

Artificial Intelligence

Probabilistic Inference

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Exact Inference in Bayesian Networks (AIMA 13.3)

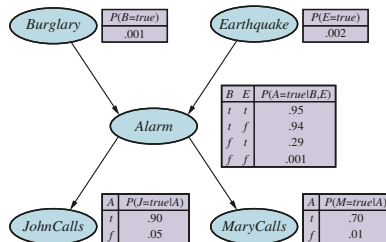
Most common task in probabilistic inference: compute the *posterior probability* of a set of **query variables** given some **event** represented as a set of **evidence variables**.

Notation:

- ▶ Query variable: X
- ▶ Set of evidence variables: $E = \{E_1, \dots, E_m\}$
- ▶ Particular observed event: e
- ▶ Hidden (nonevidence, nonquery) variables: $Y = \{Y_1, \dots, Y_l\}$
- ▶ Typical query: $Pr(X \mid e)$

Example:

- ▶ X is the boolean random variable *Burglary*
- ▶ $E = \{JohnCalls, MaryCalls\}$
- ▶ $e = \{JohnCalls = true, MaryCalls = true\}$
- ▶ $Y = \{EarthQuake, Alarm\}$



$$Pr(Buglary \mid JohnCalls = true, MaryCalls = true) = \langle 0.284, 0.716 \rangle .$$

Inference by Enumeration

Recall that we can use the full joint distribution to answer any query:

$$Pr(X|e) = \alpha Pr(X, e) = \alpha \sum_y Pr(X, e, \mathbf{y}) \quad (12.9)$$

And that a Bayes net completely represents the full joint distribution, so we can reduce the computation of a joint to:

$$Pr(x_1, \dots, x_n) = \prod_{i=1}^n Pr(x_i | parents(X_i)) \quad (13.2)$$

Using these two equations we can enumerate the appropriate probabilities to calculate the answer to any probabilistic query.

- In particular, we can get the answer by computing sums of products of conditional probabilities from a Bayes net.

Example: $Pr(\text{Burglary} \mid \text{JohnCalls} = \text{true}, \text{MaryCalls} = \text{true})$.

Using abbreviations and substituting into Eq 12.9 above (e and a are hidden):

$$Pr(B \mid j, m) = \alpha Pr(B, j, m) = \alpha \sum_e \sum_a Pr(B, j, m, e, a)$$

Then we substitute Eq 13.2 for $Pr(B, j, m, e, a)$ to get (only showing Burglary=true):

$$Pr(b \mid j, m) = \alpha \sum_e \sum_a Pr(b) Pr(e) Pr(a \mid b, e) Pr(j \mid a) Pr(m \mid a) \quad (1)$$

$$= \alpha Pr(b) \sum_e \sum_a Pr(e) Pr(a \mid b, e) Pr(j \mid a) Pr(m \mid a) \quad (2)$$

$$= \alpha Pr(b) \sum_e Pr(e) \sum_a Pr(a \mid b, e) Pr(j \mid a) Pr(m \mid a) \quad (3)$$

1. Substitute Eq 13.2 for $Pr(B, j, m, e, a)$
2. Pull out $Pr(b)$ from summations because it doesn't depend on the other variable and is thus a constant in all the summation terms.
3. Pull out $Pr(e)$ from the summation over the a values because each value of e doesn't depend on the other variables in the summation over the a values and is thus a constant in the summation terms over the values of a .

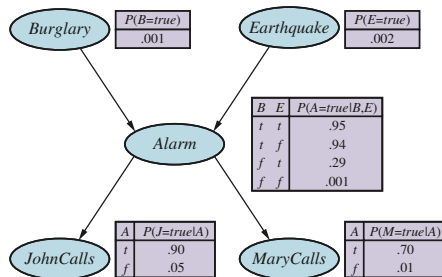
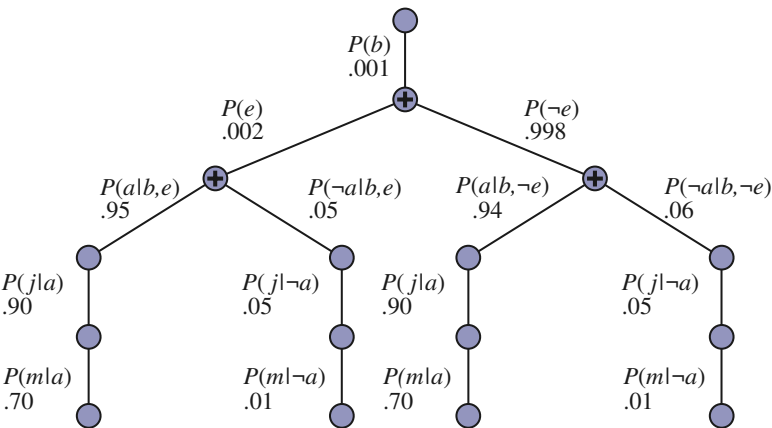
Steps 2 and 3 above reduce the complexity of the computation from $O(n2^n)$ to $O(2^n)$.

