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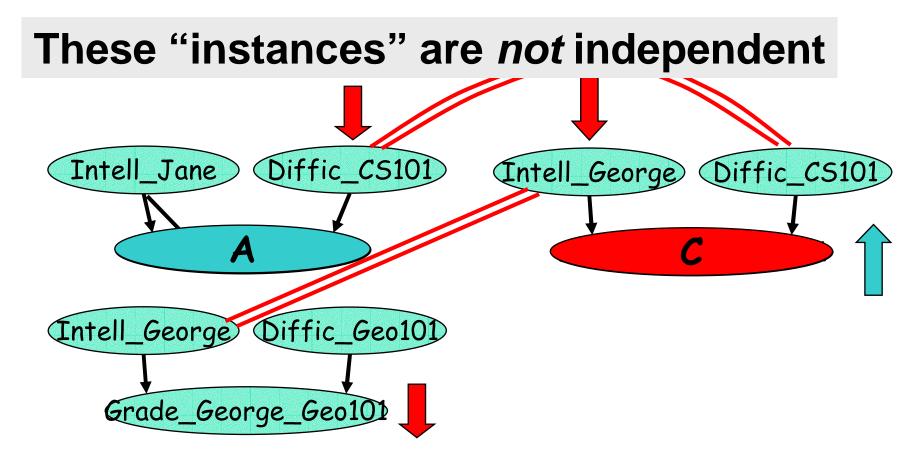


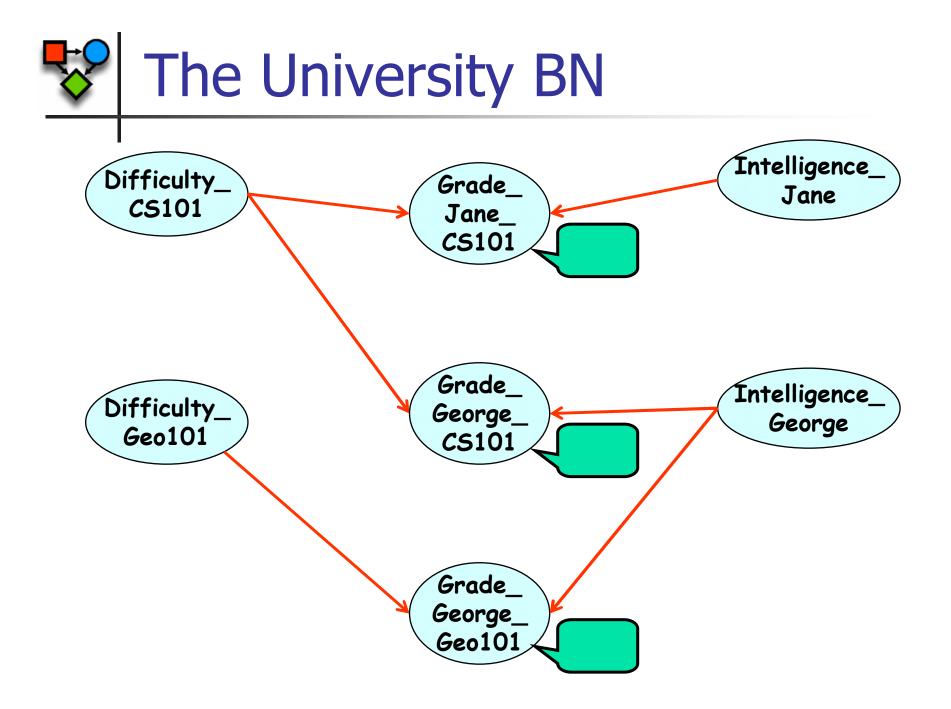
- Relational logic
- Probabilistic relational models
- Inference in PRMs
- Learning PRMs
- Uncertainty about domain structure
- Summary

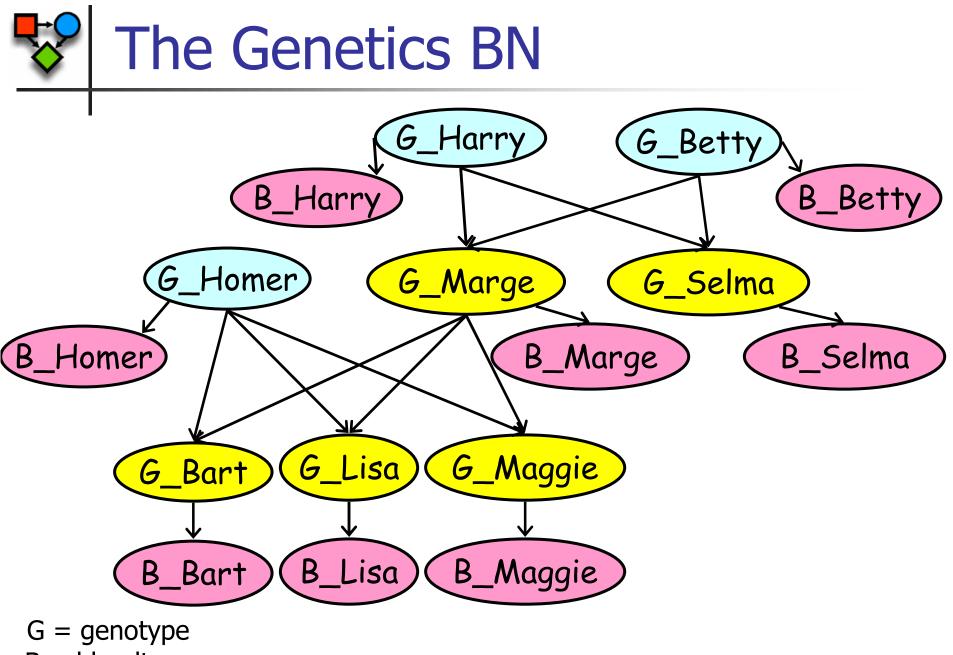


Bayesian Networks: Problem

- Bayes nets use attribute-based representation
- Real world has objects, related to each other







B = bloodtype



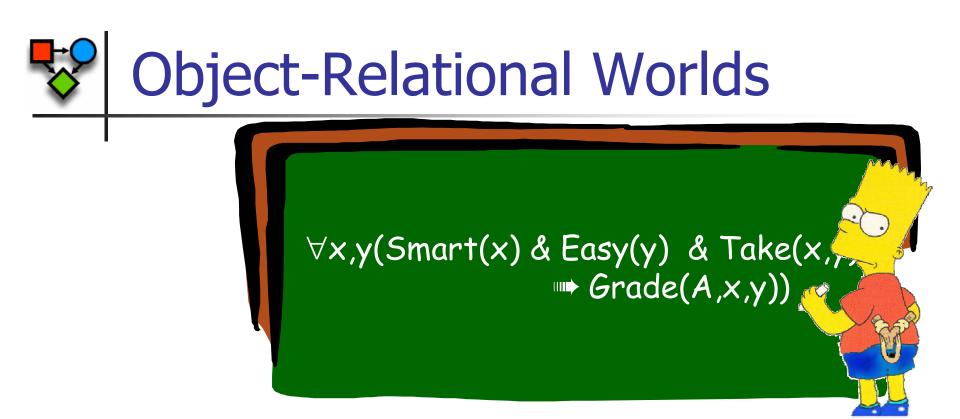
- Obvious solution:
 - Use a graphical model with shared parameters
- Nodes share not only parameters, but also local dependency structure
- Want to enforce this constraint:
 - For human knowledge engineer
 - For network learning algorithm



- How do we specify shared structure across different nodes?
 - Each person depends on his mother
 - But different people have different mothers
 - How do we specify the mapping
- We can write a special-purpose program for each domain:
 - genetic inheritance (family tree imposes constraints)
 - university (course registrations impose constraints)
- Is there something more general?



World = assignment of values to attributes
 / truth values to propositional symbols



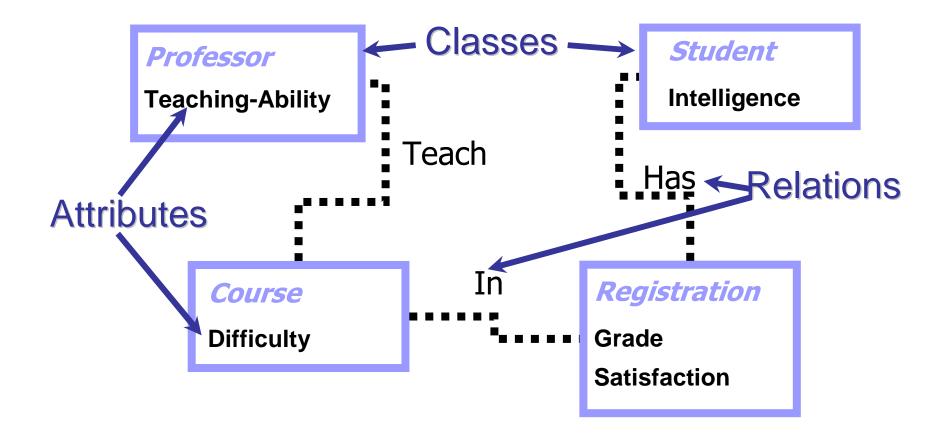
- World = relational interpretation:
 - Objects in the domain
 - Properties of these objects
 - Relations (links) between objects

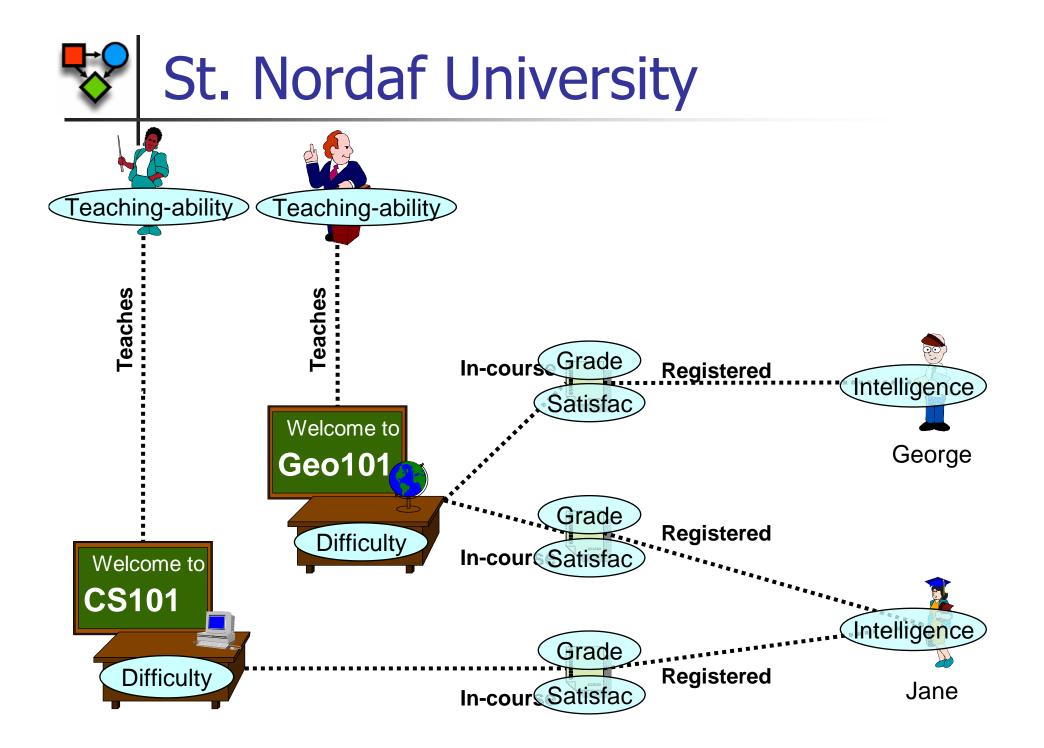


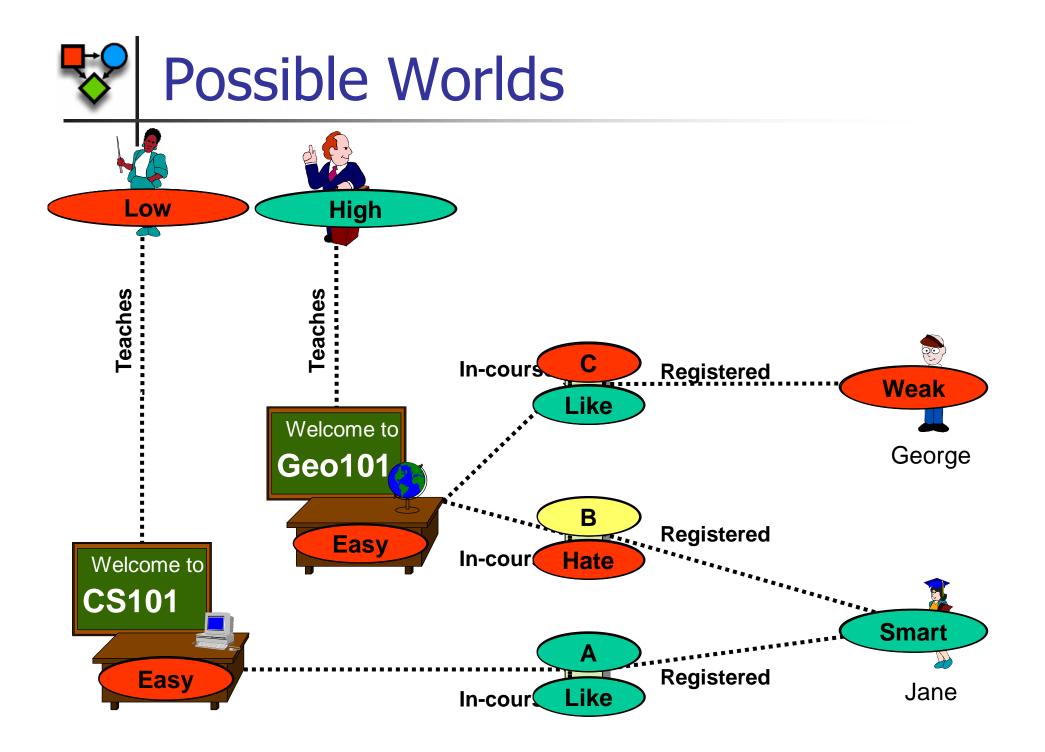
- General framework for representing:
 - objects & their properties
 - classes of objects with same model
 - relations between objects
- Represent a model at the template level, and apply it to an infinite set of domains
- Given finite domain, each instantiation of the model is propositional, but the template is not



 Specifies types of objects in domain, attributes of each type of object & types of relations between objects







Relational Logic: Summary

- Vocabulary:
 - Classes of objects:
 - Person, Course, Registration, ...
 - Individual objects in a class:
 - George, Jane, ...
 - Attributes of these objects:
 - George.Intelligence, Reg1.Grade
 - Relationships between these objects
 - Of(Reg1,George), Teaches(CS101,Smith)
- A *world* specifies:
 - A set of objects, each in a class
 - The values of the attributes of all objects
 - The relations that hold between the objects



- Any relation can be converted into an object:
 - $R(x_1, x_2, ..., x_k) \rightarrow$

new "relation" object y,

 $R_1(x_1,y), R_2(x_2,y), \dots, R_k(x_k,y)$

E.g., registrations are "relation objects"

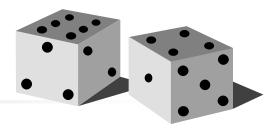
 \Rightarrow Can restrict attention to binary relations R(x,y)



- Binary relations can also be viewed as links:
- Specify the set of objects related to x via R
- $R(x,y) \rightarrow y \in x.R^1, x \in y.R^2$
- E.g., Teaches(p,c) \rightarrow
 - p.Courses = {courses c : Teaches(p,c)}
 - c.Instructor = {professors p : Teaches(p,c)}







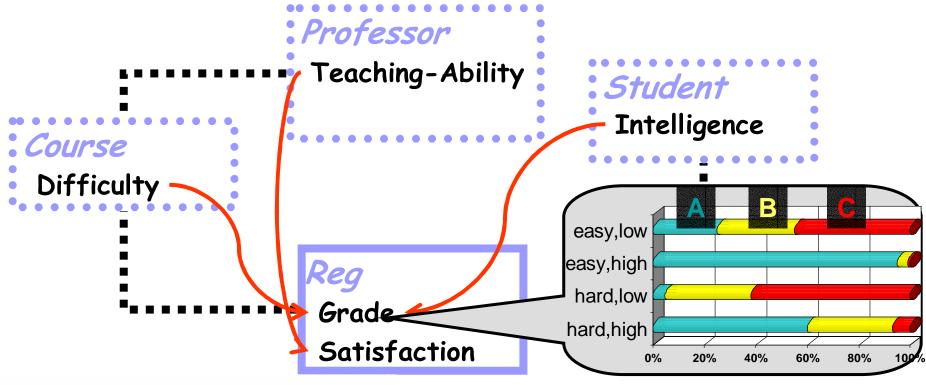
- Uncertainty model:
 - space of "possible worlds";
 - probability distribution over this space.
- In attribute-based models, world specifies
 - assignment of values to fixed set of random variables
- In relational models, world specifies
 - Set of domain elements
 - Their properties
 - Relations between them



- Entire set of relational worlds is infinite and too broad
- Assume circumscribed class of sets of worlds Ω_{ξ} consistent with some type of background knowledge ξ
- PRM Π is a template defining $P_{\Pi}(\Omega_{\xi})$ for any such ξ
- Simplest class attribute-based PRMs:
 - $\xi = relational skeleton:$
 - finite set of entities *E* and relations between them
 - Ω_{ξ} = all assignments of values to all attributes of entities in *E*
 - PRM template defines distribution over Ω_{ξ} for any such ξ

Relational Bayesian Network

- Universals: Probabilistic patterns hold for all objects in class
- Locality: Represent direct probabilistic dependencies
 - Links define potential interactions



