Machine Learning (CS 181): 19. Inference in Graphical Models

David C. Parkes and Sasha Rush

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Contents

Contents

Overview

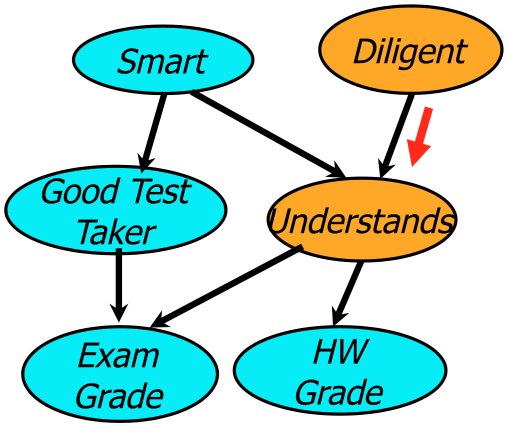
- We have seen how to construct (and learn) Bayesian Networks.
- What about reasoning patterns: which variables are conditionally independent?
- What about inference about latent variables:
  - Exact, via variable elimination and generalizations
  - Approximate, via MCMC (Gibbs sampling) and variational methods

Contents

Reasoning Patterns

(Note: assume for examples that a change in a parent has a positive effect; e.g., if GTT true then EG more likely to be better.)

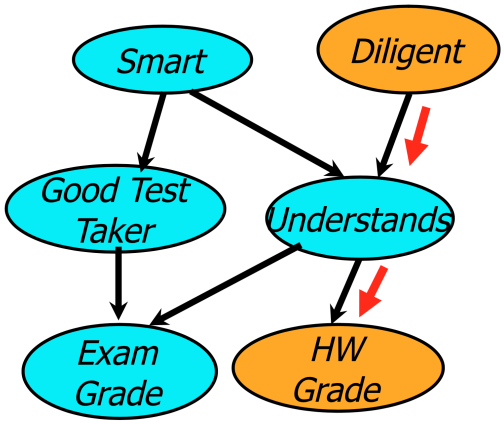
1. Causal. Observe Diligent is true. Does $p(U = true)$ go up, down, or neither?



Up. Not independent.

Reasoning Patterns

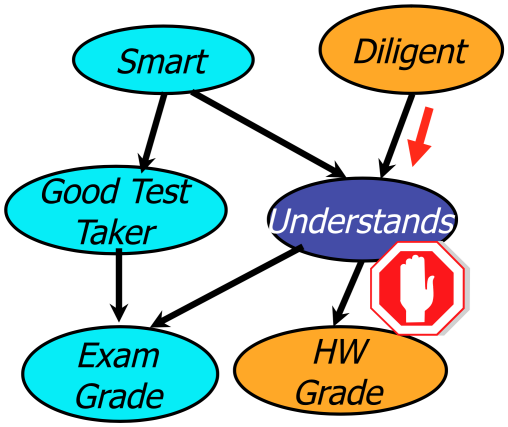
2. Chained causal. Observe Diligent is true. Does $p(HG = A)$ go up, down, or neither?



Up. Not independent.

Reasoning Patterns

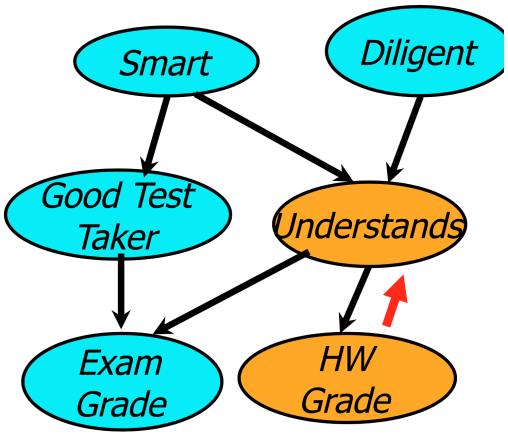
3. Chained causal. Know Understand is true. Now observe Diligent is true. Does $p(HG = A)$ go up, down, or neither?



