Pseudo-Likelihood for Relational Data

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To appear at SIAM SDM conference on data mining.



The Main Topic

- In relational data, units are interdependent
 ⇒ no product likelihood function for model.
- How to do model selection?
- Proposal of this talk: use **pseudo likelihood.**
 - Unnormalized product likelihood.
 - Like independent-unit likelihood, but with event frequencies instead of event counts.

Overview

- Define pseudo log-likelihood for *directed graphical models* (Bayes Nets).
- Interpretation as *expected log-likelihood* of random small groups of units.
- Learning Algorithms:
 - MLE solution.
 - Model Selection.
- Simulations.

Outline

- Brief intro to relational databases.
- Statistics and Relational Databases.
- Briefer intro to Bayes nets.
- Relational Random Variables.
- Relational (pseudo)-likelihoods.

Relational Databases

- 1970s: Computers are spreading. Many organizations use them to store their data.
- Ad hoc formats
 - ⇒ hard to build general data management systems.
 - \Rightarrow lots of duplicated effort.
- The Standardization Dilemma:
 - Too restrictive: doesn't fit users' needs.
 - Too loose: back to ad-hoc solutions.

The Relational Format

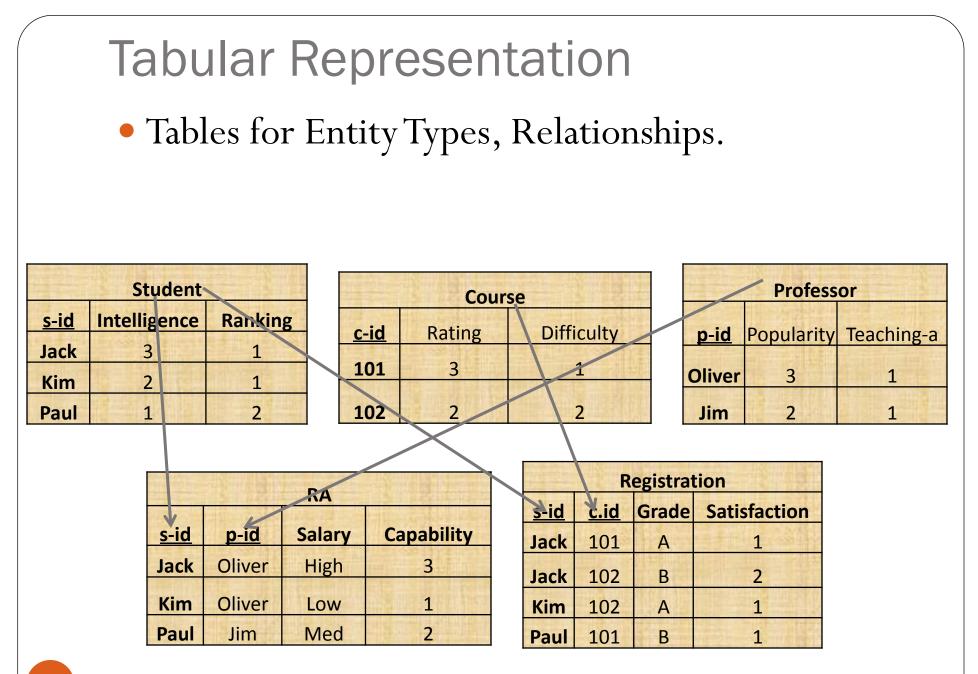
- Codd (IBM Research 1970)
- The fundamental question: What kinds of information do users need to represent?

- Answered by 1st-order predicate logic! (Russell, Tarski).
- The world consists of
 - Individuals/entities.





• Relationships/links among them.