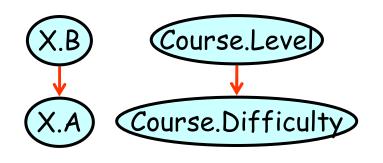
[K. & Pfeffer; Poole; Ngo & Haddawy]



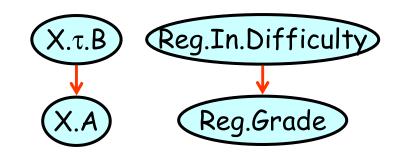
- ξ : set of objects & relations between them
- Ω_{ξ} : the set of all assignments of values to all attributes of all objects in ξ
- $P_{\Pi}(\Omega_{\xi})$ is defined by a ground Bayesian network:
 - variables: attributes of all objects
 - dependencies: determined by
 - relational links in ξ
 - dependency structure of RBN model Π



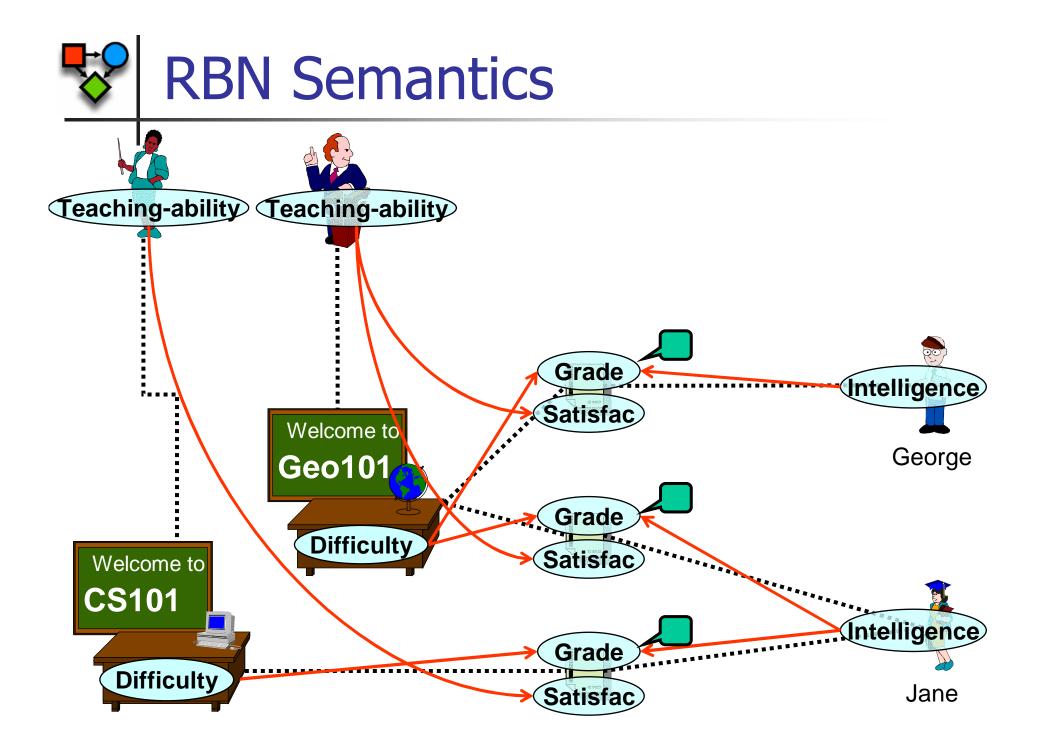
For each class X and attribute A, structure specifies parents for X.A

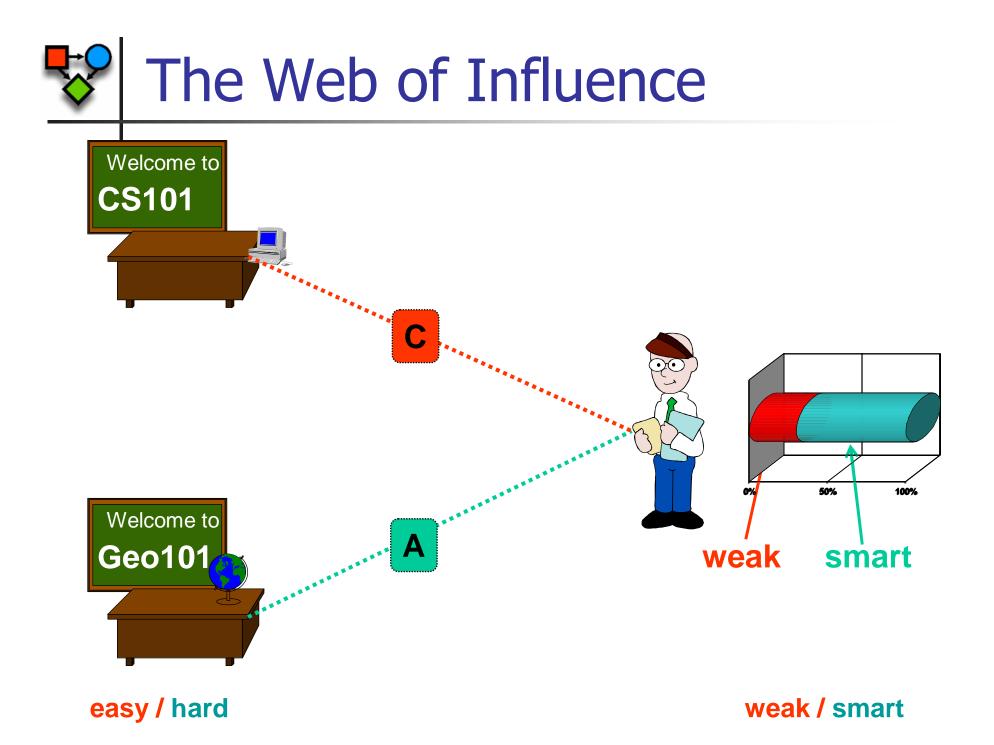


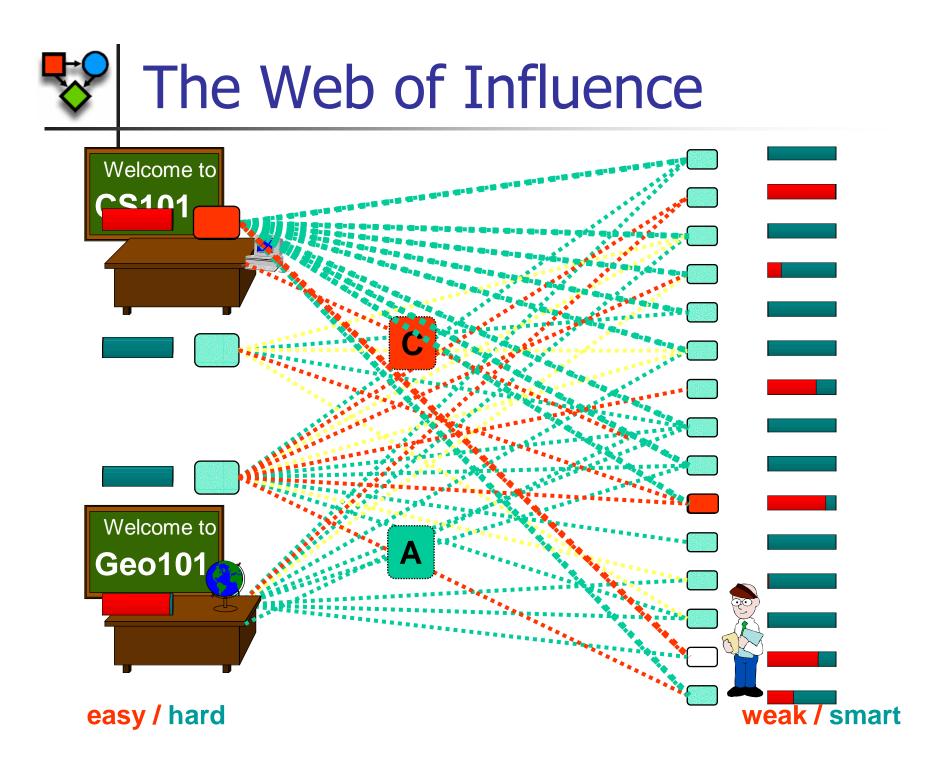
For any object x in class
 X, x.B is parent of x.A

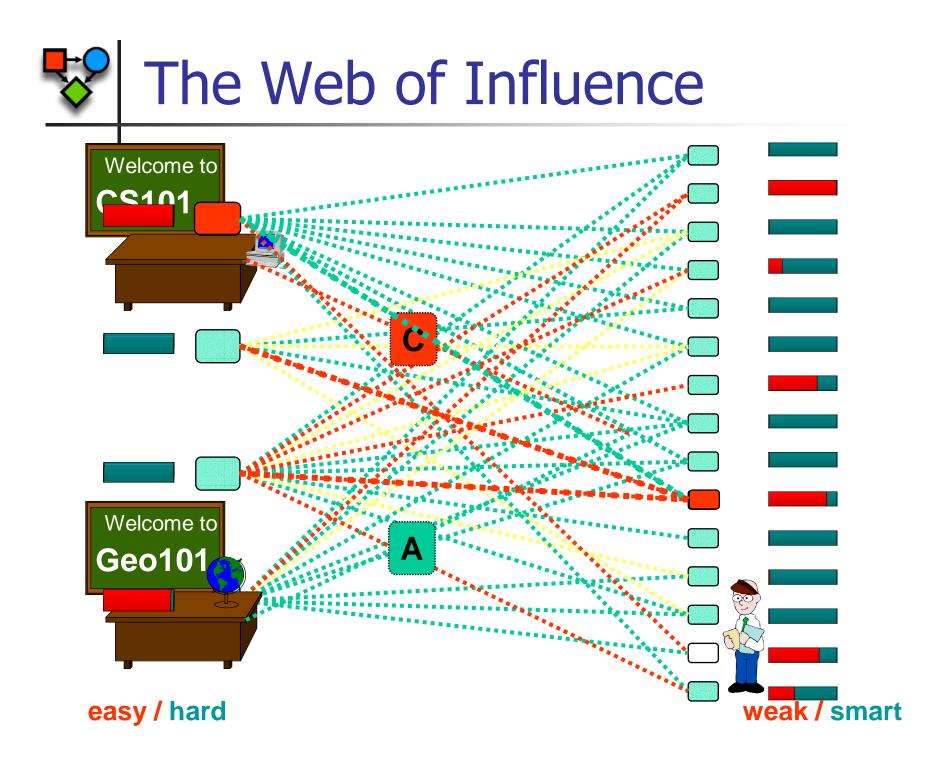


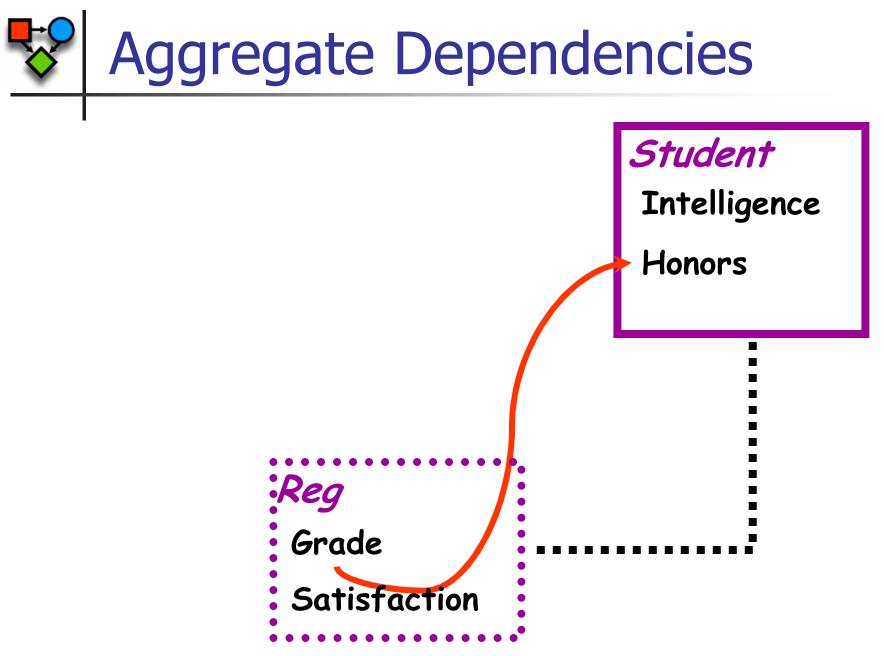
- τ : link or chain of links
- For any object x in class
 X, x.τ.B is parent of x





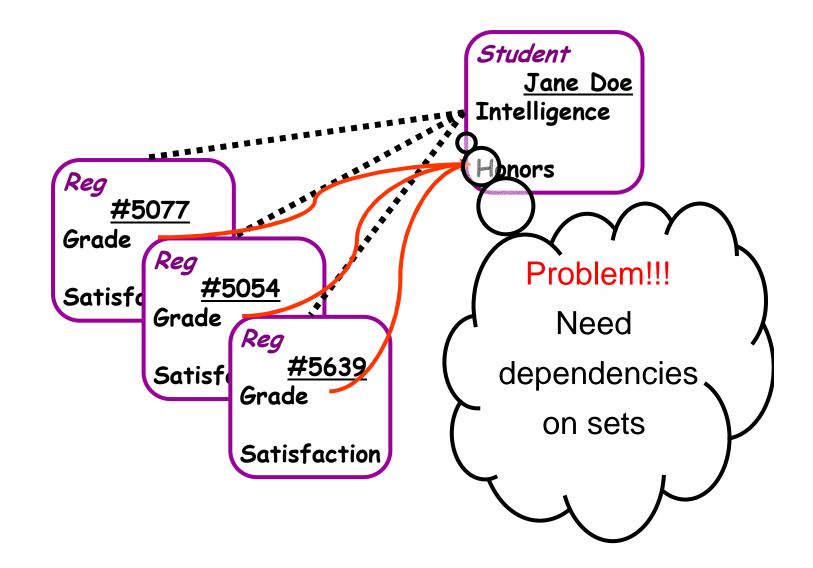


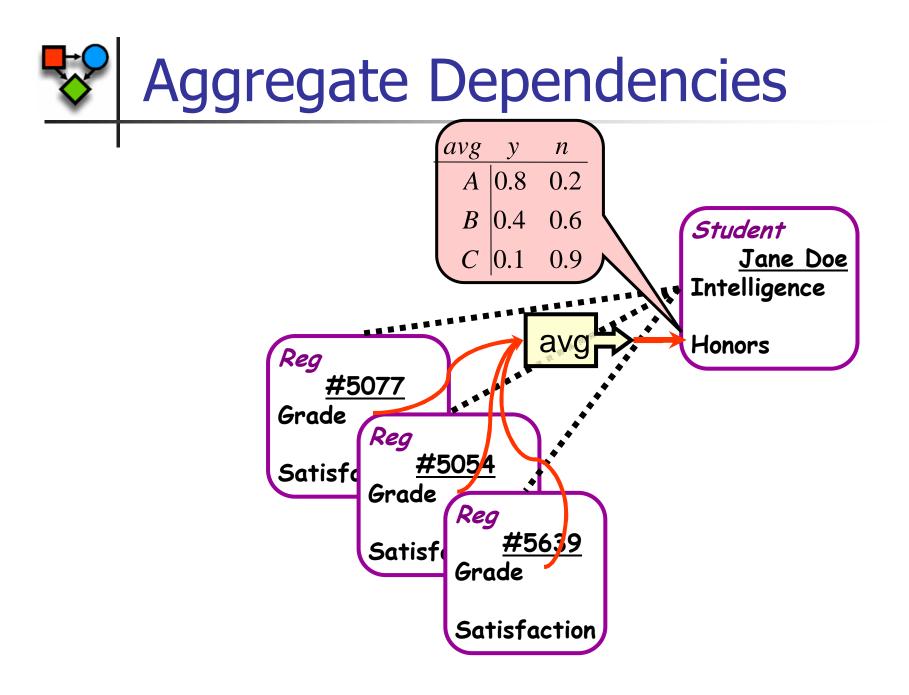


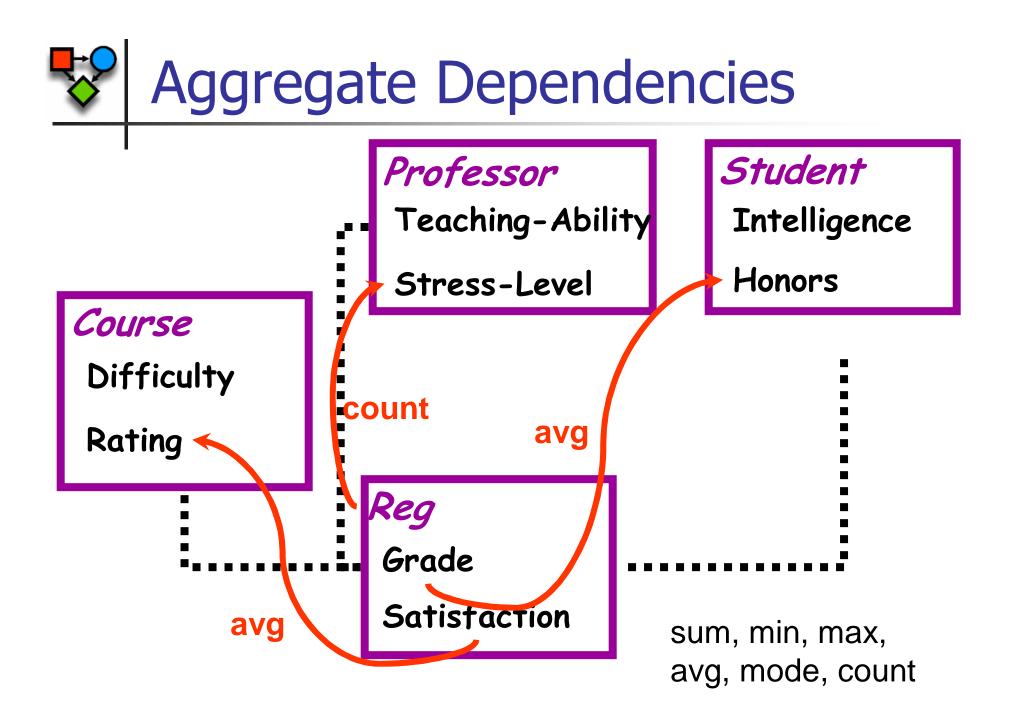


[K. & Pfeffer '98; Friedman, Getoor, K. Pfeffer '99]