Calculation of $Pr(b | j, m)$

Substituting the values from the CPTs in the Bayes net into

$$\alpha Pr(b) \sum_e Pr(e) \sum_a Pr(a | b, e) Pr(j | a) Pr(m | a)$$

we get the expression tree:



Enumeration Algorithm

The ENUMERATION-ASK algorithm evaluates these expression trees using depth-first, left-to-right recursion.

function ENUMERATION-ASK(X, \mathbf{e}, bn) **returns** a distribution over X

inputs: X , the query variable

\mathbf{e} , observed values for variables \mathbf{E}

bn , a Bayes net with variables $vars$

$\mathbf{Q}(X) \leftarrow$ a distribution over X , initially empty

for each value x_i of X **do**

$\mathbf{Q}(x_i) \leftarrow$ ENUMERATE-ALL($vars, \mathbf{e}_{x_i}$)

where \mathbf{e}_{x_i} is \mathbf{e} extended with $X = x_i$

return NORMALIZE($\mathbf{Q}(X)$)

function ENUMERATE-ALL($vars, \mathbf{e}$) **returns** a real number

if EMPTY?($vars$) **then return** 1.0

$V \leftarrow$ FIRST($vars$)

if V is an evidence variable with value v in \mathbf{e}

then return $P(v | parents(V)) \times$ ENUMERATE-ALL(REST($vars$), \mathbf{e})

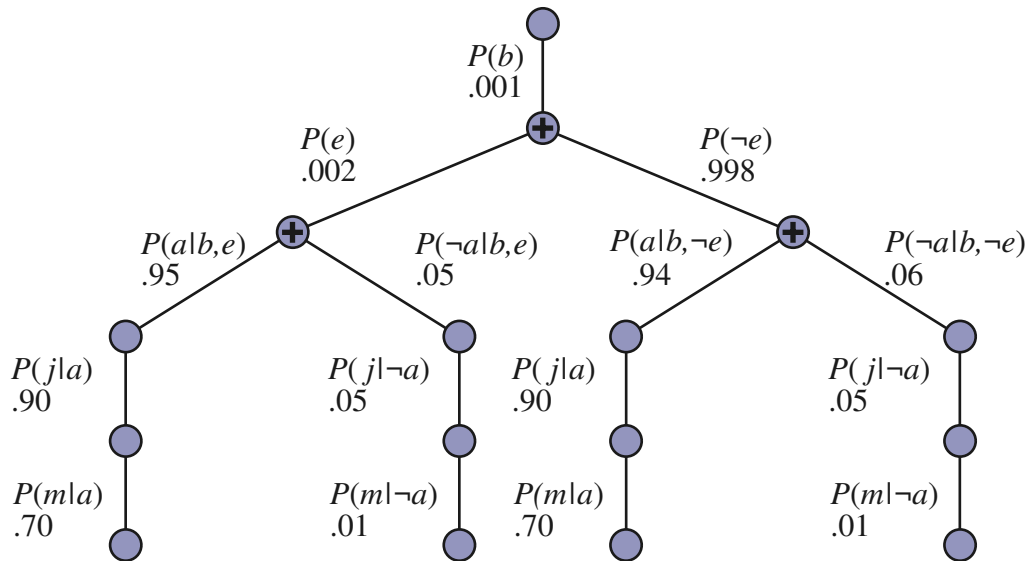
else return $\sum_v P(v | parents(V)) \times$ ENUMERATE-ALL(REST($vars$), \mathbf{e}_v)

where \mathbf{e}_v is \mathbf{e} extended with $V = v$

Unfortunately, its time complexity is $O(s^n)$. But we can improve it ...

Repeated Calculations

Notice that the subexpressions for the products $Pr(j | a)Pr(m | a)$ and $Pr(j | \neg a)Pr(m | \neg a)$ are computed twice, once for each value of E .



Variable Elimination

The enumeration algorithm can be improved substantially by eliminating repeated calculations.

- ▶ Idea: do the calculation once and save the results for later use.
- ▶ This is a form of dynamic programming.
- ▶ Several versions of this approach; variable elimination algorithm is simplest.

Variable elimination works by evaluating expressions such as

$$Pr(b \mid j, m) = \alpha Pr(b) \sum_e Pr(e) \sum_a Pr(a \mid b, e) Pr(j \mid a) Pr(m \mid a) \quad (13.5)$$

in right-to-left order (that is, bottom up in the expression tree), storing intermediate results, and only doing summations for portions of the expression that depend on the variable.

Example: Variable Elimination in Burglary Network

First, annotate the **factors** in the expression for the network:

$$Pr(B \mid j, m) = \alpha \underbrace{Pr(B)}_{f_1(B)} \sum_e \underbrace{Pr(e)}_{f_2(E)} \sum_a \underbrace{Pr(a \mid B, e)}_{f_3(A, B, E)} \underbrace{Pr(j \mid a)}_{f_4(A)} \underbrace{Pr(m \mid a)}_{f_5(A)}$$

- ▶ Each factor is a matrix indexed by the values of its argument variables.
- ▶ Notice that the factors for $Pr(j \mid a)$ and $Pr(m \mid a)$ do not include j and m . This is because the values of j and m (*JohnCalls* = *true* and *MaryCalls* = *true*) are fixed by the query.

