Inductive Logic Programming

Outline

- Predictive ILP
- Learning from entailment
- Bottom-up systems: Golem
- Top-down systems: FOIL, Progol
- 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 $article$
  $customer(john, 35, m, ca).$
  $customer(mary, 25, f, ca).$
  $customer(ann, 29, f, wa). \ldots$
  $transaction(john, bike\ \ 1, 2).$
  $transaction(ann, jacket\ \ 2, 1). \ldots$
  $article(bike\ \ 1, sport, l, 1000).$
  $article(jacket\ \ 2, clothing, l, 150). \ldots$

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
  $respond(Customer) \leftarrow$
  $transaction(Customer, Article,\ \ Quantity),$
  $article(Article, Category,\ \ Size,\ \ Price),$
  $Category = clothing$

Father Example

- Learning the definition of $father/2$
- $B = \{parent(john, mary), male(john),$
  $parent(david, steve), male(david),$
  $parent(kathy, ellen), female(kathy)\}$
- $E^+ = \{father(john, mary), father(david, steve)\}$
- $E^- = \{father(kathy, ellen), father(john, steve)\}$
- Language bias: clauses of the form $father(X, Y) : -\alpha$ with
  $\alpha \in \{parent(X, Y), parent(Y, X),$
  $male(X), male(Y), female(X), female(Y)\}$
- Possible solution

$$father(X, Y) \leftarrow parent(X, Y), male(X).$$

Intersection Example

- Learning the definition of $intersection/3$
- $B = null([]).$
  $cons(X, Y, [X|Y]).$
  $member(X, [X|Y]).$
  $member(X, [Z|Y]) \leftarrow member(X, Y).$
  $notmember(X, []).$
  $notmember(X, [Z|Y]) \leftarrow X \neq Z, notmember(X, Y).$
- $E^+ = \{int([4, 2, 6], [5, 2, 8], [2])\}$
  $E^- =$
  $\{int([4, 2, 6], [5, 2, 8], [2, 6]), int([4, 2, 6], [5, 2, 8], [4, 2, 6])\}$

Intersection Example

- Language bias: clauses of the form $int(X, Y, Z) : -\alpha$ with
  $\alpha \in \{null(X), null(Y), null(Z),$
  $cons(X1, X2, X), int(X2, Y, W) int(X2, Y, Z),$
  $cons(X1, W, Z), member(X1, Y), notmember(X1, Y)\}$
- Possible solution: $P1 =$
  $int(X, Y, Z) \leftarrow null(X), null(Z).$
  $int(X, Y, Z) \leftarrow$
  $cons(X1, X2, X), member(X1, Y), int(X2, Y, W), cons(X1, W, Z).$
  $int(X, Y, Z) \leftarrow cons(X1, X2, X), int(X2, Y, Z).$
- Beware: $P1$ derives $int([1], [1], [])$
- The program may be inconsistent with examples not in the training set

Example

- Possible solution: $P2 =$
  $int(X, Y, Z) \leftarrow null(X), null(Z).$
  $int(X, Y, Z) \leftarrow$
  $cons(X1, X2, X), member(X1, Y), int(X2, Y, W), cons(X1, W, Z).$
  $int(X, Y, Z) \leftarrow$
  $cons(X1, X2, X), notmember(X1, Y), int(X2, Y, Z).$

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 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
- $C \models D \not\Rightarrow C \geq D$

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 $\theta = \{X/john, Y/steve\}$

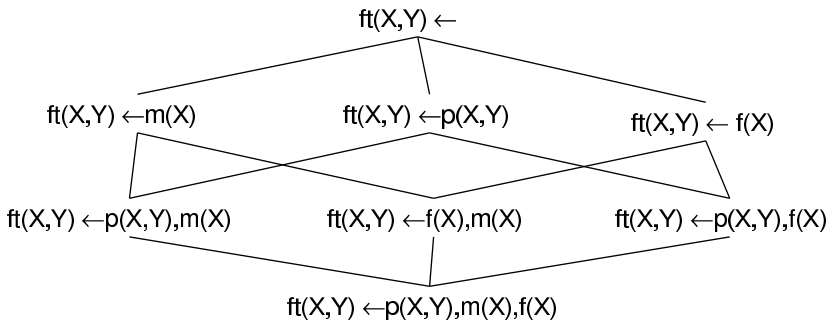
In Practice

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

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

Lattice



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 $O(s^n)$

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 $f2(t1, \ldots, tn)$ is:

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

if $f1 = f2$, otherwise

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

Least General Generalization Algorithm

- Examples

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

- 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 $L1 = (\neg)p(s1, ..., sn)$ and $L2 = (\neg)q(t1, ..., tn)$ is
  - undefined if $L1$ and $L2$ do not have the same predicate symbol and sign, otherwise

$$lgg(L1, L2) = (\neg)p(lgg(s1, t1), ...lgg(sn, tn))$$

- Examples:
  - $lgg(parent(john, mary), parent(john, steve)) = parent(john, X)$
  - $lgg(parent(john, mary),\ parent(john, steve)) = undefined$
  - $lgg(parent(john, mary), father(john, steve)) = undefined$

Least General Generalization Algorithm

- $lgg(C, D) = \{lgg\ \ lit(L, K) | L \in C, K \in D$ and $lgg\ \ lit(L, K)$ 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

- 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 $B \models \forall(C\theta \rightarrow D)$

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

$C1 = father(john, mary)$

$C2 = father(david, steve)$

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

$rlgg(C1, C2) = father(X, Y) \leftarrow parent(X, Y), male(X)$

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

Top-down Systems

- Covering loop as bottom-up systems
- Search for a clause from general to specific

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 substituted some of the constants with variables

Foil Example

- Learning the definition of $father/2$
- $B = \{parent(john, mary), male(john),$
  $parent(david, steve), male(david),$
  $parent(kathy, ellen), female(kathy)\}$
- $E^+ = \{father(john, mary), father(david, steve)\}$
- $E^- = \{father(kathy, ellen), father(john, steve)\}$
- Language bias: clauses of the form $father(X, Y) : -\alpha$ with
  $\alpha \in \{parent(X, Y), parent(Y, X),$
  $male(X), male(Y), female(X), female(Y)\}$

Foil Example

- Covering loop:
- GenerateClauseTopDown:
  - $father(X, Y) : -true.$ covers all positive and negative examples
  - $father(X, Y) : -parent(X, Y).$ covers all positive examples but also the negaive example $father(kathy, ellen)$
  - $father(X, Y) : -parent(X, Y), male(X)$ covers all positive and no negative examples
- The positive examples are removed. E^+ is now empty and the algorithm terminates generating the theory

$$father(X, Y) : -parent(X, Y), male(X).$$

Observations

- Nonexhaustive search: the algorithm explores the space of possible clauses rather than the space of possible programs.
- Once a clause is added to the theory it is never retracted
- No backtracking on clauses
- Problems in the case of recursive predicates or multiple predicates.
- We may not be able to find a solution even if one exists in the space of possible programs
- Necessary trade-off to contain the compuational complexity

Example Coverage

- Progol tests the coverage of an example e by a clause C in the following way: ask the query $\leftarrow e$ from the program $B \cup H \cup \{C\}$ where H is the set of clauses previously added
- FOIL uses *extensional coverage*:
  - resolve the example e with the clause $C = h \leftarrow B$
  - let θ be the most general unifier of e with h
  - ask the query $\leftarrow B\theta$ from the program $B \cup E^+$

Example Coverage

- With extensional coverage, the clauses are independent of each other: it does not matter the order in which they are added to the theory and the search in the space of clauses is equivalent to the serrch in the space of programs
- Good for learning recursive predicates and multiple predicates at once
- Problem: the learned programs may be extensionally complete and consistent but incomplete and inconsistent according to the definition of the ILP problem
- This may happen only when learning programs that are recursive or that contain multiple predicates

Other ILP Systems

- Aleph: similar to Progol,
  - Many tuning parameters
  - Written in Prolog
  - Available at `http://web.comlab.ox.ac.uk/activities/machinelearning/Aleph/`
- Tilde: learns logical decision trees
- ICL: learns from examples that are interpretations
- Claudien: learns from examples that are interpretations and performs descriptive induction

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

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]