- RBN specifies
 - A probabilistic dependency structure S:
 - A set of parents X.τ.B for each class attribute X.A
 - A set of *local probability models:*
 - Aggregator to use for each multi-valued dependency
 - Set of CPD parameters $\Theta_{X,A}$
- Given relational skeleton structure ξ , RBN induces a probability distribution over worlds ω
 - Distribution defined via ground BN over attributes x.A

$$P(\omega | \xi, S, \Theta) = \prod_{\substack{X, A \ x \in X_{\xi}}} P(X, A | parents_{S, \xi}(X, A), \Theta_{X, A})$$

Attributes Objects

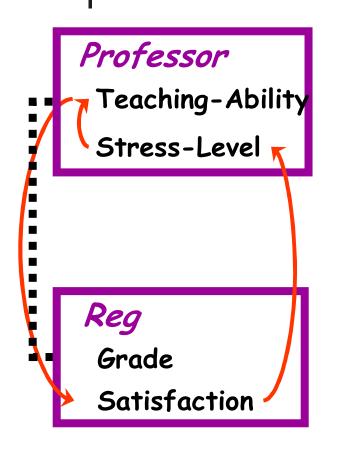
Extension: Class Hierarchy

- Subclasses inherit all attributes of parents, but may have additional ones
- For inherited attribute X.A, subclass can:
 - inherit parent's probabilistic model
 - overwrite with local probabilistic model
- Example:
 - Professor has subclasses assistant, associate, full
 - Inherit distribution over Stress-Level
 - Modify distribution over Salary



- Hierarchies allow reuse in knowledge engineering and in learning
 - Parameters and dependency models shared across more objects
- If class assignments specified in ξ, class hierarchy does not introduce complications





 For given skeleton ξ, PRM Π asserts dependencies between attributes of objects:

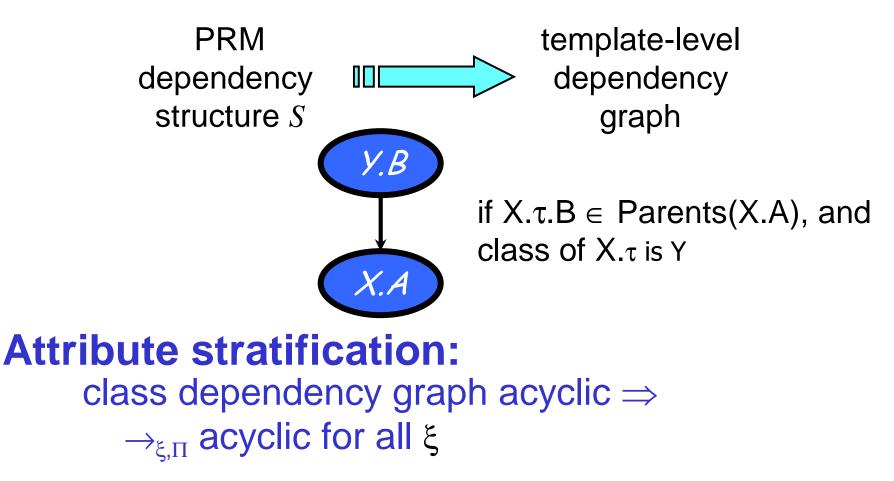
$$y.B \rightarrow_{\xi,\Pi} x.A$$

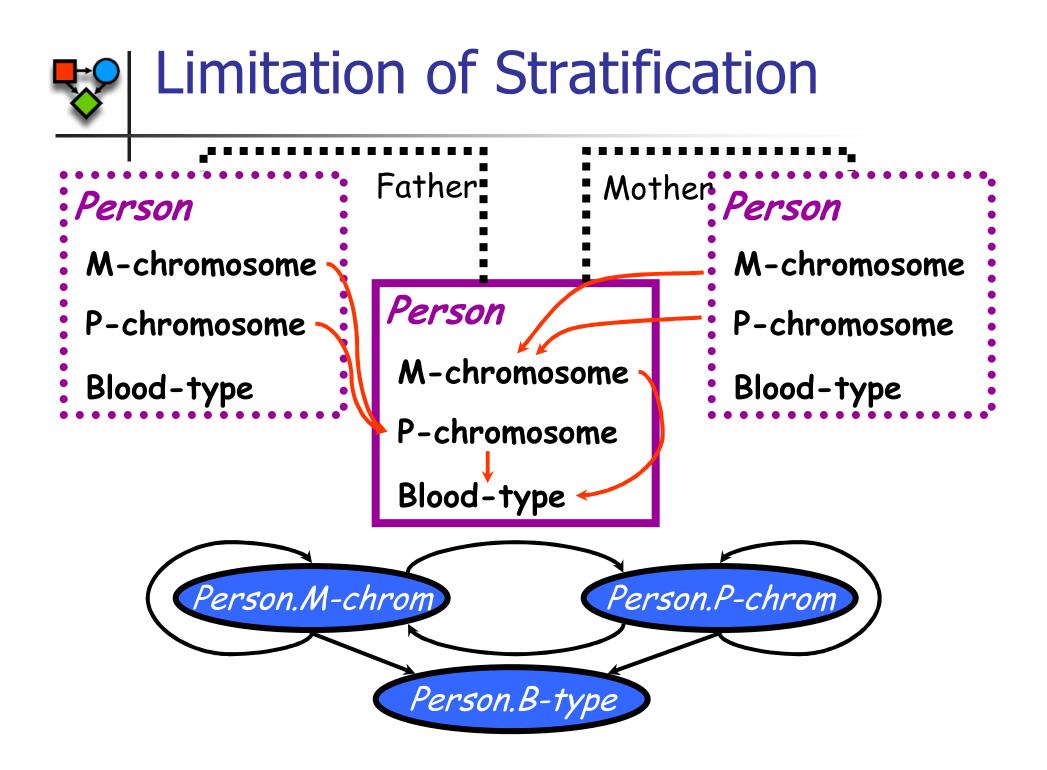
• \prod defines coherent probability model over σ if $\rightarrow_{\xi,\Pi}$ is acyclic

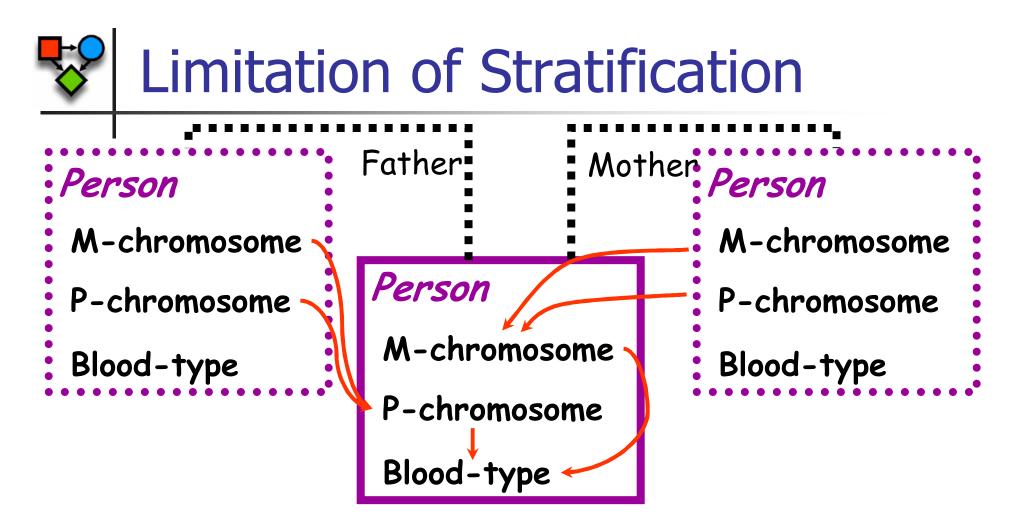
Smith.Stress-level depends probabilistically on itself [Friedman, Getoor, K. Pfeffer '99]



How do we guarantee that a PRM \prod is acyclic for *every* object skeleton ξ ?



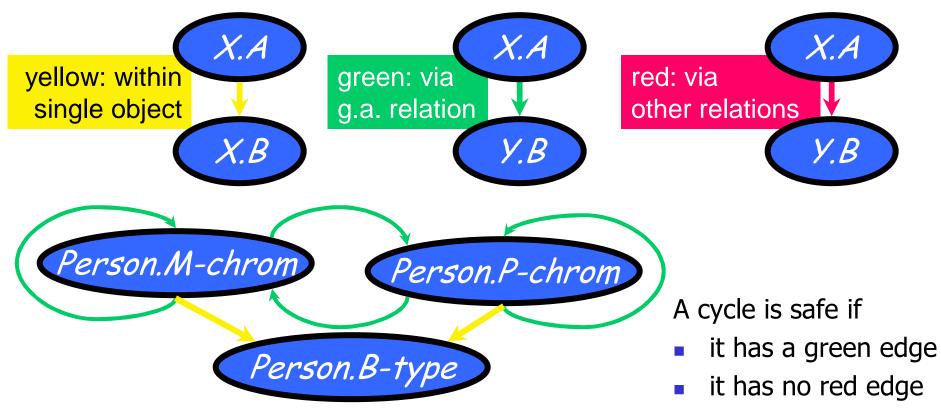




- Prior knowledge: the Father-of relation is acyclic
 - Dependence of *Person.A* on *Person.Father.B* cannot induce cycles

Guaranteeing Acyclicity

- With guaranteed acyclic relations, some cycles in the dependency graph are guaranteed to be safe.
- We color the edges in the dependency graph



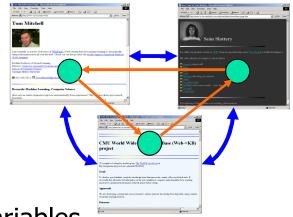
Solution Object-Oriented Bayesian Nets

- OOBNs are RBN with only one type of relation
 - One object can be a "part-of" another
 - Objects can only interact with component parts
 - Other types of relationships must be embedded into the "part-of" framework
- Defines "neat" hierarchy of related objects
- Provides clearly defined object interface
 between object x and its enclosing object y

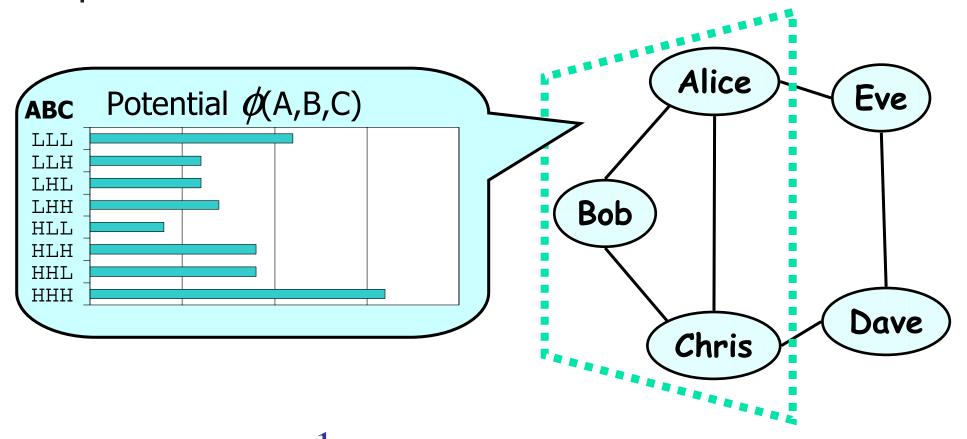


Why Undirected Models?

- Symmetric, non-causal interactions
 - E.g., web: categories of linked pages are correlated
 - Cannot introduce direct edges because of cycles
- Patterns involving multiple entities
 - E.g., web: "triangle" patterns
 - Directed edges not appropriate
- "Solution": Impose arbitrary direction
 - Not clear how to parameterize CPD for variables involved in multiple interactions
 - Impossible to do within a class-based parameterization







 $P(A,B,C,D,E) = \frac{1}{Z}\phi(A,B,C)\phi(C,D)\phi(D,E)\phi(E,A)$

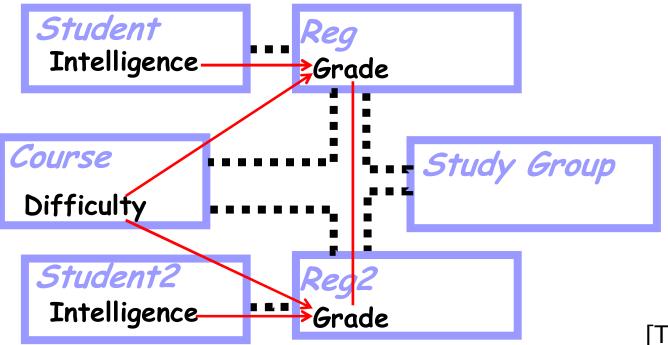
Markov Networks: Review

- A Markov network is an undirected graph over some set of variables V
- Graph associated with a set of *potentials* ϕ_i
 - Each potential is factor over subset V_i
 - Variables in \mathbf{V}_i must be a (sub)clique in network

$$\boldsymbol{P}(\boldsymbol{V}) = \frac{1}{Z} \prod_{i} \phi_{i}(\boldsymbol{V}_{i})$$

Relational Markov Networks

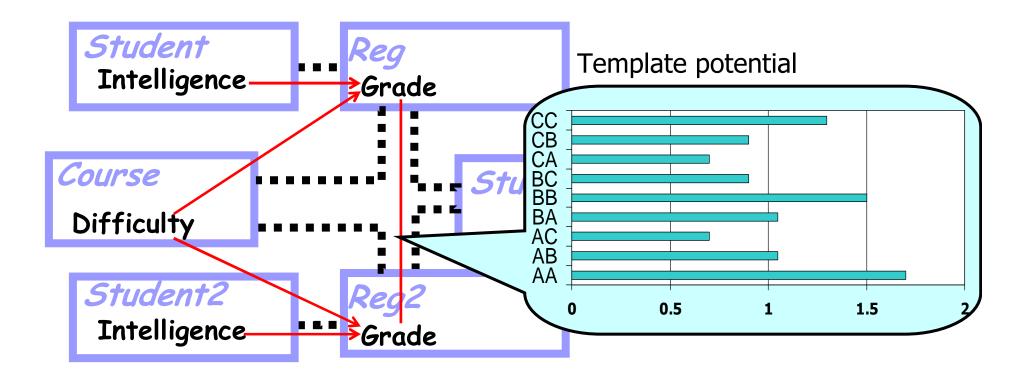
- Probabilistic patterns hold for groups of objects
- Groups defined as sets of (typed) elements linked in particular ways



[Taskar, Abbeel, K. 2002]

Relational Markov Networks

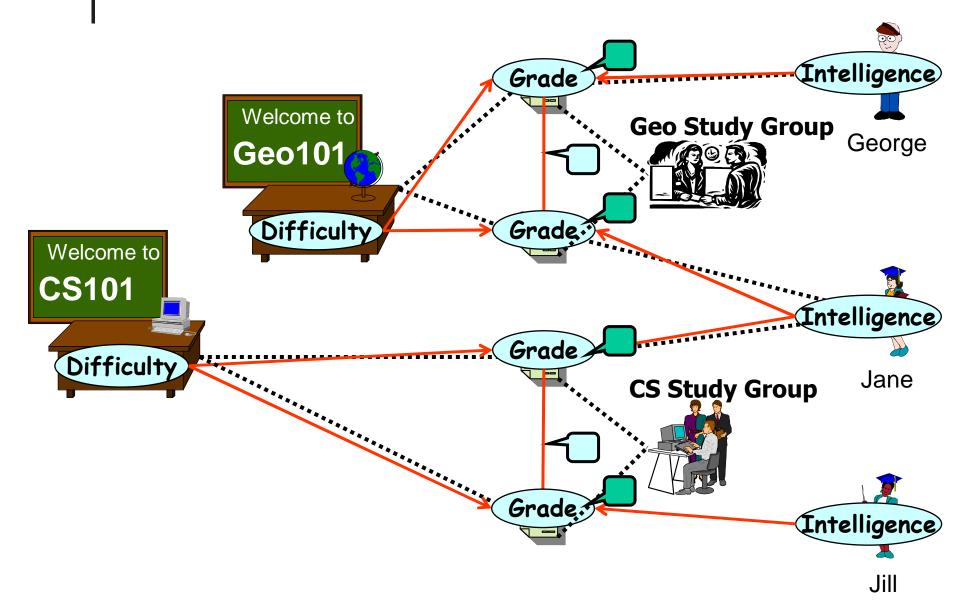
- Probabilistic patterns hold for groups of objects
- Groups defined as sets of (typed) elements linked in particular ways





- Define *clique templates*
 - All tuples {reg R₁, reg R₂, group G}
 s.t. In(G, R₁), In(G, R₂)
 - Compatibility potential
 \$\overline{R_1}\$.Grade, R_2.Grade)
- Ground Markov network contains potential φ(r₁.Grade, r₂.Grade) for all appropriate r₁, r₂

Ground MN (or Chain Graph)