Neither. $I(HWG, D \mid U)$.

Reasoning Patterns

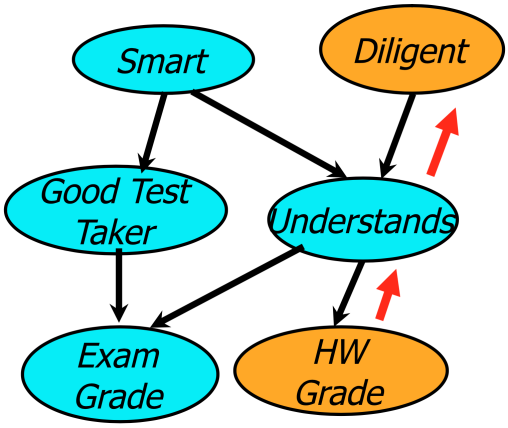
4. Evidential. Observe $HG = A$. Does $p(U = true)$ go up, down, or neither?



Up. Not independent.

Reasoning Patterns

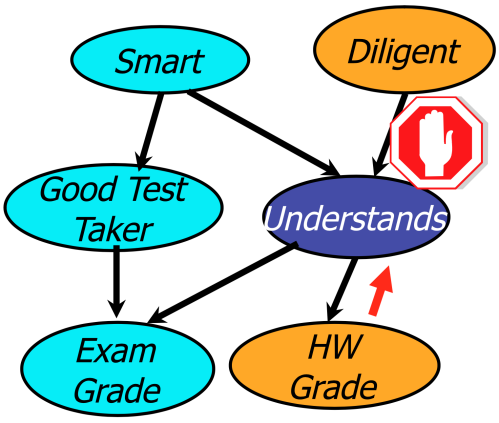
5. Chained evidential. Observe $HG = A$. Does $p(D = true)$ go up, down, or neither?



Up. Not independent.

Reasoning Patterns

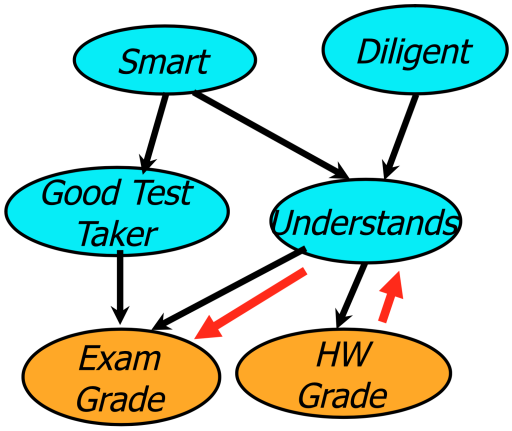
6. Chained evidential. Know that $U = true$. Observe $HG = A$. Does $p(D = true)$ go up, down, or neither?



Neither. $I(D, HWG \mid U)$.

Reasoning Patterns

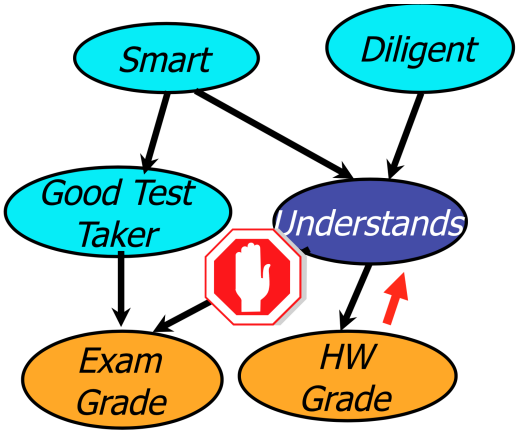
7. Mixed causal-evidential. Observe $HG = A$. Does $p(EG = A)$ go up, down, or neither?



Up. Not independent.

