
Inductive Logic Programming

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Outline of the Lecture

- Predictive ILP
 - Learning from entailment
 - Bottom-up systems: Golem
 - Top-down systems: FOIL, Progol
 - Learning from interpretations
 - ICL
- Descriptive ILP
 - Claudien
- Applications

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Predictive ILP

- Aim:
 - classifying instances of the domain, i.e.
 - predicting the class
- Two settings:
 - Learning from entailment
 - Learning from interpretations

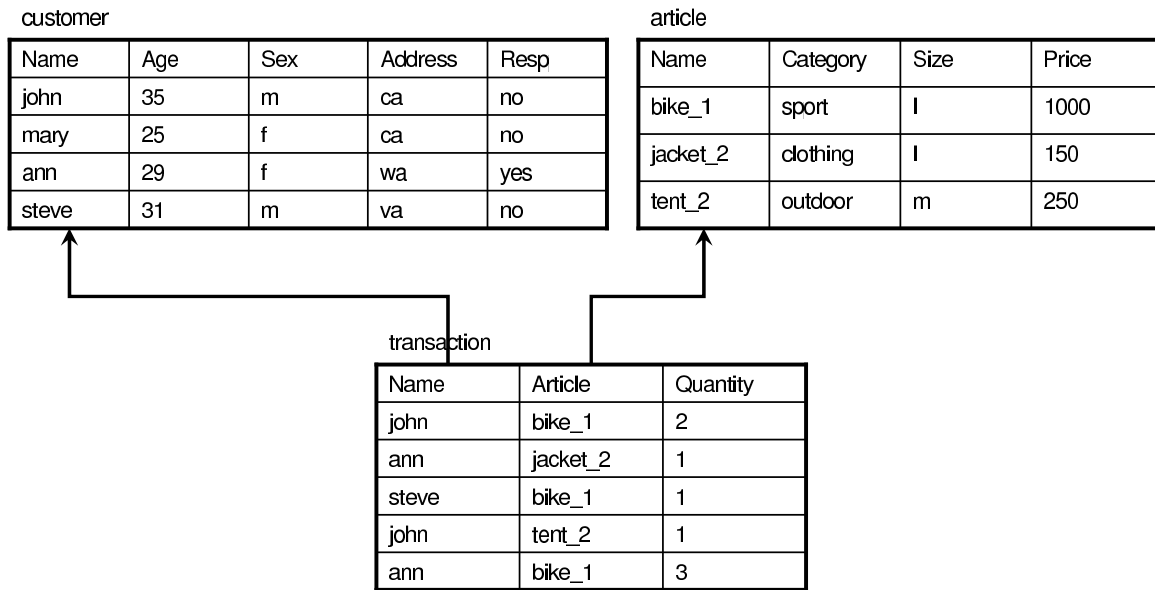
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Learning from Entailment

- Given
 - A set of positive example E^+
 - A set of negative examples E^-
 - A background knowledge B
 - A space of possible programs \mathcal{H}
- Find a program $P \in \mathcal{H}$ such that
 - $\forall e^+ \in E^+, P \cup B \models e^+$ (completeness)
 - $\forall e^- \in E^-, P \cup B \not\models e^-$ (consistency)

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Targeted Mailing



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Mailing Example

- Positive examples $E^+ = \{respond(ann)\}$
- Negative examples
 $E^- = \{respond(john), respond(mary), respond(steve)\}$
- Background $B =$ facts for relations *customer*, *transaction* and *article*
customer(john, 35, m, ca).
customer(mary, 25, f, ca).
customer(ann, 29, f, wa). . . .
transaction(john, bike_1, 2).
transaction(ann, jacket_2, 1). . . .
article(bike_1, sport, l, 1000).
article(jacket_2, clothing, l, 150). . . .

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Mailing Example

- Space of programs \mathcal{H} : programs containing clauses with
 - in the head $respond(Customer)$
 - in the body a conjunction of literals from the set $\{customer(Customer, Age, Sex, Address), transaction(Customer, Article, Quantity), article(Article, Category, Price), Age = constant, Sex = constant, \dots\}$
- Possible solution
 $respond(Customer) \leftarrow$
 $transaction(Customer, Article, _Quantity),$
 $article(Article, Category, _Size, _Price),$
 $Category = clothing$

