Relational Probabilistic Models

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Work with: `http://minervaintelligence.com`, `https://treatment.com/`

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Outline

1. Knowledge Graphs
   - Tensor Factorization and Neural Network Models
2. Representation Issues
   - Desiderata
   - How do relational models relate to probabilistic graphical models
3. Unique properties of relational models
   - Learning general knowledge vs learning about a data set
   - Varying Populations
   - What can be observed?
4. Conclusions and Challenges
5. (Exact) Lifted Inference
   - Recursive Conditioning
   - Lifted Recursive Conditioning

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With a single relation it can be implicit $\longrightarrow$ triples:
$\langle pen_7, color, red \rangle$.

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- $prop(a, type, parcel)$, where *type* is a special property and *parcel* is a class.
- $prop(a, parcel, true)$, where *parcel* is a Boolean property (characteristic function of the class *parcel*).

Triples

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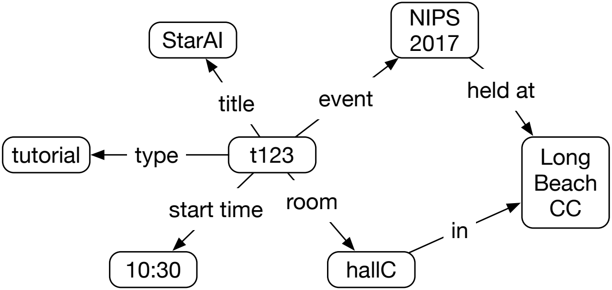
- Reify means: to make into an individual.
- How can we add extra arguments (e.g., presenters, chair)?

Triples and Knowledge Graphs

- Subject–verb–object
  Individual–property–value
  triples can be depicted as edges in graphs



- A modeller or learner needs to invent (reified) objects.

Triples are universal representations of relations

All relations can be represented in terms of triples:

$$\begin{array}{c|c|c|c|}
\cline{2-4}
 & \ldots & P_j & \ldots \\
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$prop(Individual, Property, Value)$ is the only relation needed: $\langle Individual, Property, Value \rangle$ triples, Semantic network, entity relationship model, knowledge graphs, ...

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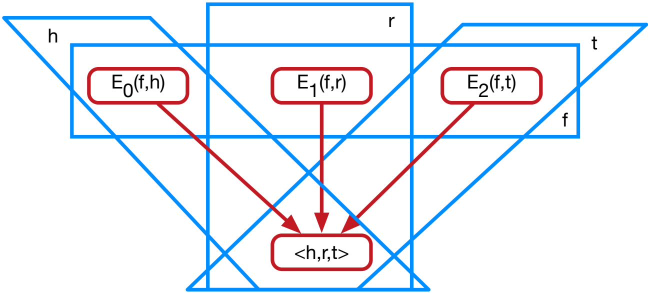

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- CompleX: the embeddings are complex numbers, tail is the conjugate of the head embedding
- SimpleE: have an embedding for r^{-1} and learn to predict both $\langle h, r, t\rangle$ and $\left\langle t, r^{-1}, h\right\rangle$

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- Which is better depends on the goals and how success is measured.
- Many of the methods try to do both; learn about specific individuals and general knowledge.

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- Difficult to learn about reified entities.

Predicting Properties

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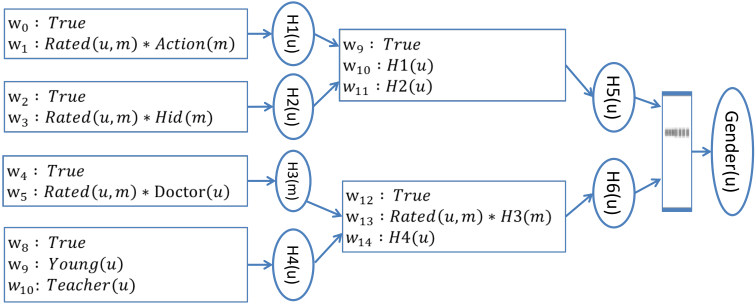
- We can build relational neural networks to solve this

[Kazemi & Poole, AAAI 2017]

Relational Neural Nets (RelNNs)



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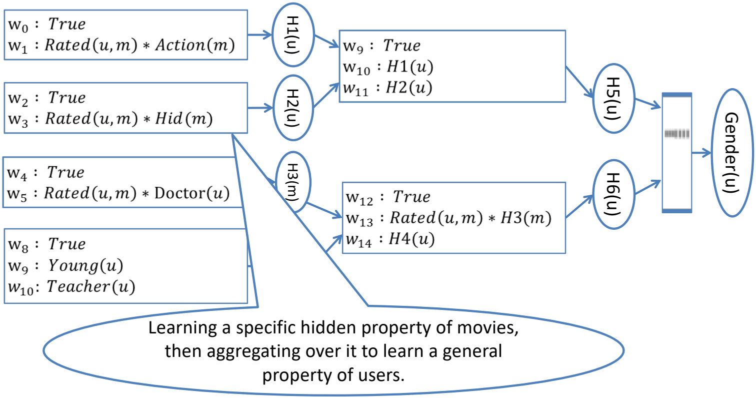

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- Modularity:
  Can independently developed parts be combined to form larger model?
  Can a larger model be decomposed into smaller parts?

