

# Relational Learning

Mark Craven and David Page  
CS 760: Machine Learning  
Spring 2019

# Goals for the lecture

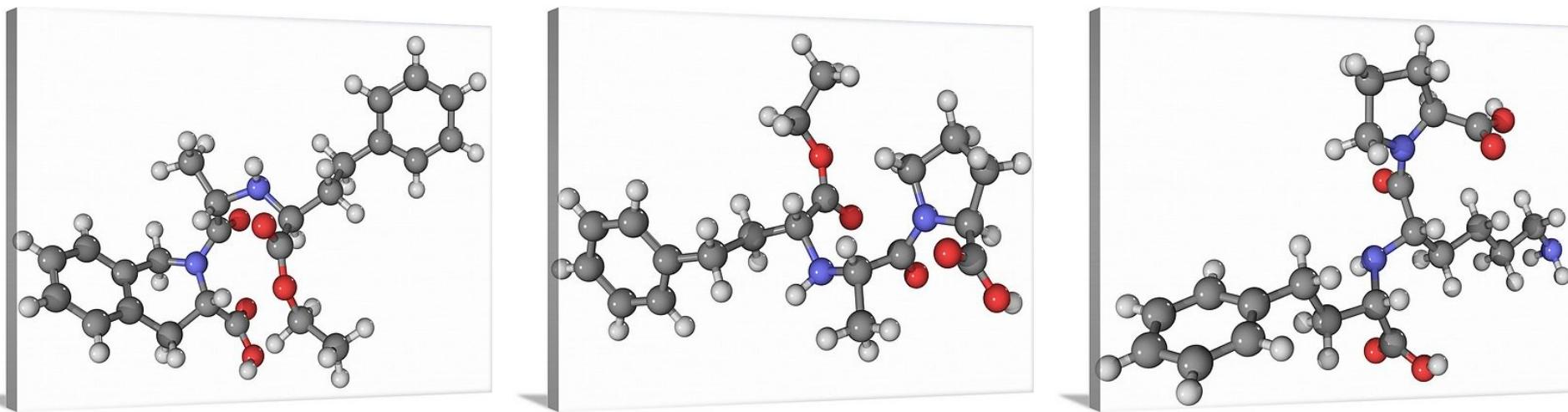
you should understand the following concepts

- relational learning
- the FOIL algorithm
- Markov logic networks
- plate models

# Relational learning example

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.

# Relational learning example

[Finn et al., *Machine Learning* 1998]

a multi-relational representation for molecules

Molecule	Target_1	...	Target_n
mol1	inactive		i nactive
mol2	active		inactive
•			
•			
•			

Molecular Bioactivity

Molecule	Bond_ID	Atom_1_ID	Atom_2_ID	Bond_Type
mol1	bond1	a1	a2	aromatic
•				
•				
•				

Bonds

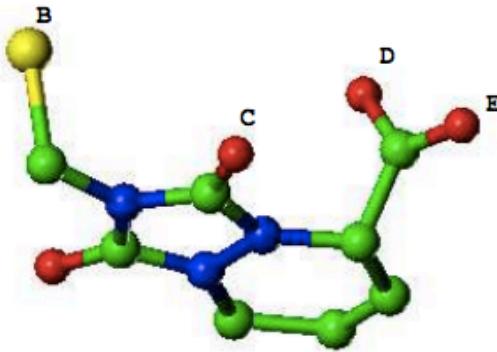
Molecule	Conformer	Atom_ID	Atom_Type	X_Coordinate	Y_Coordinate	Z_Coordinate
mol1	confl	a1	carbon	2.58	-1.23	0.69
•						
•						
•						

3D Atom Locations

# Relational learning example

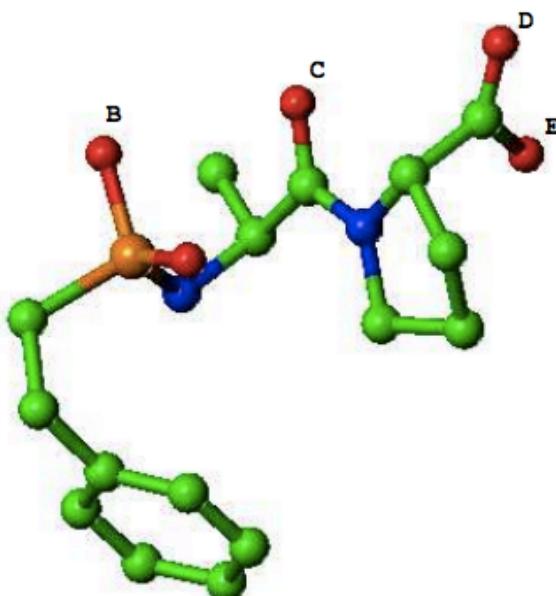
[Finn et al., *Machine Learning* 1998]

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 D and E in Conf is  $3.8 +/-.75$ .