Pseudo-Likelihood for Relational Data - Statistics Seminar

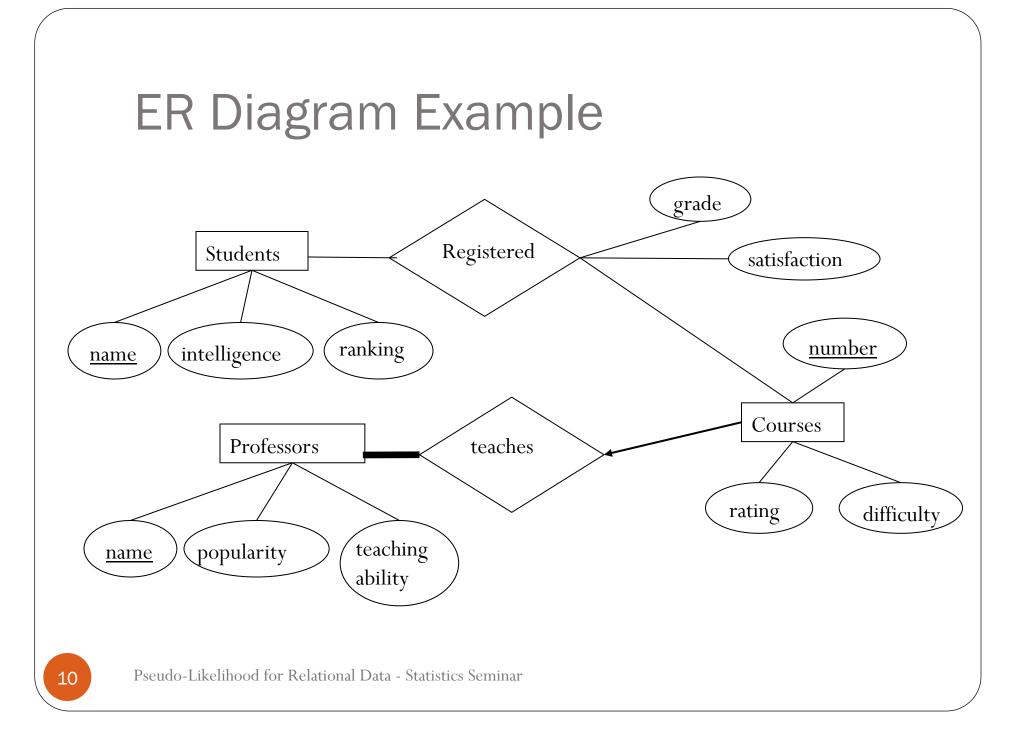
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Database Management Systems

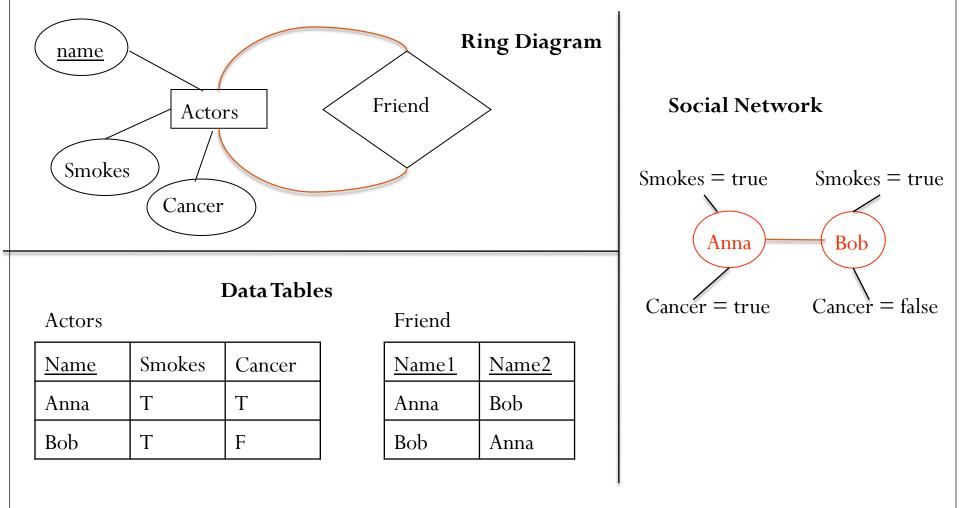
- Maintain data in linked tables.
- Structured Query Language (SQL) allows fast *data retrieval*.
 - E.g., find all SFU students who are statistics majors with gpa > 3.0.
- Multi-billion dollar industry, \$15+ bill in 2006.
- IBM, Microsoft, Oracle, SAP, Peoplesoft.