So the factors are:

$$f_1(B) = \begin{bmatrix} Pr(b) \\ Pr(\neg b) \end{bmatrix} = \begin{bmatrix} 0.001 \\ 0.999 \end{bmatrix}$$

$$f_2(E) = \begin{bmatrix} Pr(e) \\ Pr(\neg e) \end{bmatrix} = \begin{bmatrix} 0.002 \\ 0.998 \end{bmatrix}$$

$$f_4(A) = \begin{bmatrix} Pr(j \mid a) \\ Pr(j \mid \neg a) \end{bmatrix} = \begin{bmatrix} 0.090 \\ 0.05 \end{bmatrix}$$

$$f_5(A) = \begin{bmatrix} Pr(m \mid a) \\ Pr(m \mid \neg a) \end{bmatrix} = \begin{bmatrix} 0.070 \\ 0.01 \end{bmatrix}$$

$f_3(A, B, E)$ is a little more complicated ...

$$f_3(A, B, E)$$

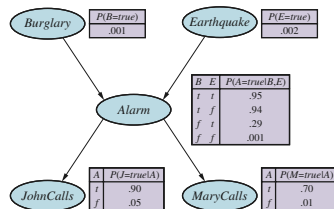
$$Pr(B | j, m) = \alpha \underbrace{Pr(B)}_{f_1(B)} \sum_e \underbrace{Pr(e)}_{f_2(E)} \sum_a \underbrace{Pr(a | B, e)}_{f_3(A, B, E)} \underbrace{Pr(j | a)}_{f_4(A)} \underbrace{Pr(m | a)}_{f_5(A)}$$

$f_3(A, B, E)$ is a $2 \times 2 \times 2$ matrix (or a rank-3 tensor). Here's one way to think about it:

- First index with A , yielding two 2×2 submatrices (one for each of the two values of A).
- Rows of each submatrix is indexed by B and columns by E .
- The entries in the submatrices are the values of $Pr(A | B, E)$

$$f_3^{(a)}(B, E) = \begin{bmatrix} Pr(a | b, e) & Pr(a | b, \neg e) \\ Pr(a | \neg b, e) & Pr(a | \neg b, \neg e) \end{bmatrix} = \begin{bmatrix} 0.95 & 0.94 \\ 0.29 & 0.001 \end{bmatrix}$$

$$f_3^{(\neg a)}(B, E) = \begin{bmatrix} Pr(\neg a | b, e) & Pr(\neg a | b, \neg e) \\ Pr(\neg a | \neg b, e) & Pr(\neg a | \neg b, \neg e) \end{bmatrix} = \begin{bmatrix} 0.05 & 0.06 \\ 0.71 & 0.999 \end{bmatrix}$$



Factorized Query

From our original query:

$$Pr(b \mid j, m) = \alpha Pr(b) \sum_e Pr(e) \sum_a Pr(a \mid b, e) Pr(j \mid a) Pr(m \mid a) \quad (13.5)$$

We annotated the factors:

$$Pr(B \mid j, m) = \alpha \underbrace{Pr(B)}_{f_1(B)} \sum_e \underbrace{Pr(e)}_{f_2(E)} \sum_a \underbrace{Pr(a \mid B, e)}_{f_3(A, B, E)} \underbrace{Pr(j \mid a)}_{f_4(A)} \underbrace{Pr(m \mid a)}_{f_5(A)}$$

And now we substitute the factor expressions for the original expressions so we can manipulate the factors using the **pointwise product** operation, denoted with \times here:

$$Pr(B \mid j, m) = \alpha f_1(B) \times \sum_e f_2(E) \times \sum_a f_3(A, B, E) \times f_4(A) \times f_5(A)$$

Now we are ready to evaluate the expression ...

Expression Evaluation

First, sum out A from the pointwise product of $f_3(A, B, E)$, $f_4(A)$, and $f_5(A)$ yielding a new 2×2 factor, $f_6(B, E)$:

$$\begin{aligned} f_6(B, E) &= \sum_a f_3(A, B, E) \times f_4(A) \times f_5(A) \\ &= (f_3(a, B, E) \times f_4(a) \times f_5(a)) + (f_3(\neg a, B, E) \times f_4(\neg a) \times f_5(\neg a)) \end{aligned}$$

Now the query expression is $Pr(B \mid j, m) = \alpha f_1(B) \times \sum_e f_2(E) \times f_6(B, E)$

Next, sum out E from the product of $f_2(E)$ and $f_6(B, E)$, yielding a new factor $f_7(B)$:

$$\begin{aligned} f_7(B) &= \sum_e f_2(E) \times f_6(B, E) \\ &= f_2(e) \times f_6(B, e) + f_2(\neg e) \times f_6(B, \neg e) \end{aligned}$$

Which leaves our final form of the query: $Pr(B \mid j, m) = \alpha f_1(B) \times f_7(B)$

This expression can be evaluated by taking the pointwise product and normalizing the result.

Operations on Factors

Two basic operations in variable elimination:

1. the pointwise product operation, and
2. summing out hidden variables from products of factors.