# Relational representation

```
ACE_inhibitor(A) ← has_zinc_binding_site(A, B) ∧  
                      has_hydrogen_acceptor(A, C) ∧  
                      distance(B, C, 7.9, 0.75) ∧  
                      has_hydrogen_acceptor(A, D) ∧  
                      distance(B, D, 8.5, 0.75) ∧  
                      distance(C, D, 8.5, 0.75) ∧  
                      has_hydrogen_acceptor(A, E) ∧  
                      distance(B, E, 4.9, 0.75) ∧  
                      distance(C, E, 3.1, 0.75) ∧  
                      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

[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

PatientID	Gender	Birthdate
P1	M	3/22/63

diagnoses

PatientID	Date	Physician	Symptoms	Diagnosis
P1	1/1/01	Smith	palpitations	hypoglycemic
P1	2/1/03	Jones	fever, aches	influenza

labs

PatientID	Date	Lab Test	Result
P1	1/1/01	blood glucose	42
P1	1/9/01	blood glucose	45

PatientID	SNP1	SNP2	...	SNP500K
P1	AA	AB		BB
P2	AB	BB		AA

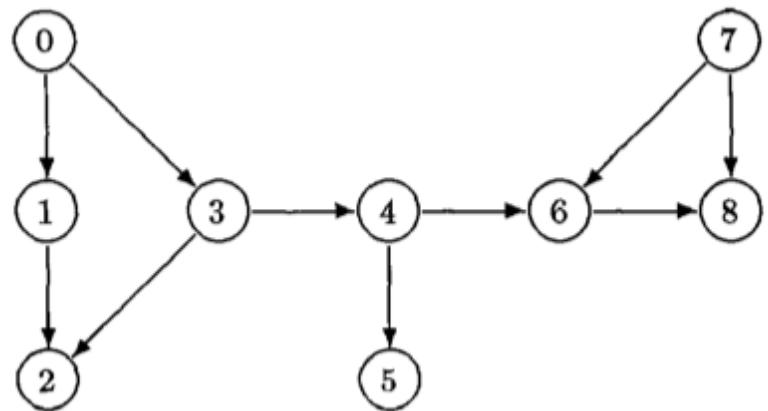
genetics

drugs

PatientID	Date Prescribed	Date Filled	Physician	Medication	Dose	Duration
P1	5/17/98	5/18/98	Jones	prilosec	10mg	3 months

# Relational learning example

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



$\oplus$ :  $\langle 0,1 \rangle \langle 0,2 \rangle \langle 0,3 \rangle \langle 0,4 \rangle \langle 0,5 \rangle \langle 0,6 \rangle \langle 0,8 \rangle \langle 1,2 \rangle \langle 3,2 \rangle \langle 3,4 \rangle \langle 3,5 \rangle \langle 3,6 \rangle \langle 3,8 \rangle \langle 4,5 \rangle \langle 4,6 \rangle \langle 4,8 \rangle \langle 6,8 \rangle \langle 7,6 \rangle \langle 7,8 \rangle$   
 $\ominus$ :  $\langle 0,0 \rangle \langle 0,7 \rangle \langle 1,0 \rangle \langle 1,1 \rangle \langle 1,3 \rangle \langle 1,4 \rangle \langle 1,5 \rangle \langle 1,6 \rangle \langle 1,7 \rangle \langle 1,8 \rangle \langle 2,0 \rangle \langle 2,1 \rangle \langle 2,2 \rangle \langle 2,3 \rangle \langle 2,4 \rangle \langle 2,5 \rangle \langle 2,6 \rangle \langle 2,7 \rangle \langle 2,8 \rangle \langle 3,0 \rangle \langle 3,1 \rangle \langle 3,3 \rangle \langle 3,7 \rangle \langle 4,0 \rangle \langle 4,1 \rangle \langle 4,2 \rangle \langle 4,3 \rangle \langle 4,4 \rangle \langle 4,7 \rangle \langle 5,0 \rangle \langle 5,1 \rangle \langle 5,2 \rangle \langle 5,3 \rangle \langle 5,4 \rangle \langle 5,5 \rangle \langle 5,6 \rangle \langle 5,7 \rangle \langle 5,8 \rangle \langle 6,0 \rangle \langle 6,1 \rangle \langle 6,2 \rangle \langle 6,3 \rangle \langle 6,4 \rangle \langle 6,5 \rangle \langle 6,6 \rangle \langle 6,7 \rangle \langle 7,0 \rangle \langle 7,1 \rangle \langle 7,2 \rangle \langle 7,3 \rangle \langle 7,4 \rangle \langle 7,5 \rangle \langle 7,7 \rangle \langle 8,0 \rangle \langle 8,1 \rangle \langle 8,2 \rangle \langle 8,3 \rangle \langle 8,4 \rangle \langle 8,5 \rangle \langle 8,6 \rangle \langle 8,7 \rangle \langle 8,8 \rangle$

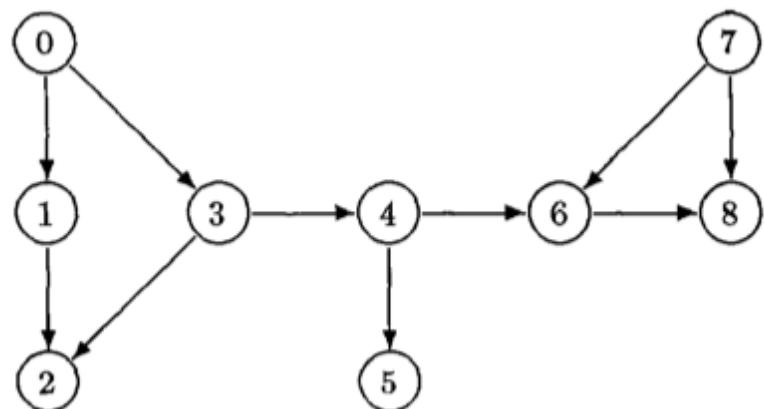
- how would you represent this task to a learner?

# Relational learning example

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

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

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



$\oplus:$   $\langle 0,1 \rangle \langle 0,2 \rangle \langle 0,3 \rangle \langle 0,4 \rangle \langle 0,5 \rangle \langle 0,6 \rangle \langle 0,8 \rangle \langle 1,2 \rangle \langle 3,2 \rangle \langle 3,4 \rangle \langle 3,5 \rangle \langle 3,6 \rangle \langle 3,8 \rangle \langle 4,5 \rangle \langle 4,6 \rangle \langle 4,8 \rangle \langle 6,8 \rangle \langle 7,6 \rangle \langle 7,8 \rangle$   
