Finding Explanations: Rules!

- Propositional Rules:
    - Rules from Decision Trees
    - Rule Sets and Lists
    - Geometrical Rules
    - CN2
- First Order Rules:
    - Inductive Logic Programming
    - FOIL

Propositional Rules

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Either true or false (under an interpretation).

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Example:

$$\text{IF} \;\; x_1 \leq 10 \;\; \text{AND} \;\; x_3 = red \;\; \text{THEN class A}$$

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Example:

$$\text{IF} \quad \underbrace{x_1 \leq 10 \;\; \text{AND} \;\; x_3 = red}_{\text{antecedent}} \quad \text{THEN} \quad \underbrace{\text{class A}}_{\text{consequent}}$$

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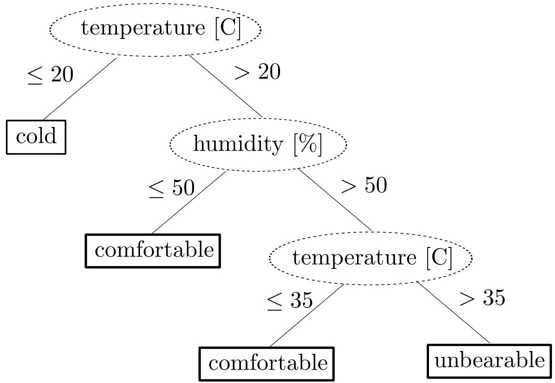
Propositional Rules

Atomic facts of propositional rules:

- constraints on numerical attributes, e.g. $<$, $\leq$, $=$, $\ldots$
- constraints on nominal attributes, e.g. $=$, $\in$ set
- constraints on ordinal attributes, e.g. $<$, $\in$ set, $\in$ range

Finding Propositional Rules in Data

Extracting Rules from Trees



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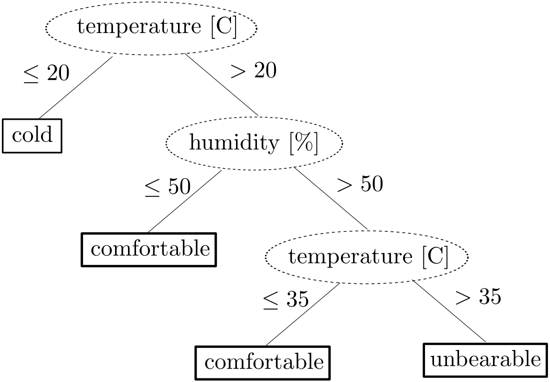

R_a : IF temperature ≤ 20 THEN class "cold"

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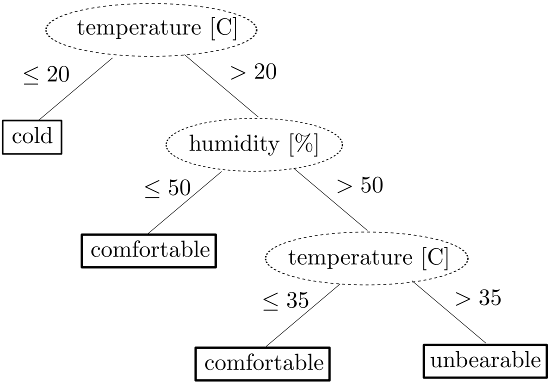

R_a : IF temperature ≤ 20 THEN class "cold"
R_b : IF temperature > 20 AND humidity ≤ 50 THEN class "comf."

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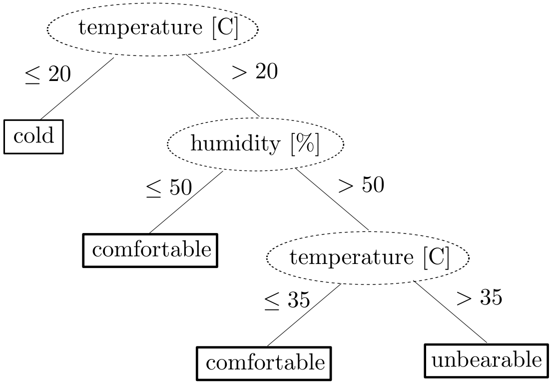

R_a : IF temperature ≤ 20 THEN class "cold"
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R_c : IF temperature $\in (20, 35]$ AND humidity > 50 THEN class "comf."