Relational Domain Models

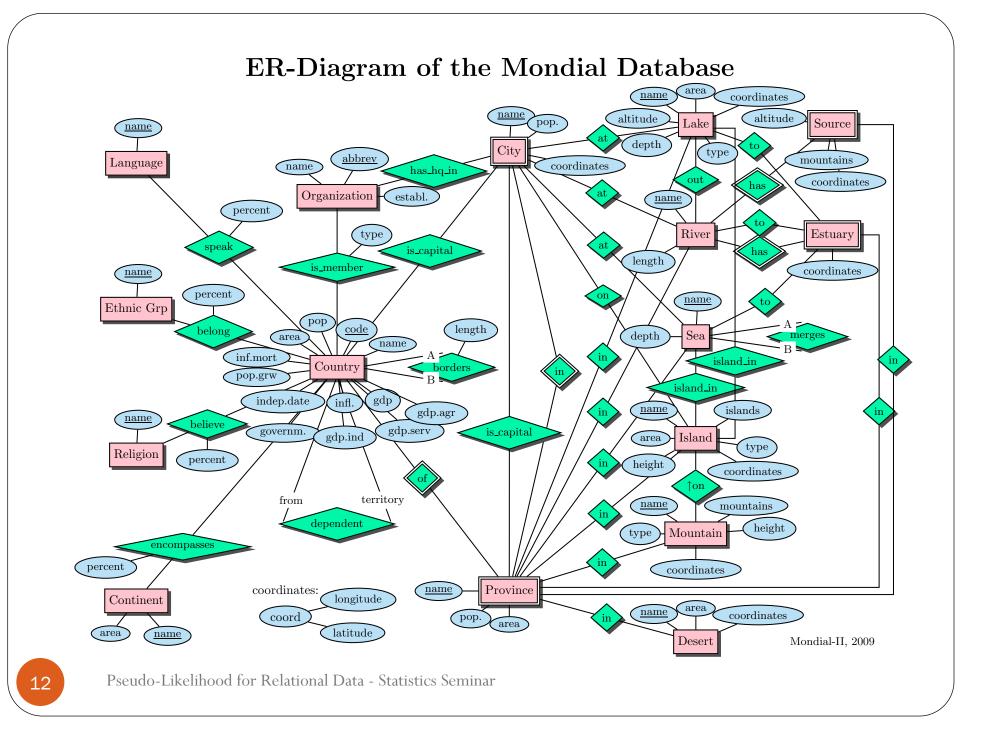
- Visualizing Domain Ontology.
- Active Area of Research.
 - Unified Modelling Language (UML).
 - Semantic Web (XML).
- Classic Tool: The Entity-Relationship (ER) Diagram.











Relationship to Social Network Analysis

- A single-relation social network is a simple special case of a relational database.
- Converse also true if you allow:
 - Different types of nodes ("actors").
 - Labels on nodes.
 - Different types of (hyper)edges.
 - Labels on edges.

• See Newman (2003) SIAM Review.

• **Observation** A relational database is equivalent to a general network as described.

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Beyond storing and retrieving data

- Much new interest in analyzing databases.
 - Data Mining.
 - Data Warehousing.
 - Business Intelligence.
 - Predictive Analytics.
- Fundamental Question: how to combine logic and probability?
- Domingos (U of W, CS): "Logic handles complexity, probability represents uncertainty."

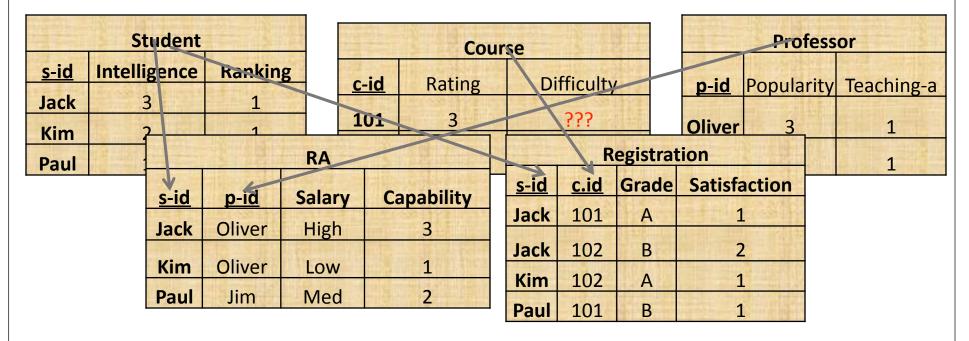


Typical Tasks for Statistical-Relational Learning (SRL)

- Link-based Classification: given the links of a target entity and the attributes of related entities, predict the class label of the target entity.
- Link Prediction: given the attributes of entities and their other links, predict the existence of a link.