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- Directed (and undirected) models are universal: can represent any probability distribution over a finite set of variables
- Algorithms developed for undirected models work for both.
- That does not mean that representations for undirected models can represent directed models.

Example

Weighted formulae about a social situation:

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If Π includes observations for all $\mathit{knows}(X, Y)$ and $\mathit{social}(Y)$:

$$P(\mathit{funFor}(X) \mid \Pi) = \mathit{sigmoid}(-5 + 10 n_T)$$

n_T is the number of individuals Y for which $\mathit{knows}(X, Y) \land \mathit{social}(Y)$ is *True* in Π.

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- Using wighted formulae to define conditional probabilities $\rightarrow$ relational logistic regression (RLR).
- Using wighted formulae to define distributiuons $\rightarrow$ Markov logic networks (MLNs).

Abstract Example

$\alpha_0 : q$
$\alpha_1 : q \wedge \neg r(x)$
$\alpha_2 : q \wedge r(x)$
$\alpha_3 : r(x)$

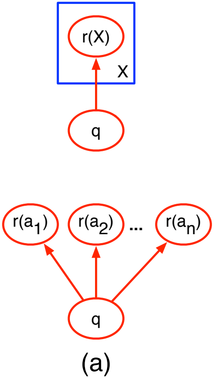
If $r(x)$ for every individual x is observed:

$$P(q \mid obs) = sigmoid(\alpha_0 + n_F\alpha_1 + n_T\alpha_2)$$

n_T is number of individuals for which $r(x)$ is true
n_F is number of individuals for which $r(x)$ is false

$$sigmoid(x) = \frac{1}{1 + e^{-x}}$$

Three Elementary Models



(a)

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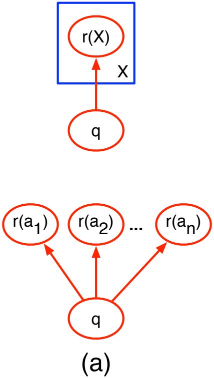

(a) Naïve Bayes
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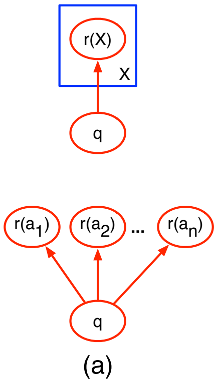

(a) Naïve Bayes
(b) (Relational) Logistic Regression
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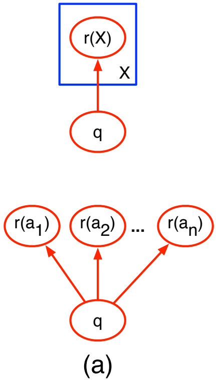

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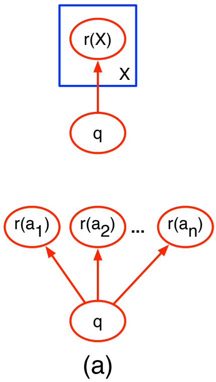

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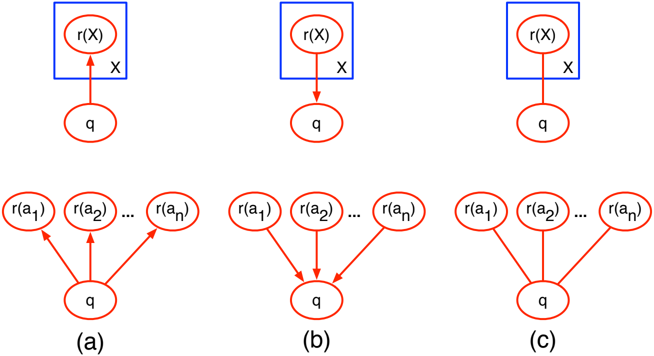
— They are identical models when all r's are observed.

Independence Assumptions



- Naïve Bayes (a) and Markov network (c): $r(a_i)$ and $r(a_j)$
  - are independent

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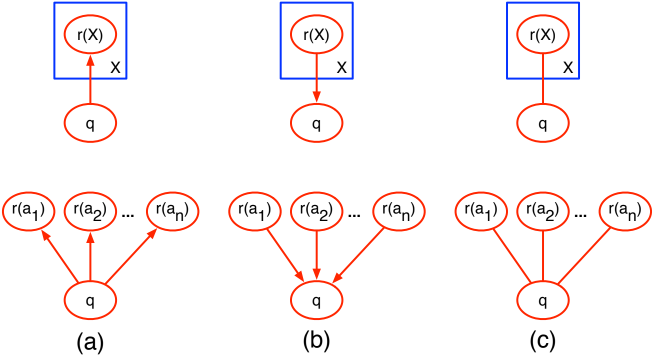

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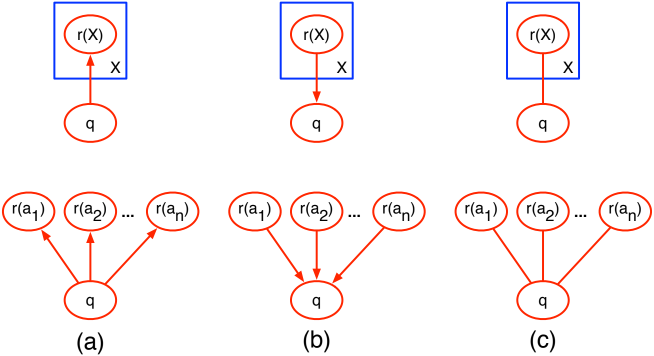