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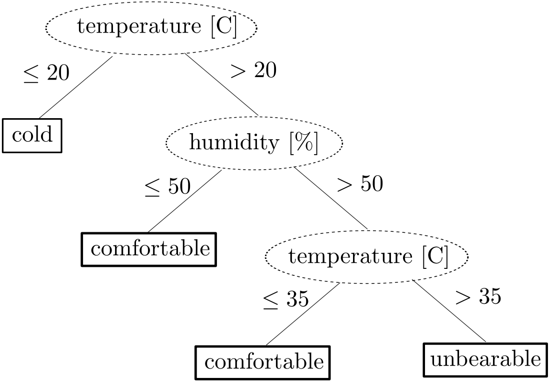

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R_b : IF temperature > 20 AND humidity ≤ 50 THEN class "comf."
R_c : IF temperature $\in (20, 35]$ AND humidity > 50 THEN class "comf."
R_d : IF temperature > 35 AND humidity > 50 THEN class "unbearable"

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Rules from Decision Tree are:

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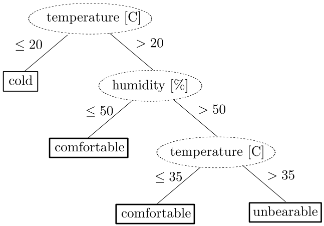

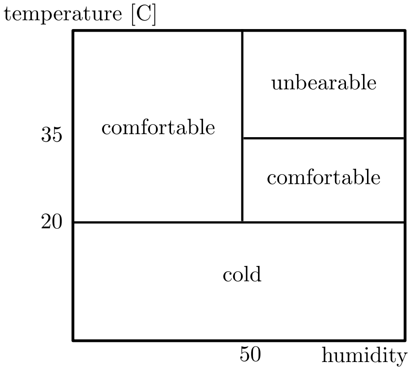

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- redundancy
  (constraints on splits appear in several rules.)

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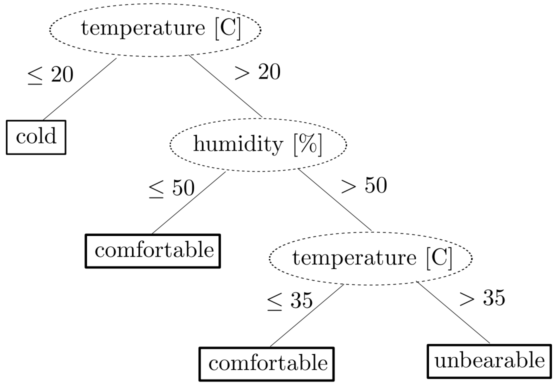

Non-redundant rule set:

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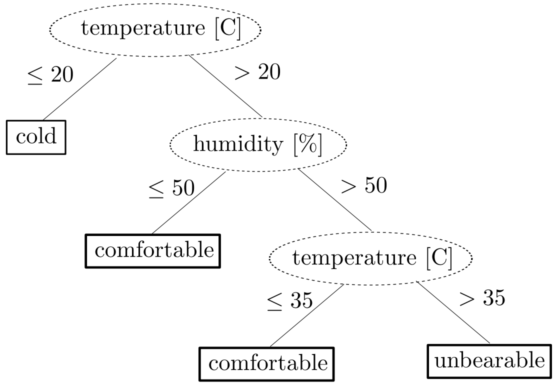

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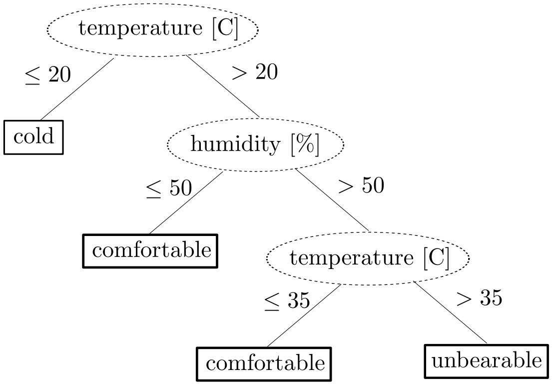

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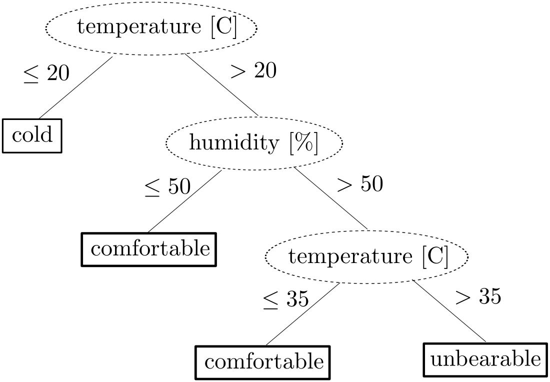

