

IN FACULTY OF ENGINEERING

E016350 - Artificial Intelligence

Reasoning under Uncertainty & Bayesian ML Inference in Bayesian networks

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Overview

- What is probabilistic inference?
- Exact inference by enumeration
- Exact inference by variable elimination
- Belief propagation
- Approximate inference by stochastic simulation

[R&N], Chapter 13 (Sec 13.3; 13.4)

This presentation is partly based on: S. Russel and P. Norvig: *Artificial Intelligence: A Modern Approach*, Fourth Ed.), denoted as [R&N] and the resource page http://aima.cs.berkeley.edu/

Inference tasks

Denote
$$\begin{split} \mathbf{X} &= \{X_1, ..., X_n\} - \text{the complete set of variables} \\ X &- \text{the query variable} \\ \mathbf{E} &= \{E_1, ..., E_n\} - \text{the set of evidence variables} \\ \mathbf{e} &= \{e_1, ..., e_n\} - \text{ an observed event (assignment to evidence variables)} \\ \mathbf{Y} &= \{Y_1, ..., Y_n\} - \text{the non-evidence, non-query variables, called hidden variables, so that } \mathbf{X} &= \{X\} \cup \mathbf{E} \cup \mathbf{Y} \end{split}$$

A typical query asks for the posterior probability distribution $\mathbf{P}(X|\mathbf{e})$

This is an example of a simple inference task. $\mathbf{P}(X|\mathbf{e})$ is called posterior marginal (because it is posterior distribution of a subset of variables, in this particular case this subset is only one variable X).

Inference tasks, contd.

- Simple queries: compute posterior marginal $P(X_i | E = e)$ e.g., P(NoGas | Gauge = empty, Lights = on, Starts = false)
- Conjunctive queries: $\mathbf{P}(X_i, X_j | \mathbf{E} = \mathbf{e}) = \mathbf{P}(X_i | \mathbf{E} = \mathbf{e})\mathbf{P}(X_j | X_i, \mathbf{E} = \mathbf{e})$
- Optimal decisions: decision networks include utility information; probabilistic inference required for P(outcome|action, evidence)
- Value of information: which evidence to seek next?
- Sensitivity analysis: which probability values are most critical?
- Explanation: why do I need a new starter motor?

Inference by enumeration: Reminder 'Dentist' example

Consider the query: $\mathbf{P}(Cavity|toothache)$

	tool	thache	\neg toothache		
	$catch \neg catch$			catch	\neg catch
cavity	.108	.012		.072	.008
¬ cavity	.016	.064		.144	.576

Denominator can be viewed as a normalization constant $\boldsymbol{\alpha}$

 $\mathbf{P}(Cavity|toothache) = \alpha \, \mathbf{P}(Cavity, toothache)$

 $= \alpha \left[\mathbf{P}(Cavity, toothache, catch) + \mathbf{P}(Cavity, toothache, \neg catch) \right]$

$$= \alpha \left[\langle 0.108, 0.016 \rangle + \langle 0.012, 0.064 \rangle \right]$$

 $= \alpha \left< 0.12, 0.08 \right> = \left< 0.6, 0.4 \right>$

Conditional probabilities can be computed by summing terms from the joint distribution: $\mathbf{P}(X|\mathbf{e}) = \alpha \mathbf{P}(X, \mathbf{e}) = \alpha \sum_{u} \mathbf{P}(X, \mathbf{e}, \mathbf{y})$

Conditional probabilities can be computed by summing terms from the joint distribution: $\mathbf{P}(X|\mathbf{e}) = \alpha \mathbf{P}(X, \mathbf{e}) = \alpha \sum_{y} \mathbf{P}(X, \mathbf{e}, \mathbf{y})$

Example: simple query on the burglary network

$$\begin{aligned} \mathbf{P}(B|j,m) &= \mathbf{P}(B,j,m)/P(j,m) \\ &= \alpha \mathbf{P}(B,j,m) \\ &= \alpha \sum_{e} \sum_{a} \mathbf{P}(B,e,a,j,m) \end{aligned}$$