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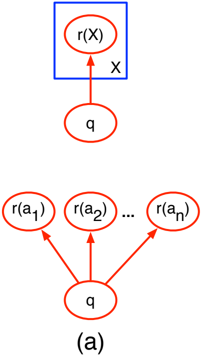

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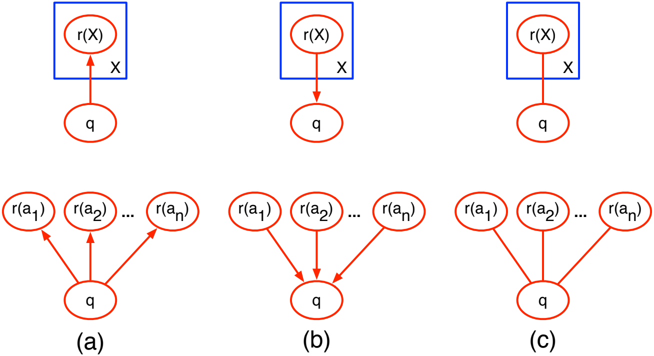

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Modularity

- Directed models are inherently modular.
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  - Why? requires factors on arbitrary subsets of $r(a_1) \dots r(a_k)$
    — pairwise (or 3-wise or ...) interactions are not adequate
    — can't marry the parents

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- MLN:

$$w : smokes(X) \leftarrow friends(X, Y) \land smokes(Y)$$

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  - ICL/Problog cannot represent negative effects: someone is less likely to smoke if their friends smoke (without there being a non-zero probability of logical inconsistency)

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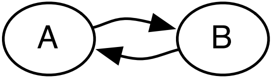
- (Relational) dependency networks: directed model,



  - $P(A, B)$ has 3 degrees of freedom,
  - $P(A \mid B), P(B \mid A)$, uses 4 numbers; typically inconsistent.
  - resulting distribution means stationary (equilibrium) distribution of Markov chain.

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- Which is better depends on the goals and how success is measured.
- Many of the methods try to do both; learn about specific individuals and general knowledge.

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- Tensor factorixation models — which learn vectors for individuals — tend to not learn generalized knowledge but about the particular individuals
- Lifted graphical models (MLNs, RLR, Problog) learn general knowledge through training weights (and structure) and specific knowledge through conditioning.
- Still open research problem

Outline

What happens as Population size n Changes: Simplest case

$\alpha_0 : q$
$\alpha_1 : q \wedge \neg r(x)$
$\alpha_2 : q \wedge r(x)$
$\alpha_3 : r(x)$

Weighted formulae define distribution:

$$P_{MLN}(q \mid n) = sigmoid(\ \alpha_0 + n \log(e^{\alpha_2} + e^{\alpha_1 - \alpha_3})\ )$$

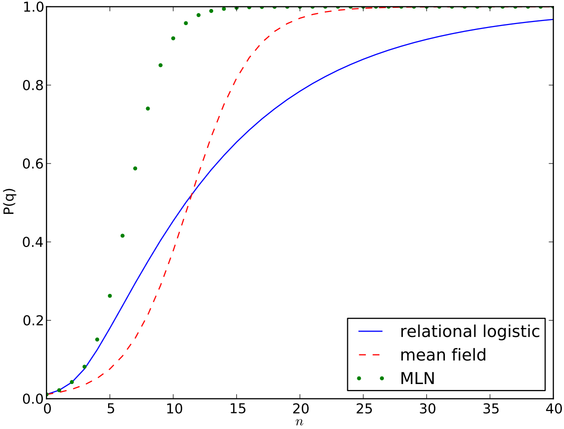
Weighted formulae define conditionals:

$$P_{RLR}(q \mid n) = \sum_{i=0}^{n} \binom{n}{i} sigmoid(\alpha_0 + i\alpha_1 + (n-i)\alpha_2)(1-p_r)^i p_r^{n-i}$$

Mean-field approximation:

$$P_{MF}(q \mid n) = sigmoid(\alpha_0 + np_r\alpha_1 + n(1-p_r)\alpha_2)$$

Population Growth: $P(q \mid n)$



All: $P(q \mid n) \rightarrow$ 0 or 1 as $n \rightarrow \infty$

Challenges of varying populations

- Example: The Movielens 100k dataset contains data about $rated(P, M, R, T)$ meaning person P gave movie M a rating of R at time T.
  Plus user demographic and movie information.
- Number of ratings per user is between 20 (arbitrary threshold) and 737; average of 106
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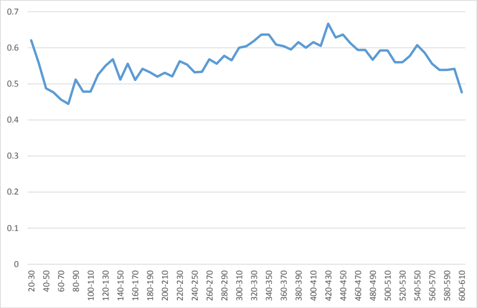
- Bigger datasets have even more variability.