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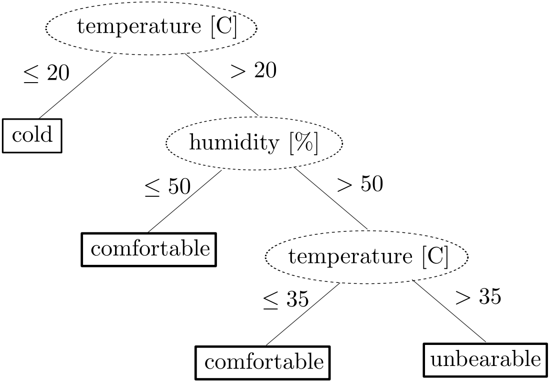

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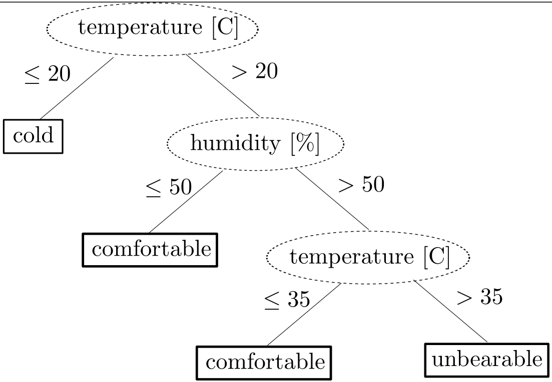
Extracting Ordered Rules from Trees



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R_4 : class = "unbearable"

↑ order of rules matters!

Extracting Ordered Rules from Trees

- previous example was heavily imbalanced tree.
- more balanced tree results in nested ordering of rules.
- in normal trees ordered rule extraction is considerably more complex.

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For a second example $(\vec{x}_2, k)$ with

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the rule is generalized:

$$\text{IF } x_1 \in [12, 12.3] \text{ AND } x_2 = 3.5 \text{ AND } x_3 \in \{'\text{red}', '\text{blue}'\} \text{ THEN class } k$$

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- and iteratively specialize the rule.

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- Many rule learning algorithms wrap the learning of one rule into an outer loop based on set covering strategy (sequential covering):
  - attempts to build most important rules first
  - iteratively adds smaller / less important rules

Geometrical Rule Learners

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- limited to numerical attributes (comparable ranges help, too)
- Goal:
  - Find rectangular (axes parallel) area(s) one by one that are occupied only by patterns of one class.
  - each such area represents a rule:

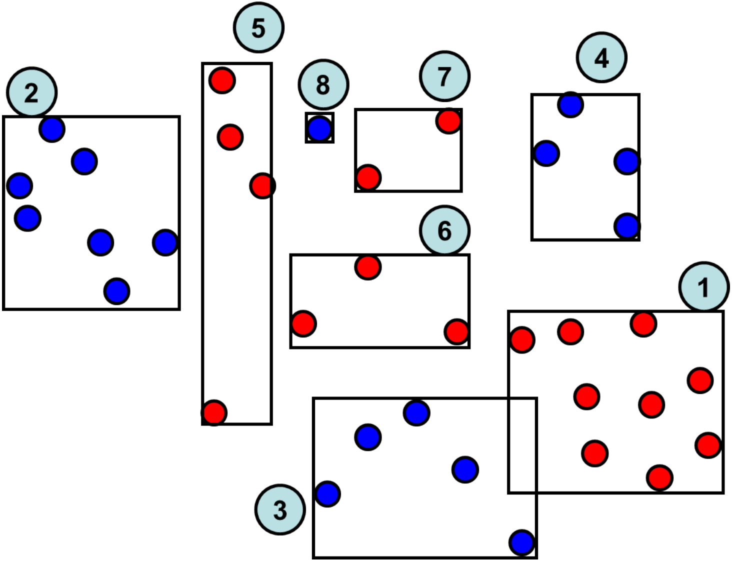
$$\text{IF } x_1 \in [a_1, b_1] \wedge \cdots \wedge x_n \in [a_n, b_n] \text{ THEN class } k$$

- Creates one rule after the other until no more useful rules can be built.

