i.e., there is a single conjunctive rule that describes the target concept)

• Properties:

- no way of knowing whether it has found the target concept (there might be more than one theory that are complete and consistent)
- \blacksquare it prefers more specific hypothesis (it will never generalize unless forced by a training example)
- **I** it only maintains one specific hypothesis (in other hypothesis languages there might be more than one)

- The Version Space V is the set of all hypotheses that
	- cover all positive examples (*completeness*)
	- do not cover any negative examples (*consistency*)
- For structured hypothesis spaces there is an efficient representation consisting of
	- the general boundary G
		- all hypotheses in V for which no generalization is in V
	- the specific boundary S
		- all hypotheses in V for which no specialization is in V
- a hypothesis that is neither in G nor in S is
	- a generalization of at least one hypothesis in S
	- a specialization of at least one hypothesis in G

Candidate Elimination Algorithm

- \overline{G} = set of maximally general hypotheses
	- S = set of maximally specific hypotheses
- For each training example e
	- \blacksquare if e is positive
		- For each hypothesis g in G that does not cover e
			- **F** remove g from G
		- For each hypothesis s in S that does not cover e
			- **F** remove s from S
			- $S = S U$ all hypotheses h such that
				- h is a minimal generalization of s
				- h covers e
				- some hypothesis in G is more general than h
			- **F** remove from S any hypothesis that is more general than another hypothesis in S

Candidate Elimination Algorithm (Ctd.)

\blacksquare if e is negative

- For each hypothesis s in S that covers e
	- **F** remove s from S
- For each hypothesis g in G that covers e
	- **F** remove g from G
	- G = G U all hypotheses h such that
		- h is a minimal specialization of g
		- h does not e
		- some hypothesis in S is more specific than h
	- **F** remove from G any hypothesis that is less general than another hypothesis in G

Example

- $S_0: \{ \langle \Theta, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset \rangle \}$ G₀: { <?, ?, ?, ?, ?, ?> }
- S_1 : { \le sunny, hot, normal, strong, warm, same > } G_1 : { <?, ?, ?, ?, ?, ?> }
- S_2 : { \langle sunny, hot, ?, strong, warm, same > } G_2 : { <?, ?, ?, ?, ?, ?> }
- S_3 : { \langle sunny, hot, ?, strong, warm, same > } G₃: { \langle sunny, ?, ?, ?, ?, ? > $\langle 2, \text{hot}, 2, 2, 2, 2 \rangle$ $\{2, 2, 2, 2, 2, 3, \text{same} > \}$
- S_4 : { <sunny, hot, ?, strong, ?, ? > } G₄: { \langle \langle sunny, ?, ?, ?, ?, ? > $\langle 2, \text{hot}, 2, 2, 2, 2 \rangle$

How to Classify these Examples?

• Version Space:

• How to Classify these Examples?

Properties

- Convergence towards target theory
	- If $S = G$
- Using partially learned concepts
	- **an example that matches all elements in S must be a member** of the target concept
	- an example that matches no element in G cannot be a member of the target concept
	- examples that match parts of S and G are undecidable
- no need to remember examples (*incremental* learning)
- **Assumptions**
	- no errors in the training set
	- the hypothesis space contains the target theory
	- **Peractical only if generality relation is (efficiently) computable**

Terminology

● training examples

- *P*: total number of positive examples
- *N*: total number of negative examples
- examples covered by the rule (predicted positive)
	- true positives *p*: positive examples covered by the rule
	- false positives *n*: negative examples covered by the rule
- examples not covered the rule (predicted negative)
	- false negatives *P-p*: positive examples not covered by the rule
	- true negatives *N-n*: negative examples not covered by the rule

Coverage Spaces

• good tools for visualizing properties of covering algorithms

● each point is a theory covering *p* positive and *n* negative examples

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
	- **a** adding a condition to a rule specializes the theory
	- **adding a new rule to a theory generalizes the theory**
- practical algorithms use different approaches
	- **COVETING OF SEPARATE-and-conquer algorithms**