Pointwise Product Example

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

Given X, Y, Z boolean variables, result of pointwise product $f(X, Y) \times g(Y, Z) = h(X, Y, Z)$ is:

X	Y	$f(X, Y)$	Y	Z	$g(Y, Z)$	X	Y	Z	$h(X, Y, Z)$
t	t	.3	t	t	.2	t	t	t	$.3 \times .2 = .06$
t	f	.7	t	f	.8	t	t	f	$.3 \times .8 = .24$
f	t	.9	f	t	.6	t	f	t	$.7 \times .6 = .42$
f	f	.1	f	f	.4	t	f	f	$.7 \times .4 = .28$
						f	t	t	$.9 \times .2 = .18$
						f	t	f	$.9 \times .8 = .72$
						f	f	t	$.1 \times .6 = .06$
						f	f	f	$.1 \times .4 = .04$

Summing out Variables

Summing out a variable from a product of factors is done by adding up the submatrices formed by fixing the variable to each of its values in turn. For example, to sum out X from $h(X, Y, Z)$, we write

$$\begin{aligned}h_2(Y, Z) &= \sum_x h(X, Y, Z) \\&= h(x, Y, Z) + h(\neg x, Y, Z) \\&= \begin{bmatrix} .06 & .24 \\ .42 & .28 \end{bmatrix} + \begin{bmatrix} .18 & .72 \\ .06 & .04 \end{bmatrix} \\&= \begin{bmatrix} .24 & .96 \\ .48 & .32 \end{bmatrix}\end{aligned}$$

Variable Elimination Algorithm

With these two basic operations, we can implement the variable elimination algorithm:

function ELIMINATION-ASK(X, \mathbf{e}, bn) **returns** a distribution over X

inputs: X , the query variable

\mathbf{e} , observed values for variables \mathbf{E}

bn , a Bayesian network with variables $vars$

$factors \leftarrow []$

for each V **in** ORDER($vars$) **do**

$factors \leftarrow [\text{MAKE-FACTOR}(V, \mathbf{e})] + factors$

if V is a hidden variable **then** $factors \leftarrow \text{SUM-OUT}(V, factors)$

return NORMALIZE(POINTWISE-PRODUCT($factors$))

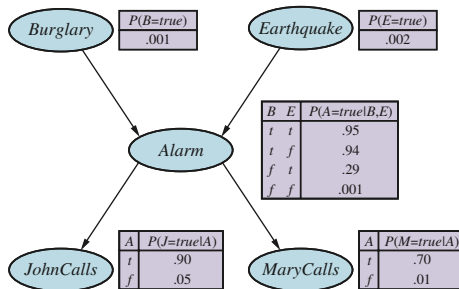
Notes about the `order` function:

- ▶ Any ordering works, some orderings lead to more efficient algorithms.
- ▶ No tractable algorithm for determining optimal ordering.
- ▶ One heuristic: eliminate whichever variable minimizes the size of the next factor to be constructed.
- ▶ General rule: every variable that is not an ancestor of a query variable or evidence variable is irrelevant to the query.

Complexity of Exact Inference in Polytrees

Notice that the Alarm Bayes net is **singly connected**, a.k.a., a **polytree**:

- ▶ there is at most one undirected path between any two nodes in the network.

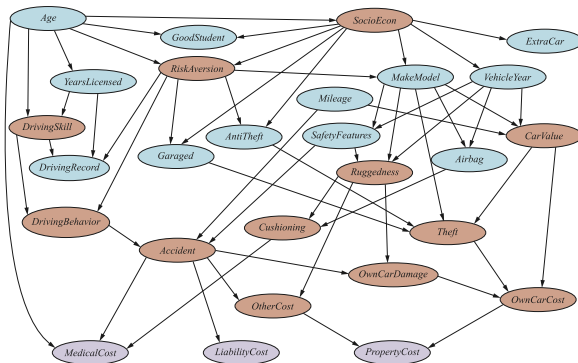


The time and space complexity of polytrees is linear in the size of the network.

- ▶ Size of network is defined as number of CPT entries.
- ▶ If $|parents(X_i)| \leq c, \forall i \in n$ for some constant c and number of nodes n , then complexity is also linear in number of nodes.

Complexity of Exact Inference in Multiply-connected Networks

Now consider **multiply-connected** networks such as the car insurance network:



- ▶ Variable elimination can have exponential worst-case time and space complexity in multiply-connected networks.
- ▶ *Since inference in Bayes nets includes inference in propositional logic as a special case, Bayes net inference is **NP-hard**.*

Approximate Inference for Bayesian Networks

Exact inference in large Bayesian networks is intractable, so we need approximate inference methods. The methods we'll learn are randomized sampling algorithms, a.k.a., **Monte Carlo** algorithms. They work by

- ▶ generating random events based on the probabilities in the Bayes net and
- ▶ counting up the different answers found in those random events.

The more the samples, the closer to the true probability distribution.

We'll learn two families of Monte carlo algorithms:

- ▶ direct sampling, and
- ▶ Markov chain sampling.

Direct Sampling Methods

The primitive element in any sampling algorithm is the generation of samples from a known probability distribution.

Feed a sample from $U(1, 1)$ to the inverse CDF of a distribution to sample the distribution.

Prior Sampling

To sample from a Bayes net with no associated evidence, sample each node in topological order.