  To find one rule:
  - draw random starting point
  - form most specific rectangular hypothesis covering this point
  - While possible
    - find nearest neighbor of same class
    - generalize hypothesis (rectangle) to include this point
      (the latter may not be possible for all neighbors of the same class)

Geometrical Rule Learners

An example:



Geometrical Rule Learners: RecBF Learner

- Goal: Finding specific and general rules
  - Allows to estimate classification certainty
- RecBF algorithm: motivated by Neural Network Learning method
- Finds most specific within each (locally) most general rule
- Iterative algorithm
- (Much) faster than rule-by-rule approach.

BuildRuleSet

Algorithm RecBF(T)

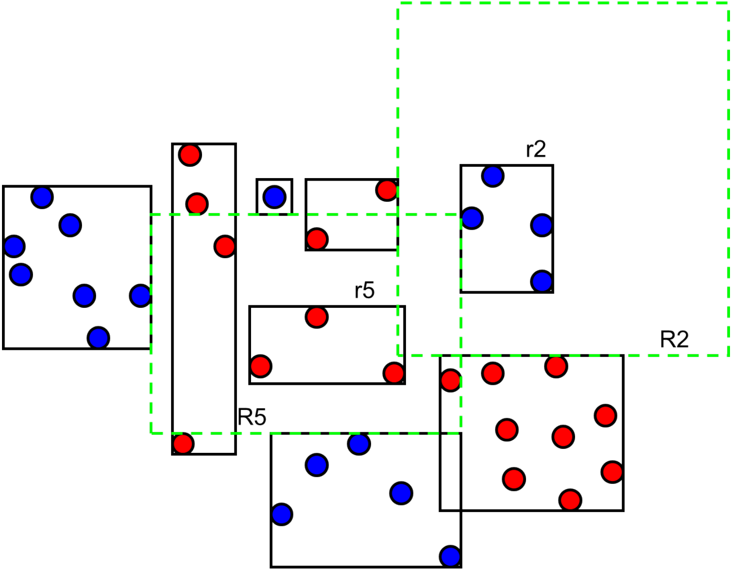
input: training data T

output: a general and specific rule set R matching T

$R = \emptyset$
while rules R are not stable
    $\forall(\vec{x}, k) \in T$
    if $\exists R^k \in R : \mathrm{covers}(R^k, \vec{x})$ **then**
        // Covered:
        $R^k.w++$ // increase weight
        $\mathrm{cover}(R^k, \vec{x})$
    else
        // Commit:
        $R = R \cup \mathrm{newRule}(\vec{x})$
    endif
    $\forall R^{k'} \in R : k \neq k' \wedge \mathrm{covers}(R^k, \vec{x})$:
        $\mathrm{shrink}(R^{k'}, \vec{x})$

RecBF Learner

An example:

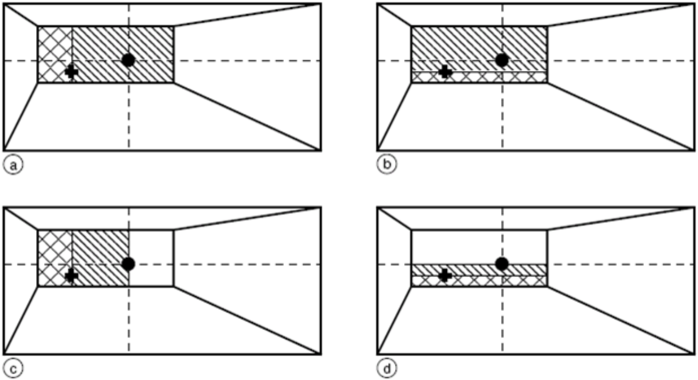


RecBF Learner: Operations

- Rule stability:
  - Algorithm converges guaranteed if training data is conflict free (Maximum: n iterations for n training patterns)
- Covered:
  - simple boundary test
  - Make sure specific rule R covers new $\vec{x}$: boundary expansion
- Commit:
  - Simple insert of most general rule R with corresponding most specific rule, centered on new training pattern
- Shrink:
  - Reducing rectangle to exclude conflicting pattern: n choices.
  - Heuristics:
    - maximize remaining volume
    - Avoid shrinkage of specific rule of R

RecBF Learner: Shrink

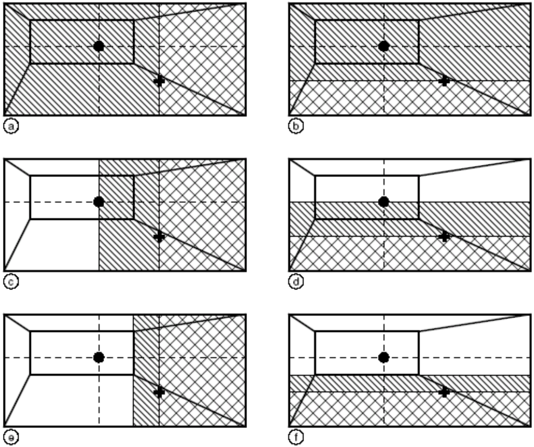
Options for Specialization of specialized rules:



(a,b): entire region considered,
(c,d): regions to anchor considered.