Link-based Classification

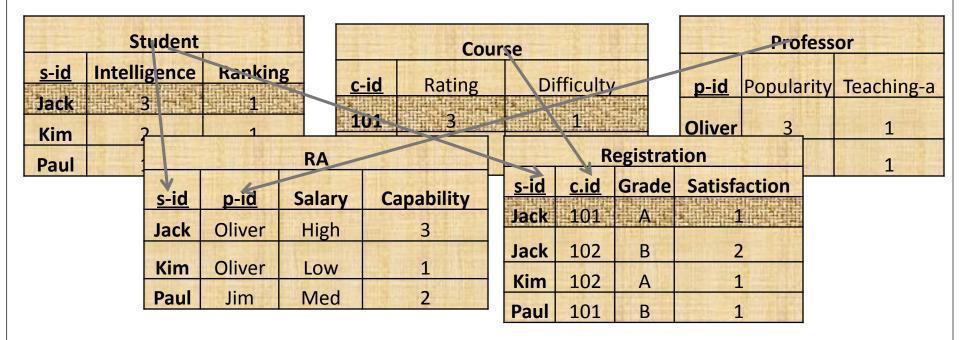
- Predict Attributes given Links, other Attributes
- E.g., P(diff(101))?



Link prediction

• Predict links given links, attributes.

• E.g., P(Registered(jack, 101))?



Generative Models

- Model the joint distribution over links and attributes.
- Today's Topic.
- We'll use Bayes nets as the model class.

What is a Bayes (belief) net? Compact representation of joint probability distributions via conditional independence

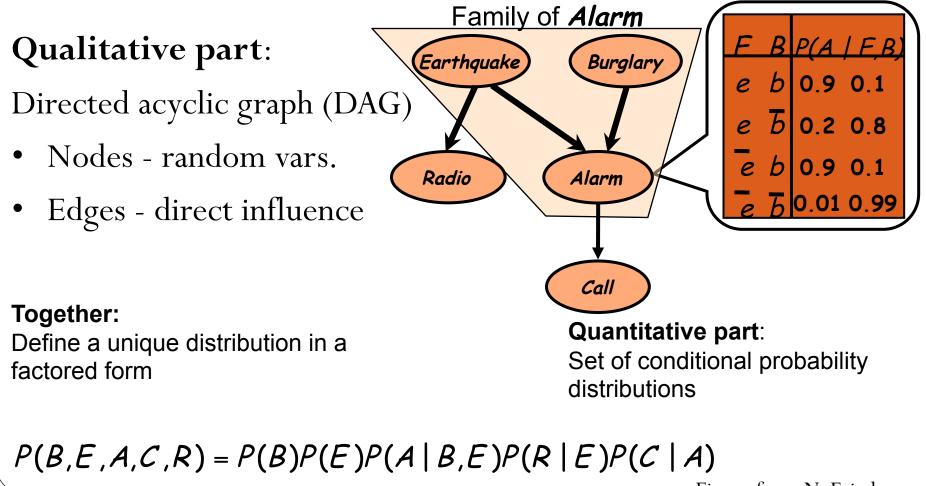


Figure from N. Friedman

Why are Bayes nets useful?

- Graph structure supports
 - Modular representation of knowledge
 - Local, distributed algorithms for inference and learning
 - Intuitive (possibly causal) interpretation
 - A solution to the relevance problem: Easy to compute "Is X relevant to Y given Z".
 - <u>Nice UBC Demo</u>.

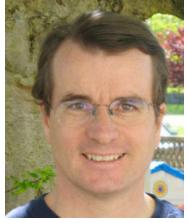
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- Relational Random Variables.
- Relational (pseudo)-likelihoods.

Relational Data: what are the random variables?

- Intuitively, the attributes and relationships in the database.
 - i.e., the columns plus link existence.
 - i.e., the components of the ER diagrams.
- Proposal from David Poole (CS UBC): apply the concept of **functors** from Logic Programming.
- I'm combining this with Halpern (CS Cornell) and Bacchus' (CS U of T) random selection probabilistic semantics for logic.