- ▶ Sample unconditioned nodes according to their prior distributions.
 - ▶ Samples become fixed values for sampling CPTs of child nodes.
- ▶ Continue sampling child nodes, in order, until all variables are sampled.

function PRIOR-SAMPLE(*bn*) **returns** an event sampled from the prior specified by *bn*

inputs: *bn*, a Bayesian network specifying joint distribution $\mathbf{P}(X_1, \dots, X_n)$

$\mathbf{x} \leftarrow$ an event with n elements

for each variable X_i **in** X_1, \dots, X_n **do**

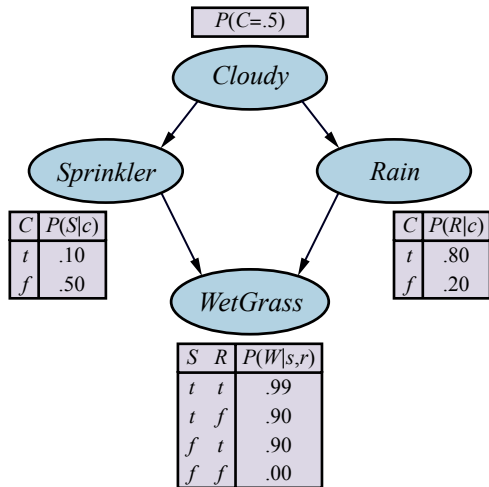
$\mathbf{x}[i] \leftarrow$ a random sample from $\mathbf{P}(X_i \mid \text{parents}(X_i))$

return \mathbf{x}

Example: Generating a Sample from Sprinkler Bayes Net

1. Sample from $Pr(Cloudy) = \langle 0.5, 0.5 \rangle$
 - ▶ Get value of true.
2. Sample from $Pr(Sprinkler | c) = \langle 0.1, 0.9 \rangle$
 - ▶ Get value of false.
3. Sample from $Pr(Rain | c) = \langle 0.8, 0.2 \rangle$
 - ▶ Get value of true.
4. Sample from $Pr(WetGrass | \neg s, r) = \langle 0.9, 0.1 \rangle$
 - ▶ Get value of true.

Full sampled event: $[true, false, true, true]$



From Sampling to Probability Estimates

A Bayes net represents a full joint distribution, so a sample generated from a Bayes net is a sample from the prior joint distribution over all the variables. So, if S_{PS} is a sample generated by the PRIOR-SAMPLE algorithm, then:

$$S_{PS}(x_1, \dots, x_n) = \prod_{i=1}^n Pr(x_i \mid \text{parents}(X_i)) = Pr(x_1, \dots, x_n)$$

To estimate these probabilities using samples, we simply generate N samples, count the number of events of interest among the N samples, and divide that number by N . This should converge to the true probability:

$$\lim_{N \rightarrow \infty} \frac{N_{PS}(x_1, \dots, x_n)}{N} = S_{PS}(x_1, \dots, x_n) = Pr(x_1, \dots, x_n)$$

From the CPTs in the Bayes net, the probability of the example event we sampled, $[true, false, true, true]$ is:

$$S_{PS}(true, false, true, true) = 0.5 \cdot 0.9 \cdot 0.8 \cdot 0.9 = 0.324.$$

So if we generated $N = 1000$ samples, we would expect to see $[true, false, true, true]$ 324 times.

Consistent Probability Estimates

An estimate that becomes exact in the large-sample limit is called **consistent**. A consistent estimate of the probability of any partially specified event x_1, \dots, x_m for $x \leq n$ is:

$$Pr(x_1, \dots, x_m) \approx \frac{N_{PS}(x_1, \dots, x_m)}{N} = \hat{Pr}(x_1, \dots, x_m)$$

That is, $\hat{Pr}(x_1, \dots, x_m)$ is an approximation of $Pr(x_1, \dots, x_m)$ that converges to the true probability as N approaches ∞

Rejection Sampling

function REJECTION-SAMPLING(X, \mathbf{e}, bn, N) **returns** an estimate of $\mathbf{P}(X | \mathbf{e})$

inputs: X , the query variable

\mathbf{e} , observed values for variables \mathbf{E}

bn , a Bayesian network

N , the total number of samples to be generated

local variables: \mathbf{C} , a vector of counts for each value of X , initially zero

for $j = 1$ **to** N **do**

$\mathbf{x} \leftarrow \text{PRIOR-SAMPLE}(bn)$

if \mathbf{x} is consistent with \mathbf{e} **then**

$\mathbf{C}[j] \leftarrow \mathbf{C}[j] + 1$ where x_j is the value of X in \mathbf{x}

return NORMALIZE(\mathbf{C})

Importance Sampling

The general statistical technique of **importance sampling** aims to emulate the effect of sampling from a distribution P^1 using samples from another distribution Q whose samples are easier to obtain.

We ensure that the answers are correct in the limit by applying a correction factor $\frac{P(\mathbf{x})}{Q(\mathbf{x})}$, also known as a **weight**, to each sample \mathbf{x} when counting up the samples.

Our query variable will always be one of the nonevidence variables, Z . The idea of importance sampling is to sample from $P(\mathbf{z} \mid \mathbf{e})$:

$$\hat{P}(\mathbf{z} \mid \mathbf{e}) = \frac{N_P(\mathbf{z})}{N} \approx P(\mathbf{z} \mid \mathbf{e})$$

but using an arbitrary distribution $Q(\mathbf{z})$:

$$\hat{P}(\mathbf{z} \mid \mathbf{e}) = \frac{N_Q(\mathbf{z})}{N} \frac{P(\mathbf{z} \mid \mathbf{e})}{Q(\mathbf{z})} \approx Q(\mathbf{z}) \frac{P(\mathbf{z} \mid \mathbf{e})}{Q(\mathbf{z})} = P(\mathbf{z} \mid \mathbf{e})$$

The question is: which Q to use? We want Q as close as possible to $P(\mathbf{z} \mid \mathbf{e})$ with $Q(\mathbf{z}) \neq 0$ whenever $P(\mathbf{z} \mid \mathbf{e}) \neq 0$. The most common approach is **likelihood weighting** ...