RecBF Learner: Shrink

Options for Specialization of general rules:



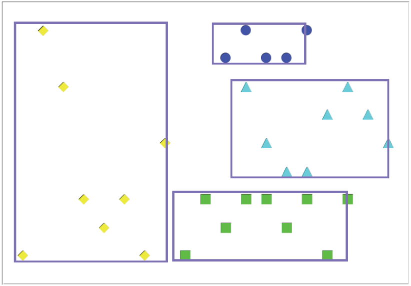
(a,b): entire region considered,
(c,d): regions to anchor considered,
(e,f): regions to “core” considered.

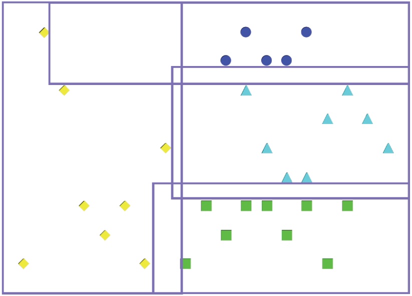
RecBF Learner: Operations

- Problems:
  - Depends on order of training examples
  - Shrink-procedure based on heuristics
- Properties
  - Explains all training pattern correctly
  - Most general rules depend on few attributes only
  - Most specific rules depend on all attributes

Note: Geometrical Sets of Rules

Examples[2] of Specialized and Generalized Rules:





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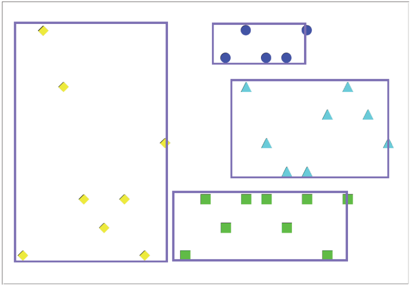

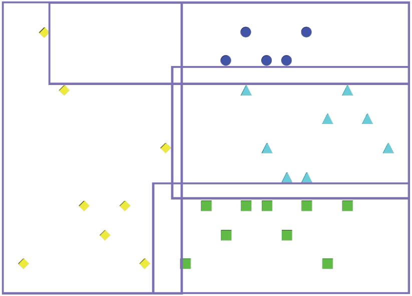

Are there more general (or special) rule sets?

[2] images from Peter Flach

Back to Propositional Rules:
CN2

The CN2 Rule Learning Algorithm

Peter Clark and Tim Niblett: **The CN2 Induction Algorithm**,
Machine Learning Journal, 3(4):261-283, 1989.

- prominent, early example of rule learning algorithm
- set covering approach
- greedy algorithm rule specialization
- simple heuristic for "most important" rule selection.

BuildRuleSet

Algorithm BuildRuleSet$(D, p_{\min})$

input:	training data D
parameter:	performance threshold $p_{\min}$
output:	a rule set R matching D with performance $\geq p_{\min}$

$R = \emptyset$
$D_{\text{rest}} = D$
while $(\text{Performance}(R, D_{\text{rest}}) < p_{\min})$
    $r = \text{FindOneGoodRule}(D_{\text{rest}})$
    $R = R \cup \{r\}$
    $D_{\text{rest}} = D_{\text{rest}} - \text{covered}(r, D_{\text{rest}})$
endwhile
return R

Alternative implementations by varying:

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```
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    R = R ∪ {r}
    D_rest = D_rest − covered(r, D_rest)
endwhile
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```

Alternative implementations by varying:

- performance measure?
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  (We could just use a decision tree learner and build only the 'best branch...)

Remark: Decision Tree Based Good Rule Finding

- Following (more than) one branch resembles a general-to-specific beam search:
  - Hypothesis (rule) is increasingly specified
  - At each branching point all possible specializations are considered
  - Choice of best branch can be made based on information gain, coverage, or mix of both
  - Class (rule post condition) depends on majority class at each point
- Greedy algorithm can produce sub-optimal solution
  - Beam search produces k candidate solutions (at each level only the k best branches are kept)
- Sometimes only learning rules of one class is sufficient (e.g. to model a minority class), default class = majority class.