Population Variables

Russell: "A good notation thinks for us".

- Consider a model with multiple populations.
- Let $X_1, X_2, Y_1, Y_2, ...$ be **population variables.**
- Each variable represents a random draw from a population.
- Population variables are jointly independent.
- A **functor** *f* is a function of one or more population variables.
- A **functor random variable** is written as $f_1(X)$ or $f_2(X, Y)$ or $f_3(X, Y, Z)$.

Unary Functors = Descriptive Attributes of Entities

- Population of Students, Professors.
- Population variables *S*,*P*.
- Attributes r.v.s *age(S)*, *gpa(S)*, *age(P)*, *rank(P)*.
- Can have several selections $age(S_1)$, $age(S_2)$.
- If *S* is uniform over students in the database:
 - P(gpa(S)=3.0) = empirical or database
 frequency of 3.0 gpa in student population.
- Can instantiate or *ground* functors with constants.
 E.g., gpa(jack) returns the gpa of Jack.

Binary Functors = Relationships

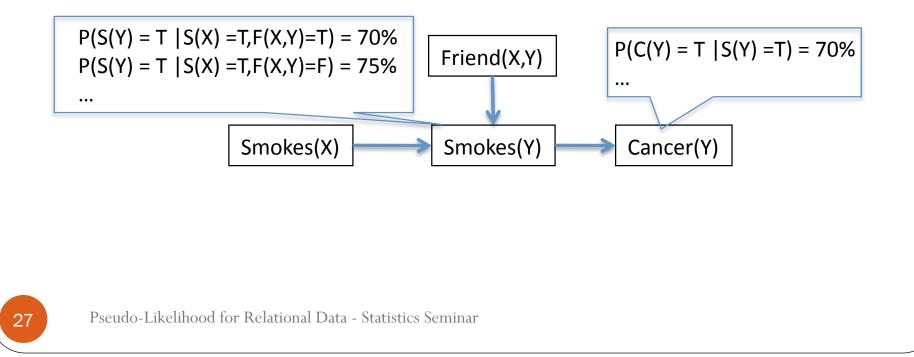
- *Registered(S,C)*: indicator function of existence of relationship.
- If *S*, *C* uniformly distributed over observed population:
 - P(Registered(S,C)=1) = #(s,c) s.t. Student s is registered in course c/ #Students x #Courses.

= Database Frequency of Registration.

Can also form chains:
 P(grade(S,C)=A, Teaches(C,P)=1).

Functor Bayes Nets

 Poole IJCAI 2003: A functor Bayes Net is a Bayes net whose nodes are functor random variables.



Likelihood Functions for Functor Bayes Nets: Latent Variables

- Problem: Given a database *D* and an FBN model *B*, how to define *P(D | B)*?
- Fundamental Issue: interdependent units, not iid.
- One approach: introduce *latent variables* such that units are independent conditional on hidden "state" (e.g., Kersting et al. IJCAI 2009).
 - Cf. social network analysis Hoff, Rafferty (U of W Stats), Linkletter SFU Stats.
 - Cf. nonnegative matrix factorization----Netflix challenge.

Likelihood Function for Single-Table Data

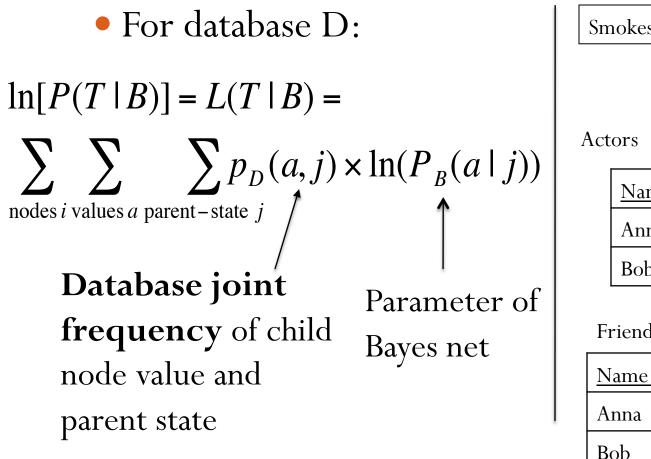
• For single table *T*: $\ln[P(T \mid B)] = L(T \mid B) =$ $\sum \sum n_T(a,j) \times \ln(P_B(a \mid j))$ nodes i values a parent-state jTable count of co-Parameter of occurrences of child Bayes net node value and parent state