Real Data



Observed $P(25 < Age(u) < 45 \mid n)$, where n is number of movies watched from the Movielens dataset.

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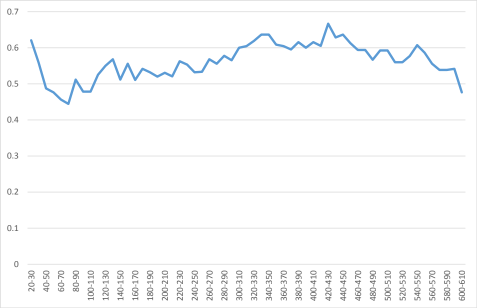

Observed $P(25 < Age(u) < 45 \mid n)$, where n is number of movies watched from the Movielens dataset.
Dont use:

$$w : middle\_age(U) \leftarrow rated(U, M) \wedge foo(M)$$

then $P(middle\_age(U)) \rightarrow$ 0 or 1 as number of movies increases.

Example of polynomial dependence of population

$\alpha_0 : q$

$\alpha_1 : q \wedge true(X)$

$\alpha_2 : q \wedge r(X)$

$\alpha_3 : true(X)$

$\alpha_4 : r(X)$

$\alpha_5 : q \wedge true(X) \wedge true(Y)$

$\alpha_6 : q \wedge r(X) \wedge true(Y)$

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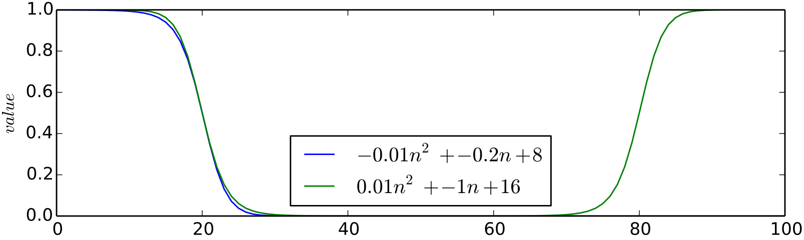
In RLR and in MLN, if all $r(a_i)$ are observed:

$$P(q \mid obs) = sigmoid(\alpha_0 + n\alpha_1 + n_1\alpha_2 + n^2\alpha_5 + n_1 n\alpha_6 + n_1^2\alpha_7)$$

$r(X)$ is true for n_1 individuals out of a population of n.

Danger of fitting to data without understanding the model

- RLR can fit sigmoid of any polynomial.
- Consider sigmoid of a polynomial of degree 2:



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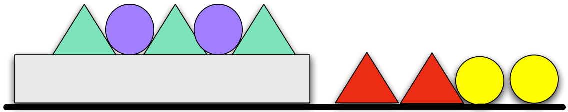
There are unboundedly many possible relations in a real-world object such as a house.

Observation Protocols

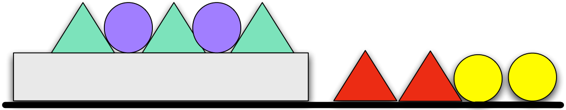


Observe a triangle and a circle touching. What is the probability the triangle is green?

$$P(green(x) \\ |triangle(x) \wedge \exists y \ circle(y) \wedge touching(x, y))$$

The answer depends on how the x and y were chosen!

Protocol for Observing



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$select(x)$	$select(y)$	$select(x, y)$
$select(y)$	$select(x)$	
$3/4$	$2/3$	$4/5$

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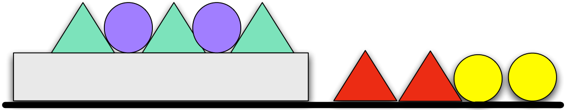

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A logical formula does not provide enough information to determine the probabilities.

Data

Real data is messy!

- Multiple levels of abstraction
- Multiple levels of detail
- Sometimes observations are abstract and lifted
  e.g., "3 people out of 300 in the audience asked a question".
- Uses the vocabulary from many ontologies
- Rich meta-data:
  - Who collected each datum? (identity and credentials)
  - Who transcribed the information?
  - What was the protocol used to collect the data? (Chosen at random or chosen because interesting?)
  - What were the controls — what was manipulated, when?
  - What sensors were used? What is their reliability and operating range?
  - What is the provenance of the data; what was done to it when?
- Errors, forgeries, . . .