Reasoning Patterns

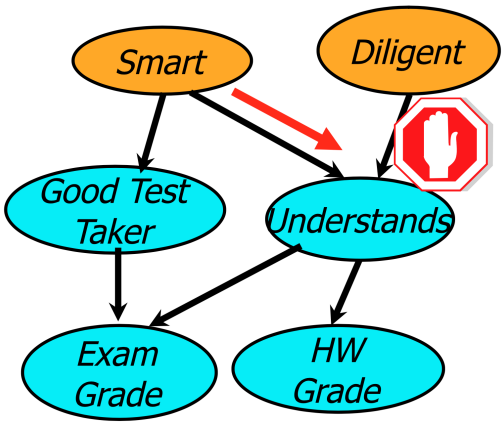
8. Mixed causal-evidential. We know $U = true$. Observe $HG = A$. Does $p(EG = A)$ go up, down, or neither?



Neither. $I(EG, HWG \mid U)$.

Reasoning Patterns

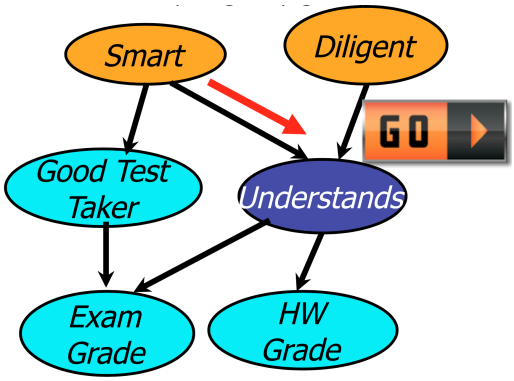
9. Inter-causal reasoning. We observe $S = true$. Does $p(D = true)$ go up, down, or neither?



Neither. Independent.

Reasoning Patterns

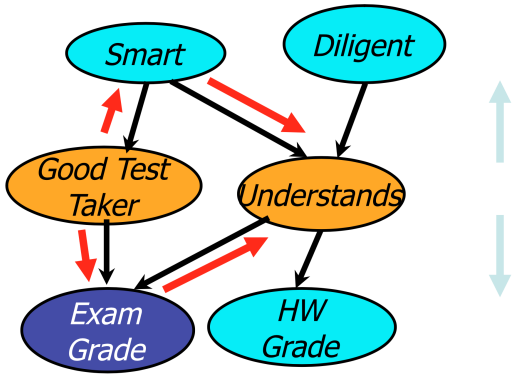
10. Inter-causal reasoning. We know that $U = true$. We observe $S = true$. Does $p(D = true)$ go up, down, or neither?



Down. not independent, conditioned on Understands!
(this is known as explaining away!)

Reasoning Patterns

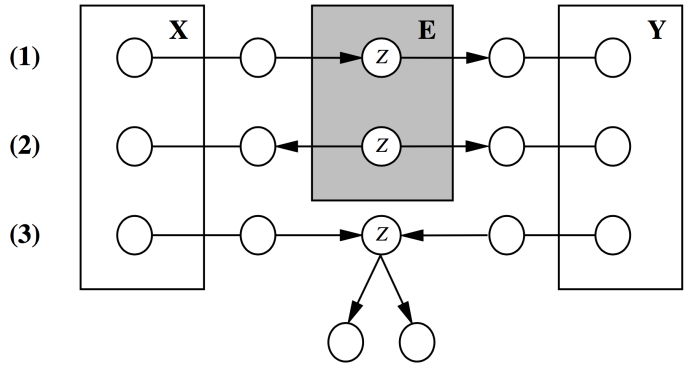
11. Conflicting pattern. We know $EG = A$. We observe $GTT = true$. Does $p(U = true)$ go up, down, or neither?



We don't know.

A Sufficient Test for Conditional Independence

One set of variables is conditionally independent of another set given evidence if every undirected path between the two sets is blocked.
Example, illustrating $I(X, Y \mid E)$:



P. Domingos

Paths (1) and (2) are blocked because Z has 'non-converging arrows' and Z is in the evidence. Path (3) is blocked because Z has 'converging arrows' and neither Z nor its descendants are in the evidence.

d-Separation

Definition (Directed separation)

X_A and X_B are d-separated by evidence X_E if every undirected path from a node in X_A to a node in X_B is blocked by X_E.