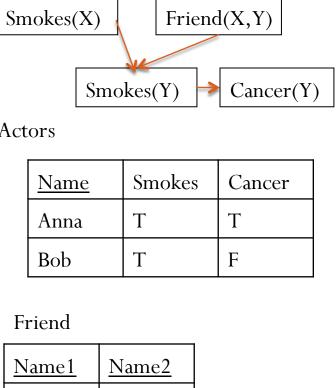
Smokes(Y)	>	Cancer(Y)

Actors

Name	Smokes	Cancer			
Anna	Т	Т			
Bob	Т	F			

Proposed Pseudo Log-Likelihood





Bob

Anna

Random Selection Log-Likelihood

- 1. Randomly select instances $X_1 = x_1, \dots, X_n = x_n$. for each variable in FBN.
- 2. Look up their properties, relationships in database.
- 3. Compute log-likelihood for the FBN assignment obtained from the instances.
- 4. L^{R} = expected log-likelihood over uniform random selection of instances.

		Hyperentity Hyperfeatures								
Smokes(X) $Friend(X,Y)$	Γ	Х	Y	F(X,Y)	S(X)	C(X)	S(Y)	C(Y)	P_B^R	$ln(P_B^R)$
	γ_1	Anna	Bob	Т	Т	Т	Т	F	0.105	-2.254
	γ_2	Bob	Anna	Т	Т	F	Т	Т	0.245	-1.406
	γ_3	Anna	Anna	F	Т	Т	Т	Т	0.263	-1.338
Smokes(Y) \rightarrow Cancer(Y)	γ_4	Bob	Bob	F	Т	F	Т	F	0.113	-2.185

 $L^{R} = -(2.254 + 1.406 + 1.338 + 2.185)/4 \approx -1.8$

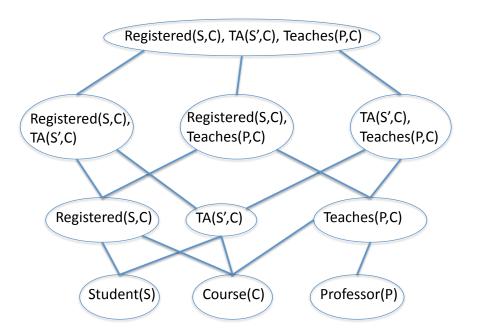
Proposition The random selection log-likelihood equals the pseudo log-likelihood.

Parameter Estimation

Proposition For a given database D, the parameter values that maximize the pseudo likelihood are the empirical conditional frequencies.

Model Selection

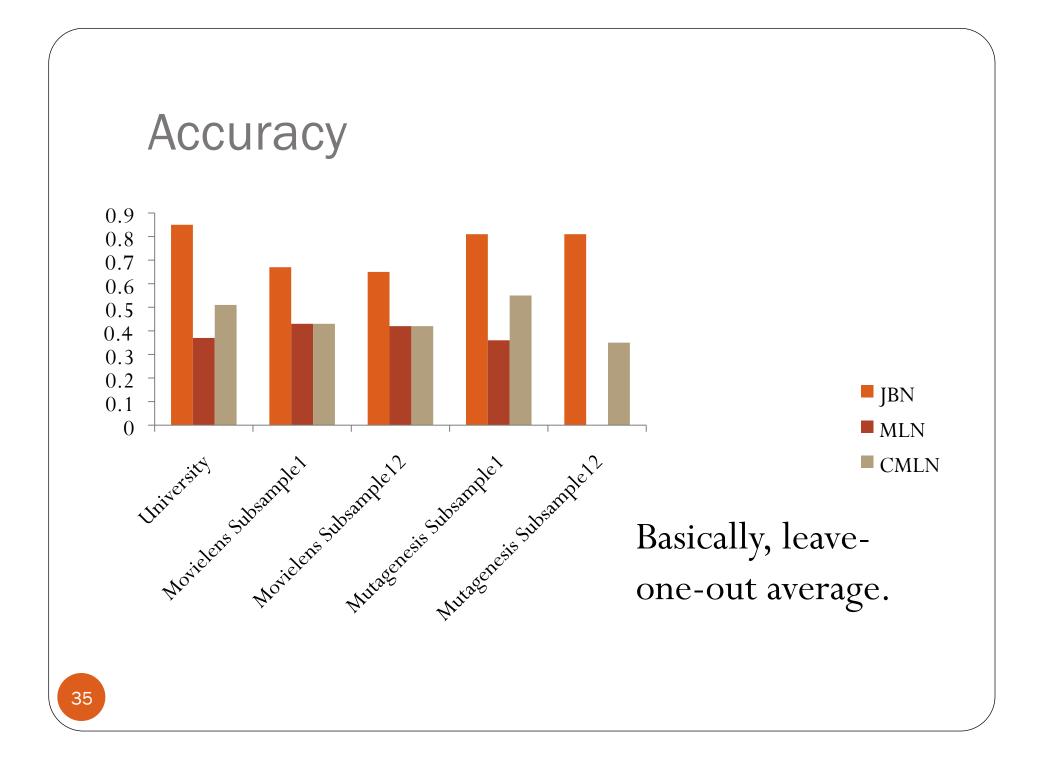
- New model selection algorithm (Khosravi, Schulte et al. AAAI 2010).
- Level-wise search through table join lattice.