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Example: simple query on the burglary network

$$\mathbf{P}(B|j,m) = \mathbf{P}(B,j,m)/P(j,m)$$

= $\alpha \mathbf{P}(B,j,m)$
= $\alpha \sum_{e} \sum_{a} \mathbf{P}(B,e,a,j,m)$



Rewrite using the actual network structure and its CPT entries:

$$\begin{aligned} \mathbf{P}(B|j,m) \\ &= \alpha \sum_{e} \sum_{a} \mathbf{P}(B) P(e) \mathbf{P}(a|B,e) P(j|a) P(m|a) \\ &= \alpha \mathbf{P}(B) \sum_{e} P(e) \sum_{a} \mathbf{P}(a|B,e) P(j|a) P(m|a) \end{aligned}$$

Recursive depth-first enumeration: O(n) space, $O(d^n)$ time

```
function ENUMERATION-ASK(X, e, bn) returns a distribution over X
   inputs: X, the query variable
              e. observed values for variables E
              bn, a Bayesian network with variables \{X\} \cup \mathbf{E} \cup \mathbf{Y}
   \mathbf{Q}(X) \leftarrow a distribution over X, initially empty
   for each value x_i of X do
        extend e with value x_i for X
        \mathbf{Q}(x_i) \leftarrow \text{ENUMERATE-ALL}(\text{VARS}[bn], \mathbf{e})
   return NORMALIZE(\mathbf{Q}(X))
function ENUMERATE-ALL(vars, e) returns a real number
   if EMPTY?(vars) then return 1.0
   Y \leftarrow \text{FIRST}(vars)
   if Y has value y in e
        then return P(y \mid Pa(Y)) \times \text{ENUMERATE-ALL}(\text{Rest}(vars), e)
        else return \Sigma_y P(y \mid Pa(Y)) \times \text{ENUMERATE-ALL}(\text{Rest}(vars), \mathbf{e}_y)
              where \mathbf{e}_{y} is e extended with Y = y
```



Inefficient: repeated computations, e.g., computes P(j|a)P(m|a) for each value of e.

Inference by variable elimination

Idea: eliminate repeated calculations carry out summations right-to-left (bottom-up) storing intermediate results for later use

$$\mathbf{P}(B|j,m) = \alpha \underbrace{\mathbf{P}(B)}_{\mathbf{f}_1(B)} \sum_{e} \underbrace{P(e)}_{\mathbf{f}_2(E)} \sum_{a} \underbrace{\mathbf{P}(a|B,e)}_{\mathbf{f}_3(A,B,E)} \underbrace{P(j|a)}_{\mathbf{f}_4(A)} \underbrace{P(m|a)}_{\mathbf{f}_5(A)}$$

Here the factors are vectors like

$$\mathbf{f}_1(B) = \begin{bmatrix} P(b) \\ P(\neg b) \end{bmatrix} \text{ ; } \mathbf{f}_4(A) = \begin{bmatrix} P(j|a) \\ P(j|\neg a) \end{bmatrix} \text{ etc.}$$

so, we have

$$\mathbf{P}(B|j,m) = \alpha \mathbf{f}_1(B) \sum_e \mathbf{f}_2(E) \sum_a \mathbf{f}_3(A, B, E) \times \mathbf{f}_4(A) \times \mathbf{f}_5(A)$$

where \times is pointwise product

Inference by variable elimination, contd.

Now, compute from right to left

$$\mathbf{P}(B|j,m) = \alpha \mathbf{f}_1(B) \sum_{e} \mathbf{f}_2(E) \underbrace{\sum_{a} \mathbf{f}_3(A, B, E) \times \mathbf{f}_4(A) \times \mathbf{f}_5(A)}_{a}$$

Inference by variable elimination, contd.

Now, compute from right to left

 $\mathbf{P}(B|j,m) = \alpha \mathbf{f}_1(B) \sum_{e} \mathbf{f}_2(E) \sum_{a} \mathbf{f}_3(A, B, E) \times \mathbf{f}_4(A) \times \mathbf{f}_5(A)$ $\mathbf{f}_6(B,E)$ $\mathbf{f}_6(B, E) = \sum_a \mathbf{f}_3(A, B, E) \times \mathbf{f}_4(A) \times \mathbf{f}_5(A) = \\ = (\mathbf{f}_3(a, B, E) \times \mathbf{f}_4(a) \times \mathbf{f}_5(a)) + (\mathbf{f}_3(\neg a, B, E) \times \mathbf{f}_4(\neg a) \times \mathbf{f}_5(\neg a))$ $\mathbf{P}(B|j,m) = \alpha \mathbf{f}_1(B) \sum \mathbf{f}_2(E) \times \mathbf{f}_6(B,E)$

Inference by variable elimination, contd.

