# Inductive Logic Programming



## 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



## Predictive ILP

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



## 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)



## Targeted Mailing

customer

| Name | Age | Sex | Address | Resp |
|---|---|---|---|---|
| john | 35 | m | ca | no |
| mary | 25 | f | ca | no |
| ann | 29 | f | wa | yes |
| steve | 31 | m | va | no |

article

| Name | Category | Size | Price |
|---|---|---|---|
| bike_1 | sport | l | 1000 |
| jacket_2 | clothing | l | 150 |
| tent_2 | outdoor | m | 250 |

transaction

| Name | Article | Quantity |
|---|---|---|
| john | bike_1 | 2 |
| ann | jacket_2 | 1 |
| steve | bike_1 | 1 |
| john | tent_2 | 1 |
| ann | bike_1 | 3 |



## Mailing Example

- Positive examples $E^+ = \{respond(ann)\}$
- Negative examples
  $E^- = \{respond(john), respond(mary), respond(steve)\}$
- Background $B =$ facts for relations $customer$, $transaction$ and $article$
  $customer(john, 35, m, ca).$
  $customer(mary, 25, f, ca).$
  $customer(ann, 29, f, wa)....$
  $transaction(john, bike\_1, 2).$
  $transaction(ann, jacket\_2, 1)....$
  $article(bike\_1, sport, l, 1000).$
  $article(jacket\_2, clothing, l, 150)....$

## 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 $\{customer(Customer, Age, Sex, Address),$ $transaction(Customer, Article, Quantity),$ $article(Article, Category, Price),$ $Age = constant, Sex = constant, \ldots\}$
- Possible solution
  $respond(Customer) \leftarrow$
  $transaction(Customer, Article, \_Quantity),$
  $article(Article, Category, \_Size, \_Price),$
  $Category = clothing$



## Definitions

- $covers(P, e) = true$ if $B \cup P \models e$
- $covers(P, E) = \{e \in E | covers(P, e) = true\}$
- 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



## Theta Subsumption

- A clause
  $h \leftarrow b_1, \ldots, b_n$
  can be seen as a set of literals $\{h, not\ b_1, \ldots, not\ b_n\}$
- A substitution $\theta$ is a replacement of variable with terms: $\theta = \{X/a, Y/b\}$
- $C$ $\theta$-subsumes $D$ ($C \geq D$) if there exists a substitution $\theta$ 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 $D$
- $C \models D \not\Rightarrow C \geq D$



## Examples of Theta Subsumption

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



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

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



## In Practice

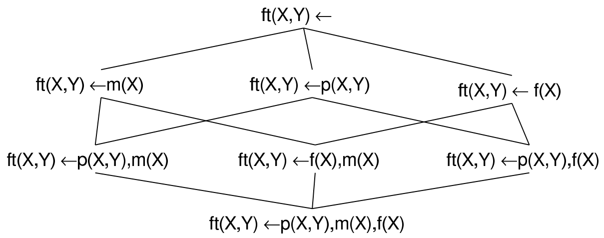
- Coverage test: SLD or SLDNF resolution
  - Try to derive $e$ from $B \cup P \cup \{C\}$
- Generality order:
  - $\theta$-subsumption

# Properties of Theta Subsumption

- $\theta$-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



# Lattice






# Least General Generalization

- $lgg(C, D)$ = least upper bound in the $\theta$-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 $O(s^n)$



# Least General Generalization Algorithm

- The algorithm keeps a set of anti-substituons $A$ that contains elements of the form $V/t1, t2$ meaning that variable $V$ replaced the term $t1$ in the first formula and the term $t2$ in the second formula
- The $lgg$ of two terms $f1(s1, \ldots, sn)$ and $f2(t1, \ldots, tm)$ is:

$$f1(lgg(s1, t1), \ldots, lgg(sn, tn))$$

  if $f1/n = f2/m$, otherwise
  - if an element of the form $V/f1(s1, \ldots, sn), f2(t1, \ldots, tm)$ is present in $A$, then the $lgg$ is $V$
  - otherwise let $V$ be a new variable, add $V/f1(s1, \ldots, sn), f2(t1, \ldots, tm)$ to $A$ and the $lgg$ is $V$



# 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



# Least General Generalization Algorithm

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

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

- Examples:
  - $lgg(parent(john, mary), parent(john, steve)) = parent(john, X)$ $A = \{X/mary, steve\}$
  - $lgg(parent(john, mary), not\ parent(john, steve)) = undefined$
  - $lgg(parent(john, mary), father(john, steve)) = undefined$

# Least General Generalization Algorithm

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

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

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



# Relative Subsumption

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



# Relative Least General Generalization

- Relative Least General Generalization (rlgg): lgg with respect to relative subsumption.
- It does not exists 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:
- $rlgg((H1 \leftarrow B1), (H2 \leftarrow B2)) = lgg((H1 \leftarrow B1, B), (H2 \leftarrow B2, B))$



# Relative Least General Generalization

- Example

$C1 = father(john, mary)$

$C2 = father(david, steve)$

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



# Relative Least General Generalization

- Example

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

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

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

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



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



## Bottom-up Systems

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

**Learn**$(E, B)$
$P := 0$
repeat /* covering loop */
    $C$ :=GenerateClauseBottomUp$(E, B)$
    $P := P \cup \{C\}$
    Remove from $E$ the positive examples covered by $P$
until Sufficiency criterion
return $P$