¹Using P instead of Pr to align with the book so we can distinguish probabilities under different distributions, e.g., P and Q .

Likelihood Weighting

Fix the values for the evidence variables \mathbf{E} and sample all the nonevidence variables in topological order, each conditioned on its parents – guarantees each sample consistent with evidence.

Let the sampling distribution be Q_{WS} and nonevidence variables be $\mathbf{Z} = \{Z_1, \dots, Z_l\}$. Then:

$$Q_{WS}(\mathbf{z}) = \prod_{i=1}^l P(z_i \mid \text{parents}(Z_i))$$

Now we need to know the weight for each sample. By general scheme for importance sampling:

$$w(\mathbf{z}) = \frac{P(\mathbf{z} \mid \mathbf{e})}{Q_{WS}(\mathbf{z})} = \alpha \frac{P(\mathbf{z}, \mathbf{e})}{Q_{WS}(\mathbf{z})}$$

where the normalizing factor $\alpha = \frac{1}{P(\mathbf{e})}$ is the same for all samples. Since \mathbf{z} and \mathbf{e} cover all the variables in the Bayes net, $P(\mathbf{z}, \mathbf{e})$ is the product of the conditional probabilities for the nonevidence variables times the product of the conditional probabilities for the evidence variables:

$$\begin{aligned} w(\mathbf{z}) &= \alpha \frac{P(\mathbf{z}, \mathbf{e})}{Q_{WS}(\mathbf{z})} = \alpha \frac{\prod_{i=1}^l P(z_i \mid \text{parents}(Z_i)) \prod_{i=1}^m P(e_i \mid \text{parents}(E_i))}{\prod_{i=1}^l P(z_i \mid \text{parents}(Z_i))} \\ &= \alpha \prod_{i=1}^m P(e_i \mid \text{parents}(E_i)) \end{aligned} \tag{14.9}$$

The name of this method comes from the fact that probabilities of evidence are generally called likelihoods.

Likelihood Weighting Algorithm

function LIKELIHOOD-WEIGHTING(X, \mathbf{e}, bn, N) **returns** an estimate of $\mathbf{P}(X | \mathbf{e})$

inputs: X , the query variable

\mathbf{e} , observed values for variables \mathbf{E}

bn , a Bayesian network specifying joint distribution $\mathbf{P}(X_1, \dots, X_n)$

N , the total number of samples to be generated

local variables: \mathbf{W} , a vector of weighted counts for each value of X , initially zero

for $j = 1$ **to** N **do**

$\mathbf{x}, w \leftarrow \text{WEIGHTED-SAMPLE}(bn, \mathbf{e})$

$\mathbf{W}[j] \leftarrow \mathbf{W}[j] + w$ where x_j is the value of X in \mathbf{x}

return NORMALIZE(\mathbf{W})

function WEIGHTED-SAMPLE(bn, \mathbf{e}) **returns** an event and a weight

$w \leftarrow 1$; $\mathbf{x} \leftarrow$ an event with n elements, with values fixed from \mathbf{e}

for $i = 1$ **to** n **do**

if X_i is an evidence variable with value x_{ij} in \mathbf{e}

then $w \leftarrow w \times P(X_i = x_{ij} | \text{parents}(X_i))$

else $\mathbf{x}[i] \leftarrow$ a random sample from $\mathbf{P}(X_i | \text{parents}(X_i))$

return \mathbf{x}, w

Likelihood Weighting Example

Given the query

► $Pr(Rain \mid Cloudy = true, WetGrass = true)$

and the ordering

► $Cloudy, Sprinkler, Rain, WetGrass$,

we initialize $w = 1.0$ and proceed as follows:

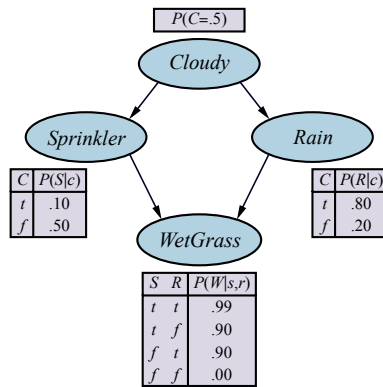
1. $Cloudy$ is an evidence variable with value true. Therefore, we set

$$w \leftarrow w \cdot Pr(c) = 0.5.$$

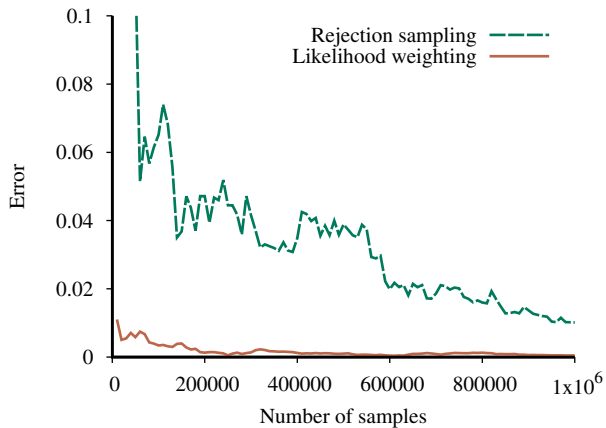
2. $Sprinkler$ is not an evidence variable, so sample from $Pr(Sprinkler \mid Cloudy = true) = \langle 0.1, 0.9 \rangle$; suppose this returns false.
3. $Rain$ is not an evidence variable, so sample from $Pr(Rain \mid Cloudy = true) = \langle 0.8, 0.2 \rangle$; suppose this returns true.
4. $WetGrass$ is an evidence variable with value true. Therefore, we set

$$w \leftarrow w \times Pr(WetGrass = true \mid \neg s, r) = 0.5 \cdot 0.9 = 0.45.$$

Here WEIGHTED-SAMPLE returns the event $[true, false, true, true]$ with weight 0.45, which we tally under $Rain = true$.