Definition (Blocked)

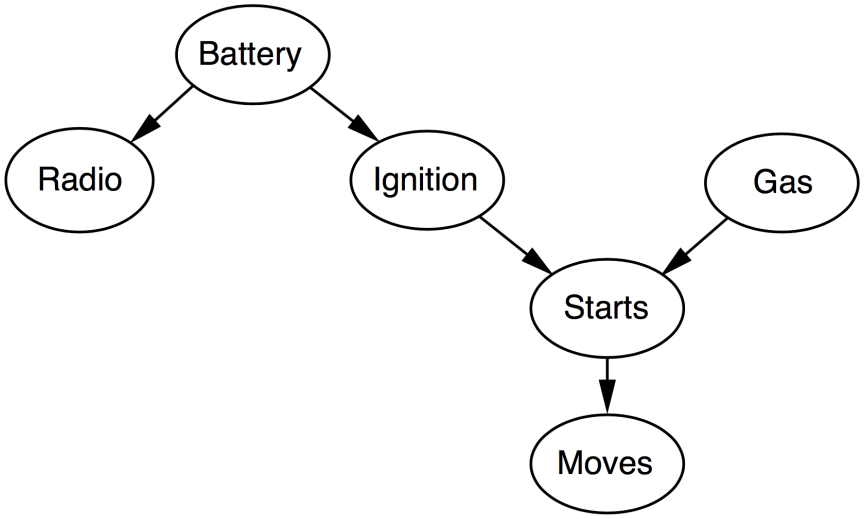
A path is blocked by evidence X_E if either:

- there is a node Z with 'non-converging arrows' on the path, and $Z \in X_E$, or
- there is a node Z with 'converging arrows' on the path, and neither Z nor its descendants are in X_E.

Theorem

If X_A and X_B are d-separated by X_E, then $I(X_A, X_B \mid X_E)$.

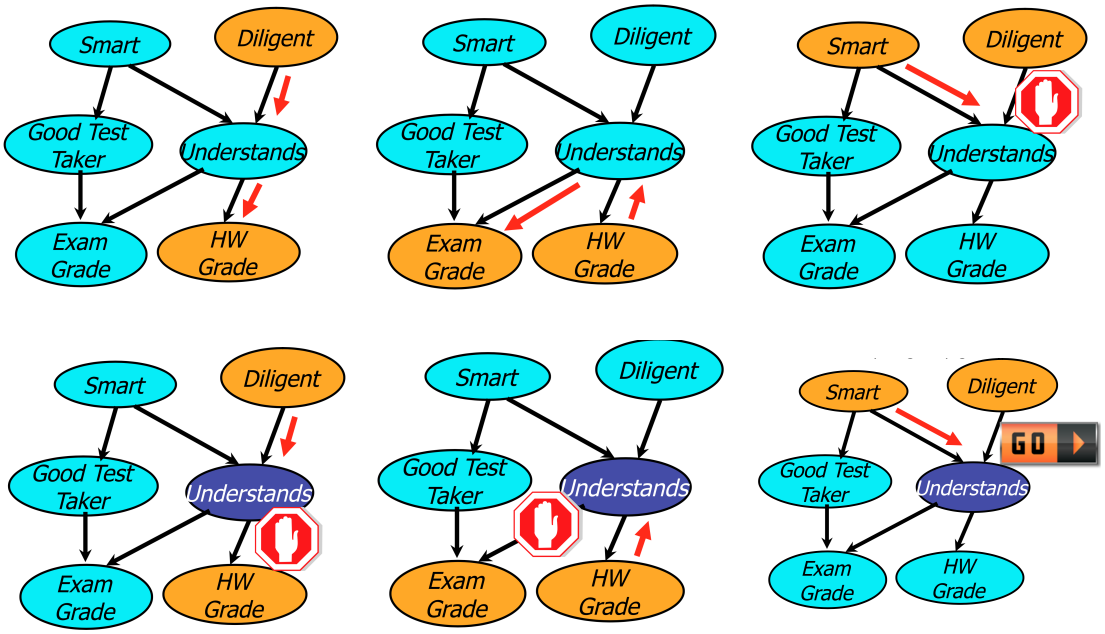
Example: Starting a Car



P. Domingos

Are Gas and Radio independent? Given Battery? Ignition? Starts? Moves?