Now, compute from right to left

 $\mathbf{P}(B|j,m) = \alpha \mathbf{f}_1(B) \sum_e \mathbf{f}_2(E) \sum_a \mathbf{f}_3(A, B, E) \times \mathbf{f}_4(A) \times \mathbf{f}_5(A)$ $\mathbf{f}_6(B,E)$ $\mathbf{f}_6(B, E) = \sum_{a} \mathbf{f}_3(A, B, E) \times \mathbf{f}_4(A) \times \mathbf{f}_5(A) = \\ = (\mathbf{f}_3(a, B, E) \times \mathbf{f}_4(a) \times \mathbf{f}_5(a)) + (\mathbf{f}_3(\neg a, B, E) \times \mathbf{f}_4(\neg a) \times \mathbf{f}_5(\neg a))$ $\mathbf{P}(B|j,m) = \alpha \mathbf{f}_1(B) \sum \mathbf{f}_2(E) \times \mathbf{f}_6(B,E)$ $\mathbf{f}_7(B)$

 $\mathbf{P}(B|j,m) = \alpha \mathbf{f}_1(B)\mathbf{f}_7(B)$

Variable elimination: Basic operations

Pointwise product of factors \mathbf{f}_1 and \mathbf{f}_2 : $\mathbf{f}_1(x_1, \dots, x_j, y_1, \dots, y_k) \times \mathbf{f}_2(y_1, \dots, y_k, z_1, \dots, z_l)$ $= \mathbf{f}(x_1, \dots, x_j, y_1, \dots, y_k, z_1, \dots, z_l)$

E.g., $f_1(a, b) \times f_2(b, c) = f(a, b, c)$

Summing out a variable from a product of factors: move any constant factors outside the summation add up submatrices in pointwise product of remaining factors:

$$\sum_{x} \mathbf{f}_{1} \times \cdots \times \mathbf{f}_{k} = \mathbf{f}_{1} \times \cdots \times \mathbf{f}_{i} \underbrace{\sum_{x} \mathbf{f}_{i+1} \times \cdots \times \mathbf{f}_{k}}_{\mathbf{f}_{\overline{X}}} = \mathbf{f}_{1} \times \cdots \times \mathbf{f}_{i} \times \mathbf{f}_{\overline{X}} \times \mathbf{f}_{i}$$
assuming $\mathbf{f}_{1}, \ldots, \mathbf{f}_{i}$ do not depend on X .

Example: pointwise product of factors

The pointwise product of two factors f_1 and f_2 yields a new factor whose variables are the union of the variables in f_1 and f_2 and whose elements are given by the product of the corresponding elements in the two factors.

A	B	$\mathbf{f}_1(A,B)$	B	C	$\mathbf{f}_2(B,C)$	A	B	C	$\mathbf{f}_3(A,B,C)$
Т	Т	.3	Т	Т	.2	Т	Т	Т	$.3 \times .2 = .06$
Т	F	.7	Т	F	.8	Т	Т	F	$.3 \times .8 = .24$
F	Т	.9	F	Т	.6	Т	F	Т	$.7 \times .6 = .42$
F	F	.1	F	F	.4	Т	F	F	$.7 \times .4 = .28$
						F	Т	Т	.9 imes.2 = .18
						F	Т	F	$.9 \times .8 = .72$
						F	F	Т	$.1 \times .6 = .06$
						F	F	F	$.1\times.4{=}.04$
Figure 14.10 Illustrating pointwise multiplication: $\mathbf{f}_1(A, B) \times \mathbf{f}_2(B, C) = \mathbf{f}_3(A, B, C)$.									