 $\ominus:$   $\langle 0,0 \rangle \langle 0,7 \rangle \langle 1,0 \rangle \langle 1,1 \rangle \langle 1,3 \rangle \langle 1,4 \rangle \langle 1,5 \rangle \langle 1,6 \rangle \langle 1,7 \rangle \langle 1,8 \rangle \langle 2,0 \rangle \langle 2,1 \rangle \langle 2,2 \rangle \langle 2,3 \rangle \langle 2,4 \rangle \langle 2,5 \rangle \langle 2,6 \rangle \langle 2,7 \rangle \langle 2,8 \rangle \langle 3,0 \rangle \langle 3,1 \rangle \langle 3,3 \rangle \langle 3,7 \rangle \langle 4,0 \rangle \langle 4,1 \rangle \langle 4,2 \rangle \langle 4,3 \rangle \langle 4,4 \rangle \langle 4,7 \rangle \langle 5,0 \rangle \langle 5,1 \rangle \langle 5,2 \rangle \langle 5,3 \rangle \langle 5,4 \rangle \langle 5,5 \rangle \langle 5,6 \rangle \langle 5,7 \rangle \langle 5,8 \rangle \langle 6,0 \rangle \langle 6,1 \rangle \langle 6,2 \rangle \langle 6,3 \rangle \langle 6,4 \rangle \langle 6,5 \rangle \langle 6,6 \rangle \langle 6,7 \rangle \langle 7,0 \rangle \langle 7,1 \rangle \langle 7,2 \rangle \langle 7,3 \rangle \langle 7,4 \rangle \langle 7,5 \rangle \langle 7,7 \rangle \langle 8,0 \rangle \langle 8,1 \rangle \langle 8,2 \rangle \langle 8,3 \rangle \langle 8,4 \rangle \langle 8,5 \rangle \langle 8,6 \rangle \langle 8,7 \rangle \langle 8,8 \rangle$

# 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

$\oplus$ :  $\langle 0,1 \rangle \langle 0,2 \rangle \langle 0,3 \rangle \langle 0,4 \rangle \langle 0,5 \rangle \langle 0,6 \rangle \langle 0,8 \rangle \langle 1,2 \rangle \langle 3,2 \rangle \langle 3,4 \rangle$   
 $\langle 3,5 \rangle \langle 3,6 \rangle \langle 3,8 \rangle \langle 4,5 \rangle \langle 4,6 \rangle \langle 4,8 \rangle \langle 6,8 \rangle \langle 7,6 \rangle \langle 7,8 \rangle$   
 $\ominus$ :  $\langle 0,0 \rangle \langle 0,7 \rangle \langle 1,0 \rangle \langle 1,1 \rangle \langle 1,3 \rangle \langle 1,4 \rangle \langle 1,5 \rangle \langle 1,6 \rangle \langle 1,7 \rangle \langle 1,8 \rangle$   
 $\langle 2,0 \rangle \langle 2,1 \rangle \langle 2,2 \rangle \langle 2,3 \rangle \langle 2,4 \rangle \langle 2,5 \rangle \langle 2,6 \rangle \langle 2,7 \rangle \langle 2,8 \rangle \langle 3,0 \rangle$   
 $\langle 3,1 \rangle \langle 3,3 \rangle \langle 3,7 \rangle \langle 4,0 \rangle \langle 4,1 \rangle \langle 4,2 \rangle \langle 4,3 \rangle \langle 4,4 \rangle \langle 4,7 \rangle \langle 5,0 \rangle$   
 $\langle 5,1 \rangle \langle 5,2 \rangle \langle 5,3 \rangle \langle 5,4 \rangle \langle 5,5 \rangle \langle 5,6 \rangle \langle 5,7 \rangle \langle 5,8 \rangle \langle 6,0 \rangle \langle 6,1 \rangle$   
 $\langle 6,2 \rangle \langle 6,3 \rangle \langle 6,4 \rangle \langle 6,5 \rangle \langle 6,6 \rangle \langle 6,7 \rangle \langle 7,0 \rangle \langle 7,1 \rangle \langle 7,2 \rangle \langle 7,3 \rangle$   
 $\langle 7,4 \rangle \langle 7,5 \rangle \langle 7,7 \rangle \langle 8,0 \rangle \langle 8,1 \rangle \langle 8,2 \rangle \langle 8,3 \rangle \langle 8,4 \rangle \langle 8,5 \rangle \langle 8,6 \rangle$   
 $\langle 8,7 \rangle \langle 8,8 \rangle$

- 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
         $R \leftarrow \text{LEARNRULE}(T, B)$ 
         $S \leftarrow S \cup R$ 
         $T \leftarrow T - \text{positive tuples covered by } R$ 
    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  $R(X_1, X_2, \dots X_k) \leftarrow L_1 \wedge L_2 \wedge \dots \wedge L_n$   
FOIL considers adding several types of literals

$$X_j = X_k$$

both  $X_j$  and  $X_k$  either appear in the LHS of the rule, or were introduced by a previous literal

$$X_j \neq X_k$$

$$Q(V_1, V_2, \dots V_a)$$

at least one of the  $V_i$ 's has to be in the LHS of the rule, or was introduced by a previous literal

$$\neg Q(V_1, V_2, \dots V_a)$$

where  $Q$  is a background relation

# Literals in FOIL (continued)

$$X_j = c$$

where  $c$  is a constant

$$X_j \neq c$$

$$X_j > a$$

$$X_j \leq a$$

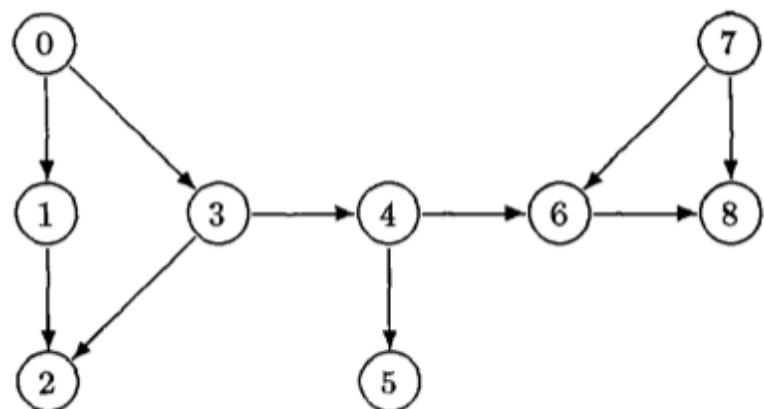
$$X_j > X_k$$

$$X_j \leq X_k$$

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



$\oplus:$   $\langle 0,1 \rangle \langle 0,2 \rangle \langle 0,3 \rangle \langle 0,4 \rangle \langle 0,5 \rangle \langle 0,6 \rangle \langle 0,8 \rangle \langle 1,2 \rangle \langle 3,2 \rangle \langle 3,4 \rangle \langle 3,5 \rangle \langle 3,6 \rangle \langle 3,8 \rangle \langle 4,5 \rangle \langle 4,6 \rangle \langle 4,8 \rangle \langle 6,8 \rangle \langle 7,6 \rangle \langle 7,8 \rangle$   