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Definitions

- $covers(P, e) = true$ if $B \cup P \models e$
- $covers(P, E) = \{e \in E \mid covers(P, e) = true\}$
- A theory P is more general than Q if $covers(P, U) \supseteq covers(Q, U)$
- If $B \cup P \models Q$ then P is more general than Q
- A clause C is more general than D if $covers(\{C\}, U) \supseteq covers(\{D\}, U)$
- If $B, C \models D$ then C is more general than D
- If a clause covers an example, all of its generalizations will ($covers$ is antimonotonic)
- If a clause does not cover an example, none of its specializations will

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Theta Subsumption

- A clause
 $h \leftarrow b_1, \dots, b_n$
can be seen as a set of literals $\{h, \text{not } b_1, \dots, \text{not } b_n\}$
- A substitution θ is a replacement of variable with terms:
 $\theta = \{X/a, Y/b\}$
- C θ -subsumes D ($C \geq D$) if there exists a substitution θ such that $C\theta \subseteq D$ [Plotkin 70]
- $C \geq D \Rightarrow C \models D \Rightarrow B, C \models D \Rightarrow C$ is more general than D
- $C \models D \not\Rightarrow C \geq D$

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Examples of Theta Subsumption

- $C1 = \text{father}(X, Y) \leftarrow \text{parent}(X, Y)$
- $C2 = \text{father}(X, Y) \leftarrow \text{parent}(X, Y), \text{male}(X)$
- $C3 = \text{father}(\text{john}, \text{steve}) \leftarrow \text{parent}(\text{john}, \text{steve}), \text{male}(\text{john})$
- $C1 = \{\text{father}(X, Y), \text{not } \text{parent}(X, Y)\}$
- $C2 = \{\text{father}(X, Y), \text{not } \text{parent}(X, Y), \text{not } \text{male}(X)\}$
- $C3 = \{\text{father}(\text{john}, \text{steve}), \text{not } \text{parent}(\text{john}, \text{steve}), \text{not } \text{male}(\text{john})\}$
- $C1 \geq C2$ with $\theta = \emptyset$
- $C1 \geq C3$ with $\theta = \{X/\text{john}, Y/\text{steve}\}$
- $C2 \geq C3$ with $\theta = \{X/\text{john}, Y/\text{steve}\}$

Example of $C \models D \not\Rightarrow C \geq D$

- $C = \text{even}(X) \leftarrow \text{even}(\text{half}(X))$.
- $D = \text{even}(X) \leftarrow \text{even}(\text{half}(\text{half}(X)))$.
- $C \models D$: we can obtain D by resolving C with itself, but
- $C \not\geq D$: there is no substitution θ such that $C\theta \subseteq D$

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In Practice

- Coverage test: SLD or SLDNF resolution
 - Try to derive e from $B \cup P \cup \{C\}$
- Generality order:
 - θ -subsumption

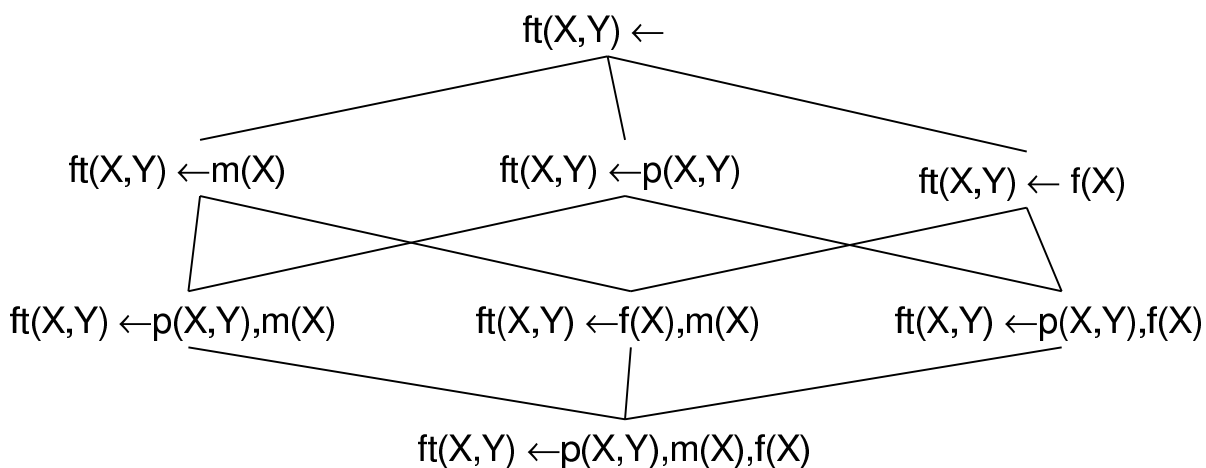
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Properties of Theta Subsumption

