Relational Learning

www.cs.wisc.edu/~page/cs760/

Goals for the lecture

you should understand the following concepts

- rule-set learning
- relational learning
- the FOIL algorithm

Rule sets as a hypothesis space

- we can use propositional rule sets as a hypothesis space for a learning algorithm
- each rule is a conjunction of tests + a class that is implied (predicted) when the conjunction is satisfied

Class=yes \leftarrow Outlook=sunny \land Humidity \leq 75%

Class=yes ← Outlook=overcast

Class=yes \leftarrow Outlook=rain \land Win ≤ 20

Decision trees and rules

Any decision tree can be converted into an equivalent set of rules



Class=yes \leftarrow Outlook=sunny \land Humidity \leq 75%

Class=yes ← Outlook=overcast

Class=yes \leftarrow Outlook=rain \land Wind \leq 20

Decision trees and rules

a small set of rules can represent a large decision tree because of the *replication problem*



Rule learning

- rule sets can be learned by extracting them from decision trees (C4.5 has a module for this)
- there are also algorithms for learning rules directly, such as SLIPPER [Cohen & Singer, AAAI 1999]

- the rules we've considered so far are expressed in propositional logic – they're not well suited to representing multiple entities and relationships among them
- let's consider *relational learning* methods, which represent their hypotheses using a subset of first-order logic

• suppose we want to learn the general concept of can-reach in a graph, given a set of training instances describing a particular graph



• how would you represent this task to a learner?

• a relational representation, such as first-order logic, can capture this concept succinctly and in a general way

 $\operatorname{can-reach}(X_1, X_2) \leftarrow \operatorname{linked-to}(X_1, X_2)$

 $\operatorname{can-reach}(X_1, X_2) \leftarrow \operatorname{linked-to}(X_1, X_3) \land \operatorname{can-reach}(X_3, X_2)$



consider the task of learning a *pharmacophore*: the substructure of a molecule that interacts with a target of interest

 instances for this task consist of interacting (+) and non-interacting molecules (-)



to represent each instance, we'd like to describe

- the (variable # of) atoms in the molecule
- the possible conformations of the molecule
- the bonds among atoms
- distances among atoms
- etc.

[Finn et al., Machine Learning 1998]

a multi-relational representation for molecules

Molecule	Target_1	 Target_n
moll	inactive	i nactive
mol2	active	inactive
•		

Molecule	Bond_ID	Atom_1_ID	Atom_2_ID	Bond_Type
mol1	bond1	al	a2	aromatic
:				
•				

Molecular Bioactivity

Bonds

Molecule	Conformer	Atom_ID	Atom_Type	X_Coordinate	Y_Coordinate	Z_Coordinate
moll	confl	al	carbon	2.58	-1.23	0.69

[Finn et al., Machine Learning 1998]

a learned relational rule characterizing ACE inhibitors

Molecule A is an ACE inhibitor if for some conformer Conf of A: molecule A contains a zinc binding site B; molecule A contains a hydrogen acceptor C; the distance between B and C in Conf is 7.9 +/- .75; molecule A contains a hydrogen acceptor D; the distance between B and D in Conf is 8.5 +/- .75; the distance between C and D in Conf is 2.1 +/- .75; molecule A contains a hydrogen acceptor E; the distance between B and E in Conf is 4.9 +/- .75; the distance between C and E in Conf is 3.1 +/- .75; the distance between C and E in Conf is 3.1 +/- .75; the distance between D and E in Conf is 3.8 +/- .75.

Relational representation

ACE_inhibitor(A) \leftarrow has_zinc_binding_site(A, B) \land has_hydrogren_acceptor(A, C) \land distance(B, C, 7.9, 0.75) \land has_hydrogen_acceptor(A, D) \land distance(B, D, 8.5, 0.75) \land distance(C, D, 8.5, 0.75) \land has_hydrogen_acceptor(A, E) \land distance(B, E, 4.9, 0.75) \land distance(C, E, 3.1, 0.75) \land distance(D, E, 3.8, 0.75)

To learn an equivalent rule with a feature-vector learner, what features would we need to represent?

has_zinc_binding_site has_hydrogen_acceptor zinc_binding_site_and hydrogen_acceptor_distance hydrogen_acceptor_hydrogen_acceptor_distance

. . .

can easily encode distance between a pair of atoms; but this pharmacophore has 4 important atoms with 6 relevant distances among them

Relational learning example [Craven et al., ECML 1998]

- consider the task of classifying web pages according their roles
- here is a learned rule for recognizing home pages for CS courses

```
course(A) \leftarrow
has-word(A, instructor),
\neg has-word(A, good),
link-from(A, B),
has-word(B, assign),
\neg link-from(B, C)
```

• test-set accuracy: 31 / 34

Relational learning example [Page et al., AAAI 2012]