 $\ominus:$   $\langle 0,0 \rangle \langle 0,7 \rangle \langle 1,0 \rangle \langle 1,1 \rangle \langle 1,3 \rangle \langle 1,4 \rangle \langle 1,5 \rangle \langle 1,6 \rangle \langle 1,7 \rangle \langle 1,8 \rangle \langle 2,0 \rangle \langle 2,1 \rangle \langle 2,2 \rangle \langle 2,3 \rangle \langle 2,4 \rangle \langle 2,5 \rangle \langle 2,6 \rangle \langle 2,7 \rangle \langle 2,8 \rangle \langle 3,0 \rangle \langle 3,1 \rangle \langle 3,3 \rangle \langle 3,7 \rangle \langle 4,0 \rangle \langle 4,1 \rangle \langle 4,2 \rangle \langle 4,3 \rangle \langle 4,4 \rangle \langle 4,7 \rangle \langle 5,0 \rangle \langle 5,1 \rangle \langle 5,2 \rangle \langle 5,3 \rangle \langle 5,4 \rangle \langle 5,5 \rangle \langle 5,6 \rangle \langle 5,7 \rangle \langle 5,8 \rangle \langle 6,0 \rangle \langle 6,1 \rangle \langle 6,2 \rangle \langle 6,3 \rangle \langle 6,4 \rangle \langle 6,5 \rangle \langle 6,6 \rangle \langle 6,7 \rangle \langle 7,0 \rangle \langle 7,1 \rangle \langle 7,2 \rangle \langle 7,3 \rangle \langle 7,4 \rangle \langle 7,5 \rangle \langle 7,7 \rangle \langle 8,0 \rangle \langle 8,1 \rangle \langle 8,2 \rangle \langle 8,3 \rangle \langle 8,4 \rangle \langle 8,5 \rangle \langle 8,6 \rangle \langle 8,7 \rangle \langle 8,8 \rangle$

- and instances of the background relation linked-to

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

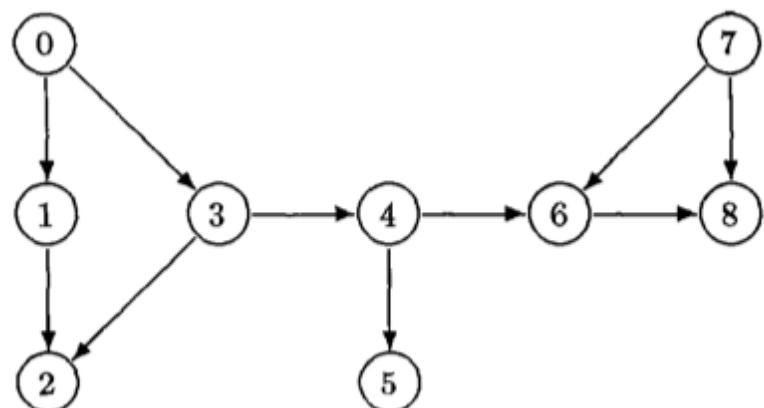
# FoIL example

- the first rule learned covers 10 of the positive instances

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

- the second rule learned covers the other 9 positive instances

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



$\oplus:$   $\langle 0,1 \rangle \langle 0,2 \rangle \langle 0,3 \rangle \langle 0,4 \rangle \langle 0,5 \rangle \langle 0,6 \rangle \langle 0,8 \rangle \langle 1,2 \rangle \langle 3,2 \rangle \langle 3,4 \rangle \langle 3,5 \rangle \langle 3,6 \rangle \langle 3,8 \rangle \langle 4,5 \rangle \langle 4,6 \rangle \langle 4,8 \rangle \langle 6,8 \rangle \langle 7,6 \rangle \langle 7,8 \rangle$   
 $\ominus:$   $\langle 0,0 \rangle \langle 0,7 \rangle \langle 1,0 \rangle \langle 1,1 \rangle \langle 1,3 \rangle \langle 1,4 \rangle \langle 1,5 \rangle \langle 1,6 \rangle \langle 1,7 \rangle \langle 1,8 \rangle \langle 2,0 \rangle \langle 2,1 \rangle \langle 2,2 \rangle \langle 2,3 \rangle \langle 2,4 \rangle \langle 2,5 \rangle \langle 2,6 \rangle \langle 2,7 \rangle \langle 2,8 \rangle \langle 3,0 \rangle \langle 3,1 \rangle \langle 3,3 \rangle \langle 3,7 \rangle \langle 4,0 \rangle \langle 4,1 \rangle \langle 4,2 \rangle \langle 4,3 \rangle \langle 4,4 \rangle \langle 4,7 \rangle \langle 5,0 \rangle \langle 5,1 \rangle \langle 5,2 \rangle \langle 5,3 \rangle \langle 5,4 \rangle \langle 5,5 \rangle \langle 5,6 \rangle \langle 5,7 \rangle \langle 5,8 \rangle \langle 6,0 \rangle \langle 6,1 \rangle \langle 6,2 \rangle \langle 6,3 \rangle \langle 6,4 \rangle \langle 6,5 \rangle \langle 6,6 \rangle \langle 6,7 \rangle \langle 7,0 \rangle \langle 7,1 \rangle \langle 7,2 \rangle \langle 7,3 \rangle \langle 7,4 \rangle \langle 7,5 \rangle \langle 7,7 \rangle \langle 8,0 \rangle \langle 8,1 \rangle \langle 8,2 \rangle \langle 8,3 \rangle \langle 8,4 \rangle \langle 8,5 \rangle \langle 8,6 \rangle \langle 8,7 \rangle \langle 8,8 \rangle$

- 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  $R \wedge L$

$n_1$  = # of negative tuples covered by  $R \wedge L$

$t$  = # of positive of tuples of  $R$  also covered by  $R \wedge L$

- 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  $R_i$

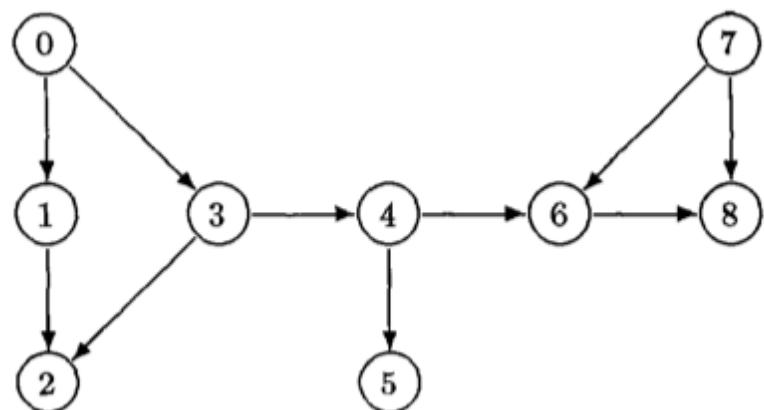
$$Info(R_i) = -\log_2 \left( \frac{p_i}{p_i + n_i} \right)$$