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- Learn general knowledge as well as about particular individuals
- Use the meta-data of how data was collected
- Model protocol used to generate the observations
- Also model what is not observed (e.g., because it was redundant information, unimportant, false or unknown)

1. Representations: Problog & MLNs
2. Representation Issues
3. **(Exact) Lifted Inference**
4. Lifted Approximate Inference and Optimization
5. Learning
6. Applications

(Exact) Lifted Inference

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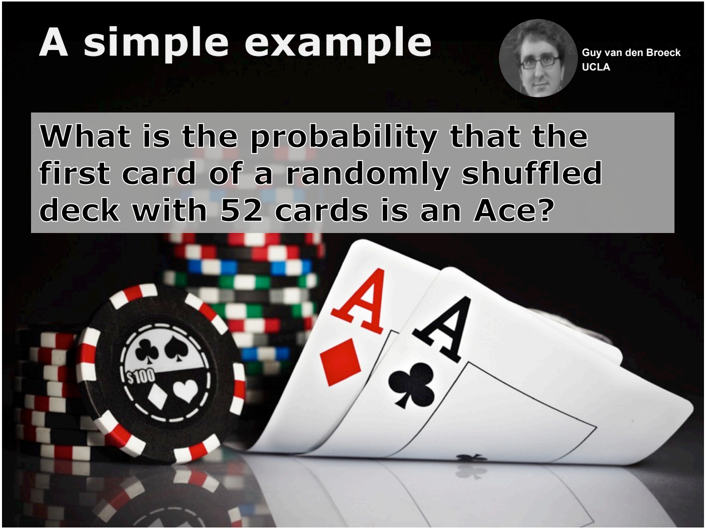
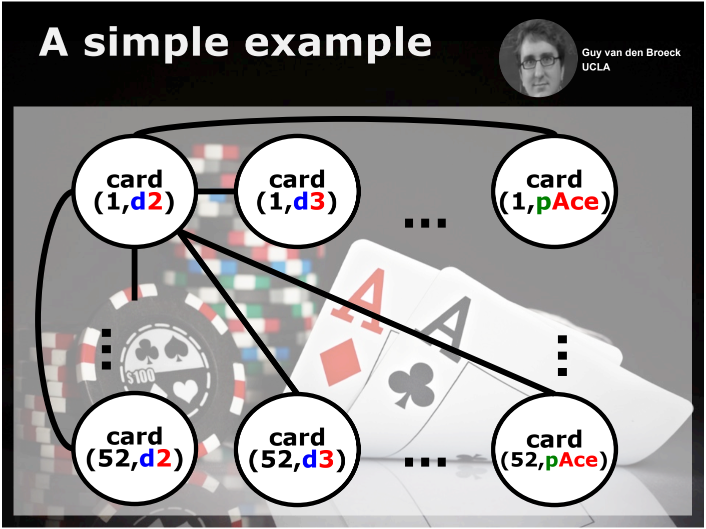
- Learning for inference
- Basis for efficient approximate inference:
    - Rao-Blackwellization
    - Variational Methods


A simple example
Guy van den Broeck
UCLA
What is the probability that the first card of a randomly shuffled deck with 52 cards is an Ace?
A
A
$100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card (1,d2)
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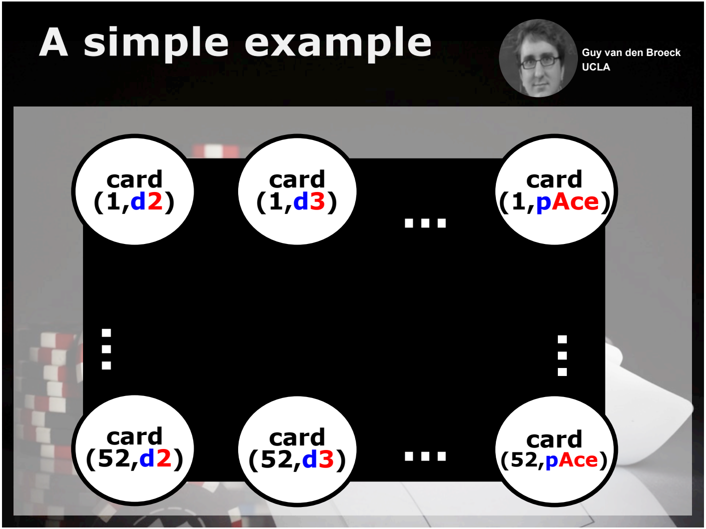
...
card (52,pAce)