- θ -subsumption induces a lattice in the space of clauses
- Every set of clauses has a least upper bound (lub) and a greatest lower bound (glb)
- This is not true for the generality relation based on logical consequence

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Lattice



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Least General Generalization

- $lgg(C, D)$ = least upper bound in the θ -subsumption order
- An algorithm exists which has complexity $O(s^2)$ where s is the size of the clauses
- Example:

$C = father(john, mary) \leftarrow parent(john, mary), male(john)$
 $D = father(david, steve) \leftarrow parent(david, steve), male(david)$
 $lgg(C, D) = father(X, Y) \leftarrow parent(X, Y), male(X)$

- For a set of n clauses the complexity is $O(s^n)$

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Least General Generalization Algorithm

- The algorithm keeps a set of anti-substitutions A that contains elements of the form $V/t_1, t_2$ meaning that variable V replaced the term t_1 in the first formula and the term t_2 in the second formula
- The lgg of two terms $f_1(s_1, \dots, s_n)$ and $f_2(t_1, \dots, t_m)$ is:

$$f_1(lgg(s_1, t_1), \dots, lgg(s_n, t_n))$$

if $f_1/n = f_2/m$, otherwise

- if an element of the form $V/f_1(s_1, \dots, s_n), f_2(t_1, \dots, t_m)$ is present in A , then the lgg is V
- otherwise let V be a new variable, add $V/f_1(s_1, \dots, s_n), f_2(t_1, \dots, t_m)$ to A and the lgg is V

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Least General Generalization Algorithm

• Examples

$$lgg(f(a, b, c), f(a, c, d)) = f(lgg(a, a), lgg(b, c), lgg(c, d)) = f(a, X, Y), A = \{X/b, c, Y/c, d\}$$

$$lgg(f(a, a), f(b, b)) = f(lgg(a, b), lgg(a, b)) = f(X, X), A = \{X/a, b\}$$

- Note that the same variable X is used in both arguments of the second example because it indicates the lgg of the same two terms

$$lgg(f(a, b), f(b, a)) = f(lgg(a, b), lgg(b, a)) = f(X, Y), A = \{X/a, b, Y/b, a\}$$

- Note that two different variables X and Y are used because the order of the terms is different

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Least General Generalization Algorithm

- The lgg of two literals $L1 = (not)p(s1, \dots, sn)$ and $L2 = (not)q(t1, \dots, tm)$ is
 - undefined if $L1$ and $L2$ do not have the same sign or if $p/n \neq q/m$, otherwise

$$lgg(L1, L2) = (not)p(lgg(s1, t1), \dots, lgg(sn, tn))$$

• Examples:

- $lgg(\text{parent}(\text{john}, \text{mary}), \text{parent}(\text{john}, \text{steve})) = \text{parent}(\text{john}, X) A = \{X/\text{mary}, \text{steve}\}$

- $lgg(\text{parent}(\text{john}, \text{mary}), \text{not parent}(\text{john}, \text{steve})) = \text{undefined}$

- $lgg(\text{parent}(\text{john}, \text{mary}), \text{father}(\text{john}, \text{steve})) = \text{undefined}$

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Least General Generalization Algorithm

- $lgg(C, D) = \{lgg(L, K) \mid L \in C, K \in D \text{ and } lgg(L, K) \text{ is defined}\}$
- Examples

$C = \text{father}(\text{john}, \text{mary}) \leftarrow \text{parent}(\text{john}, \text{mary}), \text{male}(\text{john})$
 $D = \text{father}(\text{david}, \text{steve}) \leftarrow \text{parent}(\text{david}, \text{steve}), \text{male}(\text{david})$
 $lgg(C, D) = \text{father}(X, Y) \leftarrow \text{parent}(X, Y), \text{male}(X),$
 $A = \{X/\text{john}, \text{david}, Y/\text{mary}, \text{steve}\}$

$C = \text{win}(\text{conf1}) \leftarrow \text{occ}(\text{place1}, x, \text{conf1}), \text{occ}(\text{place2}, o, \text{conf1})$
 $D = \text{win}(\text{conf2}) \leftarrow \text{occ}(\text{place1}, x, \text{conf2}), \text{occ}(\text{place2}, x, \text{conf2})$
 $lgg(C, D) = \text{win}(Conf) \leftarrow$
 $\text{occ}(\text{place1}, x, Conf), \text{occ}(L, x, Conf),$
 $\text{occ}(M, Y, Conf), \text{occ}(\text{place2}, Y, Conf)$
 $A =$
 $\{Conf/\text{conf1}, \text{conf2}, L/\text{place1}, \text{place2}, M/\text{place2}, \text{place1}, Y/o, x\}$