# Recall this example

- Definition of can-reach:

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

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



$\oplus: \langle 0,1 \rangle \langle 0,2 \rangle \langle 0,3 \rangle \langle 0,4 \rangle \langle 0,5 \rangle \langle 0,6 \rangle \langle 0,8 \rangle \langle 1,2 \rangle \langle 3,2 \rangle \langle 3,4 \rangle \langle 3,5 \rangle \langle 3,6 \rangle \langle 3,8 \rangle \langle 4,5 \rangle \langle 4,6 \rangle \langle 4,8 \rangle \langle 6,8 \rangle \langle 7,6 \rangle \langle 7,8 \rangle$   
 $\ominus: \langle 0,0 \rangle \langle 0,7 \rangle \langle 1,0 \rangle \langle 1,1 \rangle \langle 1,3 \rangle \langle 1,4 \rangle \langle 1,5 \rangle \langle 1,6 \rangle \langle 1,7 \rangle \langle 1,8 \rangle \langle 2,0 \rangle \langle 2,1 \rangle \langle 2,2 \rangle \langle 2,3 \rangle \langle 2,4 \rangle \langle 2,5 \rangle \langle 2,6 \rangle \langle 2,7 \rangle \langle 2,8 \rangle \langle 3,0 \rangle \langle 3,1 \rangle \langle 3,3 \rangle \langle 3,7 \rangle \langle 4,0 \rangle \langle 4,1 \rangle \langle 4,2 \rangle \langle 4,3 \rangle \langle 4,4 \rangle \langle 4,7 \rangle \langle 5,0 \rangle \langle 5,1 \rangle \langle 5,2 \rangle \langle 5,3 \rangle \langle 5,4 \rangle \langle 5,5 \rangle \langle 5,6 \rangle \langle 5,7 \rangle \langle 5,8 \rangle \langle 6,0 \rangle \langle 6,1 \rangle \langle 6,2 \rangle \langle 6,3 \rangle \langle 6,4 \rangle \langle 6,5 \rangle \langle 6,6 \rangle \langle 6,7 \rangle \langle 7,0 \rangle \langle 7,1 \rangle \langle 7,2 \rangle \langle 7,3 \rangle \langle 7,4 \rangle \langle 7,5 \rangle \langle 7,7 \rangle \langle 8,0 \rangle \langle 8,1 \rangle \langle 8,2 \rangle \langle 8,3 \rangle \langle 8,4 \rangle \langle 8,5 \rangle \langle 8,6 \rangle \langle 8,7 \rangle \langle 8,8 \rangle$

# FoIL example

- consider the first step in learning the second clause

can-reach( $X_1, X_2$ )  $\leftarrow$



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

$$FOIL\_Gain(L, R) = 9 \left( \log_2 \frac{18}{18 + 54} - \log_2 \frac{9}{9 + 62} \right)$$

$$= 8.8$$

$\oplus:$  [ ]  $\langle 0,2 \rangle$  [ ]  $\langle 0,4 \rangle$  [ ]  $\langle 0,5 \rangle$  [ ]  $\langle 0,6 \rangle$  [ ]  $\langle 0,8 \rangle$  [ ] [ ] [ ]  
 [ ]  $\langle 3,5 \rangle$  [ ]  $\langle 3,6 \rangle$  [ ]  $\langle 3,8 \rangle$  [ ] [ ]  $\langle 4,8 \rangle$  [ ] [ ] [ ]  
 $\ominus:$   $\langle 0,0 \rangle$   $\langle 0,7 \rangle$   $\langle 1,0 \rangle$   $\langle 1,1 \rangle$   $\langle 1,3 \rangle$   $\langle 1,4 \rangle$   $\langle 1,5 \rangle$   $\langle 1,6 \rangle$   $\langle 1,7 \rangle$   $\langle 1,8 \rangle$   
 $\langle 2,0 \rangle$   $\langle 2,1 \rangle$   $\langle 2,2 \rangle$   $\langle 2,3 \rangle$   $\langle 2,4 \rangle$   $\langle 2,5 \rangle$   $\langle 2,6 \rangle$   $\langle 2,7 \rangle$   $\langle 2,8 \rangle$   $\langle 3,0 \rangle$   
 $\langle 3,1 \rangle$   $\langle 3,3 \rangle$   $\langle 3,7 \rangle$   $\langle 4,0 \rangle$   $\langle 4,1 \rangle$   $\langle 4,2 \rangle$   $\langle 4,3 \rangle$   $\langle 4,4 \rangle$   $\langle 4,7 \rangle$   $\langle 5,0 \rangle$   
 $\langle 5,1 \rangle$   $\langle 5,2 \rangle$   $\langle 5,3 \rangle$   $\langle 5,4 \rangle$   $\langle 5,5 \rangle$   $\langle 5,6 \rangle$   $\langle 5,7 \rangle$   $\langle 5,8 \rangle$   $\langle 6,0 \rangle$   $\langle 6,1 \rangle$   
 $\langle 6,2 \rangle$   $\langle 6,3 \rangle$   $\langle 6,4 \rangle$   $\langle 6,5 \rangle$   $\langle 6,6 \rangle$   $\langle 6,7 \rangle$   $\langle 7,0 \rangle$   $\langle 7,1 \rangle$   $\langle 7,2 \rangle$   $\langle 7,3 \rangle$   
 $\langle 7,4 \rangle$   $\langle 7,5 \rangle$   $\langle 7,7 \rangle$   $\langle 8,0 \rangle$   $\langle 8,1 \rangle$   $\langle 8,2 \rangle$   $\langle 8,3 \rangle$   $\langle 8,4 \rangle$   $\langle 8,5 \rangle$   $\langle 8,6 \rangle$   
 $\langle 8,7 \rangle$   $\langle 8,8 \rangle$