Rejection vs. Importance Sampling



Markov Chain Monte Carlo (MCMC) Algorithms

Instead of generating each sample from scratch, MCMC algorithms generate a sample by making a random change to the preceding sample.

Think of an MCMC algorithm as being in a particular current state that specifies a value for every variable and generating a next state by making random changes to the current state.

We'll learn two MCMC algorithms:

- ▶ Gibbs sampling, and
- ▶ Metropolis-Hastings

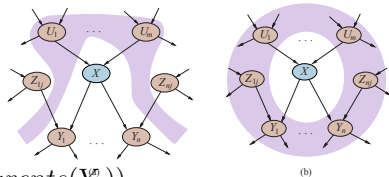
Gibbs Sampling and Markov Blankets



Gibbs Sampling

- Fix the evidence variables.
- Start in an arbitrary state sampled from the nonevidence variables.
 - Each X_i is sampled from the values in its Markov blanket, $mb(X_i)$

$$P(x_i \mid mb(X_i)) = \alpha P(x_i \mid parents(X_i)) \prod_{Y_j \in Children(X_i)} P(y_j \mid parents(Y_j)) \quad (13.10)$$



- Wander the state space randomly, keeping the evidence variables fixed and flipping one nonevidence variable by sampling from a distribution calculated Equation 14.10.

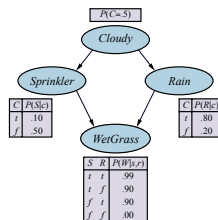
Gibbs sampling for X_i means sampling conditioned on the current values of the variables in its Markov blanket.

Gibbs Sampling Example: Step 1

Consider the query $P(\text{Rain} \mid \text{Sprinkler} = \text{true}, \text{WetGrass} = \text{true})$.

- Evidence variables *Sprinkler* and *WetGrass* fixed to observed values (true), nonevidence variables *Cloudy* and *Rain* initialized randomly to, say, true and false respectively.

- Initial state is $[\text{true}, \text{true}, \text{false}, \text{true}]$. Fixed evidence variables marked in bold.



Now the nonevidence variables Z_i are sampled repeatedly in some random order according to a probability distribution $\rho(i)$ for choosing variables. For example:

1. *Cloudy* is chosen and then sampled, given the current values of its Markov blanket: in this case, we sample from $P(\text{Cloudy} \mid \text{Sprinkler} = \text{true}, \text{Rain} = \text{false})$ whose distribution is calculated using Equation 13.10:

$$P(x_i \mid \text{mb}(X_i)) = \alpha P(x_i \mid \text{parents}(X_i)) \prod_{Y_j \in \text{Children}(X_i)} P(y_j \mid \text{parents}(Y_j)) \quad (13.10)$$

$$P(c \mid s, \neg r) = \alpha P(c) P(s \mid c) P(\neg r \mid c) = \alpha 0.5 \cdot 0.1 \cdot 0.2$$

$$P(\neg c \mid s, \neg r) = \alpha P(\neg c) P(s \mid \neg c) P(\neg r \mid \neg c) = \alpha 0.5 \cdot 0.5 \cdot 0.8$$

yielding $\alpha \langle 0.001, 0.020 \rangle \approx \langle 0.048, 0.952 \rangle$

- Suppose the result is *Cloudy* = false. Then the new current state is $[\text{false}, \text{true}, \text{false}, \text{true}]$.

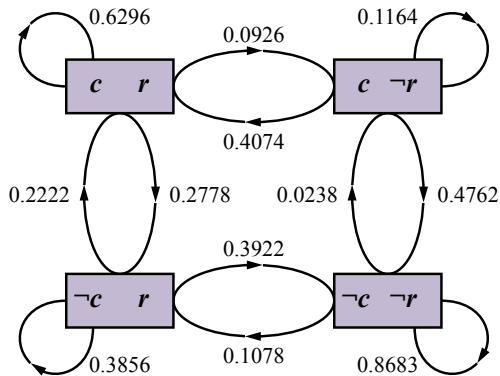
Gibbs Sampling Example: Step 2

2. Sampling $\rho(i)$ then chooses *Rain* as next variable. We sample from $P(\text{Rain} \mid \text{Cloudy} = \text{false}, \text{Sprinkler} = \text{true}, \text{WetGrass} = \text{true})$ using Equation 13.10 (just like Step 1, not shown here).

- Suppose this yields *Rain* = *true*. The new current state is [*false*, **true**, *true*, **true**].

Figure on the right shows the complete Markov chain for the case where variables are chosen uniformly, i.e., $\rho(\text{Cloudy}) = \rho(\text{Rain}) = 0.5$.