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Relative Subsumption

- θ subsumption does not take into account background knowledge
- $C \geq D \Leftrightarrow \models \forall (C\theta \rightarrow D)$
- Relative Subsumption [Plotkin 71]: C θ subsume D relative to background B ($C \geq_B D$) if there exists a substitution θ such that $B \models \forall (C\theta \rightarrow D)$

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Relative Least General Generalization

- Relative Least General Generalization (rlgg): lgg with respect to relative subsumption.
- It does not exist in the general case of B a set of Horn clauses
- It exists in the case that B is a set of ground atoms and can be computed in this way:
- $rlgg((H1 \leftarrow B1), (H2 \leftarrow B2)) =$
 $lgg((H1 \leftarrow B1, B), (H2 \leftarrow B2, B))$

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Relative Least General Generalization

● Example

$C1 = \text{father}(\text{john}, \text{mary})$

$C2 = \text{father}(\text{david}, \text{steve})$

$B = \{\text{parent}(\text{john}, \text{mary}), \text{parent}(\text{david}, \text{steve}),$
 $\text{parent}(\text{kathy}, \text{mary}), \text{female}(\text{kathy}),$
 $\text{male}(\text{john}), \text{male}(\text{david})\}$

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Relative Least General Generalization

● Example

$$C1 \leftarrow B = fa(j, m) \leftarrow p(j, m), p(d, s), p(k, m), f(k), m(j), m(d)$$

$$C2 \leftarrow B = fa(d, s) \leftarrow p(j, m), p(d, s), p(k, m), f(k), m(j), m(d)$$

$$rlgg(C1, C2) = fa(X, Y) \leftarrow p(j, m), p(X, Y), p(Z, m), \\ p(W, U), p(d, s), p(S, U), p(T, m), p(R, Y), p(k, m), \\ f(k), m(j), m(X), m(W), m(d)$$

$$A =$$

$$\{X/j, d, Y/m, s, Z/j, k, W/d, j, U/s, m, S/d, k, T/k, j, R/k, d\}$$

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Reduced clause

- Two clauses C and D are equivalent (relative to B) if $C \geq D$ and $D \geq C$ ($C \geq_B D$ and $D \geq_B C$)
- A clause C is reduced (relative to B) if it does not contain any subset D that is equivalent to C (relative to B)
- $C = rlgg(C1, C2) = fa(X, Y) \leftarrow p(j, m), p(X, Y), p(Z, m), p(W, U), p(d, s), p(S, U), p(T, m), p(R, Y), p(k, m), f(k), m(j), m(X), m(W), m(d)$ is equivalent to $D = fa(X, Y) \leftarrow p(j, m), p(X, Y), p(d, s), p(k, m), f(k), m(j), m(X), m(d)$ and is equivalent relative to B to $D = fa(X, Y) \leftarrow p(X, Y), m(X)$

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- Predictive ILP
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 - **Bottom-up systems: Golem**
 - Top-down systems: FOIL, Progol
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 - ICL
- Descriptive ILP
 - Claudien
- Applications

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Bottom-up Systems

- Covering loop
- Search for a clause from specific to general

Learn(E, B)

$P := 0$

repeat /* covering loop */

$C := \text{GenerateClauseBottomUp}(E, B)$

$P := P \cup \{C\}$

 Remove from E the positive examples covered by P

until Sufficiency criterion

return P

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Golem [Muggleton, Feng 90]

- Bottom-up system
- Generalization by means of rlgg
- Sufficiency criterion: $E^+ = \emptyset$

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Golem

GolemGenerateClause(E, B)

select randomly some couples of examples from E^+

compute their rlgg

let C be the rlgg that covers most positive examples

while covering no negative

repeat

randomly select some examples from E^+

compute the rlgg between C and each selected example

let C be the rlgg that covers most positive examples

while covering no negative

remove from E^+ the examples covered by C

while C covers no negatives

remove literals from the body of C until C covers

some negative examples

return C

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Top-down Systems

- Covering loop as bottom-up systems
- Search for a clause from general to specific using beam search
- Score clauses using a heuristic function