$\oplus:$   $\langle 0,2,1 \rangle$   $\langle 0,2,3 \rangle$   $\langle 0,4,1 \rangle$   $\langle 0,4,3 \rangle$   $\langle 0,5,1 \rangle$   $\langle 0,5,3 \rangle$   $\langle 0,6,1 \rangle$   
 $\langle 0,6,3 \rangle$   $\langle 0,8,1 \rangle$   $\langle 0,8,3 \rangle$   $\langle 3,5,2 \rangle$   $\langle 3,5,4 \rangle$   $\langle 3,6,2 \rangle$   $\langle 3,6,4 \rangle$   
 $\langle 3,8,2 \rangle$   $\langle 3,8,4 \rangle$   $\langle 4,8,5 \rangle$   $\langle 4,8,6 \rangle$   
 $\ominus:$   $\langle 0,0,1 \rangle$   $\langle 0,0,3 \rangle$   $\langle 0,7,1 \rangle$   $\langle 0,7,3 \rangle$   $\langle 1,0,2 \rangle$   $\langle 1,1,2 \rangle$   $\langle 1,3,2 \rangle$   
 $\langle 1,4,2 \rangle$   $\langle 1,5,2 \rangle$   $\langle 1,6,2 \rangle$   $\langle 1,7,2 \rangle$   $\langle 1,8,2 \rangle$   $\langle 3,0,2 \rangle$   $\langle 3,0,4 \rangle$   
 $\langle 3,1,2 \rangle$   $\langle 3,1,4 \rangle$   $\langle 3,3,2 \rangle$   $\langle 3,3,4 \rangle$   $\langle 3,7,2 \rangle$   $\langle 3,7,4 \rangle$   $\langle 4,0,5 \rangle$   
 $\langle 4,0,6 \rangle$   $\langle 4,1,5 \rangle$   $\langle 4,1,6 \rangle$   $\langle 4,2,5 \rangle$   $\langle 4,2,6 \rangle$   $\langle 4,3,5 \rangle$   $\langle 4,3,6 \rangle$   
 $\langle 4,4,5 \rangle$   $\langle 4,4,6 \rangle$   $\langle 4,7,5 \rangle$   $\langle 4,7,6 \rangle$   $\langle 6,0,8 \rangle$   $\langle 6,1,8 \rangle$   $\langle 6,2,8 \rangle$   
 $\langle 6,3,8 \rangle$   $\langle 6,4,8 \rangle$   $\langle 6,5,8 \rangle$   $\langle 6,6,8 \rangle$   $\langle 6,7,8 \rangle$   $\langle 7,0,6 \rangle$   $\langle 7,0,8 \rangle$   
 $\langle 7,1,6 \rangle$   $\langle 7,1,8 \rangle$   $\langle 7,2,6 \rangle$   $\langle 7,2,8 \rangle$   $\langle 7,3,6 \rangle$   $\langle 7,3,8 \rangle$   $\langle 7,4,6 \rangle$   
 $\langle 7,4,8 \rangle$   $\langle 7,5,6 \rangle$   $\langle 7,5,8 \rangle$   $\langle 7,7,6 \rangle$   $\langle 7,7,8 \rangle$

# Another Approach – Extend Markov Networks... Recall:

$$\Pr(\vec{V}) = \frac{1}{Z} \exp \sum_i w_i f_i(\vec{V})$$

- In this formulation, the  $w$ 's are just weights and the  $f$ 's are just features
- As such, we can throw the graph out if we want – we have everything we need in the  $w$ 's and  $f$ 's
- In this view, parameter learning is just weight learning

Assume: Data set  $D$  consists of  $d_1, \dots, d_m$

Features are  $f_1, \dots, f_n$

Weights on features are  $W = \langle w_1, \dots, w_n \rangle$

Let  $n_i(D)$  denote the number of times (data points where)  
 $f_i$  is true in  $D$

With slight abuse of notation, let  $E_W(n_i(m))$  denote the expected number  
of times  $f_i$  is true in  $m$  examples under the distribution defined by  $W$

Let  $ll$  denote the log-likelihood of  $W$  given  $D$ :  $\ln P(D|W)$

$$ll = \sum_j \ln \frac{1}{Z} e^{\sum_i w_i f_i(d_j)}$$

$$ll = \sum_{i,j} w_i f_i(d_j) - \ln Z$$

$$\frac{\partial ll}{\partial w_i} = \sum_j f_i(d_j) - \frac{1}{Z} \sum_V e^{\sum_i w_i f_i(V)} f_i(V)$$

$$\frac{\partial ll}{\partial w_i} = n_i(D) - E_W(n_i(m))$$

Assume: Data set  $D$  consists of  $d_1, \dots, d_m$

Features are  $f_1, \dots, f_n$

Weights on features are  $W = \langle w_1, \dots, w_n \rangle$

Let  $n_i(D)$  denote the number of times (data points where)  
 $f_i$  is true in  $D$

With slight abuse of notation, let  $E_W(n_i(m))$  denote the expected number  
of times  $f_i$  is true in  $m$  examples under the distribution defined by  $W$

Let  $ll$  denote the log-likelihood of  $W$  given  $D$ :  $\ln P(D|W)$

$$ll = \sum_j \ln \frac{1}{Z} e^{\sum_i w_i f_i(d_j)}$$

$$ll = \sum_{i,j} w_i f_i(d_j) - \ln Z$$

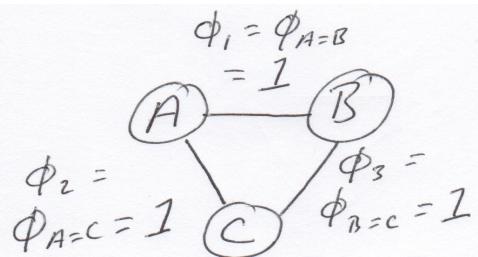
$$\frac{\partial ll}{\partial w_i} = \sum_j f_i(d_j) - \frac{1}{Z} \sum_V e^{\sum_i w_i f_i(V)} f_i(V)$$

$$\frac{\partial ll}{\partial w_i} = [n_i(D)] - [E_W(n_i(m))]$$

Target value

To be changed

# Example: Ising Model



$$Z = \sum_{\vec{v}} e^{\sum_i \phi_i(\vec{v})}$$