- The algorithm wanders around in this graph, following links with stated probabilities.
- Each state visited during this process is a sample that contributes to the estimate for the query variable *Rain*.
- If the process visits 20 states where *Rain* is true and 60 states where *Rain* is false, then the answer to the query is $\text{NORMALIZE}(\langle 20, 60 \rangle) = \langle 0.25, 0.75 \rangle$.



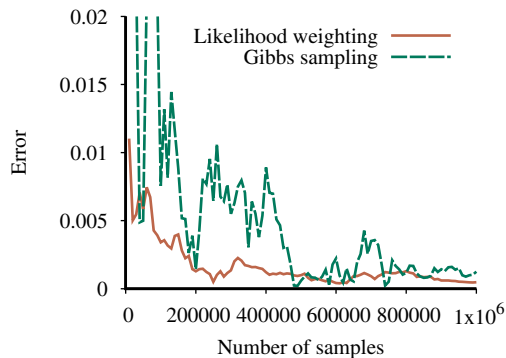
Gibbs Sampling Algorithm

function GIBBS-ASK(X, \mathbf{e}, bn, N) **returns** an estimate of $\mathbf{P}(X | \mathbf{e})$
 local variables: \mathbf{C} , a vector of counts for each value of X , initially zero
 \mathbf{Z} , the nonevidence variables in bn
 \mathbf{x} , the current state of the network, initialized from \mathbf{e}

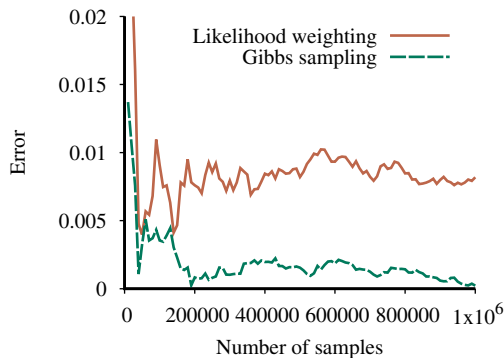
 initialize \mathbf{x} with random values for the variables in \mathbf{Z}
 for $k = 1$ **to** N **do**
 choose any variable Z_i from \mathbf{Z} according to any distribution $\rho(i)$
 set the value of Z_i in \mathbf{x} by sampling from $\mathbf{P}(Z_i | mb(Z_i))$
 $\mathbf{C}[j] \leftarrow \mathbf{C}[j] + 1$ where x_j is the value of X in \mathbf{x}
 return NORMALIZE(\mathbf{C})

Gibbs Sampling vs. Importance Sampling

Performance of Gibbs sampling compared to likelihood weighting on the car insurance network.



(a)

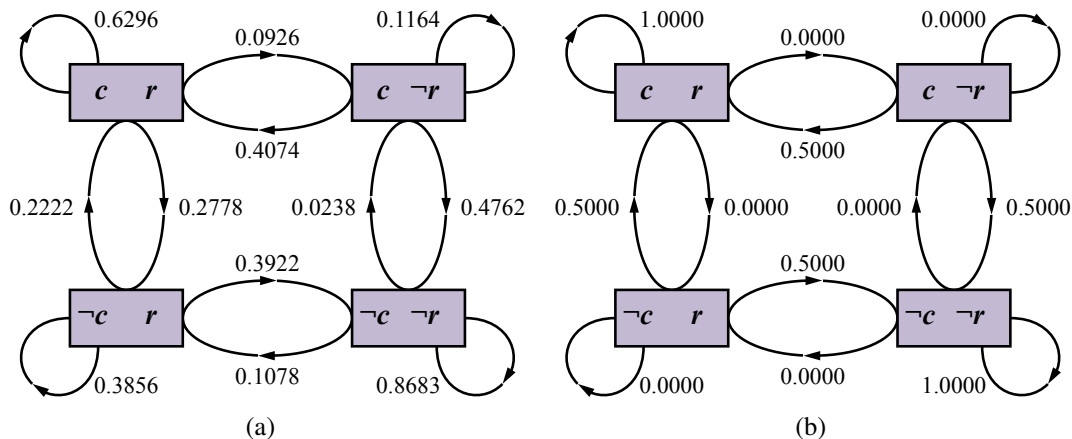


(b)

- ▶ (a) for the standard query on *PropertyCost*, and
- ▶ (b) for the case where the output variables are observed and *Age* is the query variable.

Gibbs sampling typically outperforms likelihood weighting when evidence is mostly downstream.

Markov Chains



- ▶ (a) The states and transition probabilities of the Markov chain for the query $P(Rain|Sprinkler = true, WetGrass = true)$. Note the self-loops: the state stays the same when either variable is chosen and then resamples the same value it already has.
- ▶ (b) The transition probabilities when the CPT for $Rain$ constrains it to have the same value as $Cloudy$.

Metropolis



Metropolis-Hastings Sampling

Like simulated annealing, MH has two stages in each iteration of the sampling process:

1. Sample a new state x' from a **proposal distribution** $q(x'|x)$, given the current state x .
2. Probabilistically accept or reject x' according to the **acceptance probability**

$$a(x'|x) = \min \left(1, \frac{\pi(x')q(x|x')}{\pi(x)q(x'|x)} \right)$$

If the proposal is rejected, the state remains at x .

$q(x'|x)$ could be defined as follows:

- ▶ With probability 0.95, perform a Gibbs sampling step to generate x' .
- ▶ Otherwise, generate x' by running WEIGHTED-SAMPLE using likelihood weighting.

This has the effect of getting MH “unstuck.”