Example: summing out a variable from a product of factors

A	В	$\mathbf{f}_1(A,B)$	B	C	$\mathbf{f}_2(B,C)$	A	B	C	$\mathbf{f}_3(A, B, C)$
Т	Т	.3	Т	Т	.2	Т	Т	Т	$.3 \times .2 = .06$
Т	F	.7	Т	F	.8	Т	Т	F	$.3 \times .8 = .24$
F	Т	.9	F	Т	.6	Т	F	Т	$.7 \times .6 = .42$
F	F	.1	F	F	.4	Т	F	F	$.7 \times .4 = .28$
						F	Т	Т	$.9 \times .2 = .18$
						F	Т	F	$.9 \times .8 = .72$
						F	F	Т	$.1 \times .6 = .06$
						F	F	F	$.1\times.4{=}.04$
Figure 14.10 Illustrating pointwise multiplication: $\mathbf{f}_1(A, B) \times \mathbf{f}_2(B, C) = \mathbf{f}_3(A, B, C)$.									

$$\mathbf{f}(B,C) = \sum_{a} \mathbf{f}_{3}(A,B,C) = \mathbf{f}_{3}(a,B,C) + \mathbf{f}_{3}(\neg a,B,C)$$
$$= \begin{bmatrix} 0.06 & 0.24\\ 0.42 & 0.28 \end{bmatrix} + \begin{bmatrix} 0.18 & 0.72\\ 0.06 & 0.04 \end{bmatrix} = \begin{bmatrix} 0.24 & 0.96\\ 0.48 & 0.32 \end{bmatrix}$$

Variable elimination algorithm

```
function ELIMINATION-Ask(X, e, bn) returns a distribution over X
   inputs: X, the query variable
             e, evidence specified as an event
             bn, a belief network specifying joint distribution \mathbf{P}(X_1, \ldots, X_n)
   factors \leftarrow []; vars \leftarrow ORDER (VARS[bn])
   for each var in vars do
        factors \leftarrow [MAKE-FACTOR(var, e)] factors]
        if var is a hidden variable then factors \leftarrow \text{SUM-OUT}(var, factors)
   return NORMALIZE(POINTWISE-PRODUCT(factors))
```

Think of variable ordering.

Variable relevance - Example



$$\mathbf{P}(J|b) = \alpha \sum_{e} \sum_{a} \sum_{m} P(J, b, e, a, m)$$

= $\alpha \sum_{e} \sum_{a} \sum_{m} P(b)P(e)P(a|b, e)P(J|a)P(m|a)$
= $\alpha P(b) \sum_{e} P(e) \sum_{a} P(a|b, e)P(J|a) \underbrace{\sum_{m} P(m|a)}_{1}$

So, there was no need to include m!

Every variable that is not an ancestor of a query variable or evidence variable is irrelevant to the query!

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Belief propagation

- Belief propagation algorithm was introduced by Judea Pearl, 1982
- Exact inference in networks without loops; time complexity linear in the number of nodes
- Became very popular after it was shown that the same computations are in turbo codes and the same principles in the Viterbi algorithm
- Main idea: inference by local **message passing** among neighboring nodes; The message can loosely be interpreted as "I (node *i*) think that you (node *j*) are that much likely to be in a given state".





Message passing revisited

Distributed soldier counting:



Distributed soldier counting with leader in line:



Do we need the leader for this process? Think of leaderless soldier counting.

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Belief propagation

Problem: express the probability of X given the set of old evidences $e_n = \{e_1 \dots e_n\}$ and a new piece of evidence e_{n+1}

Belief propagation

Problem: express the probability of X given the set of old evidences $e_n = \{e_1 \dots e_n\}$ and a new piece of evidence e_{n+1}

$$P(x|\mathbf{e}_n, e_{n+1}) = \frac{P(x, \mathbf{e}_n, e_{n+1})}{P(\mathbf{e}_n, e_{n+1})} = \frac{P(e_{n+1}|x, \mathbf{e}_n)P(x, \mathbf{e}_n)}{P(\mathbf{e}_n, e_{n+1})}$$
$$= \frac{P(e_{n+1}|x, \mathbf{e}_n)P(x|\mathbf{e}_n)P(\mathbf{e}_n)}{P(e_{n+1}|\mathbf{e}_n)P(\mathbf{e}_n)}$$
$$= \underbrace{P(e_{n+1}|\mathbf{e}_n)^{-1}}_{\alpha}P(e_{n+1}|x, \mathbf{e}_n)P(x|\mathbf{e}_n)$$

Belief propagation in chains



Note: we assumed here that all available evidence \mathbf{E} is split into \mathbf{E}^+ and \mathbf{E}^- , i.e., $\mathbf{E} = \mathbf{E}^+ \cup \mathbf{E}^-$, and \mathbf{e}^+ and \mathbf{e}^- are assignments to \mathbf{E}^+ and \mathbf{E}^- , respectively.