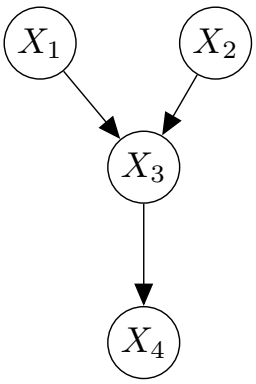
Checking d-separation on the Reasoning Patterns



(a) (b) (c)

Contents

Exact Inference (1 of 9)



Suppose we want to calculate the marginal probability:

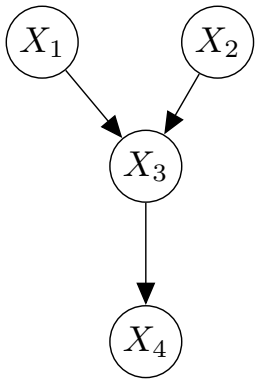
$$p(x_4) = \sum_{x_1,x_2,x_3} p(x_1)p(x_2)p(x_3 \mid x_1, x_2)p(x_4 \mid x_3)$$

Let $k =$ max domain size. This requires k^4 steps (k^3 steps for each x_4.)
Generally, with $m = \#$ variables, we have k^m steps.

Exact Inference (2 of 9)

Use variable elimination procedure, build intermediate g terms:

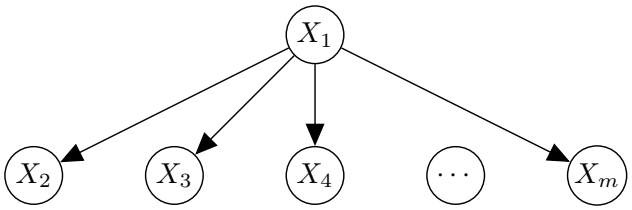
$$
\begin{aligned}
p(x_4) &= \sum_{x_1,x_2,x_3} p(x_1)p(x_2)p(x_3 \mid x_1, x_2)p(x_4 \mid x_3) \\
&= \sum_{x_2,x_3} p(x_2)p(x_4 \mid x_3) \underbrace{\sum_{x_1} p(x_1)p(x_3 \mid x_1, x_2)}_{g_1(x_2,x_3)} \\
&= \sum_{x_3} p(x_4 \mid x_3) \underbrace{\sum_{x_2} p(x_2)g_1(x_2, x_3)}_{g_2(x_3)} \\
&= \sum_{x_3} p(x_4 \mid x_3)g_2(x_3) = g_3(x_4)
\end{aligned}
$$



Now: $k^2(k) + k(k) + k(k)$ steps vs k^4 steps. Order here is x_1, x_2, x_3: leaves first, working towards query.

Exact Inference (3 of 9)

order of elimination matters



If eliminate x_1 first, get

$$p(x_m) = \sum_{x_2,\ldots,x_{m-1}} \sum_{x_1} p(x_1)p(x_2 \mid x_1) \ldots p(x_m \mid x_1) = \sum_{x_2,\ldots,x_{m-1}} g_1(x_2, \ldots, x_m)$$

With 'leaves-first' order $x_2, \ldots, x_{m-1}, x_1$, get

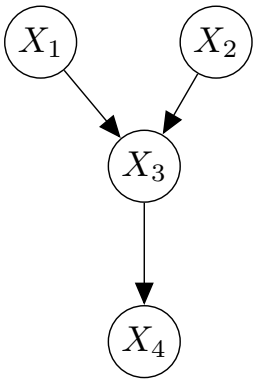
$$
\begin{aligned}
p(x_m) &= \sum_{x_3,\ldots,x_{m-1},x_1} p(x_1)p(x_3 \mid x_1) \ldots p(x_m \mid x_1) \underbrace{\sum_{x_2} p(x_2 \mid x_1)}_{g_1(x_1)} \\
&= \sum_{x_4,\ldots,x_{m-1},x_1} p(x_1) \ldots p(x_m \mid x_1) \underbrace{\sum_{x_3} p(x_3 \mid x_1)g_1(x_1)}_{g_2(x_1)} = \cdots
\end{aligned}
$$

This requires mk^2 steps vs k^m steps (!).