- Data from electronic health records (EHRs) is being used to learn models for risk assessment, adverse event detection, etc.
- A patient's record is described by multiple tables in a relational DB

demographics

diagnoses

	PatientID P1	Gender M	Birthdate 3/22/63	PatientID P1 P1	Da 1/1 2/1	/01 /03	Physic Smith Jones	ian S h pa s fe	ympt alpita ver, a	oms tions ches	hy in	Diagnosis /poglycemic fluenza	
labs	PatientID P1 P1 P1	Date 1/1/01 1/9/01	Lab Test blood gluco blood gluco	Result ose 42 ose 45		Patio	entID P1 P2	SNP AA AB	1 SN A B	P2 B B		SNP500K BB AA	genetics
drugs	PatientID P1	Date	Prescribed 5/17/98	Date Filled 5/18/98	Physici		ician Med les pri		edication D prilosec 10		bse Duration mg 3 months		

The FOIL algorithm for relational learning [Quinlan, Machine Learning 1990]

given:

- tuples (instances) of a target relation
- extensionally represented background relations

do:

 learn a set of rules that (mostly) cover the positive tuples of the target relation, but not the negative tuples

Input to FOIL

• instances of target relation

 $\begin{array}{c} \textcircledleft : \langle 0,1\rangle \ \langle 0,2\rangle \ \langle 0,3\rangle \ \langle 0,4\rangle \ \langle 0,5\rangle \ \langle 0,6\rangle \ \langle 0,8\rangle \ \langle 1,2\rangle \ \langle 3,2\rangle \ \langle 3,4\rangle \\ \langle 3,5\rangle \ \langle 3,6\rangle \ \langle 3,8\rangle \ \langle 4,5\rangle \ \langle 4,6\rangle \ \langle 4,8\rangle \ \langle 6,8\rangle \ \langle 7,6\rangle \ \langle 7,8\rangle \\ \hlineleft : \langle 0,0\rangle \ \langle 0,7\rangle \ \langle 1,0\rangle \ \langle 1,1\rangle \ \langle 1,3\rangle \ \langle 1,4\rangle \ \langle 1,5\rangle \ \langle 1,6\rangle \ \langle 1,7\rangle \ \langle 1,8\rangle \\ \langle 2,0\rangle \ \langle 2,1\rangle \ \langle 2,2\rangle \ \langle 2,3\rangle \ \langle 2,4\rangle \ \langle 2,5\rangle \ \langle 2,6\rangle \ \langle 2,7\rangle \ \langle 2,8\rangle \ \langle 3,0\rangle \\ \langle 3,1\rangle \ \langle 3,3\rangle \ \langle 3,7\rangle \ \langle 4,0\rangle \ \langle 4,1\rangle \ \langle 4,2\rangle \ \langle 4,3\rangle \ \langle 4,4\rangle \ \langle 4,7\rangle \ \langle 5,0\rangle \\ \langle 5,1\rangle \ \langle 5,2\rangle \ \langle 5,3\rangle \ \langle 5,4\rangle \ \langle 5,5\rangle \ \langle 5,6\rangle \ \langle 5,7\rangle \ \langle 5,8\rangle \ \langle 6,0\rangle \ \langle 6,1\rangle \\ \langle 6,2\rangle \ \langle 6,3\rangle \ \langle 6,4\rangle \ \langle 6,5\rangle \ \langle 6,6\rangle \ \langle 6,7\rangle \ \langle 7,0\rangle \ \langle 7,1\rangle \ \langle 7,2\rangle \ \langle 7,3\rangle \\ \langle 7,4\rangle \ \langle 7,5\rangle \ \langle 7,7\rangle \ \langle 8,0\rangle \ \langle 8,1\rangle \ \langle 8,2\rangle \ \langle 8,3\rangle \ \langle 8,4\rangle \ \langle 8,5\rangle \ \langle 8,6\rangle \\ \langle 8,7\rangle \ \langle 8,8\rangle \end{array}$

• extensionally defined background relations

$$linked-to = \{ \langle 0,1 \rangle, \langle 0,3 \rangle, \langle 1,2 \rangle, \langle 3,2 \rangle, \langle 3,4 \rangle, \\ \langle 4,5 \rangle, \langle 4,6 \rangle, \langle 6,8 \rangle, \langle 7,6 \rangle, \langle 7,8 \rangle \}$$

The FOIL algorithm for relational learning

FOIL uses a covering approach to learn a set of rules

LEARNRULESET(set of tuples *T* of target relation, background relations *B*) { $S = \{ \}$ repeat $R \leftarrow \text{LEARNRULE}(T, B)$ $S \leftarrow S \cup R$ $T \leftarrow T$ – positive tuples covered by *R* until there are no (few) positive tuples left in *T* return *S* }