$\approx 56.2$

A	B	C	$e^{\sum_i \phi_i(\vec{v})}$	$P_{\vec{\phi}}(\vec{v})$
0	0	0	$e^3 \approx 20$	.35
0	0	1	$e \approx 2.7$	.05
0	1	0	:	:
0	1	1	:	:
1	0	0	:	:
1	0	1	:	:
1	1	0	:	:
1	1	1	$e^3 \approx 20$	.35

Data		
A	B	C
1	1	0
0	1	1
1	1	1
0	0	0
1	0	1

$$\#_{A=B} = 3$$

$$\#_{B=C} = 3$$

$$\#_{A=C} = 3$$

$$E_{\vec{\phi}, 101=5} [\#_{A=B}] = .8(5) = 4$$

same for  $\#_{A=C}$ ,  $\#_{B=C}$

Gradient:  $\langle -1, -1, -1 \rangle$

$$\text{New } \vec{\phi}: \langle 1, 1, 1 \rangle + \eta \langle -1, -1, -1 \rangle$$

$$(\text{e.g., } .05) = \langle .95, .95, .95 \rangle$$

# Alternative: Markov logic



- a logical knowledge base is a set of **hard constraints** on the set of possible worlds
- let's make them **soft constraints**: when a world violates a formula, it becomes less probable, not impossible
- give each formula a weight (higher weight → stronger constraint)

$$P(\text{world}) \propto \exp\left(\sum \text{weights of formulas it satisfies}\right)$$

# MLN definition

- a *Markov Logic Network* (MLN) is a set of pairs  $(F, w)$  where  
 $F$  is a formula in first-order logic  
 $w$  is a real number
- together with a set of constants, it defines a Markov network with
  - one node for each grounding of each predicate in the MLN
  - one feature for each grounding of each formula  $F$  in the MLN, with the corresponding weight  $w$

# MLN example: friends & smokers

Smoking causes cancer.

Friends have similar smoking habits.

# MLN example: friends & smokers

$$\forall x \text{ Smokes}(x) \Rightarrow \text{Cancer}(x)$$
$$\forall x, y \text{ Friends}(x, y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$$

# MLN example: friends & smokers

1.5  $\forall x \text{ Smokes}(x) \Rightarrow \text{Cancer}(x)$

1.1  $\forall x, y \text{ Friends}(x, y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$

# MLN example: friends & smokers

1.5  $\forall x \text{ Smokes}(x) \Rightarrow \text{Cancer}(x)$

1.1  $\forall x, y \text{ Friends}(x, y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$

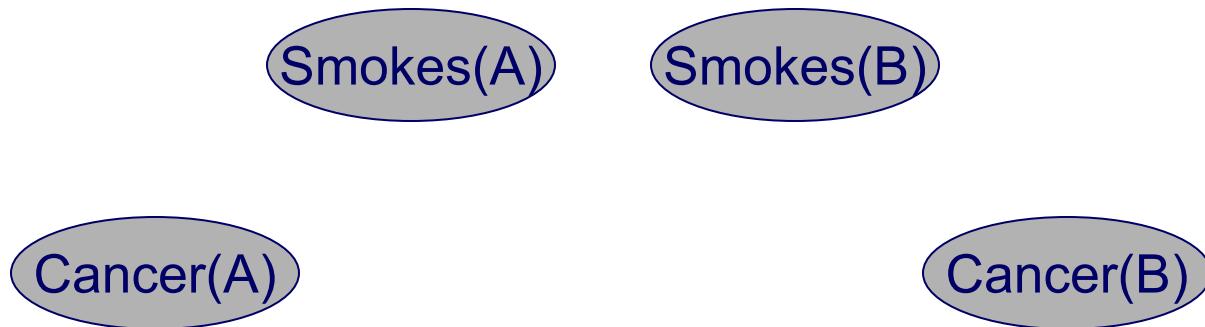
Two constants: **Anna** (A) and **Bob** (B)

# MLN example: friends & smokers

1.5  $\forall x \text{ Smokes}(x) \Rightarrow \text{Cancer}(x)$

1.1  $\forall x, y \text{ Friends}(x, y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$

Two constants: **Anna** (A) and **Bob** (B)

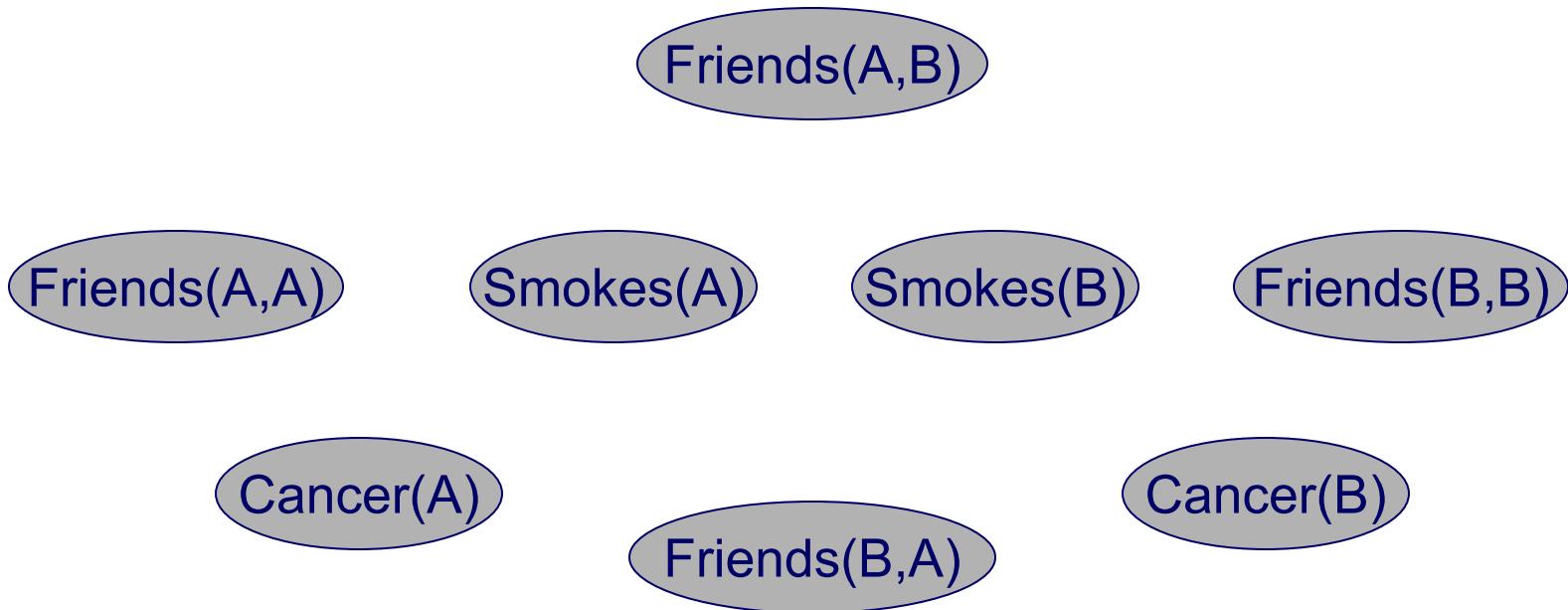


# MLN example: friends & smokers

1.5  $\forall x \text{ Smokes}(x) \Rightarrow \text{Cancer}(x)$

1.1  $\forall x, y \text{ Friends}(x, y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$

Two constants: **Anna** (A) and **Bob** (B)

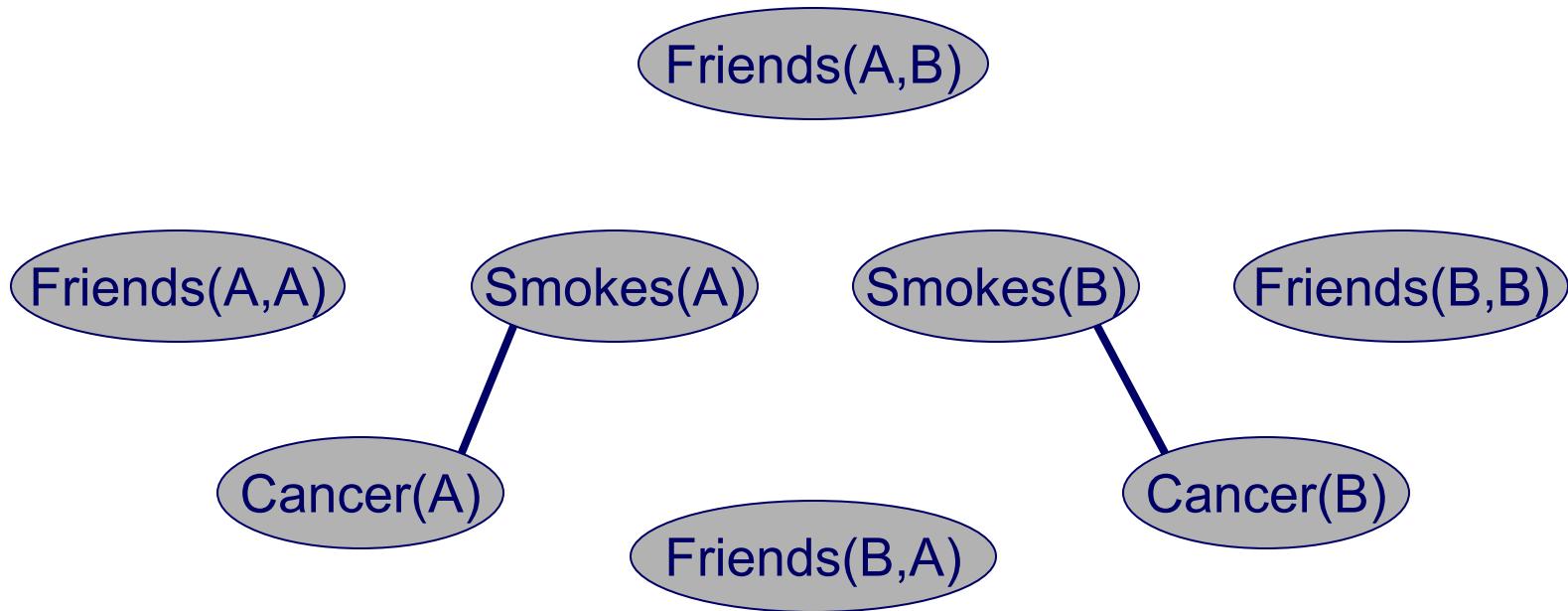


# MLN example: friends & smokers

1.5  $\forall x \text{ Smokes}(x) \Rightarrow \text{Cancer}(x)$

1.1  $\forall x, y \text{ Friends}(x, y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$

Two constants: **Anna** (A) and **Bob** (B)

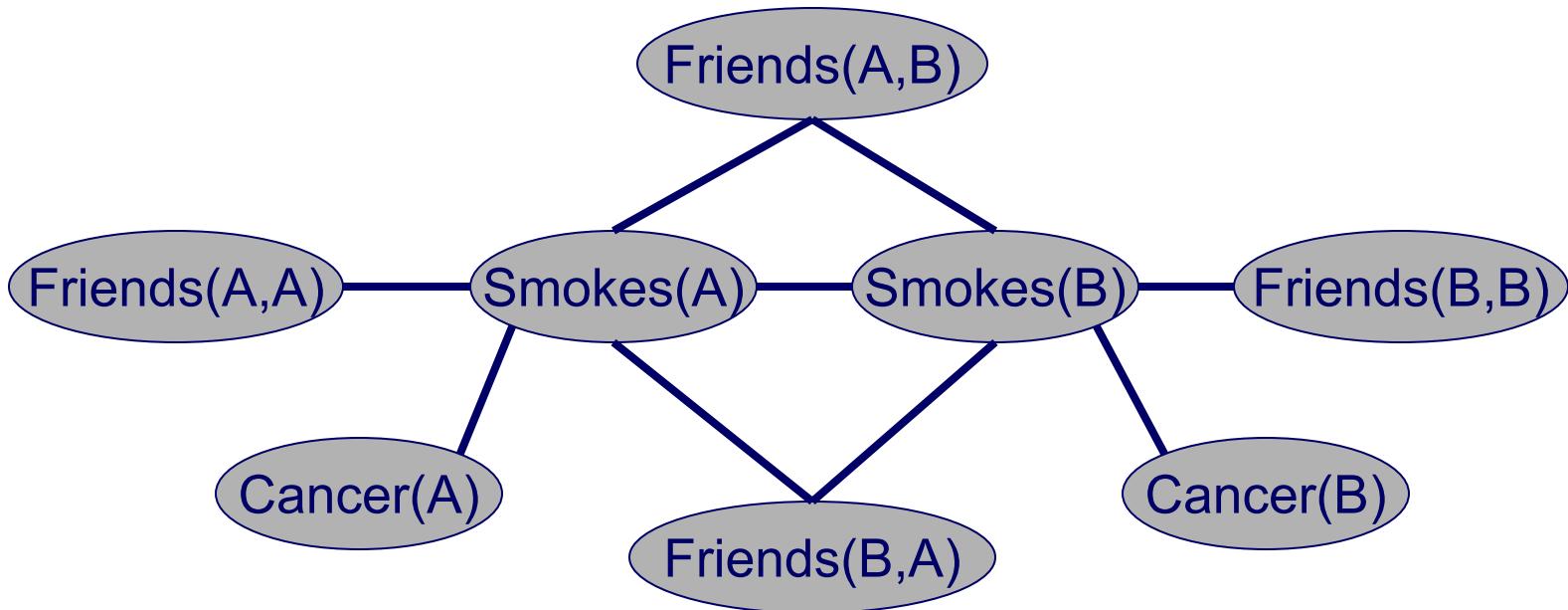


# MLN example: friends & smokers

1.5  $\forall x \text{ Smokes}(x) \Rightarrow \text{Cancer}(x)$

1.1  $\forall x, y \text{ Friends}(x, y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$

Two constants: **Anna** (A) and **Bob** (B)



# Markov logic networks

- a MLN is a **template** for ground Markov nets
  - the logic determines the form of the cliques
  - but if we had one more constant (say, **Larry**), we'd get a different Markov net
- we can determine the probability of a world  $\nu$  (assignment of truth values to ground predicates) by

$$P(\nu) = \frac{1}{Z} \exp\left( \sum_i w_i n_i(\nu) \right)$$

weight of formula  $i$

# of true groundings of formula  $i$  in  $\nu$

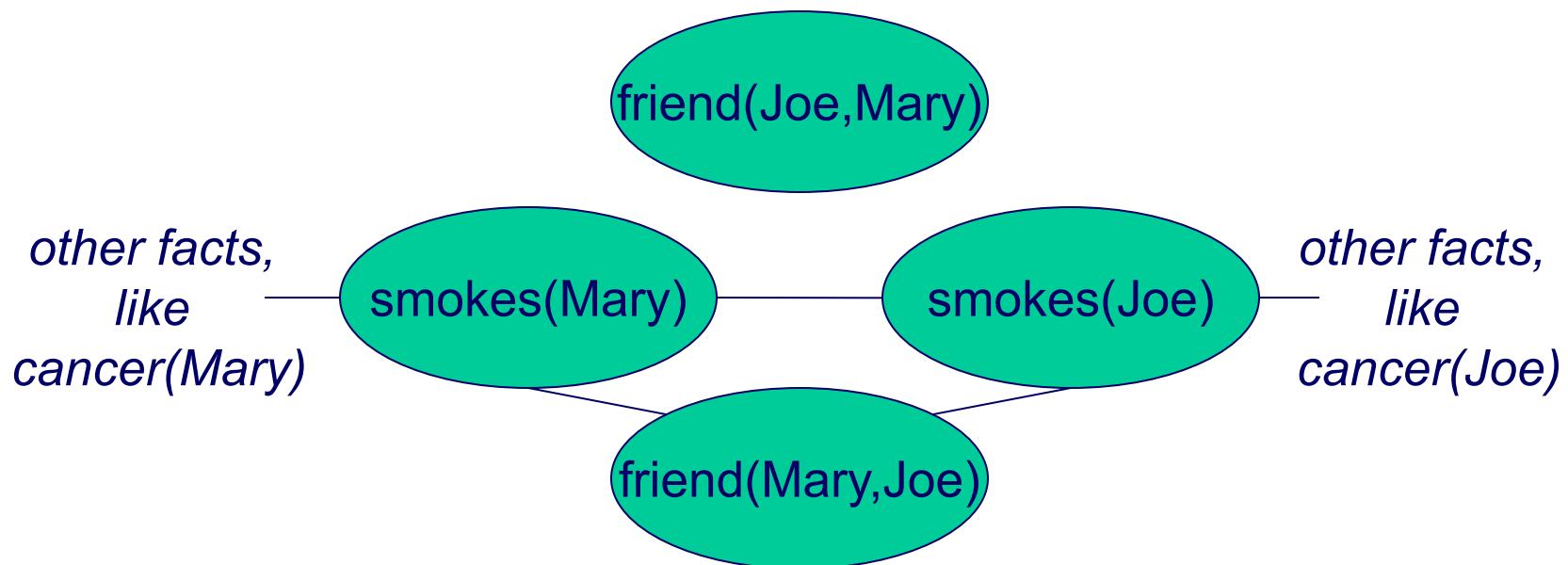
# Example translated to Markov Network

- **Facts:**

smokes(Mary)  
smokes(Joe)  
friend(Joe, Mary)

- **Rules:**