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Top-down Systems

GenerateClauseTopDown(E,B)

$Beam := \{p(X) \leftarrow true\}$

$BestClause := null$

repeat /* specialization loop */

 Remove the first clause C of $Beam$

 compute $\rho(C)$

 score all the refinements

 update $BestClause$

 add all the refinements to the beam

 order the beam according to the score

 remove the last clauses that exceed the dimension d

until the Necessity criterion is satisfied

return $BestClause$

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Typical Stopping Criteria

● Sufficiency criteria:

- $E^+ = \emptyset$
- GenerateClauseTopDown returns $null$
- a disjunction of the above

● Necessity criteria

- the number of negative examples covered by $BestClause$ is 0
- the number of negative examples covered by $BestClause$ is below a threshold
- $Beam$ is empty
- a disjunction of the above

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Refinement Operator

- $\rho(C) = \{D \mid D \in L, C \geq D\}$
- where L is the space of possible clauses
- A refinement operator usually generates only minimal specializations
- A typical refinement operator applies two syntactic operations to a clause
 - it applies a substitution to the clause
 - it adds a literal to the body

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Heuristic Functions

- n^+, n^- number of positive and negative examples in the training set, $n = n^+ + n^-$
- $n^+(C), n^-(C)$ number of positive and negative examples covered by clause C
- $n(C) = n^+(C) + n^-(C)$
- Accuracy: $Acc = P(+|C)$ (more accurately Precision), $P(+|C)$ can be estimated by
 - relative frequency: $P(+|C) = \frac{n^+(C)}{n(C)}$
 - m-estimate: $P(+|C) = \frac{n^+(C) + mP(+)}{n(C) + m}$, where $P(+)=n^+/n$
 - Laplace: m-estimate with $m = 2, P(+)=0.5$
 $P(+|C) = \frac{n^+(C)+1}{n(C)+2}$

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Heuristic Functions

- Coverage: $Cov = n^+(C) - n^-(C)$
- Informativity: $Inf = \log_2(Acc)$
- Weighted relative accuracy:
 $WRAcc = P(C)(P(+|C) - P(+))$

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FOIL [Quinlan 90]

- Top-down system with
 - Dimension of the beam: 1
 - Heuristic: (approximately) weighted gain of Inf :
 $H = n(C')(Inf(C') - Inf(C))$
 - Refinement operator: addition of a literal or unification
 - Sufficiency criterion: $E^+ = \emptyset$
 - Necessity criterion: $n^-(BestClause) = 0$

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Progol [Muggleton 95]

- Top-down system with
 - Dimension of the beam: user defined
 - Heuristic: Compression:
 $Comp = n^+(C) - n^-(C) - |C|$
 - Refinement operator: see next slides
 - Sufficiency criterion: $E^+ = \emptyset$
 - Necessity criterion: $Beam = \emptyset$ or a maximum number of iterations of the loop is reached

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Progol Refinement Operator

- Progol refinement operator
 - adds a literal from the most specific clause \perp after having replaced some of the constants with variables

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Learning from Interpretations

- Interpretation = set of ground atoms.
- Aim: learning a classifier for logical interpretations
- Classifier: a set of disjunctive clauses
- Disjunctive clause
 - $C = h_1 \vee h_2 \vee \dots \vee h_n \leftarrow b_1, b_2, \dots, b_m$
 - can be seen as a set of literals
 - $\{h_1, \dots, h_n, \text{not } b_1, \dots, \text{not } b_m\}$
- $\text{head}(C) = h_1 \vee h_2 \vee \dots \vee h_n$ or $\{h_1, \dots, h_n\}$
- $\text{body}(C) = b_1, b_2, \dots, b_m$ or $\{b_1, \dots, b_m\}$
- $\text{body}^+(C) =$ set of positive literals of $\text{body}(C)$
- $\text{body}^-(C) =$ set of atoms of negative literals of $\text{body}(C)$

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Learning from Interpretations

- Set of clauses as a classifier
 - an interpretation is positive if all the clauses are true in the interpretation
 - an interpretation is negative if there exists at least one clause that is false in it
- A clause C is true in an interpretation I if for all grounding substitutions θ of C :
 $I \models body(C)\theta \rightarrow head(C)\theta \cap I \neq \emptyset$
or
 $body^+(C)\theta \subseteq I \wedge body^-(C)\theta \cap I = \emptyset \rightarrow head(C)\theta \cap I \neq \emptyset$