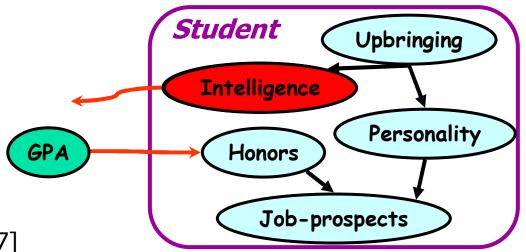


Inference: Simple Method

- Define ground network as in semantics
- Apply standard inference methods
- Problem:
 - Very large models can be specified very easily
 - Resulting ground network often highly connected
 - Exact inference is typically intractable
- In practice, often must resort to approximate methods such as belief propagation

Exploiting Structure: Encapsulation

- Objects interact only in limited ways
- Can define *object interface*:
 - Outputs: Object attributes influencing other objects
 - Inputs: External attributes influencing object
- Object is independent of everything given interface
- Inference can be encapsulated within objects, with "communication" limited to interfaces



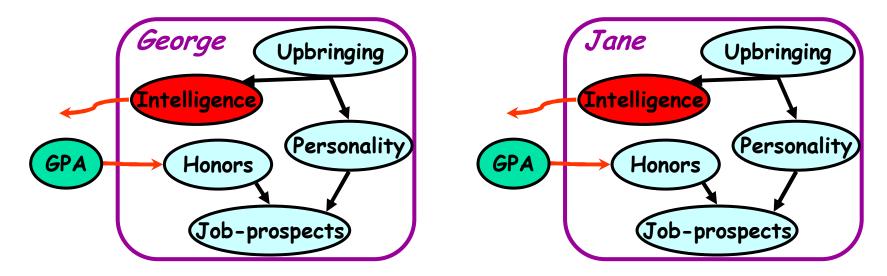
[K. & Pfeffer, 1997]

Exploiting Structure: Encapsulation

- Marginalize object distribution onto interface
- Dependency graph over interfaces induced by
 - Inter-object dependencies
 - And hence by the relational structure
- Perform inference over interfaces
 - If interaction graph has low tree-width, can use exact inference
 - E.g., part-of hierarchy in OOBNs
 - If relational structure is more complex, can use BP
 - A form of Kikuchi BP, where cluster selection is guided by relational structure

Exploiting Structure: Reuse

- Objects from same class have same model
- For *generic* objects no internal evidence marginalize interface is the same
- Can reuse inference a form of "lifting"



[Pfeffer & K. 1998]

Exploiting Structure: Reuse

- Generic objects often play same role in model
 - Multiple students that all take the same class
- Reuse: compute interface once
- Combinatorics: compute total contribution to probability in closed form

P(*k* students like the class | teaching-ability = low) =

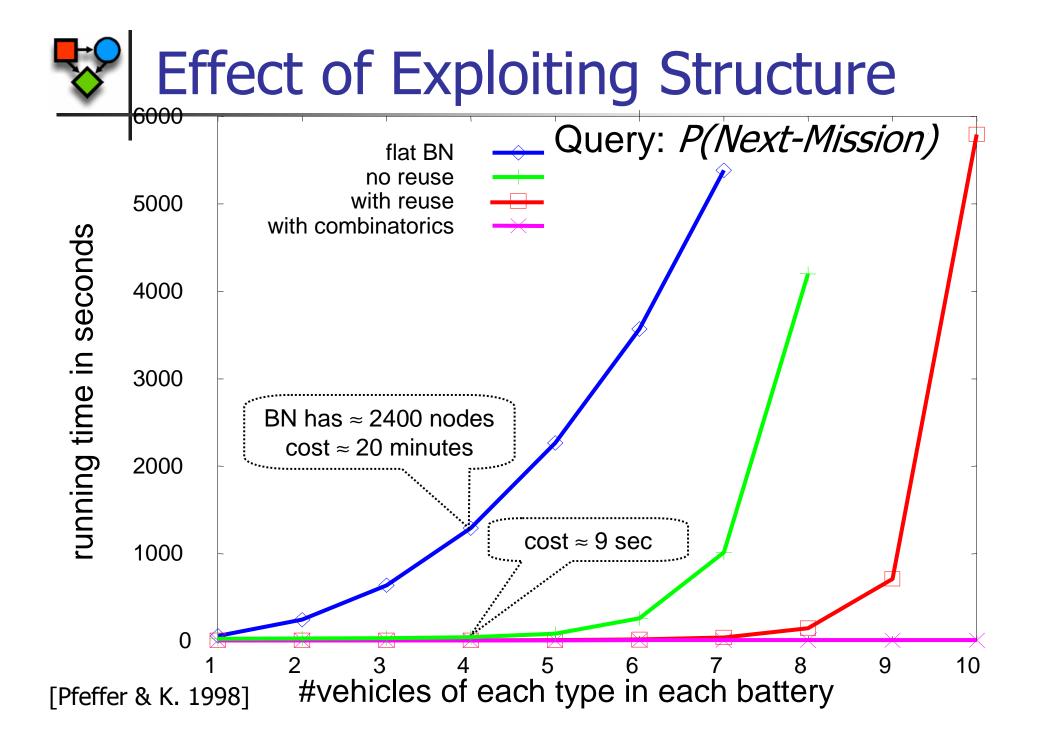
P(generic student likes the class | teaching ability = low)



Battlefield situation assessment for missile units

- several locations
- many units
- each has detailed model
- Example object classes:
 - Battalion
 - Battery
 - Vehicle
 - Location
 - Weather.

- Example relations:
 - At-Location
 - Has-Weather
 - Sub-battery/In-battalion
 - Sub-vehicle/In-battery

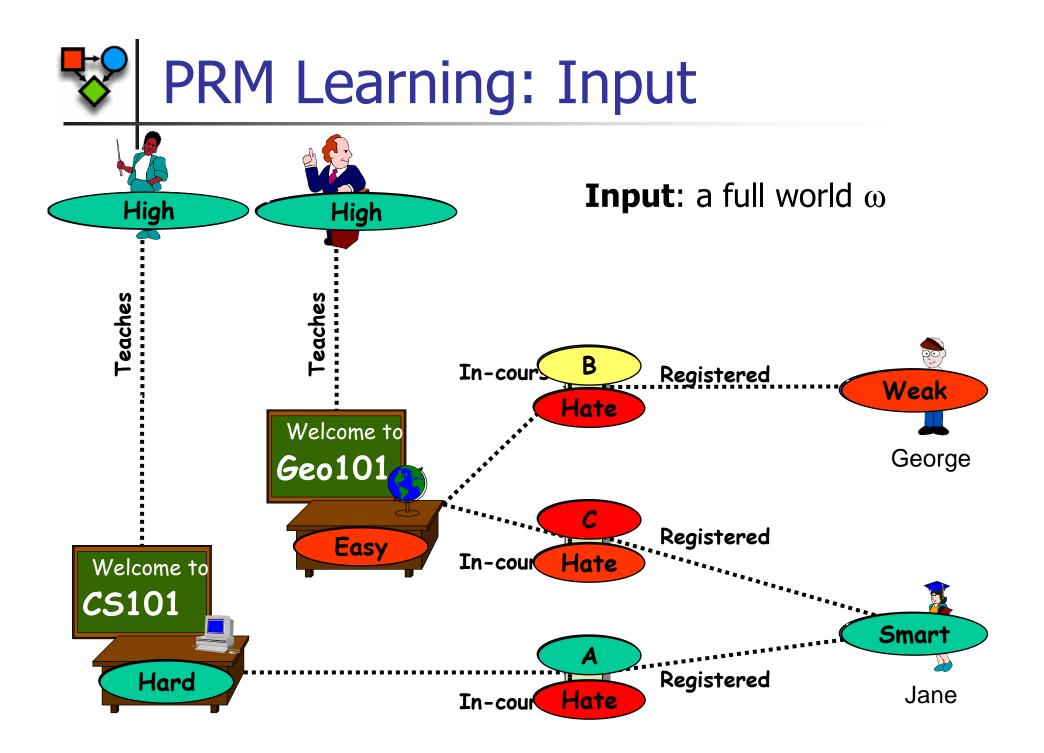






Relational Bayesian networks

- Likelihood function
- ML parameter estimation
- EM
- Structure learning
- Relational Markov networks
 - Parameter estimation
- Applications:
 - Collective classification web data
 - Relational clustering biological data





$$\mathcal{L}(\mathcal{S}, \Theta: \omega) = \mathcal{P}(\omega \,|\, \xi, \mathcal{S}, \Theta)$$

 $= \prod_{\substack{X.A \ x \in X_{\xi}}} P(X.A \mid parents_{S,\sigma}(X.A), \Theta_{X.A})$ Attributes Objects

- Likelihood of a BN with shared parameters
- Joint likelihood is a product of likelihood terms
 One for each attribute X.A and its family
- For each X.A, the likelihood function aggregates counts from all occurrences x.A in world $\boldsymbol{\omega}$



Log-likelihood:

 $\log P(\omega | \xi, S, \Theta) =$

 $\sum \mathcal{M}(a, u) \log \theta_{x|u}$ $X.A \quad u \in Va/(Pa(X.A)) \quad a \in Va/(X.A)$

Sufficient statistics:

 $M(a, \mathbf{u}) =$

 $|\{x \in X_{\omega} : x : A = a, parents_{S,\omega}(x : A) = u\}|$



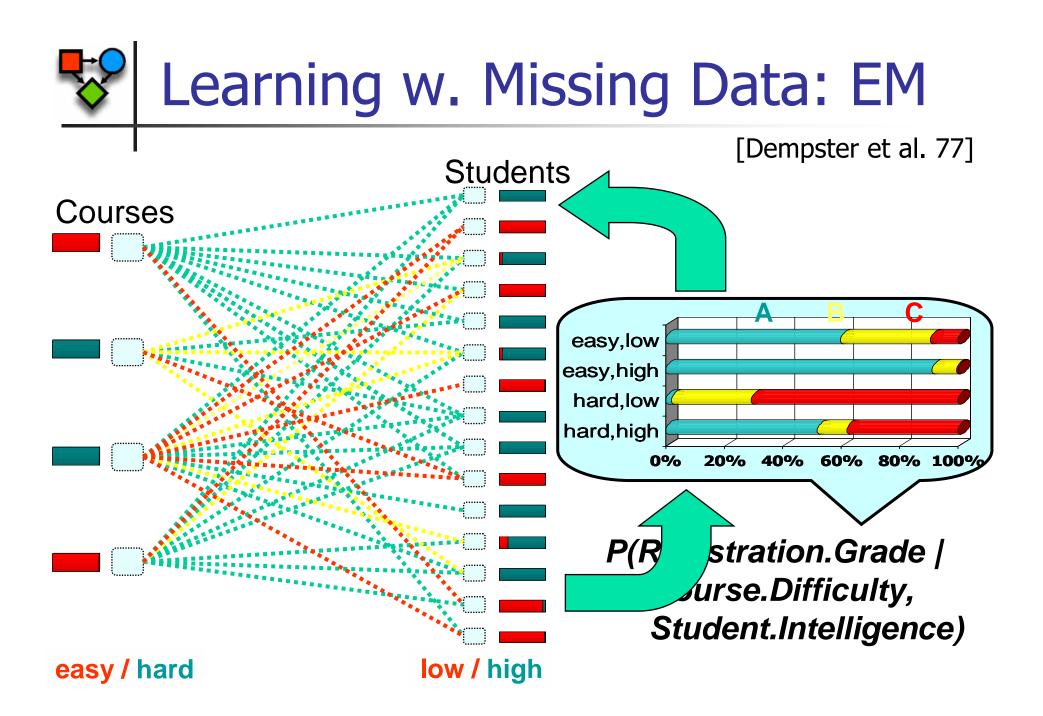
MLE parameters:

 $\hat{P}(Reg.Grade = A | Student.Intell = hi, Course.Diff = lo) \\ = \frac{M(Reg.Grade = A, Student.Intell = hi, Course.Diff = lo)}{M(Reg.Grade = *, Student.Intell = hi, Course.Diff = lo)}$

- Bayesian estimation:
 - Prior for each attribute X.A
 - Posterior uses aggregated sufficient statistics

Learning w. Missing Data

- EM Algorithm applies essentially unchanged
 - E-step computes expected sufficient statistics, aggregated over all objects in class
 - M-step uses ML (or MAP) parameter estimation
- Key difference:
 - In general, the hidden variables are **not** independent
 - Computation of expected sufficient statistics requires inference over entire network
 - [Same reasoning as for forward-backward algorithm in temporal models]





- Define set of legal RBN structures
 Ones with legal class dependency graphs
- Define scoring function Bayesian score

$$Score(S:\omega) = \log[P(\omega|S,\xi)P(S)]$$

$$P(\omega|S,\xi) = \int \mathcal{L}(S,\Theta_{S}:\omega)P(\Theta_{S})d\Theta_{S}$$

- Product of family scores:
 - One for each X.A
 - Uses aggregated sufficient statistics

Search for high-scoring legal structure

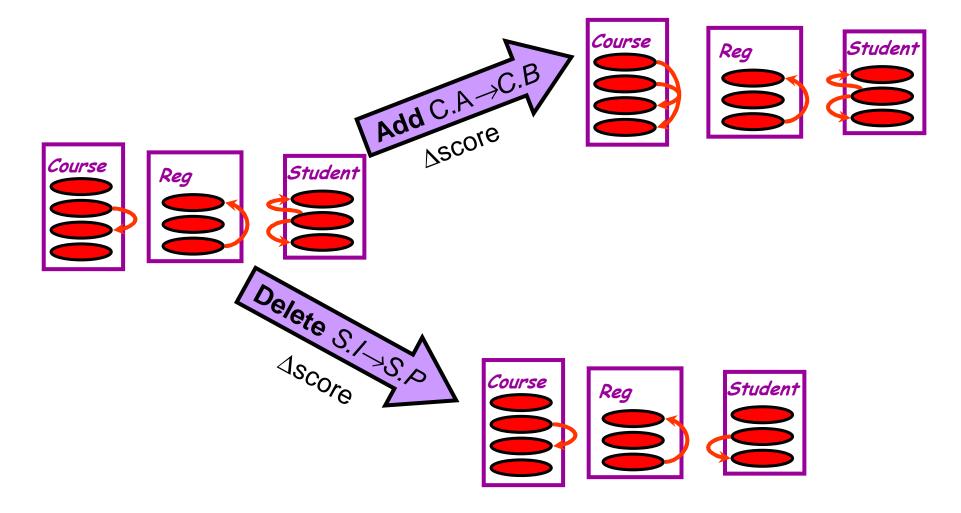
[Friedman, Getoor, K., Pfeffer, 1999]

Learning RBN Structure

- All operations done at class level
 - Dependency structure = parents for X.A
 - Acyclicity checked using class dependency graph
 - Score computed at class level
- Individual objects only contribute to sufficient statistics
 - Can be obtained efficiently using standard DB queries

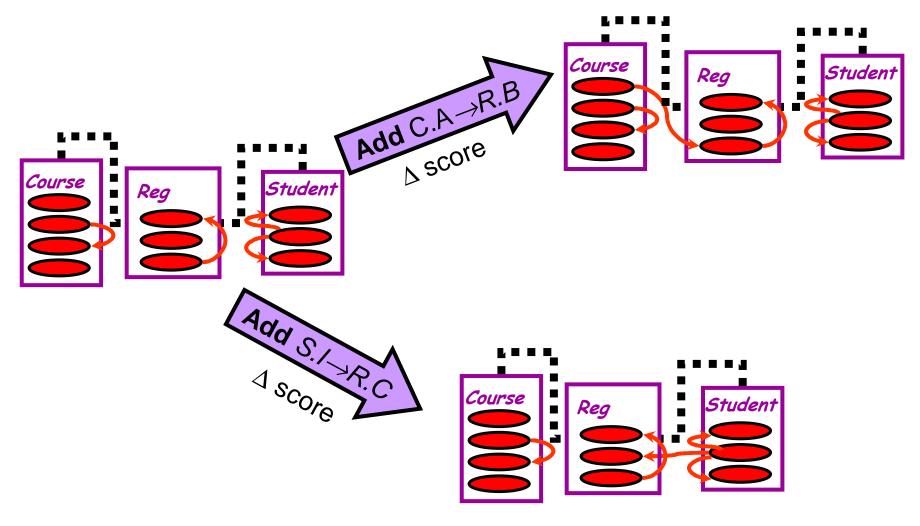


Phase 0: consider only dependencies within a class



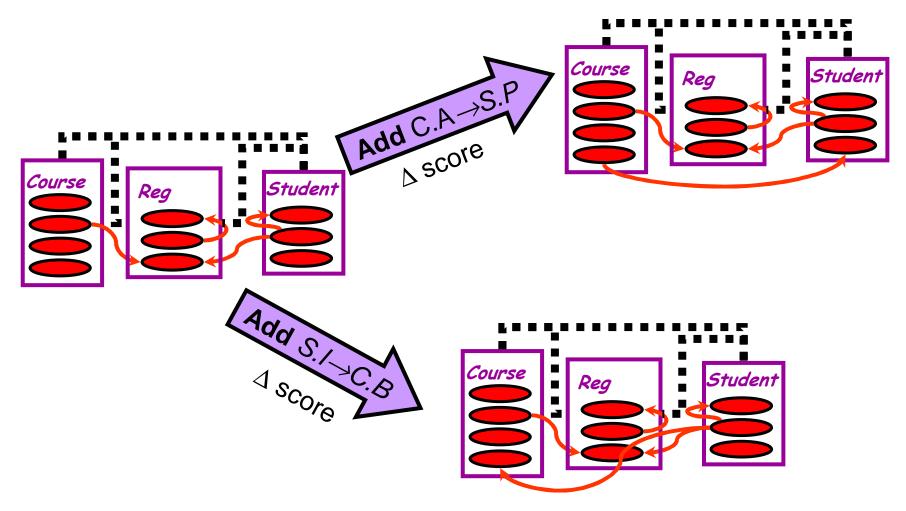


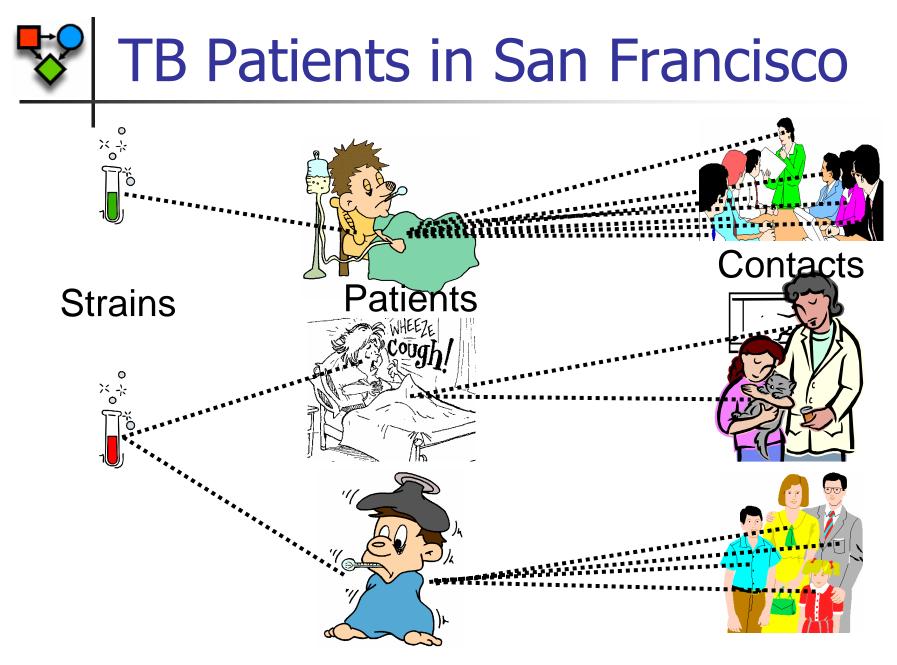
Phase 1: consider dependencies one link away