Running time on benchmarks

Dataset	JBN	MLN	CMLN
University	$0.03 {+} 0.032$	5.02	11.44
MovieLens	1.2+120	NT	NT
MovieLens Subsample 1	0.05 + 0.33	44	121.5
MovieLens Subsample 2	0.12 + 5.10	2760	1286
Mutagenesis	0.5 + NT	NT	NT
Mutagenesis subsample 1	0.1 + 5	3360	900
Mutagenesis subsample 2	0.2 + 12	NT	3120

- Time in Minutes. NT = did not terminate.
- x + y = structure learning + parametrization (with Markov net methods).
- JBN: Our join-based algorithm.
- MLN, CMLN: standard programs from the U of Washington (Alchemy)



Future Work: Inference

Prediction is usually based on *knowledge-based model construction* (Ngo and Haddaway, 1997; Koller and Pfeffer, 1997; Haddaway, 1999).

- Basic Idea: instantiate population variables with all population members. Predict using instantiated model.
- With Bayes nets, can lead to cycles.
- My conjecture: cycles can be handled with a normalization constant that has a closed form.
- Help?!

Summary: Likelihood for relational data.

- Combining relational databases and statistics.
 - Very important in practice.
 - Combine logic and probability.
- Interdependent units → hard to define model likelihood.
- Proposal: Consider a randomly selected small group of individuals.
- Pseudo log-likelihood = expected log-likelihood of randomly selected group.

Summary: Statistics with Pseudo-Likelihood

- Theorem: Random pseudo log-likelihood equivalent to standard single-table likelihood, replacing table counts with database frequencies.
- Maximum likelihood estimates = database frequencies.
- Efficient Model Selection Algorithm based on lattice search.
- In simulations, very fast (minutes vs. days), much better predictive accuracy.

Thank you!

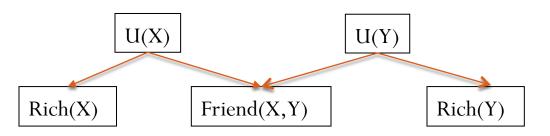
• Any questions?



Choice of Functors

- Can have complex functors, e.g.
 - Nested: wealth(father(father(X))).
 - Aggregate: AVG_C{grade(S,C): Registered(S,C)}.
- In remainder of this talk, use functors corresponding to
 - Attributes (columns), e.g., *intelligence(S)*, *grade(S,C)*
 - Boolean Relationship indicators, e.g. *Friend(X,Y)*.

Hidden Variables Avoid Cycles



• Assign unobserved values *u(jack)*, *u(jane)*.

- Probability that Jack and Jane are friends depends on their unobserved "type".
- In ground model, *rich(jack)* and *rich(jane)* are correlated given that they are friends, but neither is an ancestor.
- Common in social network analysis (Hoff 2001, Hoff and Rafferty 2003, Fienberg 2009).
- \$1M prize in Netflix challenge.
- Also for multiple types of relationships (Kersting et al. 2009).
- Computationally demanding.

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