A simple example
Guy van den Broeck
UCLA
card (1,d2)
card (1,d3)
...
card (1,pAce)
card (52,d2)
card (52,d3)
...
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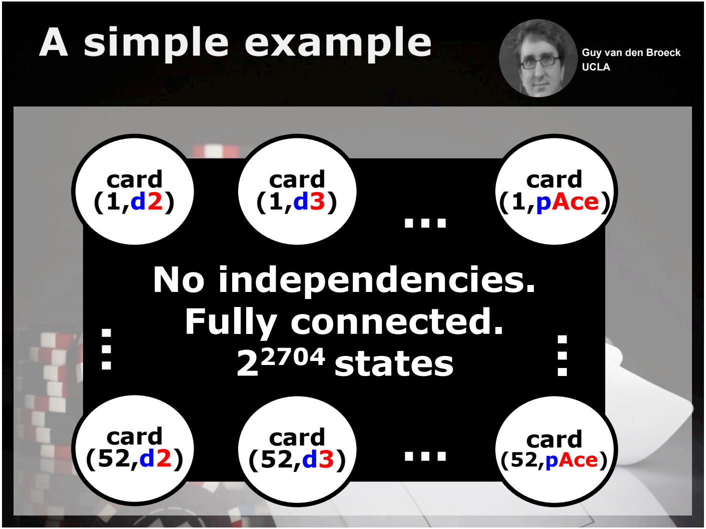
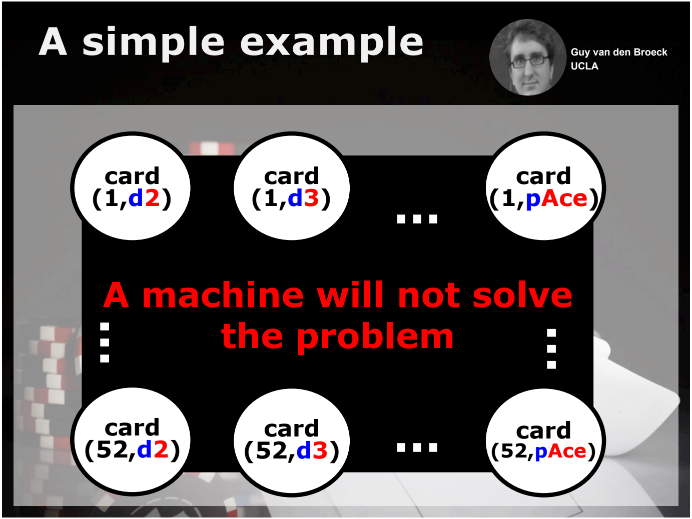
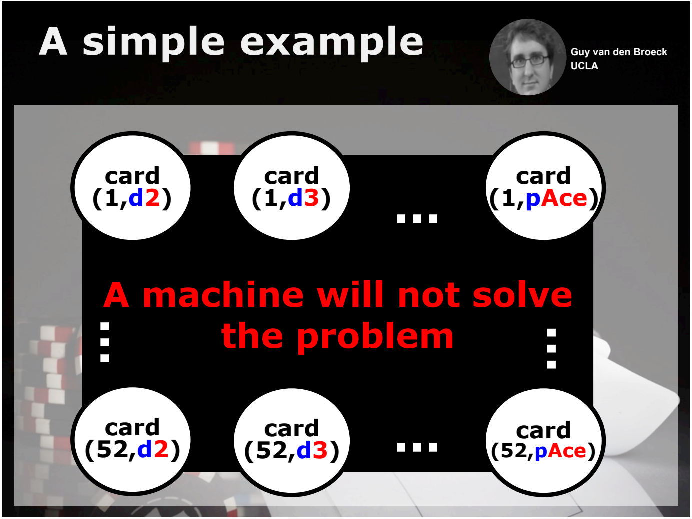

A simple example
Guy van den Broeck
UCLA
card (1,d2)
card (1,d3)
...
card (1,pAce)
No independencies.
Fully connected.
2^{2704} states
card (52,d2)
card (52,d3)
...
card (52,pAce)


A simple example
Guy van den Broeck
UCLA
card (1,d2)
card (1,d3)
...
card (1,pAce)
A machine will not solve the problem
card (52,d2)
card (52,d3)
...
card (52,pAce)



... unless it can represent and exploit symmetry.

Example: lifted inference

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- Suppose the probability of someone at random matching the description is one in a million.

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- We don't need to reason about all of the other individuals separately, but can count over them.

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- Suppose someone is giving a presentation, and three people out of 100 people in the audience asked a question (so 97 people were observed to not ask a question).
- A reasonable model about the eloquence of the speaker might depend on the questions asked
- each of the people who didn't ask a question, their silence might depend on the questions asked, but not on the questions not asked.
- Rather than reasoning separately about each person who was observed to not ask a question, it is reasonable to just count over them.

Example: lifted inference

- The spread of a malaria (or other diseases) may depend on the number of people and the number of mosquitoes.
- Individual mosquitoes are important in such a model, but we don't want to model each mosquito separately.

Lifted Inference

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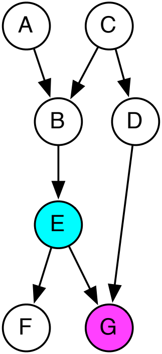
Lifted Inference

- Idea: treat those individuals about which you have the same information as a block; just count them.
- Use the ideas from lifted theorem proving - no need to ground.
- Potential to be exponentially faster in the number of non-differentialed individuals.
- Relies on knowing the number of individuals (the population size).

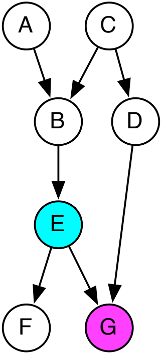
Outline

Inference via factorization in graphical models

$$P(E \mid g) = \frac{P(E \wedge g)}{\sum_E P(E \wedge g)}$$



Inference via factorization in graphical models



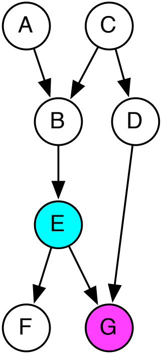
$$P(E \mid g) = \frac{P(E \wedge g)}{\sum_E P(E \wedge g)}$$

$$P(E \wedge g)$$

$$= \sum_F \sum_B \sum_C \sum_A \sum_D P(A)P(B \mid AC) P(C)P(D \mid C)P(E \mid B)P(F \mid E)P(g \mid ED)$$

$$=$$

Inference via factorization in graphical models



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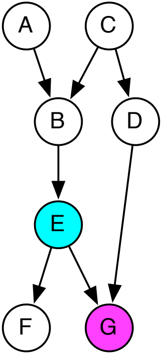
$$=$$

$$\left(\sum_D P(D \mid C)P(g \mid ED)\right)\Bigg)\Bigg)$$

Inference via factorization in graphical models



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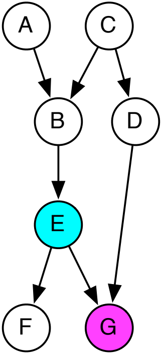
Inference via factorization in graphical models