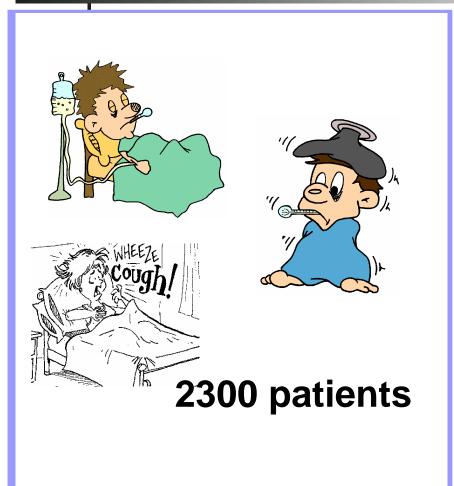
Phase *k*: consider dependencies *k* links away

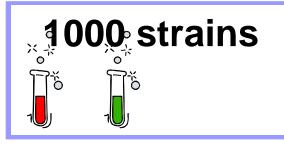




[[]Getoor, Rhee, K., Small, 2001]

TB Patients in San Francisco

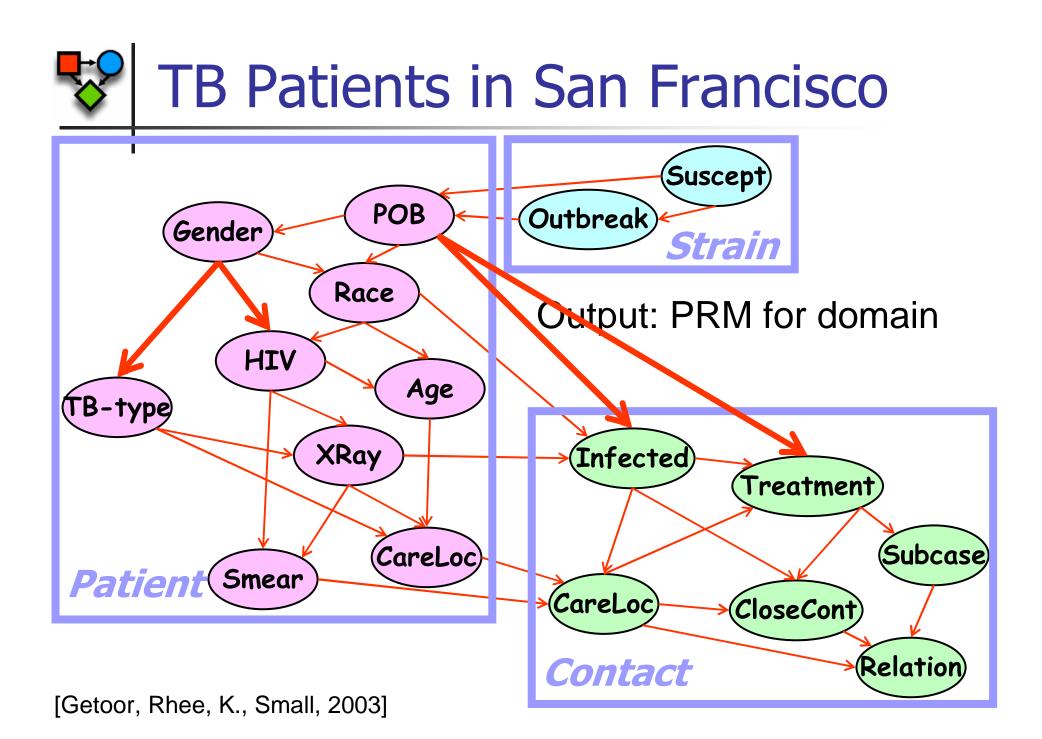




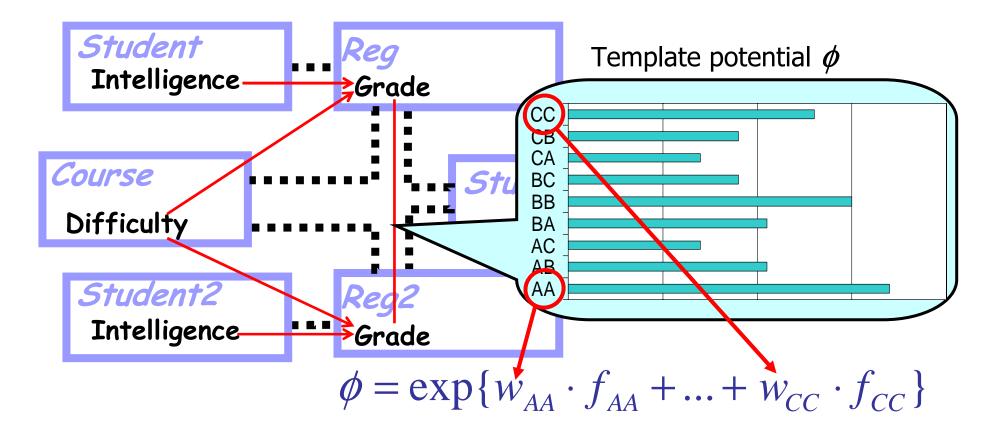
Input: Relational database



20000 contacts







Parameterize potentials as log-linear model

[Taskar, Abbeel, K., 2002]



$$\ell(\boldsymbol{w}:\boldsymbol{\omega}) = \log P_{\boldsymbol{w}}(\boldsymbol{\omega} \mid \boldsymbol{w}) = \sum_{i} W_{i} \cdot f_{i}(\boldsymbol{\omega}) - \log Z$$

Counts in $\boldsymbol{\omega}$

For example:

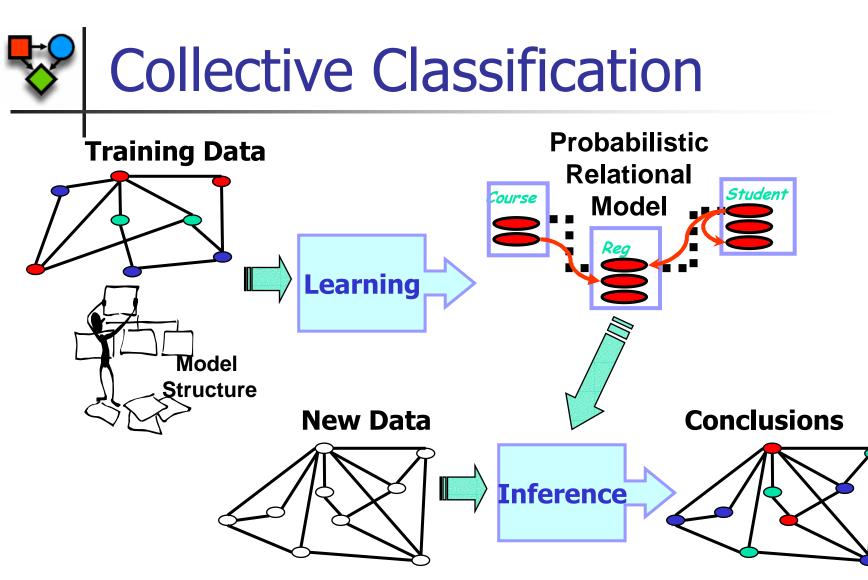
 $f_{AA}(\omega) = # \text{ of tuples } \{\text{reg } r_1, \text{ reg } r_2, \text{ group } g\} \text{ s.t.}$ In(g, r₁), In(g, r₂); r₁.Grade=A, r₂.Grade=A

Learning RMN Parameters

- Parameter estimation is not closed form
- Convex problem \Rightarrow unique global maximum
- Can use methods such as conjugate gradient

$$\frac{\partial \ell}{\partial w_{AA}} = \#(Grade = A, Grade = A) \quad \text{actual count} \\ -\sum P(Grade = A, Grade = A) \quad -\text{expected count}$$

- Gradient process tries to find parameters s.t.
 expected counts = actual counts
- Computing expected counts requires inference over ground Markov network



Example:

- Train on one year of student intelligence, course difficulty, and grades
- Given only grades in following year, predict all students' intelligence

Discriminative Training

- Goal: Given values of observed variables ω.O=o, predict desired target values ω.T=t*
- Do not necessarily want the model to fit the joint distribution P(ω.O=o, ω.T=t*)
- To maximize classification accuracy, we can consider other optimization criteria
 - Maximize conditional log likelihood

$$P(\omega.T = t^* | \omega.O = o)$$

Maximize margin

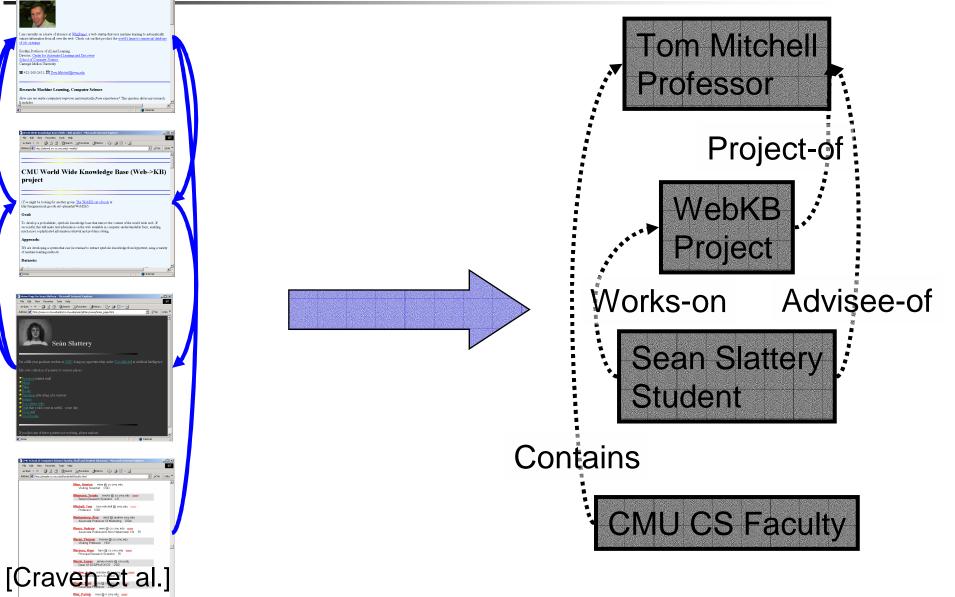
$$\log P(\omega.T = t^* | \omega.O = o)$$

$$-\log[\max_{t\neq t^*} P(\omega.T = t \mid \omega.O = o)]$$

[Taskar, Abbeel, K., 2002; Taskar, Guestrin, K. 2003]

P(second highest probability label)





Web Classification Experiments

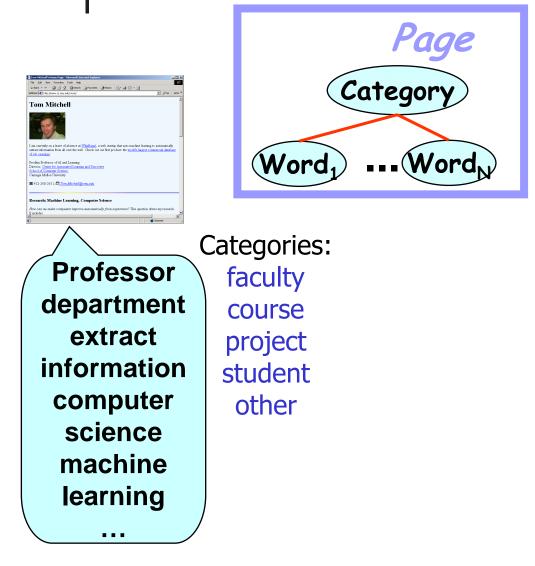
- WebKB dataset
 - Four CS department websites
 - Bag of words on each page
 - Links between pages
 - Anchor text for links
- Experimental setup
 - Trained on three universities
 - Tested on fourth
 - Repeated for all four combinations