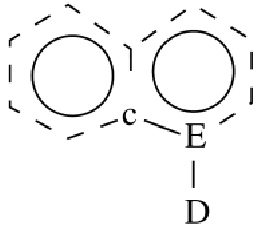
SAR

- 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

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

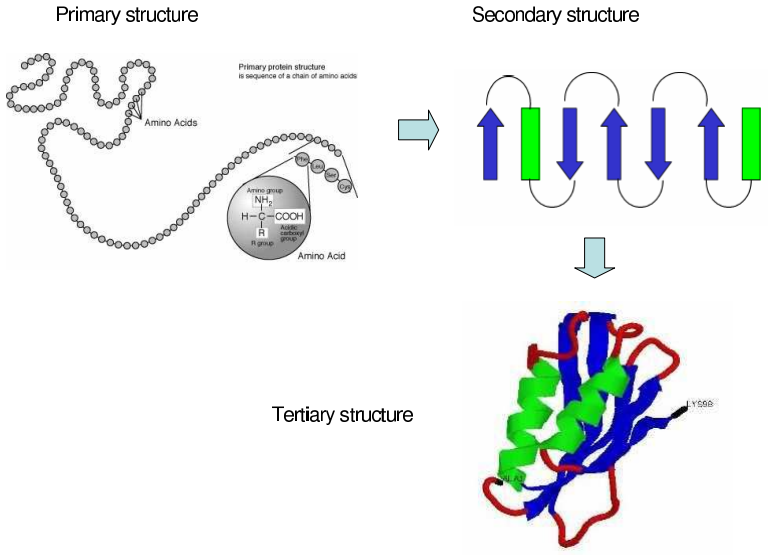
A carbon atom of type 27 merges two six-membered aromatic rings.
A bond of type 7 is an aromatic bond.
This rule identifies compounds of two fused six-membered aromatic rings, one of which has a further single bond with an atom of any type.



Biology

- Description of the binding sites (pharmacophores) of ACE inhibitors (hypertension drug) and an HIV-protease inhibitor (an anti-AIDS drug)
  - Progol: rediscovered a pharmacophore found by experts [Finn et al. 98]
- Biological classification of river water quality
  - Golem: comprehensibility [Dzeroski et al. 94]
  - Claudien: intuitive rules [De Raedt, Dehaspe 97]

Proteins



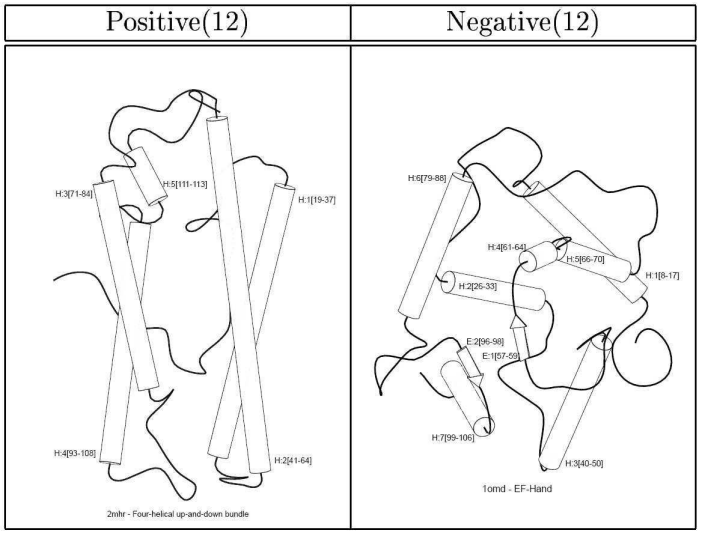
Protein Secondary Structure

- 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



Chemistry

- Identification of the structure of diterpene from spectral information
  - FOIL: 78.3% [Dzeroski et al. 96]
  - Tilde: 90.4% [Blockeel, De Raedt 98]
- Predicting the half-time of aqueous biodegradation of a compound from its chemical structure
  - ICL: 58.1% [Van Laer et al. 97]
- Judging whether a molecule is a musk
  - Tilde: 79.4% [Blockeel, De Raedt 98]

Engineering

- Learning rules for finite element mesh design
  - Claudien: 34% from pos. ex. only [De Raedt, Dehaspe 97]
  - ICL: 66.5% [Van Laer et al. 97]
  - Golem: 78% [Dolsak et al. 94]

Various

- Identifying document components
  - FOIL: 96.3%-100% [Quinlan, Cameron-Jones 95]
- Recovering program loop invariants from program traces
  - Claudien: found true invariants [De Raedt, Dehaspe 97]

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 on the web
  - [Bergadano et al. 96]
  - [Dzeroski, Lavrac 01]

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