Separate-and-Conquer Rule Learning

- **Learn a set of rules, one by one**
	- 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: If E is non-empty, goto 2.
- One of the oldest family of learning algorithms
	- goes back AQ (Michalski, 60s)
	- FRINGE, PRISM and CN2: relation to decision trees (80s)
	- popularized in ILP (FOIL and PROGOL, 90s)
	- RIPPER brought in good noise-handling
- Different learners differ in how they find a single rule

• language bias:

- ◆ which type of conditions are allowed (static)
- which combinations of condictions are allowed (dynamic)
- search bias:
	- ◆ search heuristics
	- ◆ search algorithm (greedy, stochastic, exhaustive)
	- ◆ search strategy (topdown, bottom-up)
- overfitting avoidance bias:
	- ◆ pre-pruning (stopping criteria)
	- ◆ post-pruning

Covering Strategy

- Covering or Separate-and-Conquer rule learning learning algorithms learn one rule at a time
- This corresponds to a path in coverage space:
	- 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)

Top-Down Hill-Climbing

■ Top-Down: A rule is successively *specialized*

- 1. Start with an empty rule R that covers all examples
- 2. Evaluate all possible ways to add a condition to R
- 3. Choose the best one (according to some heuristic)
- 4. If R is satisfactory, return it
- 5. Else goto 2.

Almost all greedy s&c rule learning systems use this strategy

Top-Down Hill-Climbing

Successively extends a rule by adding conditions

- This corresponds to a path in coverage space:
	- \blacksquare The rule p: -true covers all examples (universal theory)
	- **Adding a condition never** increases *p* or *n* (specialization)
	- \blacksquare The rule $p:$ -false covers no examples (empty theory)

which conditions are selected depends on a *heuristic function* that estimates the quality of the rule

Rule Learning Heuristics

• Adding a rule should

- **EXT** increase the number of covered negative examples as little as possible (do not decrease *consistency*)
- **nd increase the number of covered positive examples as much** as possible (increase *completeness*)
- An evaluation heuristic should therefore trade off these two extremes
	- **Example: Laplace heuristic**

$$
h_{Lap} = \frac{p+1}{p+n+2}
$$

- grows with *p*∞
- \bullet grows with $n{\rightarrow}0$
- Note: Precision is not a good heuristic. Why?

$$
h_{\text{Prec}} = \frac{p}{p+n}
$$

Example

- Heuristics Precision and Laplace
	- add the condition Outlook= Overcast to the (empty) rule
	- **stop and try to learn the next rule**
- Heuristic Accuracy / p-n
	- \blacksquare adds Humidity = Normal
	- **E** continue to refine the rule (until no covered negative)

Isometrics in Coverage Space

● Isometrics are lines that connect points for which a function in p and n has equal values

 Examples: Isometrics for heuristics *h p = p* and *h n* $= -n$

Precision (Confidence)

$$
h_{Prec} = \frac{p}{p+n}
$$

- *basic idea:* percentage of positive examples among covered examples
- *effects:*
	- **•** rotation around origin (0,0)
	- all rules with same angle equivalent
	- **n** in particular, all rules on P/N axes are equivalent

Entropy and Gini Index

 $\big)$

$$
h_{Ent} = -\left(\frac{p}{p+n}\log_2\frac{p}{p+n} + \frac{n}{p+n}\log_2\frac{n}{p+n}\right)
$$

$$
h_{Gini} = 1 - \left(\frac{p}{p+n}\right)^2 - \left(\frac{n}{p+n}\right)^2 \approx \frac{pn}{(p+n)^2}
$$

effects:

- **E** entropy and Gini index are equivalent
- like precision, isometrics rotate around (0,0)
- **EX isometrics are symmetric** around 45° line
- a rule that only covers negative examples is as good as a rule that only covers positives

Accuracy

$$
h_{Acc} = \frac{p + (N - n)}{P + N} \simeq p - n
$$

● *basic idea:* percentage of correct classifications (*covered positives* plus *uncovered negatives*)

● *effects:*

- **E** isometrics are parallel to 45° line
- **covering one positive** example is as good as not covering one negative example

Weighted Relative Accuracy

$$
h_{Acc} = \frac{p+n}{P+N} \left(\frac{p}{p+n} - \frac{P}{P+N}\right) \approx \frac{p}{P} - \frac{n}{N}
$$