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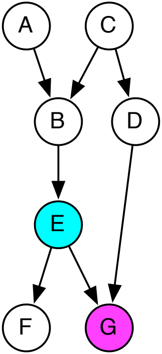
$$=$$

$$\sum_C \left(P(C) \left(\sum_A P(A)P(B \mid AC) \right) \left(\sum_D P(D \mid C)P(g \mid ED) \right) \right)$$

Inference via factorization in graphical models



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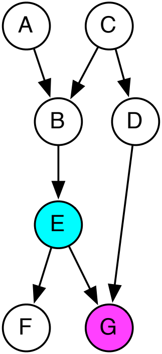

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$$\begin{aligned}
P(E \wedge g) & \\
&= \sum_F \sum_B \sum_C \sum_A \sum_D P(A)P(B \mid AC) \\
&\quad P(C)P(D \mid C)P(E \mid B)P(F \mid E)P(g \mid ED) \\
&= \left(\sum_F P(F \mid E)\right) \\
&\quad \sum_B P(E \mid B) \sum_C \left(P(C)\left(\sum_A P(A)P(B \mid AC)\right)\right. \\
&\quad \left.\left(\sum_D P(D \mid C)P(g \mid ED)\right)\right)
\end{aligned}$$

Recursive Conditioning

- Computes sum (partition function) from outside in

Input:

- Context - assignment of values to variables
- Set of factors

Output: value of summing out other variables (partition function)

- Evaluate a factor as soon as all its variables are assigned
- Cache values already computed
- Recognize disconnected components
- Recursively branch on a variable

Variable Elimination and Recursive Conditioning

- Variable elimination is the dynamic programming variant of recursive conditioning.
- Recursive Conditioning is the search variant of variable elimination
- They do the same additions and multiplications.
- Complexity $O(nr^t)$, for n variables, range size r, and treewidth t.

Outline

1. Knowledge Graphs
   - Tensor Factorization and Neural Network Models
2. Representation Issues
   - Desiderata
   - How do relational models relate to probabilistic graphical models
3. Unique properties of relational models
   - Learning general knowledge vs learning about a data set
   - Varying Populations
   - What can be observed?
4. Conclusions and Challenges
5. (Exact) Lifted Inference
   - Recursive Conditioning
   - Lifted Recursive Conditioning

Weighted Formula

A Weighted formula is a pair $\langle F, v \rangle$ where

- F a formula on parametrized random variables
- v number

Example:

$\langle X \neq Y \wedge likes(X, Y) \wedge rich(Y), 0.001 \rangle$
$\langle likes(X, X) \wedge rich(X), 0.7 \rangle$

...

Lifted Recursive Conditioning

LiftedRC(*Context*, *WeightedFormulas*)

- *Context* is a set of assignments to random variables and counts to assignments of instances of relations. e.g.:

$$\begin{aligned}\{\neg a,\ & \#_X f(X) \wedge g(X) = 7,\\ & \#_X f(X) \wedge \neg g(X) = 5,\\ & \#_X \neg f(X) \wedge g(X) = 18,\\ & \#_X \neg f(X) \wedge \neg g(X) = 0\}\end{aligned}$$

- *WeightedFormulas* is a set of weighted formulae, e.g.,

$$\begin{aligned}\{ & \langle \neg a \wedge \neg f(X) \wedge g(X), 0.1\rangle,\\ & \langle a \wedge \neg f(X) \wedge g(X), 0.2\rangle,\\ & \langle f(X) \wedge g(Y), 0.3\rangle,\\ & \langle f(X) \wedge h(X), 0.4\rangle\}\end{aligned}$$

Evaluating Weighted Formulae

Context:

$$\{\neg a, \quad \#_X f(X) \land g(X) = 7,$$
$$\#_X f(X) \land \neg g(X) = 5,$$
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WeightedFormulas:

$$\{ \quad \langle \neg a \land \neg f(X) \land g(X), 0.1\rangle\,,$$
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$$\langle f(X) \land g(Y), 0.3\rangle\,,$$
$$\langle f(X) \land h(X), 0.4\rangle\}$$

$LiftedRC(Context, WeightedFormulas)$ returns:

Evaluating Weighted Formulae

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$$0.1^{18} *$$

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LiftedRC(*Context*, *WeightedFormulas*) returns:

$$0.1^{18} * 1 *$$

Evaluating Weighted Formulae

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WeightedFormulas:

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$LiftedRC(Context, WeightedFormulas)$ returns:

$$0.1^{18} * 1 * 0.3^{12*}$$

Evaluating Weighted Formulae

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$LiftedRC(Context, WeightedFormulas)$ returns:

$$0.1^{18} * 1 * 0.3^{12*25} *$$

Evaluating Weighted Formulae

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$LiftedRC(Context, WeightedFormulas)$ returns:

$$0.1^{18} * 1 * 0.3^{12*25} * LiftedRC(Context, \{\langle f(X) \wedge h(X), 0.4 \rangle\})$$

Branching

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WeightedFormulas: $\{\langle f(X) \wedge h(X), 0.4\rangle, \dots\}$
Branching on H for the 7 "X" individuals s.th. $f(X) \wedge g(X)$:
$LiftedRC(Context, WeightedFormulas) =$

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Branching

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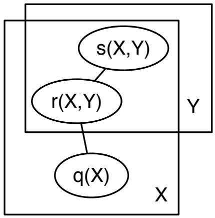
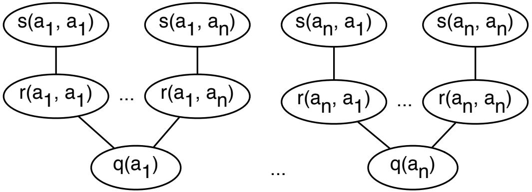
Recognizing Disconnectedness



Relational Model

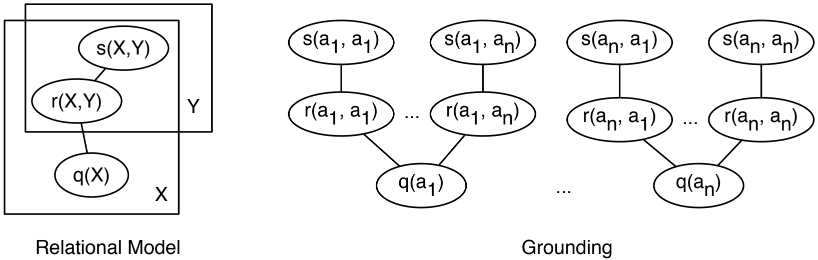


Grounding

Weighted formulae *WeightedFormulas*:

$$\{\ \langle\{s(X,Y)\wedge r(X,Y)\},t_1\rangle$$
$$\langle\{q(X)\wedge r(X,Y)\},t_2\rangle\}$$

Recognizing Disconnectedness



Weighted formulae *WeightedFormulas*:

$$\{\langle\{s(X,Y)\wedge r(X,Y)\}, t_1\rangle$$
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$$LiftedRC(Context, WeightedFormulas)$$
$$= LiftedRC(Context, WeightedFormulas\{X/c\})^n$$

...now we only have unary predicates

Observations and Queries

- Observations become the initial context.
  Observations can be ground or lifted.
-
$$P(q|obs) = \frac{LiftedRC(q \wedge obs, WFs)}{LiftedRC(q \wedge obs, WFs) + LiftedRC(\neg q \wedge obs, WFs)}$$

  calls can share the cache
- "How many?" queries are also allowed

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As the population size n of undifferentiated individuals increases:

- If grounding is polynomial — instances must be disconnected — lifted inference is constant in n (taking r^n for real r)

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- Otherwise, ground one individual from population, recurse. Sometimes this domain recursion is linear, but is typically exponential (as is grounding the population).

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- If non-unary relations become unary, above holds.
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Always exponentially faster than grounding everything.

What we can and cannot lift

We can lift a model that consists just of

$$\langle\{f(X) \land g(Z)\}, \alpha_4\rangle$$

What we can and cannot lift

We can lift a model that consists just of

$$\langle \{ f(X) \wedge g(Z) \}, \alpha_4 \rangle$$

or just of

$$\langle \{ f(X,Z) \wedge g(Y,Z) \}, \alpha_2 \rangle$$

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or just of

$$\langle\{f(X,Z) \wedge g(Y,Z)\}, \alpha_2\rangle$$

or just of

$$\langle\{f(X,Z) \wedge g(Y,Z) \wedge h(Y)\}, \alpha_3\rangle$$

What we can and cannot lift

We can lift a model that consists just of

$$\langle\{f(X) \land g(Z)\}, \alpha_4\rangle$$

or just of

$$\langle\{f(X,Z) \land g(Y,Z)\}, \alpha_2\rangle$$

or just of

$$\langle\{f(X,Z) \land g(Y,Z) \land h(Y)\}, \alpha_3\rangle$$

We cannot lift (still exponential) a model that consists just of:

$$\langle\{f(X,Z) \land g(Y,Z) \land h(Y,W)\}, \alpha_3\rangle$$

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or

$$\langle\{f(X,Z) \land g(Y,Z) \land h(Y,X)\}, \alpha_3\rangle$$

Compilation

- The computation reduces to products and sums
- The structure can be determined at compile time
- Orders of magnitude faster than lifted recursive conditioning
- Often abstracted as weighted model counting (WMC)

Take Home

- Lifted inference exploits symmetries ("for all")
- Instead of considering which individuals a predicate is true for, count how many individuals it is true for, and determine appropriate probabilities.
- Always exponentially better in the number of undifferentiated individuals than grounding everything.
- Open problem: finding a dichotomy of those problems we know we can lift and those we know it is impossible to lift.