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Test of the Truth of a Clause

- Range restricted clause: all the variables in the head appear in the body
- Range restricted clause C , finite interpretation I : run the query $? - body(C), not head(C)$ against a logic program containing I
- If $C = h_1 \vee h_2 \vee \dots \vee h_n \leftarrow b_1, b_2, \dots, b_m$ then the query is $? - b_1, b_2, \dots, b_m, not h_1, not h_2, \dots, not h_n$
- If the query succeeds, C is false in I . If the query fails, C is true in I [De Raedt, Bruynooghe 93]

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Example

- $I = \{female(liz), male(richard), gorilla(liz), gorilla(richard)\}$
- $C = male(X) \vee female(X) \leftarrow gorilla(X)$: the clause is true in I because the query
? – $gorilla(X), not\ male(X), not\ female(X)$ fails
- $C = male(X) \leftarrow gorilla(X)$: the clause is false in I because the query
? – $gorilla(X), not\ male(X)$ succeeds with $\theta = \{X/liz\}$.

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Learning from Interpretations

- **Given**
 - a space of possible clausal theories \mathcal{H}
 - a set P of interpretations
 - a set N of interpretations
- **Find:** a clausal theory $H \in \mathcal{H}$ such that
 - for all $p \in P, p \models H$
 - for all $n \in N, n \not\models H$
- Less expressive than learning from entailment: no recursive definitions

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Test with Background

- Background: a normal program B
- Truth of a clause C in the interpretation $M(B \cup I)$ where M is the model according to the chosen semantics and I is an interpretation (i.e. $B \cup I \models C$)
- Range restricted clause C , normal program B containing only range restricted clauses, interpretation I : run the query $? - body(C), not head(C)$ against the logic program $B \cup I$.
- If the query succeeds, C is false in $M(B \cup I)$ ($B \cup I \not\models C$). If the query fails, C is true in $M(B \cup I)$ ($B \cup I \models C$)

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Learning from Int. with Background

Given

- a space of possible clausal theories \mathcal{H}
- a set P of interpretations
- a set N of interpretations
- a background theory B

Find: a clausal theory $H \in \mathcal{H}$ such that

- for all $p \in P$, $B \cup p \models H$
- for all $n \in N$, $B \cup n \not\models H$

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Generality Relation

- $cover(\{C\}, e) = true$ if $e \models C$
- $C \geq D \Rightarrow C \models D \Rightarrow D$ is more general than C
- the relation is reversed
- $C \geq D \Rightarrow D$ is more general than C
- Example:

$false \leftarrow true$

$false \leftarrow gorilla(X)$

$female(X) \leftarrow gorilla(X)$

$female(X) \vee male(X) \leftarrow gorilla(X)$

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ICL [De Raedt, Van Laer, 95]

- Dual version of a top down entailment algorithm:
 - coverage loop is performed on negative examples
- Updates CN2 to first order

ICL(P, N, B)

$H := \emptyset$

repeat

$C := \text{FindBestClause}(P, N, B)$

 if $C \neq null$ then

 add C to H

 remove from N all interpretations that are false for C

until $C = null$ or N is empty

return H

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ICL FindBestClause

FindBestClause(P, N, B)

$Beam := \{false \leftarrow true\}$, $BestClause := null$

while $Beam$ is not empty do

$NewBeam := \emptyset$

 for each clause C in $Beam$ do

 for each refinement Ref of C do

 if Ref is better than $BestClause$ and Ref is statistically significant then

$BestClause := Ref$

 if Ref is not to be pruned then

 add Ref to $NewBeam$

 if size of $NewBeam > MaxBeamSize$ then
 remove worst clause from $NewBeam$

$Beam := NewBeam$

return $BestClause$

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ICL Heuristics

- $n(\overline{C})$ = number of interpretations (positive and negative) where C is false
- $n^-(\overline{C})$ = number of negative interpretation where C is false
- $H(C) = p(-|\overline{C}) = \frac{n^-(\overline{C})+1}{n(\overline{C})+2}$ = precision over negative class

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Descriptive ILP

- Discovering regularities, patterns
- Example tasks:
 - finding association rules
 - clustering
 - subgroup discovery

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Claudien [De Raedt, Dehaspe 97]

- Learning problem: Given
 - a space of possible clausal theories \mathcal{H}
 - a set P of interpretations
 - a background theory B
- **Find:** a clausal theory $H \in \mathcal{H}$ such that
 - $\forall p \in P, B \cup p \models H$
 - H is maximally specific