- *basic idea:* normalize accuracy with the class distribution
- *effects:*
	- **E** isometrics are parallel to diagonal
	- covering $x%$ of the positive examples is as good as not covering *x%* of the negative examples

Linear Cost Metric

- Accuracy and weighted relative accuracy are only two special cases of the general case with linear costs:
	- **Costs c mean that covering 1 positive example is** equivalent to not covering (1-*c*)/*c* negative examples

- The general form is then $h_{cost} = cp-(1-c)n$
	- \bullet the isometrics of h_{cost} are parallel lines with slope $(1\text{-}c)/c$

Laplace-Estimate

$$
h_{Lap} = \frac{p+1}{p+n+2}
$$

- *basic idea:* precision, but count coverage for positive and negative examples starting with 1 instead $of $0$$
- *effects:*
	- origin at $(-1,-1)$
	- **different values on** $p=0$ or $n=0$ axes
	- not equivalent to precision

m-Estimate

● *basic idea:* initialize the counts with *m* examples in total, distributed according to the prior distribution *P/(P+N)* of *p* and *n*.

● *effects:*

- **•** origin shifts to (*-mP*/(*P+N*)*,-mN*/(*P+N*))
- with increasing *m*, the lines become more and more parallel
- **can be re-interpreted as a** trade-off between WRA and confidence

Generalized m-Estimate

- One can re-interpret the m-Estimate:
	- Re-interpret $c = N/(P+N)$ as a cost factor like in the general cost metric
	- Re-interpret *m* as a trade-off between precision and costmetric
		- \bullet $m = 0$: precision (independent of cost factor)
		- *m*→∞: the isometrics converge towards the parallel isometrics of the cost metric
- Thus, the m-Estimate may be viewed as a means of trading off between precision and the cost metric

Optimizing Precision

- Precision tries to pick the steepest continuation of the curve
	- **does not assume any costs**

Optimizing Accuracy

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

Summary of Rule Learning Heuristics

- There are two basic types of (linear) heuristics.
	- **Pariciple 1 precision:** rotation around the origin
	- **Cost metrics**: parallel lines
- They have different goals
	- **Periculary Precision picks the steepest continuation for the curve for** unkown costs
	- linear cost metrics pick the best point according to known or assumed costs
- The m-heuristic may be interpreted as a trade-off between the two prototypes
	- **Perameter c chooses the cost model**
	- **•** parameter *m* chooses the "degree of parallelism"

Foil Gain

(*c* is the precision of the parent clause)

A Pathology for Top-Down Learning

- Parity problems (e.g. XOR)
	- *r* relevant binary attributes
	- *s* irrelevant binary attributes
	- **e** each of the $n = r + s$ attributes has values 0/1 with probability $\frac{1}{2}$
	- **an example is positive if the number of 1's in the relevant** attributes is even, negative otherwise
- **Problem for top-down learning:**
	- by construction, each condition of the form $a_i = 0$ or $a_i = 1$ covers approximately 50% positive and 50% negative examples
	- **•** irrespective of whether a_i is a relevant or an irrelevant attribute
	- ➔ top-down hill-climbing cannot learn this type of concept
- **Typical recommendation:**
	- use bottom-up learning for such problems

Bottom-Up Approach: Motivation

Bottom-Up Hill-Climbing

- Simple inversion of top-down hill-climbing
- A rule is successively *generalized*

1. Start with an empty rule R that covers all examples 2. Evaluate all possible ways to add a condition to R 3. Choose the best one 4. If R is satisfactory, return it a fully specialized a single example delete

5. Else goto 2.

A Pathology of Bottom-Up Hill-Climbing

- Target concept att1 = 1 not (reliably) learnable with bottom-up hill-climbing
- **•** because no generalization of a seed example will increase coverage
- **Hence you either stop or make an arbitrary choice (e.g.,** delete attribute 1)

Bottom-Up Rule Learning Algorithms

- AQ-type:
	- **select a seed example and search the space of its** generalizations
	- **BUT: search this space top-down**
	- Examples: AQ (Michalski 1969), Progol (Muggleton 1995)
- based on least general generalizations (Iggs)
	- **greedy bottom-up hill-climbing**
	- **BUT: expensive generalization operator** (*lgg/rlgg* of *pairs* of seed examples)
	- **Examples: Golem (Muggleton & Feng 1990), DLG (Webb 1992), RISE** (Domingos 1995)
- Incremental Pruning of Rules:
	- greedy bottom-up hill-climbing via deleting conditions
	- BUT: start at point previously reached via top-down specialization
	- Examples: I-REP (Fürnkranz & Widmer 1994), Ripper (Cohen 1995)