The FOIL algorithm for relational learning

```
LEARNRULE(set of tuples T of target relation, background relations B)

{

R = \{ \}

repeat

L \leftarrow best literal, based on T and B, to add to right-hand side of R

R \leftarrow R \cup L

T \leftarrow new set of tuples that satisfy L

until there are no (few) negative tuples left in T

return R

}
```

Literals in FOIL

• Given the current rule $R(X_1, X_2, ..., X_k) \leftarrow L_1 \land L_2 \land ... \land L_n$ FOIL considers adding several types of literals

$X_j = X_k$ $X_j \neq X_k$	both X_j and X_k either appear in the LHS of the rule, or were introduced by a previous literal
$Q(V_1, V_2,, V_a)$	at least one of the V_i 's has to be in the LHS of the rule, or was introduced by
$\neg Q(V_1, V_2, \dots V_a)$	a previous literal

where Q is a background relation

Literals in FOIL (continued)

 $X_j = c$ where *c* is a constant $X_j \neq c$

 $X_{j} > a$ $X_{j} \le a$ $X_{j} > X_{k}$ $X_{j} \le X_{k}$

where X_j and X_k are numeric variables and a is a numeric constant

Foil example

- suppose we want to learn rules for the target relation can-reach (X_1, X_2)
- we're given instances of the target relation from the following graph



• and instances of the background relation linked-to

$$linked-to = \{ \langle 0,1 \rangle, \langle 0,3 \rangle, \langle 1,2 \rangle, \langle 3,2 \rangle, \langle 3,4 \rangle, \\ \langle 4,5 \rangle, \langle 4,6 \rangle, \langle 6,8 \rangle, \langle 7,6 \rangle, \langle 7,8 \rangle \}$$

Foil example

- the first rule learned covers 10 of the positive instances can-reach $(X_1, X_2) \leftarrow \text{linked-to}(X_1, X_2)$
- the second rule learned covers the other 9 positive instances can-reach(X_1, X_2) \leftarrow linked-to(X_1, X_3) \land can-reach(X_3, X_2)



• note that these rules generalize to other graphs

Evaluating literals in FOIL

• FOIL evaluates the addition of a literal *L* to a rule *R* by

FOIL_Gain(L,R) =
$$t \left(\log_2 \frac{p_1}{p_1 + n_1} - \log_2 \frac{p_0}{p_0 + n_0} \right)$$

• where

 p_0 = # of positive tuples covered by R n_0 = # of negative tuples covered by R p_1 = # of positive tuples covered by $R \land L$ n_1 = # of negative tuples covered by $R \land L$ t = # of positive of tuples of R also covered by $R \land L$

- like information gain, but takes into account
 - we want to cover positives, not just get a more "pure" set of tuples
 - the size of the tuple set grows as we add new variables

Evaluating literals in FOIL

$$FOIL_Gain(L,R) = t\left(Info(R_0) - Info(R_1)\right)$$

- where R_0 represents the rule without L and R_1 is the rule with L added
- *Info*(*R_i*) is the number of bits required to encode a positive in the set of tuples covered by *R_i*

$$Info(R_i) = -\log_2\left(\frac{p_i}{p_i + n_i}\right)$$

Recall this example

• Definition of can-reach:

 $\operatorname{can-reach}(X_1, X_2) \leftarrow \operatorname{linked-to}(X_1, X_2)$

 $\operatorname{can-reach}(X_1, X_2) \leftarrow \operatorname{linked-to}(X_1, X_3) \wedge \operatorname{can-reach}(X_3, X_2)$



Foil example

 consider the first step in learning the second clause

 $\operatorname{can-reach}(X_1, X_2) \leftarrow$

 $can-reach(X_1, X_2) \leftarrow \\ linked-to(X_1, X_3)$

Additional refinements of FOIL

- early stopping to prevent overfitting
- using *m*-estimates of rule precision to guide search [Džeroski & Bratko, *ILP* 1992]
- type constraints on variables
- relational pathfinding to guide search for binary target relations [Craven, Slattery & Nigam, ECML 1998]
- using *intensional* background relations [Pazzani & Kibler, *Machine Learning* 1992]

between(X, Y, Z) \leftarrow less-than(X, Y) \land less-than(Y, Z) between(X, Y, Z) \leftarrow less-than(Z, Y) \land less-than(Y, X)

Comments on relational learning

- enables learning with more expressive hypothesis spaces
- but this comes at the cost of having <u>large hypothesis</u> spaces
 - harder to search
 - easier to overfit
- can take advantage of background knowledge represented as extensional relations or logical clauses (rules)
- one branch of research in this area *inductive logic programming* focuses on learning hypotheses in a logic programming framework
- search can be top-down (like FOIL) or bottom-up
- many relational learning methods not well suited to handling noisy data, representing uncertainty
 - but in the next lecture we'll discuss *statistical relational learning* methods which are designed to address these limitations