Exact Inference (4 of 9)

- Cost of variable elimination is exponential in the number of variables mentioned by the intermediate factors $g(\cdot)$.
- Example (g_1 mentions two variables):

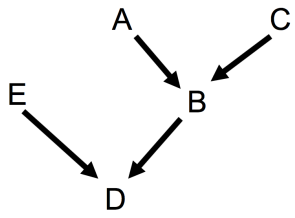
$$
\begin{aligned}
p(x_4) &= \sum_{x_1,x_2,x_3} p(x_1)p(x_2)p(x_3 \mid x_1, x_2)p(x_4 \mid x_3) \\
&= \sum_{x_2,x_3} p(x_2)p(x_4 \mid x_3) \underbrace{\sum_{x_1} p(x_1)p(x_3 \mid x_1, x_2)}_{g_1(x_2, x_3)}
\end{aligned}
$$



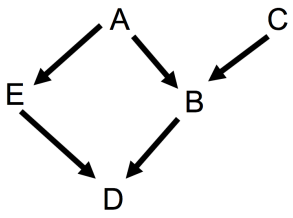
- The tree width of a BN is the minimum over all elimination orders of the largest number of mentions in intermediate factors.

Exact Inference (5 of 9)

Inference is easy for polytrees.



polytree



not polytree

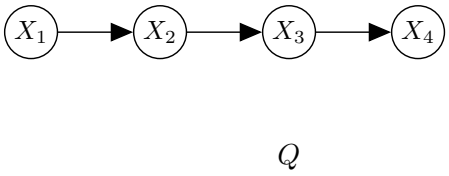
Let d = max # parents

Theorem

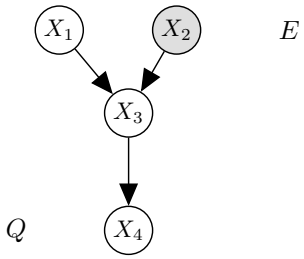
For Bayesian Networks that are polytrees ($\equiv$ no undirected cycles) then 'leaves first ordering' is optimal and gives $O(mk^{d+1})$ steps.

Linear in the size of the representation!

Exact Inference (6 of 9)



(a)



(b)

Additional observations:

(a) We can prune vars that are not ancestors to Q or E:

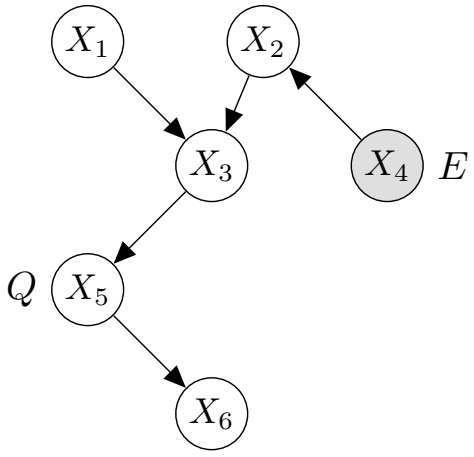
$$p(x_3) = \sum_{x_1,x_2,x_4} p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_2)p(x_4 \mid x_3)$$
$$= \sum_{x_1,x_2} p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_2) \underbrace{\sum_{x_4} p(x_4 \mid x_3)}_{=1}$$

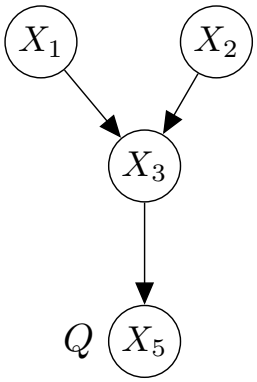
(b) For $p(x_Q \mid \mathbf{x}_E)$, we can instantiate the evidence $\mathbf{x}_E$ in the BN and then reduce the network.