Overfitting

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

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

 \bigcirc ... Literals

WWW ... Post-Pruning Decisions

Pre-Proming Decisions

Pre-Pruning Heuristics

- Threshold
	- **Part and the require a certain minimum value of the search heuristic**
	- e.g.: Laplace > 0.8 .
- 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
	- **E** lengths are measured in bits (information content)
- CN2's Significance Test
	- **the set is whether the distribution of the examples covered by a** rule deviates significantly from the distribution of the examples in the entire training set
	- **n** if not, discard the rule

Minimum Coverage Filtering

filter rules that do not cover a minimum number of

positive examples all examples

Support/Confidence Filtering

- 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

CN2's likelihood ratio statistics

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

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

- *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)

Fossil's Correlation

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

- *basic idea:* measure correlation coefficient of predictions with target
- *effects:*
	- non-linear isometrics
	- **n** 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

Foil's MDL-based Stopping Criterion

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

- *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

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
	- the rule covering fewer positive examples is acceptable
	- but the rule covering more positive examples is not!

Pre-Pruning Systems

● Foil:

- **Search heuristic: Foil Gain**
- **Pruning: MDL-Based**
- CN2:
	- Search heuristic: Laplace/m-heuristic
	- **Pruning: Likelihood Ratio**
- Fossil:
	- **Search heuristic: Correlation**
	- **Pruning: Threshold**

How Foil Works

- → Foil (almost) implements Support/Confidence Filtering
- **Filtering of rules with no** information gain
	- \bullet after each refinement ste the region of acceptable rules is adjusted as in precision/confidence filtering
- **Filtering of rules that** exceed the rule length
	- \bullet after each refinement ste the region of acceptable rules is adjusted as in support filtering

Post Pruning

- simplify a theory after it has been learned
- Reduced Error Pruning
	- **anaologous to decision trees**
		- Reserve part of the data for validation (pruning set)
		- Learn a rule set
		- Simplify rule set by deleting rules and conditions as long as this does not decrease accuracy on the validation set
- **accurate but not efficient**

$$
\bullet \ \ O(n^4)
$$

Reduced Error Pruning

Incremental Reduced Error Pruning

- Prune each rule right after it is learned:
	- 1. split data into a training 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 it to the rule set and goto 1.
- More accurate, much more efficient
	- **EXTERN** because it does not learn overly complex intermediate concept
	- REP: $O(n^4)$ I-REP: $O(n \log^2 n)$
- Subsequently used in the RIPPER (JRip in Weka) rule learner (Cohen, 1995)

Accuracy

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
- Ordered
	- sort classes learn first against rest remove first repeat
	- Ripper (Cohen 1995)
- Error Correcting Output Codes (Dietterich & Bakiri, 1995)
	- **generalized by (Allwein, Schapire, & Singer, JMLR 2000)**

One-against-all binarization

Treat each class as a separate concept:

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

Round Robin Learning (aka *Pairwise Classification*)

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

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

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

Yes, but isn't that expensive?

YES:

We have $O(c^2)$ learning problems...

but NO:

the total *training* effort is smaller than for the *c* learning problems in the one-against-all setting!

● Fine Print :

- single round robin
	- more rounds add a constant factor
- **training effort only**
	- test-time and memory are still quadratic
	- BUT: theories to test may be simpler

Advantages of Round Robin

- Accuracy
	- **never lost against one**against-all
	- **often significantly more** accurate
- Efficiency
	- **proven to be faster than,** e.g., one-against-all, ECOC, boosting...
	- **higher gains for slower** base algorithms
- Understandability
	- simpler boundaries/concepts
	- **similar to pairwise ranking as** recommended by Pyle (1999)
- Example Size Reduction
	- \blacksquare each binary task is considerably smaller than original data
	- **subtasks might fit into** memory where entire task does not
- Easily parallelizable
	- \blacksquare each task is independent of all other tasks