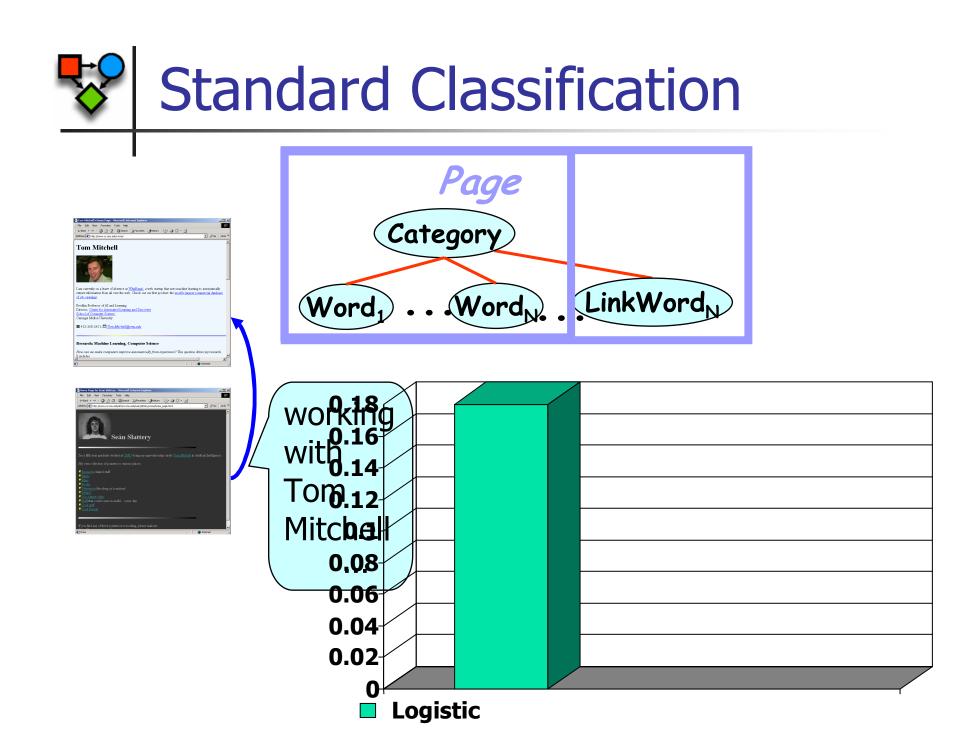


Standard Classification

Logistic

Regression





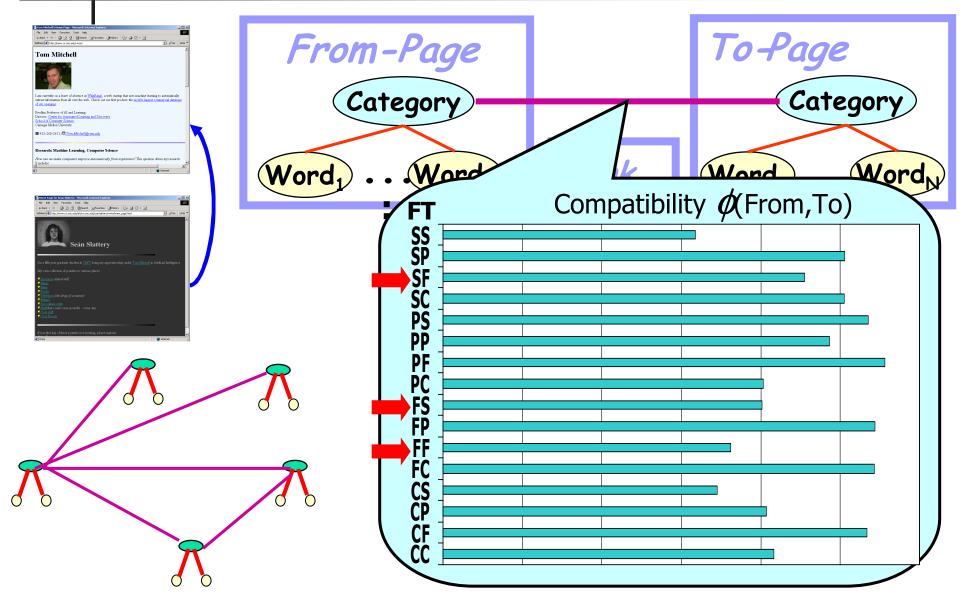


Power of Context

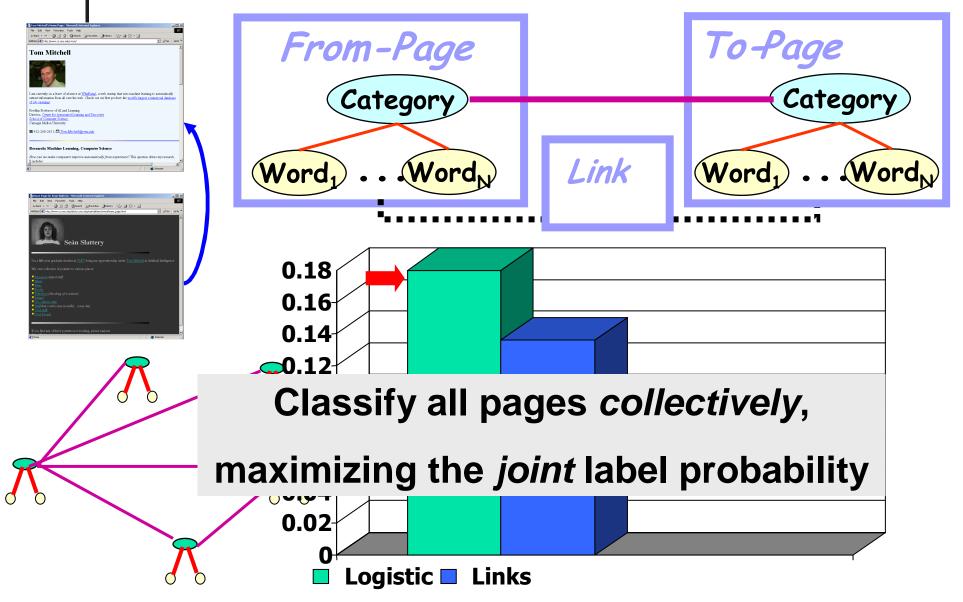
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CMU World Wide Knowledge Base (Web->KB)	🖥 Home Page for Sean Slattery - Microsoft Internet Englaner	
project	File Edit View Favorites Tools Help ↓→Book - → - ④ ② ① ③ ② South ⓐFavorites ④Hezory ♀ ④ ③ • ●	
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(You might be looking for another group: <u>The WebKB set of tools</u> at http://ineganetia.int.gu.edu.au/-pénnathr/WebKB/		
Goal:		
To develop a probabilitie, symbolic knowledge suce that mirrors the content of the world wide web. If successful, this will make test information on the web senable in computer-understandable form, enabling much more spoteinated a formation terrors and	Seán Slattery	
Approach:	Trn a fifth year graduate student at <u>CMU</u> doing my apprenticeship under <u>Tom Marched</u> in Artificial Intelligence.	
We are developing a system that case be trained to extract symbolic knowledge from hypertext, using a variety of machine learning methods.	My own collection of pointers to various places:	
Datasets:	● <u>Respearch</u> selated stuff ● Munic	
El torne	Paras Booka	
	♥ <u>Television</u> (<i>the drug of a nation</i>) ♥ <u>iseland</u> ♥ So cubare exhic	
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	Cool People	

Professor? Student? Post-doc?

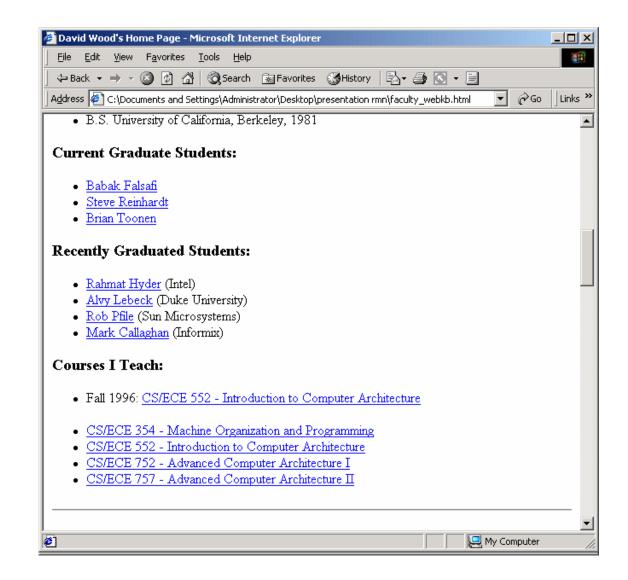




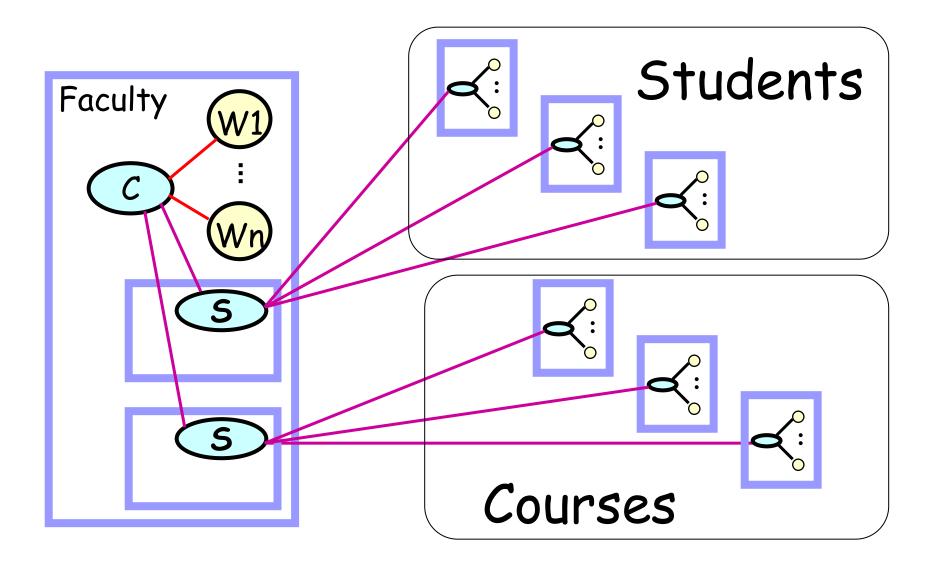


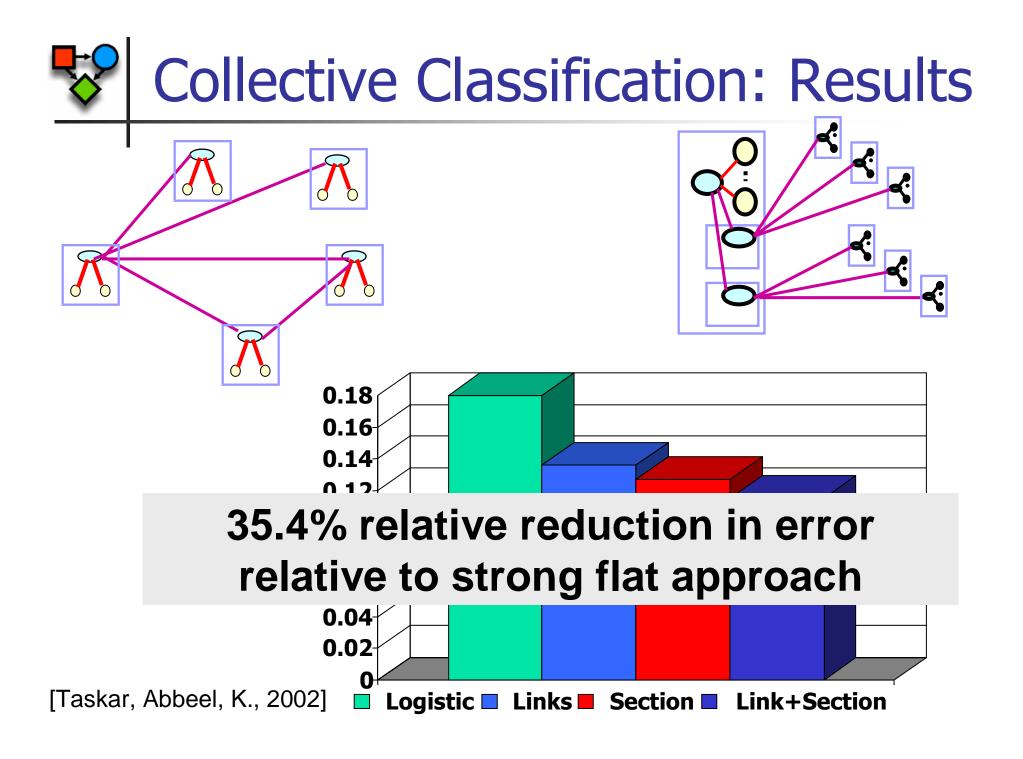


More Complex Structure

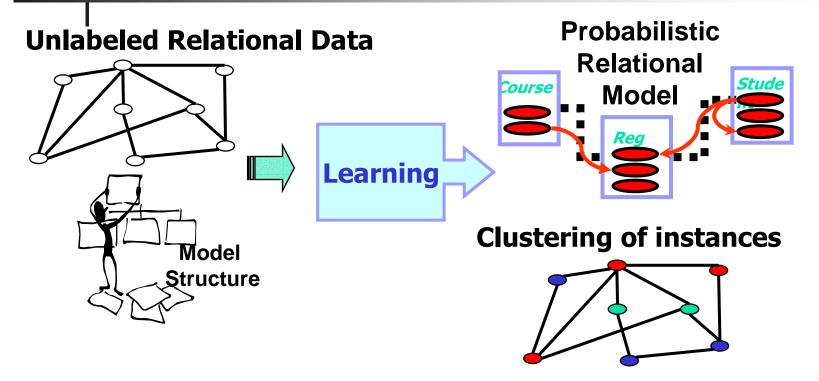








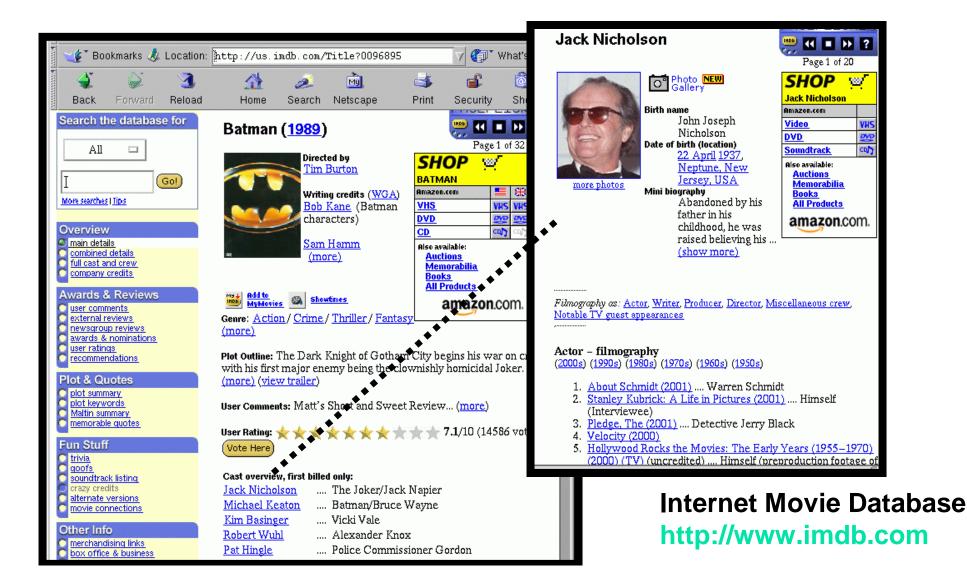




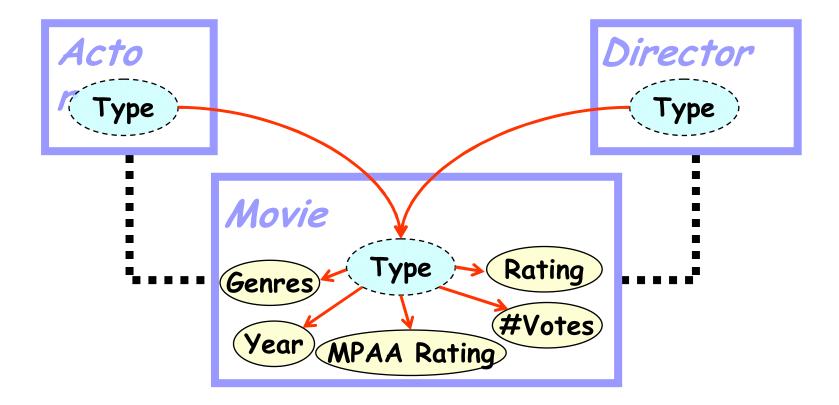
Example:

• Given only students' grades, cluster similar students









[Taskar, Segal, K., 2001]



Discovering Hidden Types

Movies

Wizard of Oz Cinderella Sound of Music The Love Bug Pollyanna The Parent Trap **Mary Poppins**



Swiss Family Robinson

Terminator 2 Batman Batman Forever GoldenEye Starship Troopers **Mission: Impossible** Hunt for Red October

. . .



Actors

Sylvester Stallone Bruce Willis Harrison Ford Steven Seagal Kurt Russell Kevin Costner Jean-Claude Van Damme Arnold Schwarzenegger

Harvey Keitel

Gary Oldman

. . .

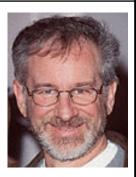


Directors

Alfred Hitchcock **Stanley Kubrick David Lean Milos Forman Terry Gilliam Francis Coppola**



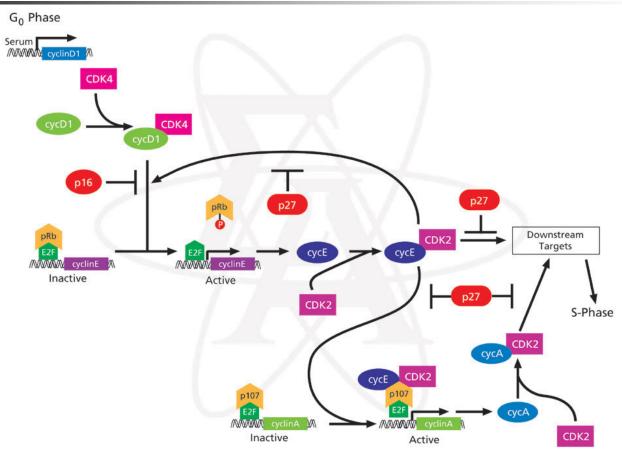
Steven Spielberg Tim Burton Tony Scott James Cameron John McTiernan **Joel Schumacher**



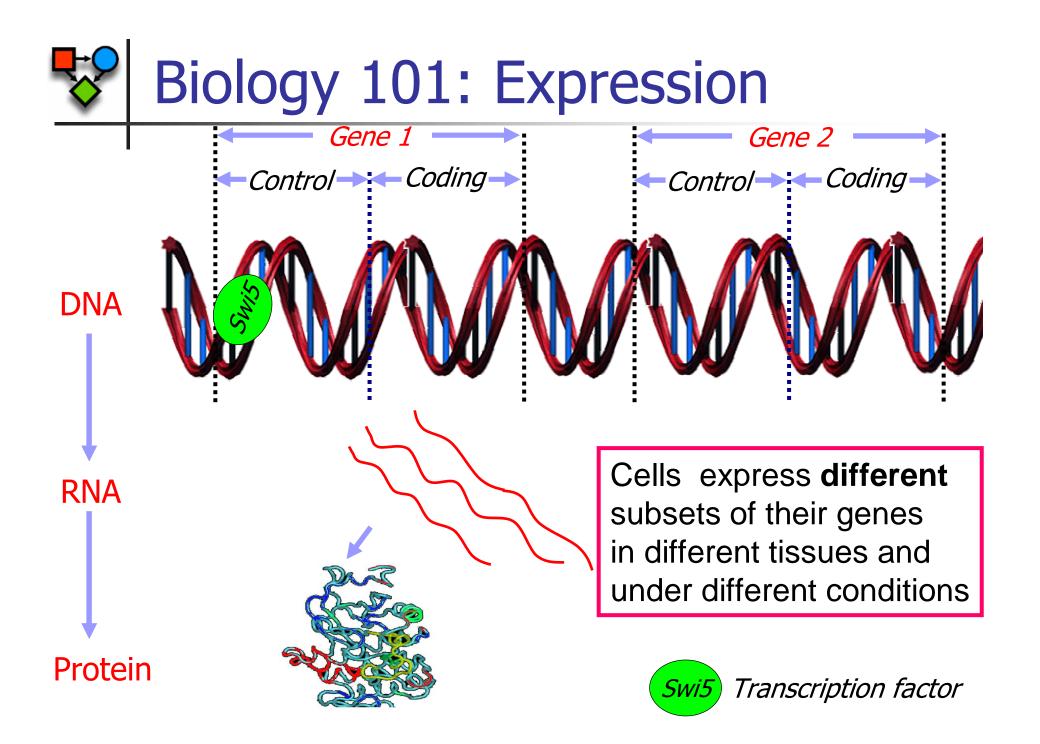




Biology 101: Pathways

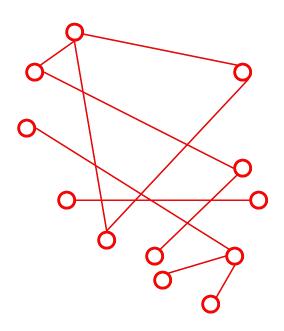


 Pathways are sets of genes that act together to achieve a common function





Use protein-protein interaction data





Finding Pathways: Attempt I

Use protein-protein interaction data

Problems:

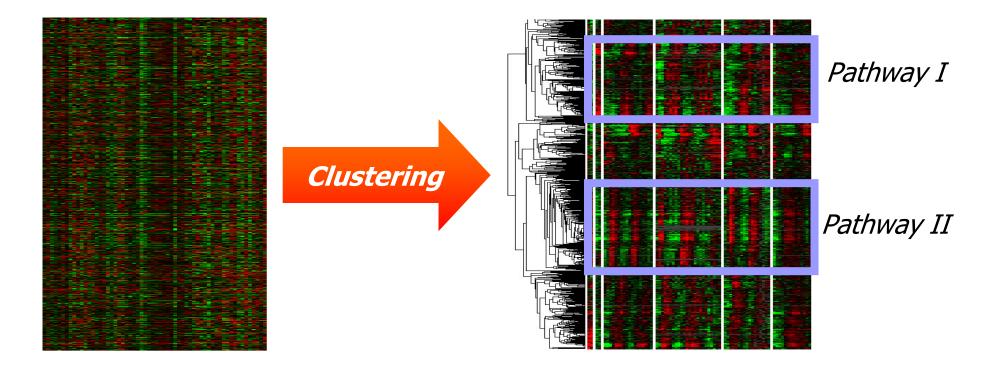
- Data is very noisy
- Structure is lost:
 - Large connected component (3527/3589 genes) in interaction graph



Finding Pathways: Attempt II

Use gene expression data

Thousands of arrays available under different conditions



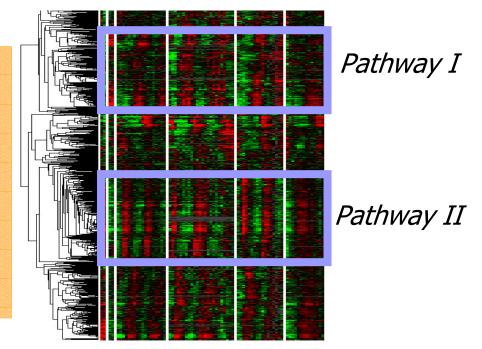
Finding Pathways: Attempt II

Use gene expression data

Thousands of arrays available under different conditions

Problems:

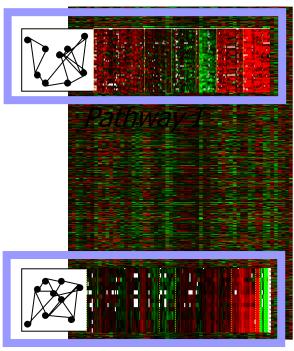
- Expression is only 'weak' indicator of interaction
- Data is noisy
- Interacting pathways are not separable



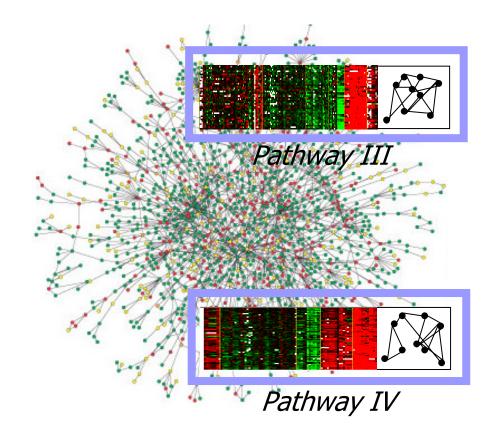
Finding Pathways: Our Approach

Use both types of data to find pathways

- Find "active" interactions using gene expression
- Find pathway-related co-expression using interactions



Pathway II

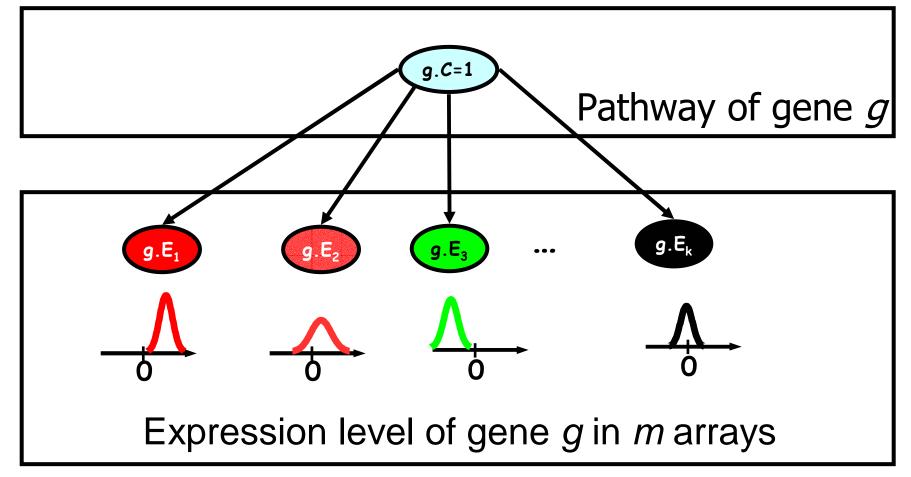




- Genes are partitioned into "pathways":
 - Every gene is assigned to one of `k' pathways
 - Random variable for each gene with domain {1,...,k}
- Expression component:
 - Model likelihood is higher when genes in the same pathway have similar expression profiles
- Interaction component:
 - Model likelihood is higher when genes in the same pathway interact

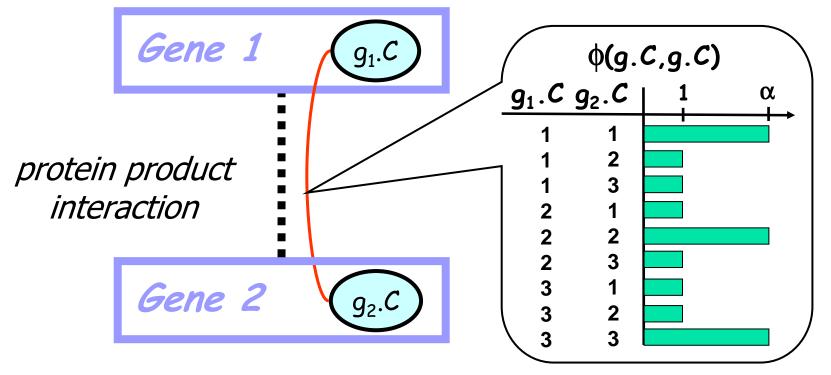


Naïve Bayes

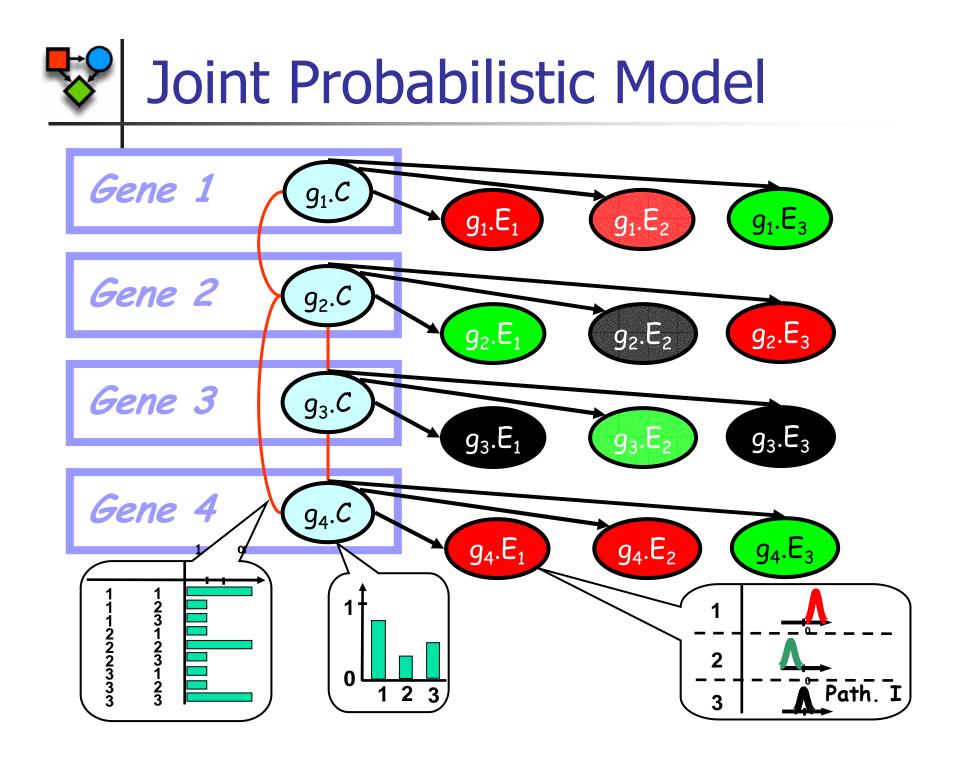


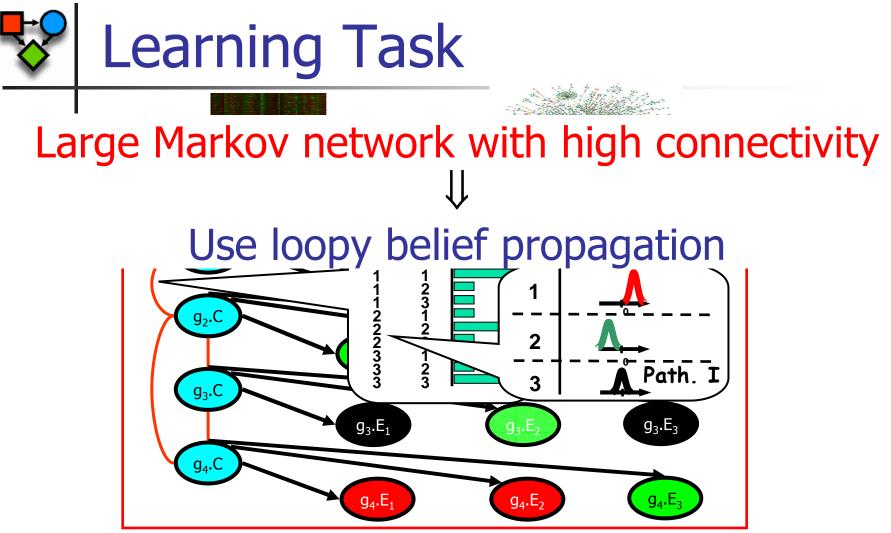


Interacting genes are more likely to be in the same pathway



Compatibility potential

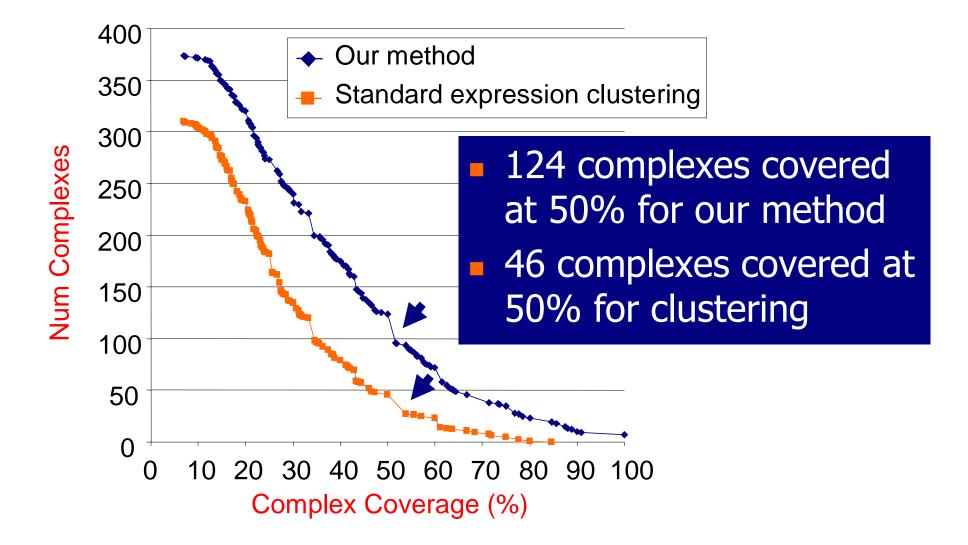


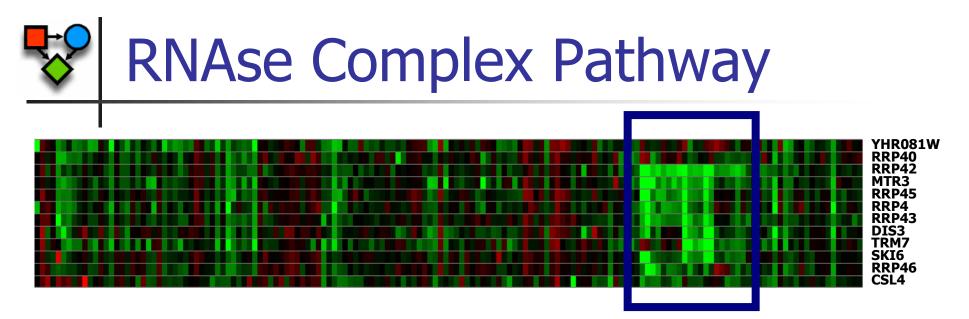


- E-step: compute pathway assignments
- M-step: Estimate Gaussian distribution parameters
- Estimate compatibility potentials using cross-validation

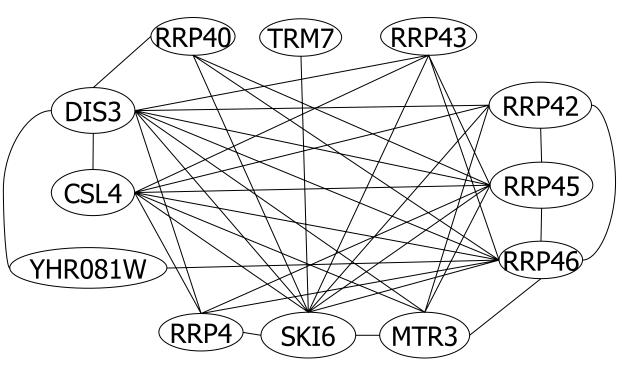
Capturing Protein Complexes

Independent data set of interacting proteins



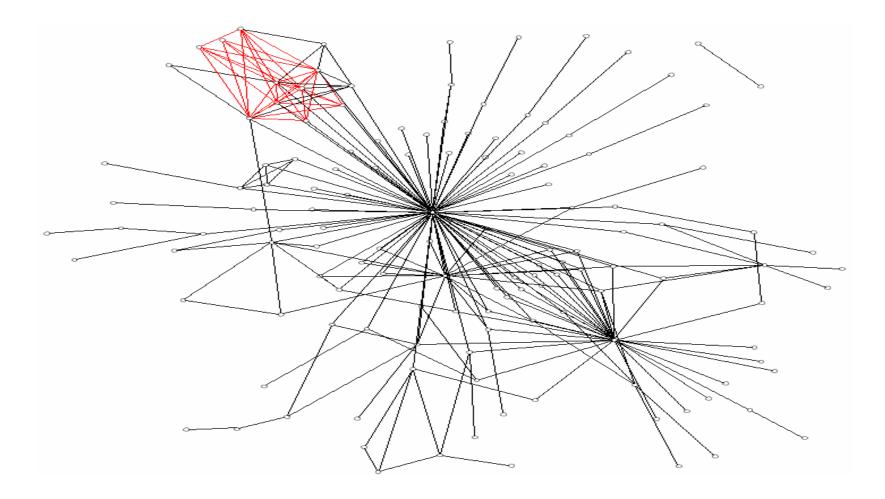


- Includes all 10 known pathway genes
- Only 5 genes found by clustering





 RNAse complex found by interaction clustering as part of cluster with 138 genes





Or PRMs are not just template BNs/MNs



- Class uncertainty:
 - To which class does an object belong
- Relational uncertainty:
 - What is the relational (link) structure
- Identity uncertainty:
 - Which "names" refer to the same objects
 - Also covers data association

Relational Uncertainty

Probability distribution over graph structures

- Link existence model
 - E.g., hyperlinks between webpages
 - Each potential link is a separate event
 - Its existence is a random variable
- Link reference model
 - E.g., instructors teaching a course
 - Fix set of outgoing links per object
 - Distribution over # of endpoints for outgoing link
 - Each link has distribution over link endpoint
 - e.g., instructor link for CS course likely to point to CS prof
- Many other models possible

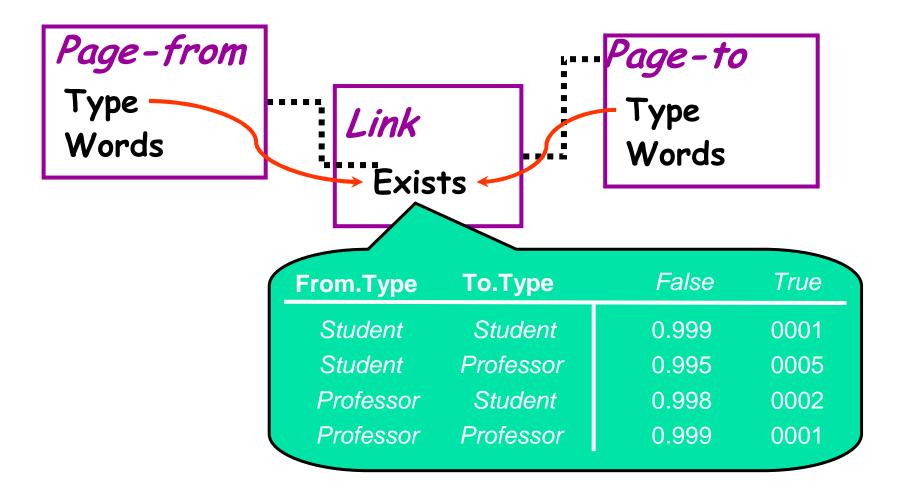
[Getoor, Friedman, K. Taskar, 2002]



- Background knowledge ξ is an *object skeleton*
 - A set of entity objects
- PRM defines distribution over worlds ω
 - Assignments of values to all attributes
 - Existence of links between objects
- Define objects for any potential links
 - E.g., a potential link object for any pair of webpages w1, w2
- Each potential link object has *link existence* attribute, denoting whether the link exists or not

Link existence variables have probabilistic model [Getoor, Friedman, K. Taskar, 2002]



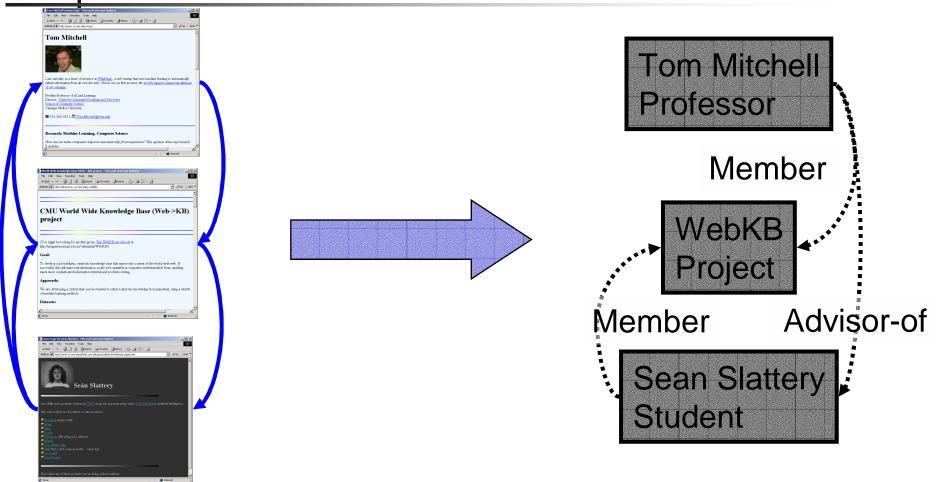


Why Are Link Models Useful?