Exact Inference (7 of 9)

General polytree inference procedure:

- Prune any non-ancestors of query or evidence variables
- Instantiate evidence variables
- Find leaves, and do variable elimination in order of leaves, working back towards the query





Exact Inference (8 of 9)

- Exact inference is #P-hard in general BNs.
  - #P problems are counting problems, e.g., number of subsets of lists of integers that add to zero.
  - Solving in poly time would imply $P = NP$.
- NP-hard to determine whether there exists an elimination order where no intermediate function mentions more than ℓ variables.
  - NP problems are decision problems for which 'yes'-instances are easy to verify, e.g., "is there a solution to a traveling salesperson problem with cost $\leq c$?" NP-hard are the hardest problems in NP.
  - Conjectured that P $\neq$ NP.
- Typical to use a greedy heuristic, select as next var to eliminate the one that generates a g function with as few vars as possible.

Exact Inference (9 of 9)

- Variable elimination is for computing the marginal probability of one variable, e.g. $p(x_4 \,|\, \mathbf{x}_E)$.
- What if we want to perform multiple inference tasks with the same evidence?
- Use the sum-product message passing algorithm on polytrees. This is a generalization of the 'forward-backward' algorithm. (Generalizes, via junction-tree algorithm to general networks.)

Contents

Approximate Inference (1 of 8)

Because exact inference on general BNs is #P-hard, it is also important to have methods of approximate inference.

Two common approaches:

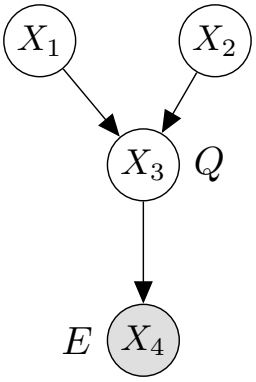
- Stochastic approximations via Markov Chain Monte Carlo methods.
- Variational methods.

We give a sketch of the ideas.

Approximate inference (2 of 8)

One idea: rejection sampling to estimate posterior, $p(\mathbf{x}_Q \mid \mathbf{x}_E)$:

- Sample $\mathbf{x}$ from the joint distribution $p(\mathbf{x})$ (recall: use top. order)
- Reject any sample where evidence $\mathbf{x}_E$ is not satisfied. Use other samples to estimate posterior.



Pro: very simple. Con: fraction of samples rejected grows exponentially as the size of E grows.

Approximate inference (3 of 8)

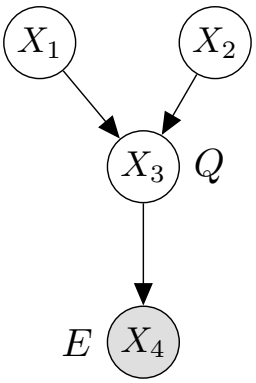
Markov chain Monte Carlo (MCMC) methods:

- An approach for generating samples from the posterior distribution
- Construct a Markov chain, where each state ($\mathbf{x}^{(t)}$ at step t) corresponds to an instantiation of the variables.
- Let $P^{(t)}$ denote the distribution on states after t steps. Idea is that $P^{(t)}$ will converge, for large t, to the posterior.
- The next state is sampled $q(\mathbf{x}^{(t+1)} \mid \mathbf{x}^{(t)})$. Define q such that:
  - stationary distr. of chain is equal to posterior
  - convergence is fast
  - q is tractable to sample from

Approximate inference (4 of 8)

Gibbs sampling is a useful MCMC method for BNs:

- Fix evidence variables throughout. Initialize rest of variables arbitrarily.
- Sample each of the non-evidence variables at random, sampling each variable given the current values of the other variables.