$\forall x \forall y \text{ friend}(x,y) \wedge \text{Smokes}(x) \rightarrow \text{Smokes}(y)$



# Computing weights

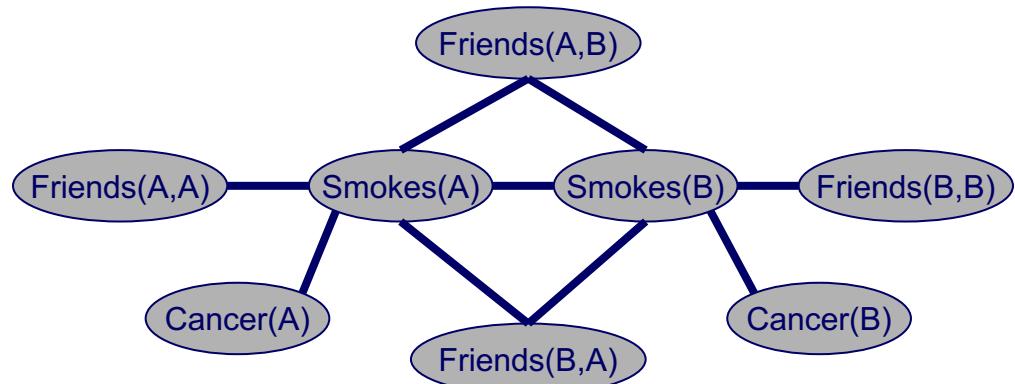
Consider the effect of rule R:  $\text{Friends}(x,y) \wedge \text{Smokes}(x) \rightarrow \text{Smokes}(y)$  weight  
1.1

	smokes(Mary)		$\neg\text{smokes}(Mary)$
	smokes(Joe)	$\neg\text{smokes}(Joe)$	smokes(Joe)
friends(Mary,Joe)	$e^{1.1}$	1	$e^{1.1}$
$\neg\text{friends}(Mary,Joe)$	$e^{1.1}$	$e^{1.1}$	$e^{1.1}$

This is the only setting that does not satisfy R  
Thus, it is given value 1, while the others are  
Given value  $\exp(\text{weight}(R))$

# Probability of a world in an MLN

$$v = \left[ \begin{array}{l} \text{Friends(A,A)} = T \\ \text{Friends(A,B)} = T \\ \text{Friends(B,A)} = T \\ \text{Friends(B,B)} = T \\ \text{Smokes(A)} = F \\ \text{Smokes(B)} = T \\ \text{Cancer(A)} = F \\ \text{Cancer(B)} = F \end{array} \right]$$



$$\forall x \text{Smokes}(x) \Rightarrow \text{Cancer}(x)$$

$$x = A \quad T$$

$$x = B \quad F$$

$$n_1(v) = 1$$

$$\forall x,y \text{Friends}(x,y) \Rightarrow (\text{Smokes}(x) \Leftrightarrow \text{Smokes}(y))$$

$$x = A, y = A \quad T$$

$$x = A, y = B \quad F$$

$$x = B, y = A \quad F$$

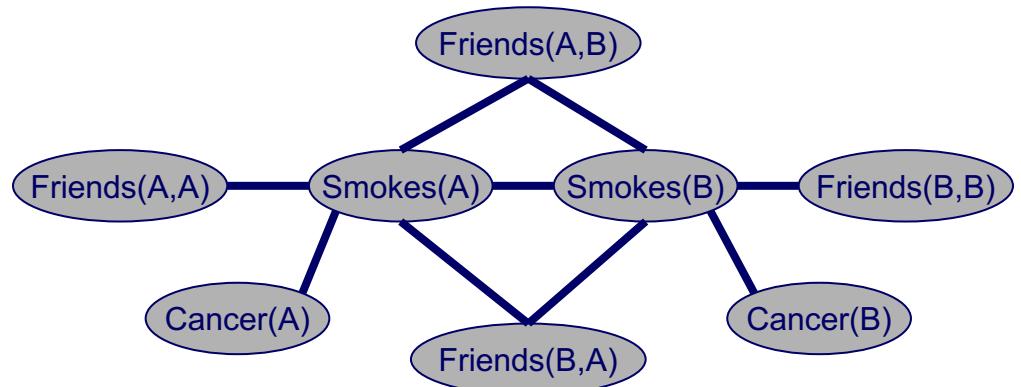
$$x = B, y = B \quad T$$

$$n_2(v) = 2$$

# of true groundings of formula 1 in  $v$

# Probability of a world in an MLN

$$\nu = \begin{bmatrix} \text{Friends(A,A)} = T \\ \text{Friends(A,B)} = T \\ \text{Friends(B,A)} = T \\ \text{Friends(B,B)} = T \\ \text{Smokes(A)} = F \\ \text{Smokes(B)} = T \\ \text{Cancer(A)} = F \\ \text{Cancer(B)} = F \end{bmatrix}$$



$$\begin{aligned} P(\nu) &= \frac{1}{Z} \exp\left( \sum_i w_i n_i(\nu) \right) \\ &= \frac{1}{Z} \exp\left( 1.5(1) + 1.1(2) \right) \end{aligned}$$

# For Learning, Input is Relational DB

- the input to the learning process is a relational database of ground atoms

$\text{Friends}(x, y)$

---

Anna, Anna  
Anna, Bob  
Bob, Anna  
Bob, Bob

$\text{Smokes}(x)$

---

Bob

$\text{Cancer}(x)$

---

Bob

- the closed world assumption is used to infer the truth values of atoms not present in the DB

# Parameter learning

- parameters (weights on formulas) can be learned as in Markov network

$$\frac{\partial}{\partial w_i} \log P_w(\boldsymbol{v}) = n_i(\boldsymbol{v}) - E_w[n_i(\boldsymbol{v})]$$

# of times clause  $i$  is true in data

Expected # times clause  $i$  is true according to MLN

- approximation methods may be needed to estimate *both* terms

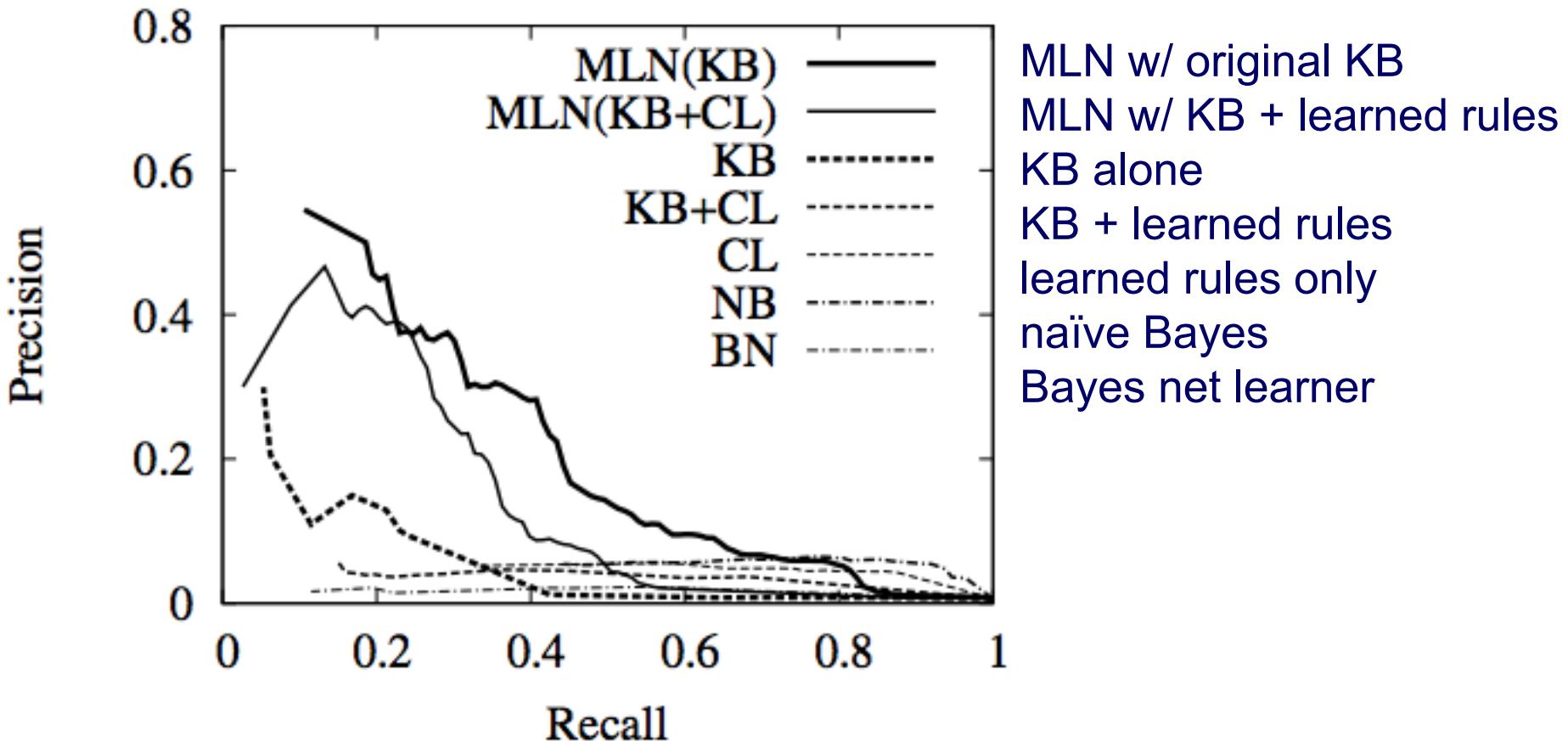
# MLN experiment

- testbed: a DB describing Univ. of Washington CS department
  - 12 predicates
    - $\text{Professor}(person)$
    - $\text{Student}(person)$
    - $\text{Area}(x, area)$
    - $\text{AuthorOf}(publication, person)$
    - $\text{AdvisedBy}(person, person)$
    - etc.
  - 2707 constants
    - publication (342)
    - person (442)
    - course (176)
    - project (153)
    - etc.

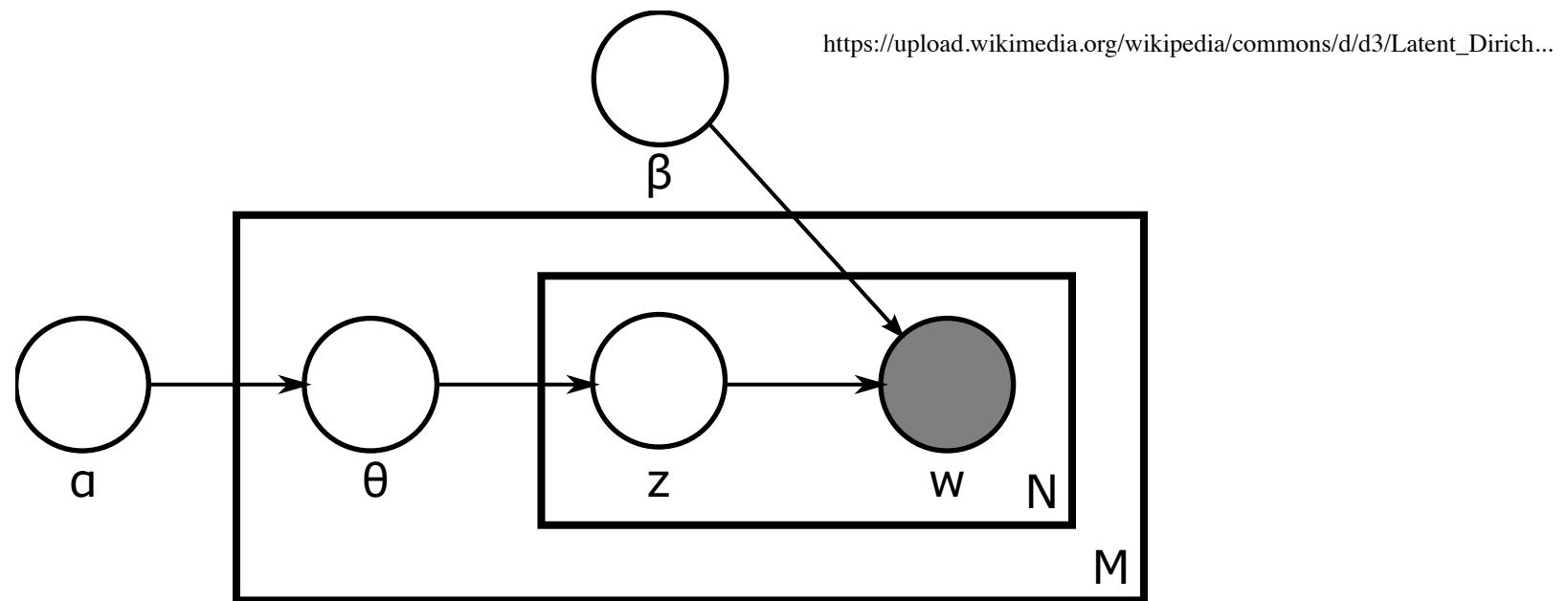
# MLN experiment

- obtained knowledge base by having four subjects provide a set of formulas in first-order logic describing the domain
- the formulas in the KB represent statements such as
  - students are not professors
  - each student has at most one advisor
  - if a student is an author of a paper, so is her advisor
  - at most one author of a given publication is a professor
  - etc.
- note that the KB is not consistent

# Learning to predict the AdvisedBy( $x, y$ ) relation

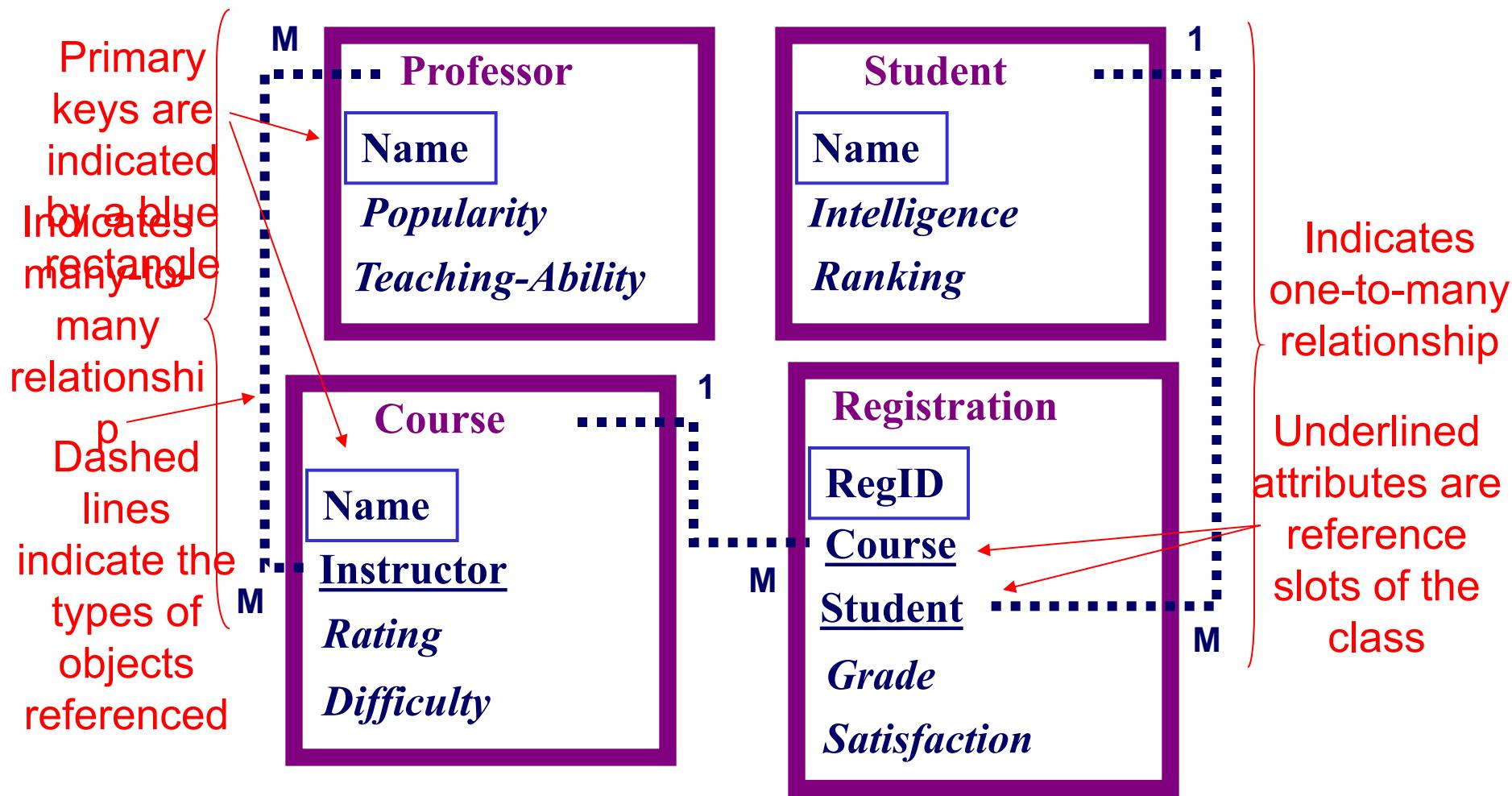


# Alternative for Relational Learning: Plates

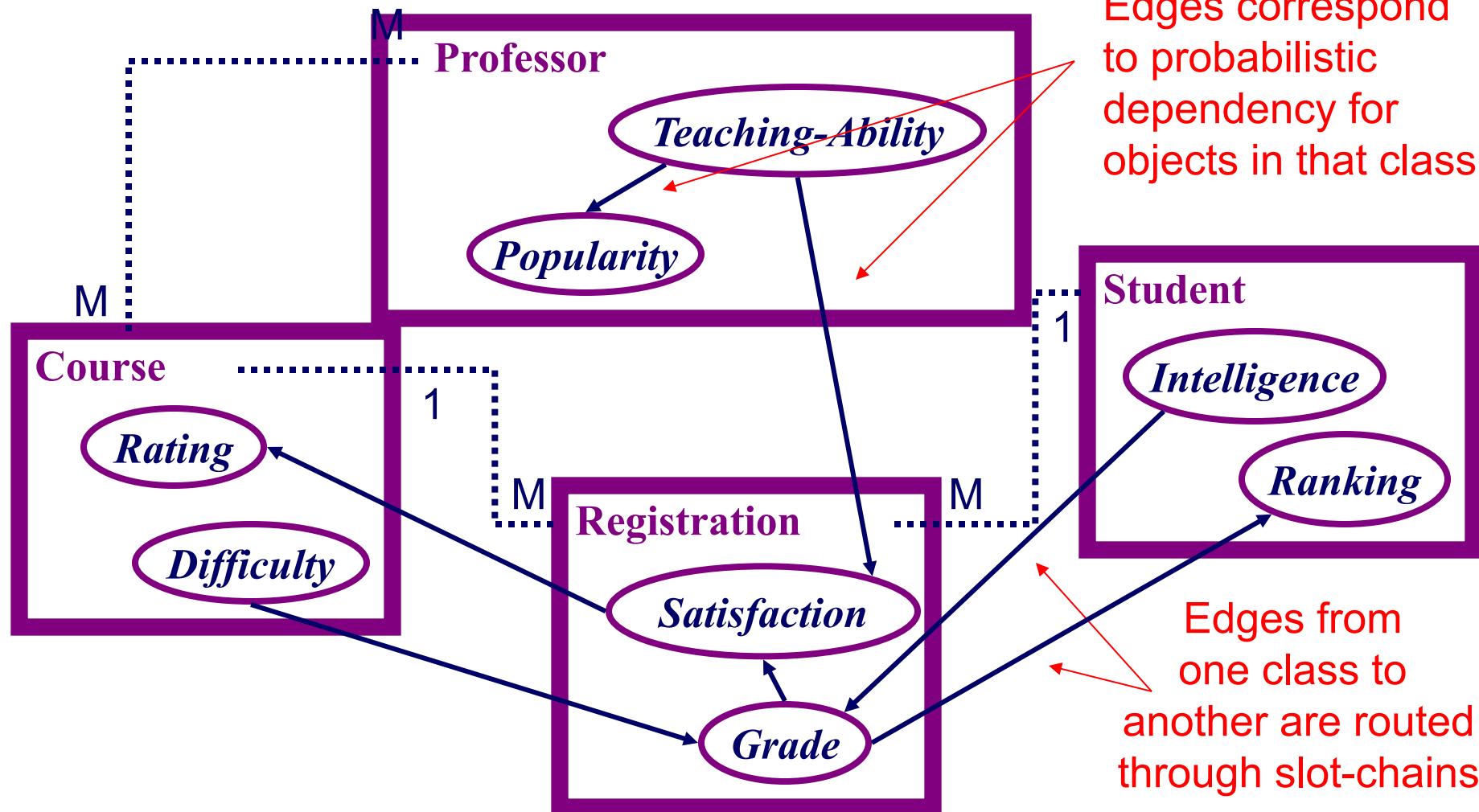


A rectangle labeled “N” denotes N copies of the Bayes net inside.  
Typically arcs go *into* rectangles, but we relax to allow outgoing next...

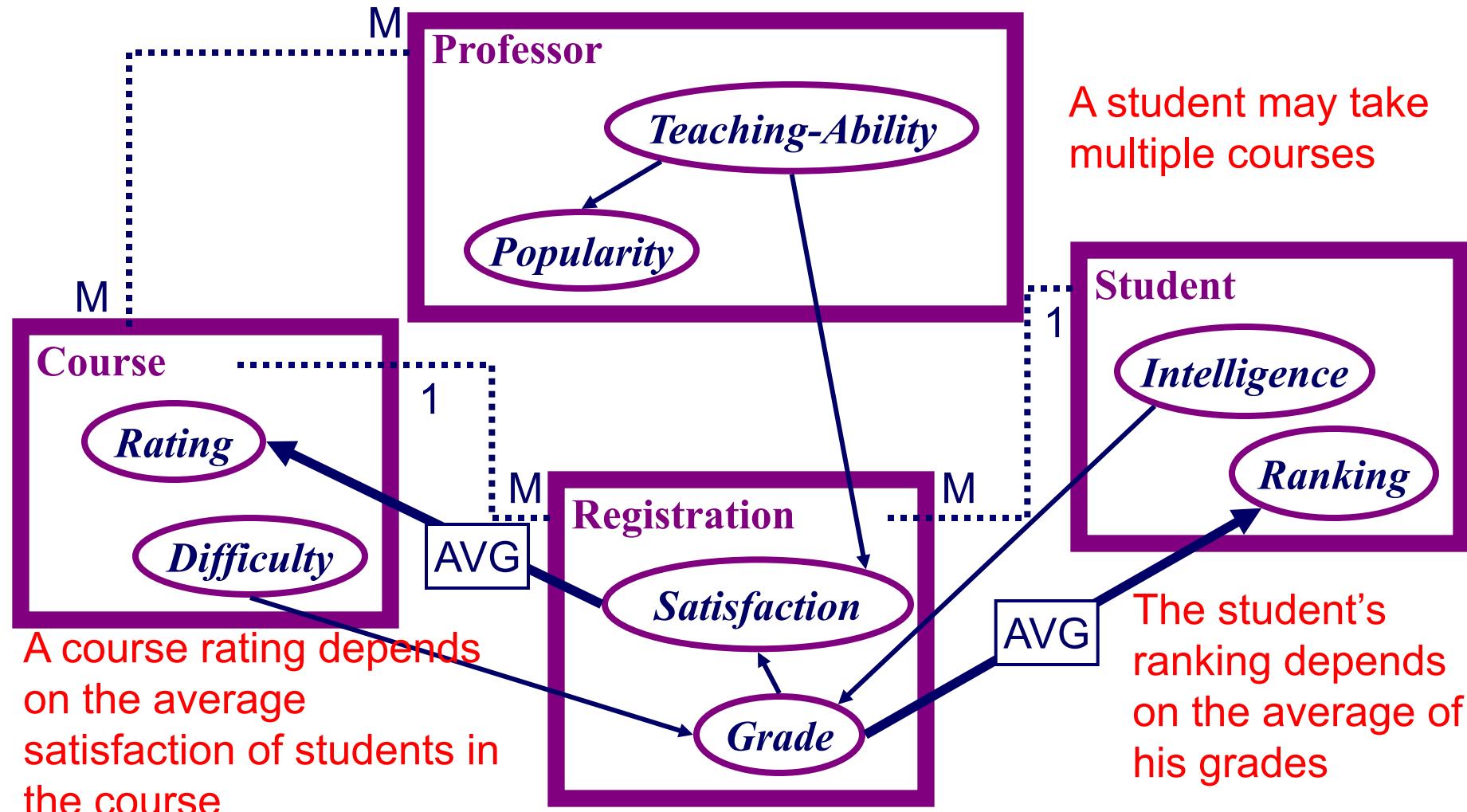
# Alternative: Probabilistic Relational Models (PRMs)



# PRM Dependency Structure for the University Domain



# PRM Dependency Structure



# CPDs in PRMs