FindOneGoodRule

Algorithm FindOneGoodRule(D_{rest})

input: (subset of) training data D_{rest}

output: one good rule r explaining some instances of the training data

```
h_best = true   // most general hypothesis
H_candidates = {h_best}
while H_candidates ≠ ∅
    H_candidates = specialize(H_candidates)
    h_best = arg max_{h ∈ H_candidates ∪ {h_best}} {Performance(h, D_rest)}
    update(H_candidates)   // clean up
endwhile
return 'IF h_best THEN arg max_k{|covered_k(h_best, D_rest)|}'
```

$h_{\text{best}} = \text{true}$ // most general hypothesis

$H_{\text{candidates}} = \{h_{\text{best}}\}$

while $H_{\text{candidates}} \neq \emptyset$

$\quad H_{\text{candidates}} = \text{specialize}\,(H_{\text{candidates}})$

$\quad h_{\text{best}} = \arg\max_{h \in H_{\text{candidates}} \cup \{h_{\text{best}}\}} \{\text{Performance}(h, D_{\text{rest}})\}$

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endwhile

return $'\text{IF } h_{\text{best}} \text{ THEN } \arg\max_k\{|\text{covered}_k(h_{\text{best}}, D_{\text{rest}})|\}'$

Heuristics for FindOneGoodRule

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- Estimating the probability using relative frequencies:

$$p(k|\text{Conditions}) = \frac{\#\text{covered correct}}{\#\text{covered total}}$$

Probability Estimates

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- Relative frequency of covered correctly:

$$p(k|R) = \frac{\#\text{covered correct}}{\#\text{covered total}}$$

Problems with small samples.

Probability Estimates

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Probability Estimates (cont.)

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  - special case: $p(k) = 1/\#\text{classes}$, $m = \#\text{classes}$
  - takes into account prior class probabilities
  - independent of number of classes
  - m is domain dependent (more noise, larger m)

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- Weighted measures in order to favor more general rules:

$$W\_G(R', R) = \frac{\#\text{correct covered by } R'}{\#\text{correct covered by } R} \cdot \_G(R', R)$$

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  - $\Rightarrow$ Fuzzy Rules
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- Propositional Rules not very expressive...

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For this, other types of rules are more approriate.

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  (Reminder:

  - $\forall$: the universal quantifier, e.g. $\forall x, y : \mathrm{Daughter}(x, y) \rightarrow \mathrm{female(x)}$
  - $\exists$: existential quantifier, e.g. $\forall x : \exists y : \mathrm{female(x)} \rightarrow \mathrm{Daughter}(x, y)$

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Horn clauses are also used to express Prolog programs ⇒ Learning First Order Rules is often called "Inductive Logic Programming" (ILP).

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- Recursive rules:
  IF x is Parent of z AND z is Anchestor of y
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  IF x is Parent of y THEN x is Anchestor of y

Learning First Order Rules: FOIL

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- one (easy) extension: literals in body can be negated.

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  - negating of either of the above forms of literals.
- How does FOIL pick the “best” specialization?

FOIL: Guiding the Search

FoilGain used to evaluation contribution of new literal L to rule R:

$$\text{FoilGain}(L, R) = t\left(-\log_2 \frac{p'}{p'+n'} - \log_2 \frac{p}{p+n}\right)$$

- R: rule
- p: number of positive bindings of R
- n: number of negative bindings of R
- L: new literal
- R': new rule (R with added L)
- p': number of positive bindings of R'
- n': number of negative bindings of R'

If L introduces a new variable, any original binding is considered to be covered if at least some of the (extended) binding of R is present in the bindings of R'.

FOIL: Example

- Target literal: GrandDaughter(x, y)
  (the grand daughter of x is y)
- Training "data" (assertions):
  - GrandDaughter(Victor, Sharon)
  - Father(Sharon, Bob)
  - Father(Tom, Bob)
  - Female(Sharon)
  - Father(Bob, Victor)
- Closed world assumption:
  all other bindings of predicates above are implicitly false, e.g.
  - ¬Father(Bob, Tom)
  - ¬Female(Victor)
  - ¬GrandDaugher(Bob, Sharon), ...
- Available predicates:
  - Father(x, y)
  - Female(x)

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- Final result:

  GrandDaughter(x,y) :- Father(y,z), Father(z,x), Female(y)

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- Extensions of FOIL also handle noisy data
  - Stopping criteria considers description-length principle to avoid adding lengthy rules to explain few examples.

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- Applicable for special types of data (e.g. structured or mainly nominal values)