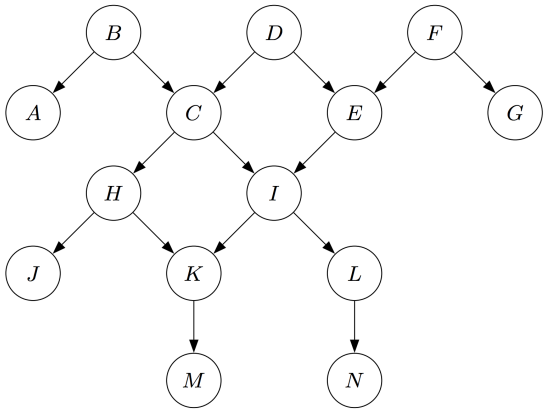
Need: $p(x_3 \mid x_1, x_2, x_3), p(x_2 \mid x_1, x_3, x_4), p(x_1 \mid x_2, x_3, x_4)$.

How can we compute these conditional distributions?

Approximate inference (5 of 8)

A: via the Markov blanket of a variable. This is the set of parents, children and childrens' parents.

Theorem: Each variable is conditionally independent of all others given its Markov blanket (via d-separation arguments.)



T. Nielsen and F. Verner Jensen

The Markov blanket of I is $\{C, E, H, K, L\}$. Leads to fast calculation of conditional distr. on any variable, given values of rest of variables.

Approximate inference (6 of 8)

Still, Gibbs sampling can be too slow for large BNs because the successive samples are highly correlated, and thus it can take a large number of samples to achieve an unbiased estimate of the posterior.

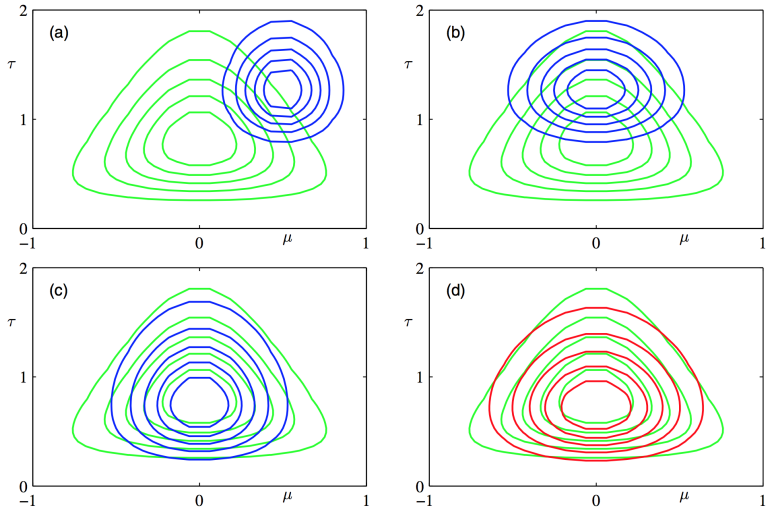
Approximate inference (7 of 8)

Leads to variational methods. Estimate posterior.

$$\min_{\mathbf{w}} ||p'(\mathbf{x}_Q; \mathbf{w}), p(\mathbf{x}_Q \mid \mathbf{x}_E)||$$

where p' is a simpler distribution, and for some measure of distance.

Choose family p' to allow for fast optimization, but close approximation.



Approximate inference (8 of 8)

Variational approximations are a very active area at the moment, and being coupled with probabilistic programming languages such as Stan.

Automatic Variational Inference in Stan

Alp Kucukelbir
Columbia University
alp@cs.columbia.edu

Rajesh Ranganath
Princeton University
rajeshr@cs.princeton.edu

Andrew Gelman
Columbia University
gelman@stat.columbia.edu

David M. Blei
Columbia University
david.blei@columbia.edu

Abstract

Variational inference is a scalable technique for approximate Bayesian inference. Deriving variational inference algorithms requires tedious model-specific calculations; this makes it difficult for non-experts to use. We propose an automatic variational inference algorithm, automatic differentiation variational inference (ADVI); we implement it in Stan (code available), a probabilistic programming system. In

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Conclusion

- Bayesian networks provide a compact representation of distributions on lots of variables.
- We can understand conditional independence via d-separation.
- For exact inference in polytrees, variable elimination is fast and effective.
- For approximate inference, both MCMC via Gibbs sampling and variational methods are in wide effect.