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Example

$p1 = \{female(liz), male(richard),$
 $gorilla(liz), gorilla(richard)\}$

$p2 = \{female(ginger), male(fred),$
 $gorilla(ginger), gorilla(fred)\}$

If \mathcal{H} contains only range-restricted, constant-free clauses a solution is:

$gorilla(X) \leftarrow female(X)$

$gorilla(X) \leftarrow male(X)$

$male(X) \vee female(X)$

$\leftarrow male(X), female(X)$

Claudien Algorithm

ClausalDiscovery(E, B)

$H := \emptyset$

$Beam := \{false \leftarrow true\}$

while $Beam$ is not empty do

 delete from $Beam$ the first clause C

 if C is true on E then

$H := H \cup \{C\}$

 else

 for all $C' \in \rho(C)$ for which not prune(C') do

$Beam := Beam \cup \{C'\}$

return H

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 - Claudien
- Applications

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Applications

- Biology
- Chemistry
- Engineering
- Various

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Algorithm Evaluation

- Notation:
 - $n^+(P)$ number of positive examples covered by P
 - $n^-(\bar{P})$ number of negative examples not covered by P
 - $n = |E|$
- Accuracy:

$$Acc(P) = \frac{n^+(P) + n^-(\bar{P})}{n}$$

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Structure Activity Relationships (SARs)

- Predicting the activity of a chemical compound on humans based on its structure and properties
 - Drugs: whether they are effective
 - Compounds, drugs: whether they are toxic

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Description of Chemical Compounds

Basic structure:

atom(compound, atom, element, atomType, charge)

e.g. *atom(d2, d2_1, c, 22, 0.067)*

bond(compound, atom1, atom2, bondType)

e.g. *bond(d2, d2_1, d2_2, 7)*

Structures:

benzene(compound, listOfAtoms)

e.g. *benzene(d4, [d4_6, d4_1, d4_2, d4_3, d4_4, d4_5])*

phenanthrene(compound, listOfListsOfAtoms)

nitro(compound, listOfAtoms)

...

Properties:

polar(atom, polarity)

polar(d2_1, polar3)

...

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- Drugs against Alzheimer's disease
 - Golem: not significantly different from propositional, comprehensibility [King et al. 95]
- Drugs for inhibition of E. Coli Dihydrofolate Reductase
 - Golem: not significantly different from propositional, comprehensibility [King et al. 95]
- Predicting carcinogenicity
 - Progol: 72%, highest machine accuracy [Srinivasan et al. 97]

- Predicting mutagenicity
 - regression friendly compounds
 - FOIL: 82% [Srinivasan et al 95]
 - ICL: 86.2% [Van Laer et al. 97]
 - Progol: 88% [Srinivasan et al 95]
 - Claudien: found alternative explanations [De Raedt, Dehaspe 97]
 - regression unfriendly compounds
 - Progol: 85.7% [King et al. 96]

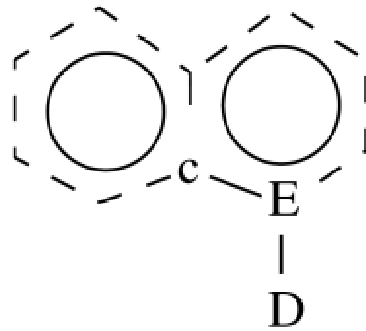
Progol on Mutagenesis

$active(A) \leftarrow$
 $atom(A, B, c, 27, C),$
 $bond(A, D, E, 1), bond(A, E, B, 7)$

A carbon atom of type 27 merges two six-membered aromatic rings.

A bond of type 7 is an aromatic bond.

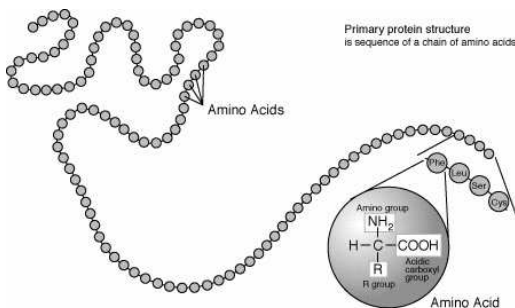
This rule identifies compounds of two fused six-membered aromatic rings, one of which has a further single bond with an atom of any type.