- Predict which links exist in the world
 - Which professor teaches each course
 - Which student will register for which course
- Use known links to infer values of attributes
 - Given that student registered for a hard class, is she more likely to be a graduate student
 - Given that one page points to another, is it more likely to be a faculty page?

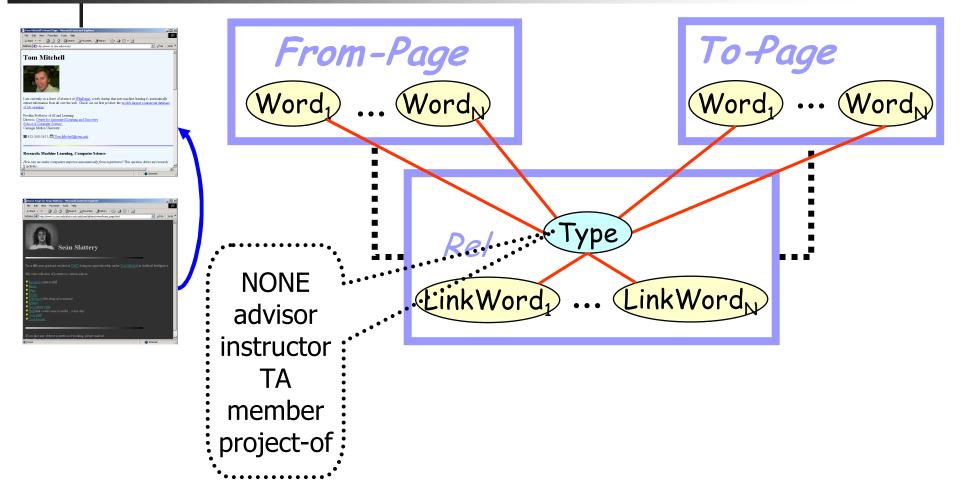


Predicting Relationships

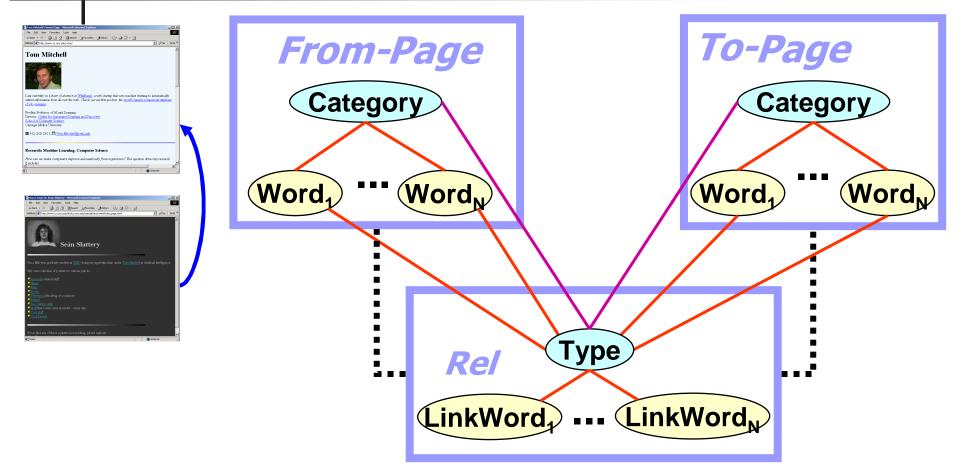


Predict and classify relationships between objects



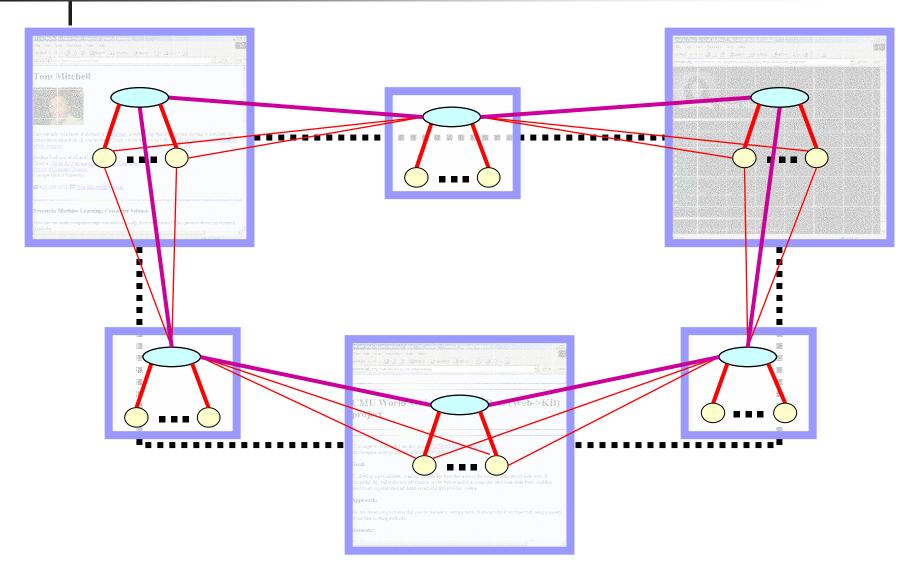


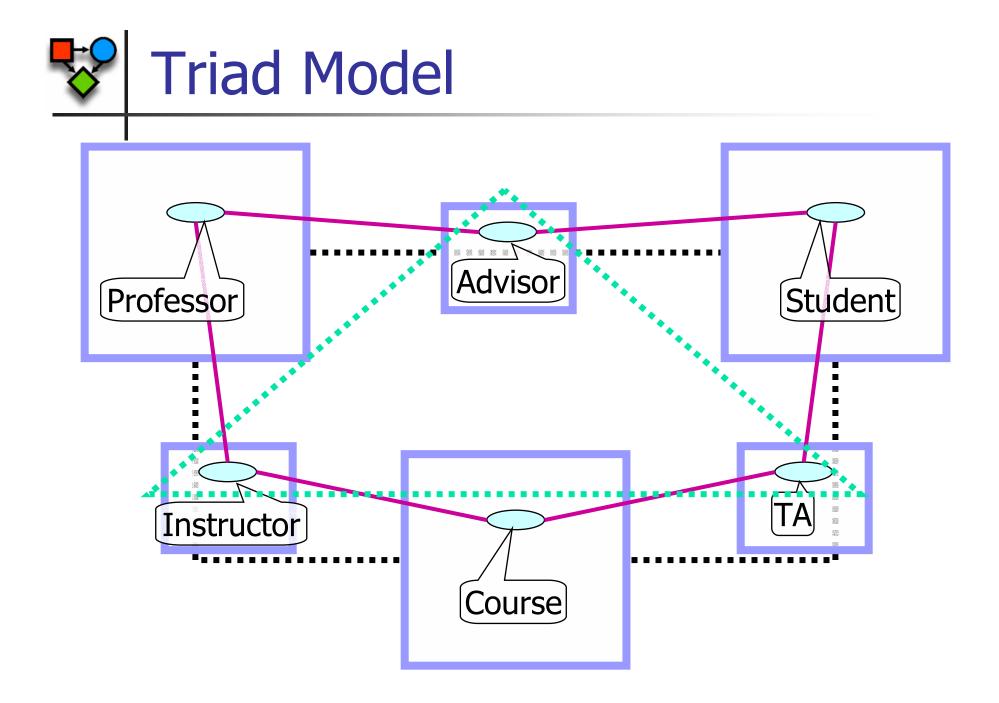
Collective Classification: Links

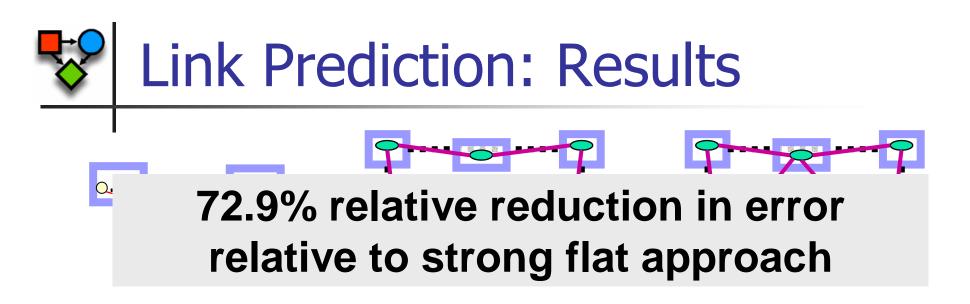


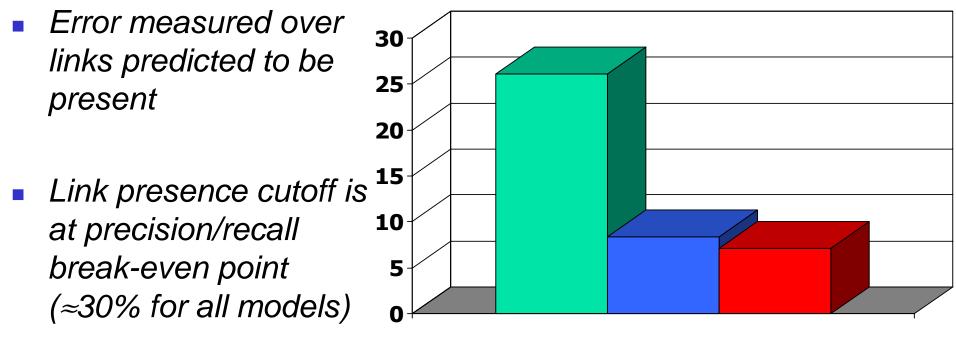
[Taskar, Wong, Abbeel, K., 2002]









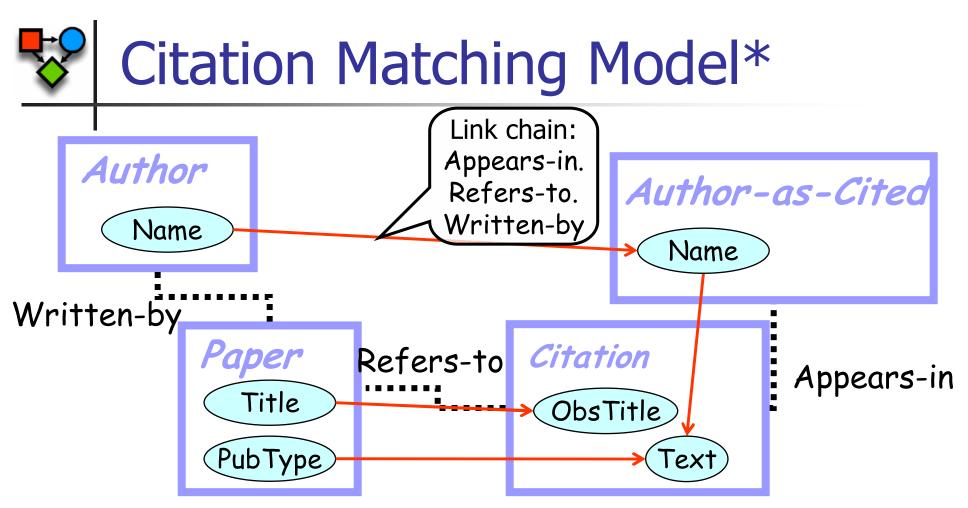


[Taskar, Wong, Abbeel, K., 2002]

🗖 Flat 🔲 Links 📕 Triad

V Identity Uncertainty Model

- Background knowledge ξ is an *object universe*
 - A set of potential objects
- \blacksquare PRM defines distribution over worlds ω
 - Assignments of values to object attributes
 - Partition of objects into equivalence classes
 - Objects in same class have same attribute values



- Each citation object associated with paper object
- Uncertainty over equivalence classes for papers

Title, PubType

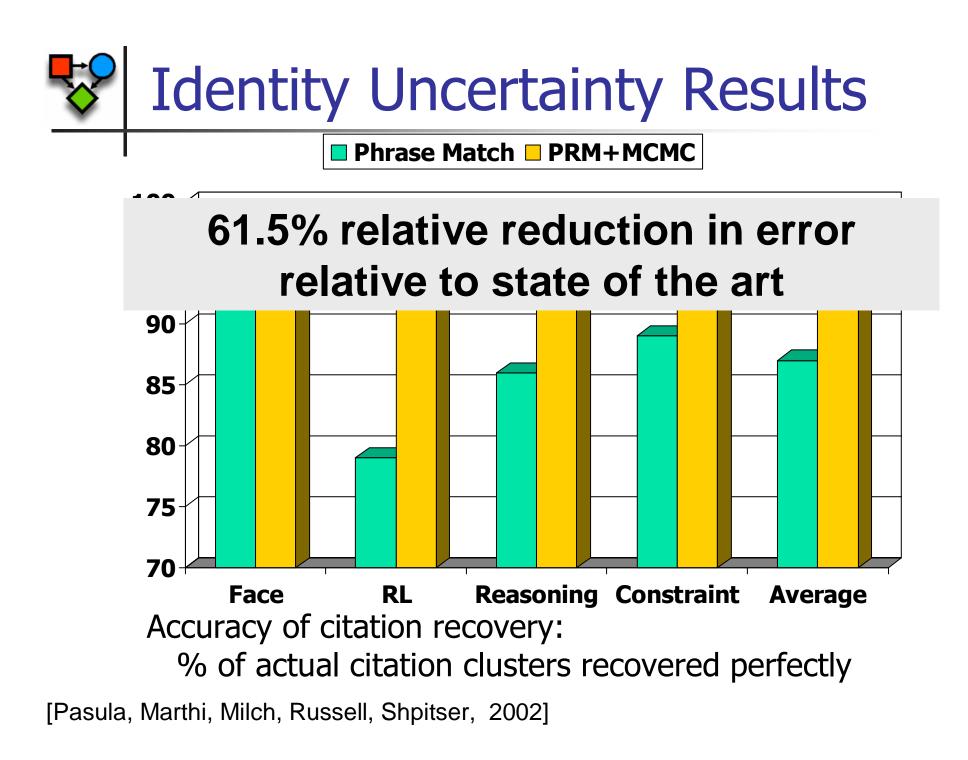
Authors

- If P₁=P₂, have same attributes & links
- * Simplified

V Identity Uncertainty

- Depending on choice of equivalence classes:
 - Number of objects changes
 - Dependency structure changes
- No "nice" corresponding ground BN
- Algorithm:
 - Each partition hypothesis defines simple BN
 - Use MCMC over equivalence class partition
 - Exact inference over resulting BN defines acceptance probability for Markov chain

[Pasula, Marthi, Milch, Russell, Shpitser, 2002]





- Inherit the advantages of graphical models:
 - Coherent probabilistic semantics
 - Exploit structure of local interactions

- Allow us to represent the world in terms of:
 - Objects
 - Classes of objects
 - Properties of objects
 - Relations



- Convenient language for specifying complex models
- "Web of influence": subtle & intuitive reasoning
- A mechanism for tying parameters and structure
 - within models
 - across models
- Framework for learning from relational and heterogeneous data



New way of thinking about models & problems

- Incorporating heterogeneous data by connecting related entities
- New problems:
 - Collective classification
 - Relational clustering
- Uncertainty about richer structures:
 - Link graph structure
 - Identity

But What Do We *Really* Gain?

Are PRMs just a convenient language for specifying attribute-based graphical models?

- Simple PRMs \approx relational logic w. fixed domain and \forall only
 - Induce a "propositional" BN
- Can augment language with additional expressivity
 - Existential quantifiers & functions
 - Equality
- Resulting language is inherently more expressive, allowing us to represent distributions over
 - worlds where dependencies vary significantly [Getoor et al., Pasula et al.]
 - worlds with different numbers of objects [Pfeffer et al., Pasula et al.]
 - worlds with infinitely many objects [Pfeffer & K.]

Big questions: Inference & Learning



http://robotics.stanford.edu/~koller/