Belief propagation in chains, contd.

$$(e^+ \longrightarrow T \longrightarrow U \longrightarrow X \longrightarrow Y \longrightarrow Z \longrightarrow e^-$$

$$P(x|\mathbf{e}^+, \mathbf{e}^-) = \alpha \lambda(x) \pi(x)$$

$$\lambda(x) = P(\mathbf{e}^-|x), \ \pi(x) = P(x|\mathbf{e}^+)$$

Notice how $\pi(x)$ propagates down the chain:

$$\pi(x) = P(x|\mathbf{e}^+) = \sum_{u} \underbrace{P(x|u, \mathbf{e}^+)}_{P(x|u)} \underbrace{P(u|\mathbf{e}^+)}_{\pi(u)} = \sum_{u} P(x|u)\pi(u)$$

Belief propagation in chains, contd.

$$(e^+ \longrightarrow T \longrightarrow U) \longrightarrow (X) \longrightarrow (Y) \longrightarrow (Z) \longrightarrow (e^-)$$

 $P(x|\mathbf{e}^+,\mathbf{e}^-) = \alpha\lambda(x)\pi(x)$

$$\lambda(x) = P(\mathbf{e}^-|x), \ \pi(x) = P(x|\mathbf{e}^+)$$

Similarly, $\lambda(x)$ propagates in the other direction:

$$\lambda(x) = P(\mathbf{e}^{-}|x) = \sum_{y} \underbrace{P(\mathbf{e}^{-}|y,x)}_{P(\mathbf{e}^{-}|y) = \lambda(y)} P(y|x) = \sum_{y} \lambda(y) P(y|x)$$

Belief propagation in chains, contd.

$$\xrightarrow{\pi(t)}_{\lambda(t)} \underbrace{T}_{\lambda(u)}^{\pi(t)} \underbrace{U}_{\lambda(x)}^{\pi(u)} \underbrace{X}_{\lambda(y)}^{\pi(x)} \underbrace{Y}_{\lambda(z)}^{\pi(y)} \underbrace{Z}_{\lambda(z)}^{\pi(y)}$$

 $BEL(x) = P(x|\mathbf{e}) = P(x|\mathbf{e}^+, \mathbf{e}^-) = \alpha\lambda(x)\pi(x)$

 $\lambda(x) = P(\mathbf{e}^-|x), \ \pi(x) = P(x|\mathbf{e}^+)$

BEL(x) - belief accorded to proposition X = x by all evidence **e** so far received. $\pi(x)$ - causal or predictive support attributed to the assertion X = x by all non-descendants of X, mediated by X's parent. $\chi(x)$ - diagnostic or retrospective support that X = x receives from X's descendent

 $\lambda(x)$ – diagnostic or retrospective support that X = x receives from X's descendents.

Belief propagation in trees



- Let the query be $BEL(x) = P(x|\mathbf{e})$
- Divide e into e_X⁻ and e_X⁺. Suppose e_X⁻ is in the network rooted at X and e_X⁺ is in the rest of the network.
- Like with the chain, we can show $BEL(x) = P(x|\mathbf{e}) = \alpha\lambda(x)\pi(x)$, with $\lambda(x) = P(\mathbf{e}_X^{-}|x), \ \pi(x) = P(x|\mathbf{e}_X^{+});$ $\alpha = P(\mathbf{e}_X^{-}|\mathbf{e}_X^{+})^{-1}$

$$\lambda(x) = P(\mathbf{e}_X^-|x) = P(\mathbf{e}_Y^-, \mathbf{e}_Z^-|x) = P(\mathbf{e}_Y^-|x)P(\mathbf{e}_Z^-|x) = \underbrace{\lambda_Y(x)\lambda_Z(x)}_{\text{messages from children}}$$

$$\pi(x) = P(x|\mathbf{e}_X^+) = \sum_u P(x|\mathbf{e}_X^{\not\leftarrow}, u) P(u|\mathbf{e}_X^+) = \sum_u P(x|u)\pi_X(u)$$

message from the parent

Belief propagation in trees, contd.