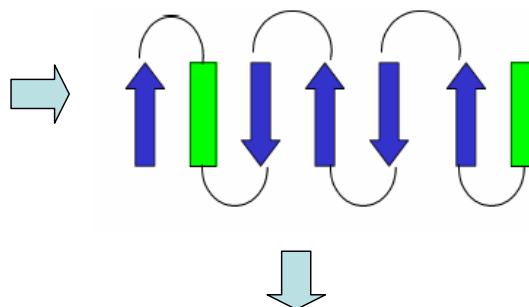
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Proteins

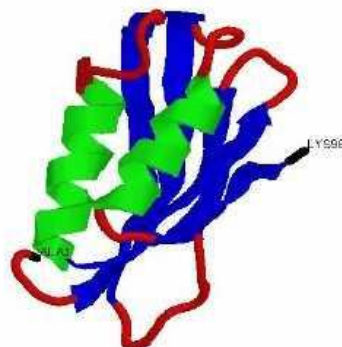
Primary structure



Secondary structure



Tertiary structure



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Protein Secondary Structure

- Predicting protein secondary structure from the amino-acid sequence
- Structures
 - helices, of various types and length
 - strands, of various orientations and length
- Results:
 - Golem: 80% [Muggleton et al. 92]
 - FOIL: 65% [Quinlan, Cameron-Jones 95]

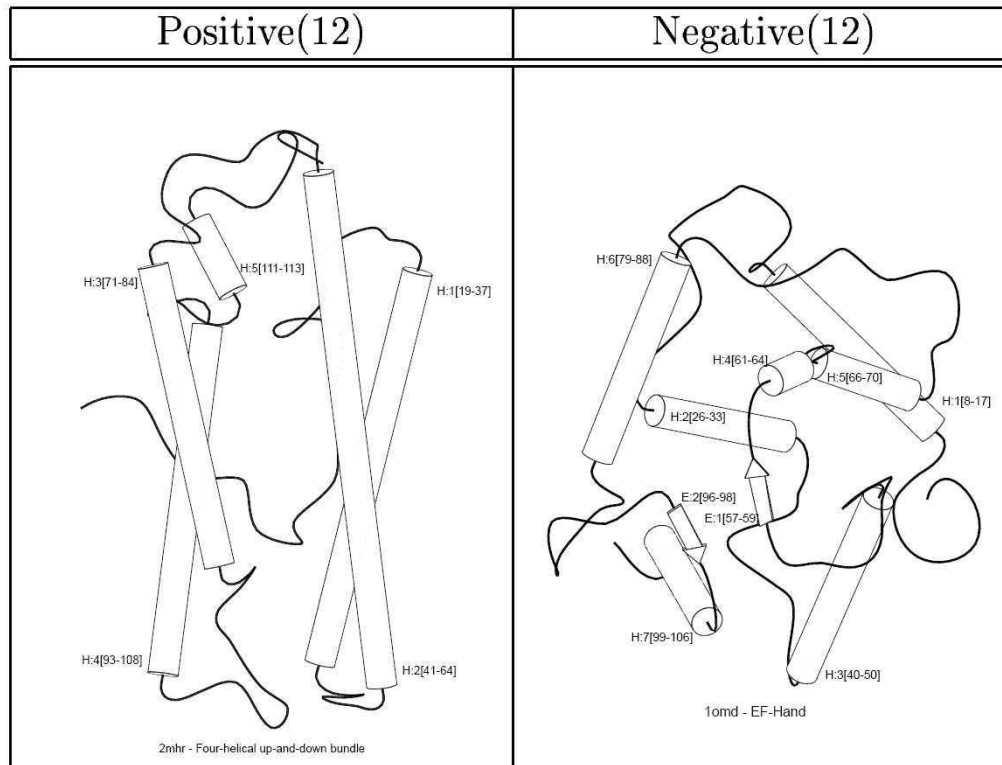
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Protein Tertiary Structure

- Predicting the tertiary structure of proteins by classifying them into one of the SCOP classes
- Proteins represented as a sequence of secondary structure elements
- Results:
 - Progol: 78.28% [Turcotte et al. 01]

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Protein Tertiary Structure



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Pointers

- ILPnet2
 - <http://www.cs.bris.ac.uk/~ILPnet2/>
 - <http://www-ai.ijs.si/~ilpnet2/>
- KDnet <http://www.kdnet.org/>
- Books:
 - [Lavrac, Dzeroski 94]: freely available in pdf from <http://www-ai.ijs.si/SasoDzeroski/ILPBook/>
 - [Bergadano et al. 96]
 - [Dzeroski, Lavrac 01]

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