## Golem [Muggleton, Feng 90]

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



## 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

# 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 $BestClause$



# 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



# Refinement Operator

- $\rho(C) = \{D | D \in L, C \geq D\}$
- 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



# 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 $m = 2, P(+) = 0.5$ $P(+|C) = \frac{n^+(C)+1}{n(C)+2}$



# Heuristic Functions

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



# 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: $n^-(BestClause) = 0$

## 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



## 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
  $C = h_1 \vee h_2 \vee \ldots \vee h_n \leftarrow b_1, b_2, \ldots, b_m$
  can be seen as a set of literals
  $\{h_1, \ldots, h_n, not\ b_1, \ldots, not\ b_m\}$
- $head(C) = h_1 \vee h_2 \vee \ldots \vee h_n$ or $\{h_1, \ldots, h_n\}$
- $body(C) = b_1, b_2, \ldots, b_m$ or $\{b_1, \ldots, b_m\}$
- $body^+(C) =$ set of positive literals of $body(C)$
- $body^-(C) =$ set of atoms of negative literals of $body(C)$



## 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 $\theta$ of $C$:
  $I \models body(C)\theta \rightarrow head(C)\theta \cap I \neq \emptyset$
  or
  $body^+(C)\theta \subseteq I \wedge body^-(C)\theta \cap I = \emptyset \rightarrow head(C)\theta \cap I \neq \emptyset$



## 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 $C = h_1 \vee h_2 \vee \ldots \vee h_n \leftarrow b_1, b_2, \ldots, b_m$ then the query is $? - b_1, b_2, \ldots, b_m, not\ h_1, not\ h_2, \ldots, not\ h_n$
- If the query succeeds, $C$ is false in $I$. If the query fails, $C$ is true in $I$ [De Raedt, Bruynooghe 93]

## 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 $\theta = \{X/liz\}$.



## 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



## 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 $M(B \cup I)$ ($B \cup I \models C$)



## 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 $n \in N$, $B \cup n \not\models H$



## 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:

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



## 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
    $C :=$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 $H$

## 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 $BestClause$



## 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



## 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



## 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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## Applications

- Biology
- Chemistry
- Engineering
- Various



## Algorithm Evaluation

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

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



## 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



## 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. $benzene(d4, [d4\_6, d4\_1, d4\_2, d4\_3, d4\_4, d4\_5])$
$phenanthrene(compound, listOfListsOfAtoms))$
$nitro(compound, listOfAtoms)$
$\ldots$
Properties:
$polar(atom, polarity)$
$polar(d2\_1, polar3)$
$\ldots$

# SAR

- 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]



# SAR

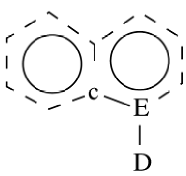
- Predicting mutagenicity
  - regression friendly compounds
    - FOIL: 82% [Srinivasan et al 95]
    - ICL: 86.2% [Van Laer et al. 97]
    - Progol: 88% [Srinivasan et al 95]
    - Claudien: found alternative explanations [De Raedt, Dehaspe 97]
  - regression unfriendly compounds
    - Progol: 85.7%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



# Progol on Mutagenesis

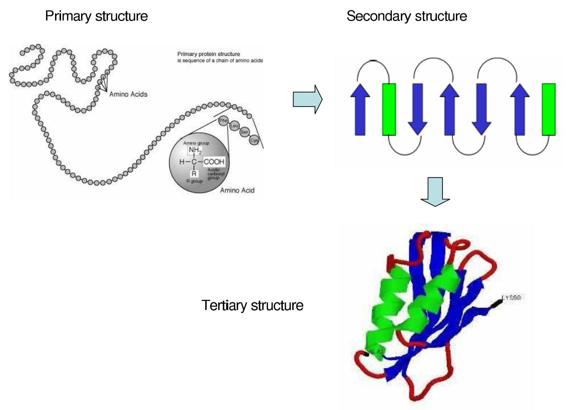
$$
\begin{aligned}
& active(A) \leftarrow \\
& \quad atom(A, B, c, 27, C), \\
& \quad bond(A, D, E, 1), bond(A, E, B, 7)
\end{aligned}
$$

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.






# Proteins






# Protein Secondary Structure

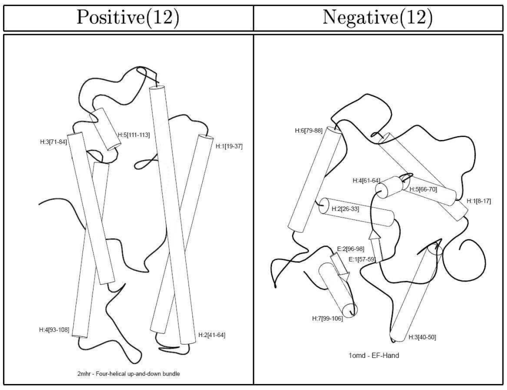
- Predicting protein secondary structure from the amino-acid sequence
- Structures
  - helices, of various types and length
  - strands, of various orientations and length
- Results:
  - Golem: 80% [Muggleton et al. 92]
  - FOIL: 65% [Quinlan, Cameron-Jones 95]



# 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]

# Protein Tertiary Structure






# 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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