• Belief updating

 $BEL(x) = P(x|\mathbf{e}) = \alpha\lambda(x)\pi(x)$ $\lambda(x) = \prod_{i} \lambda_{Y_{j}}(x)$ $\pi(x) = \sum_{u}^{j} P(x|u)\pi_{X}(u)$ $\alpha \text{ is const. such that } \sum_{i} BEL(x) = 1$

- Bottom-up propagation $\lambda_X(u) = \sum_x \lambda(x) P(x|u)$
- Top-down propagation $\pi_{Y_j}(x) = \alpha \pi(x) \prod_{k \neq j} \lambda_{Y_k}(x)$

For more details, see (optional):

Judea Pearl, *Probabilistic reasoning in intelligence Systems: Networks of Plausible Inference*, (2nd Edition, Section 4.2)

Belief propagation in trees, contd.



Inference by stochastic simulation

- Basic idea
 - Draw samples from a sampling distribution
 - Compute an approximate posterior probability
 - Show this converges to the true probability
- Different methods from this class:
 - Sampling from an empty network
 - ► Rejection sampling: reject samples disagreeing with evidence
 - Likelihood weighting: use evidence to weight samples
 - Markov chain Monte Carlo (MCMC): sample from a stochastic process whose stationary distribution is the true posterior
- Applicable to arbitrary network topologies and arbitrary combinations of discrete and continuous r.v.s
- Convergence can be very slow

Network separation

A **simple path** through a graph (or a **simple chain**) is a sequence of vertices and edges where no vertices (and hence no edges) are repeated.

In other words, a simple chain contains no loops.



The internal nodes of a simple path can be classified as:



We investigate (conditional) independence in three simple networks featuring these types of nodes. Let $a \perp b \mid c$ denote "a and b are conditionally independent given c"



$$P(a,b) = \sum_{c} P(a)P(c \mid a)P(b \mid c) = P(a)P(b \mid a)$$

$$\neq P(a)P(b) \implies a \not \perp b \mid \emptyset$$

(in this network a and b are in general **not** independent)

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Consider now evidence in *c*:



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Consider now evidence in c:

$$P(a,b | c) = \frac{P(a,b,c)}{P(c)} = \frac{P(a)P(c | a)P(b | c)}{P(c)} =$$

$$= P(a | c)P(b | c)$$

$$\Rightarrow a \perp b \mid c$$

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- We also say that the chain is blocked by the corresponding node.

Examples:





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Chain from X to Y is **NOT** blocked.



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Examples:

Chain from X to Y is **NOT** blocked.



Let's see the cases where nodes are connected with multiple chains

The nodes X and Y are **d-separated** by evidence $A = \{U, D\}$.



All the chains between X and Y are blocked

- Chain [X, U, D, Y] is blocked by the divergent node D
- Chain [X, L, V, Y] is blocked by the convergent node V

We use the same principle in larger networks

A, B and C are non-overlapping sets



The sets A and B are d-separated by C if each node in A is d-separated from each node in B by C

We denote this by: A **I** B | C

Collider

Here is an easy way to remember the (conditional) independence structure. A **collider** contains two or more incoming arrows along a chosen path.



If C has more than one incoming link, then $A \perp\!\!\!\perp B$ and $A \not\!\!\perp B \mid C$. In this case C is called collider.



If C has at most one incoming link, then $A \perp\!\!\!\perp B \mid C$ and $A \not\!\!\perp B$. In this case C is called non-collider.

Summary

- Probabilistic inference computes the posterior probability distribution for a set of query variables, given some observed event (i.e., some assignment of values to a set of evidence variables)
- Exact inference
 - Inference by enumeration is conceptually simple, but inefficient
 - Variable elimination smarter approach avoids recalculations
 - Belief propagation (exact on networks without loops)
- Approximate inference
 - Stochastic simulation
 - Can handle arbitrary combinations of discrete and continuous r.v.s
 - Convergence can be very slow
 - We will learn about this later in the context of general graphical models
- Use the network separation where possible!