Inference in belief networks

Chapter 15.3–4 + New

Outline

- \diamondsuit Exact inference by enumeration
- \diamond Exact inference by variable elimination
- \diamondsuit Approximate inference by stochastic simulation
- \diamondsuit Approximate inference by Markov chain Monte Carlo

Inference tasks

<u>Simple queries</u>: compute posterior marginal $\mathbf{P}(X_i | \mathbf{E} = \mathbf{e})$ e.g., P(NoGas | Gauge = empty, Lights = on, Starts = false)

<u>Conjunctive queries</u>: $\mathbf{P}(X_i, X_j | \mathbf{E} = \mathbf{e}) = \mathbf{P}(X_i | \mathbf{E} = \mathbf{e})\mathbf{P}(X_j | X_i, \mathbf{E} = \mathbf{e})$

<u>Optimal decisions</u>: decision networks include utility information; probabilistic inference required for P(outcome|action, evidence)

<u>Value of information</u>: 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

Slightly intelligent way to sum out variables from the joint without actually constructing its explicit representation

Simple query on the burglary network:

$$\mathbf{P}(B|J = true, M = true)$$

$$= \mathbf{P}(B, J = true, M = true) / P(J = true, M = true)$$

$$= \alpha \mathbf{P}(B, J = true, M = true)$$

$$= \alpha \Sigma_e \Sigma_a \mathbf{P}(B, e, a, J = true, M = true)$$

Rewrite full joint entries using product of CPT entries: P(B = true | J = true, M = true) $= \alpha \sum_{e} \sum_{a} P(B = true) P(e) P(a | B = true, e) P(J = true | a) P(M = true | a)$ $= \alpha P(B = true) \sum_{e} P(e) \sum_{a} P(a | B = true, e) P(J = true | a) P(M = true | a)$

Enumeration algorithm

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

```
ENUMERATIONASK(X, \mathbf{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)
    \mathbf{Q}(x) \leftarrow a distribution over X
   for each value x_i of X do
         extend e with value x_i for X
         \mathbf{Q}(x_i) \leftarrow \text{ENUMERATEALL}(\text{VARS}[bn], \mathbf{e})
   return NORMALIZE(\mathbf{Q}(X))
ENUMERATEALL(vars, e) returns a real number
   if EMPTY?(vars) then return 1.0
   else do
          Y \leftarrow \text{FIRST}(vars)
         if Y has value y in e
               then return P(y \mid Pa(Y)) \times \text{ENUMERATEALL}(\text{Rest}(vars), \mathbf{e})
               else return \sum_{y} P(y \mid Pa(Y)) \times \text{ENUMERATEALL}(\text{Rest}(vars), \mathbf{e}_{y})
                     where \mathbf{e}_{y} is \mathbf{e} extended with Y = y
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Inference by variable elimination

Enumeration is inefficient: repeated computation e.g., computes P(J = true|a)P(M = true|a) for each value of e

Variable elimination: carry out summations right-to-left, storing intermediate results (<u>factors</u>) to avoid recomputation

$$\begin{split} \mathbf{P}(B|J = true, M = true) \\ &= \alpha \underbrace{\mathbf{P}(B)}_{B} \underbrace{\sum_{e} \underbrace{P(e)}_{E} \sum_{a} \underbrace{\mathbf{P}(a|B,e)}_{A} \underbrace{P(J = true|a)}_{J} \underbrace{P(M = true|a)}_{M}}_{M} \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{E} \sum_{a} \mathbf{P}(a|B,e) P(J = true|a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{a} \mathbf{P}(a|B,e) f_{J}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{a} \underbrace{\sum_{a} f_{A}(a,b,e)}_{J}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{a} f_{A}(a,b,e) f_{J}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{a} f_{A}(a,b,e) f_{J}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{J}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{A}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{A}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{A}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{A}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{A}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{A}(a) f_{M}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{A}(a,b,e) f_{A}(a) f_{A}(a) \\ &= \alpha \mathbf{P}(B) \underbrace{\sum_{e} P(e)}_{A} f_{A}(a,b,e) f_{A}($$

Variable elimination: Basic operations

$$\begin{array}{l} \underline{\text{Pointwise product}} \text{ of factors } f_1 \text{ and } f_2: \\ f_1(x_1, \dots, x_j, y_1, \dots, y_k) \times f_2(y_1, \dots, y_k, z_1, \dots, z_l) \\ &= f(x_1, \dots, x_j, y_1, \dots, y_k, z_1, \dots, z_l) \\ \text{E.g., } f_1(a, b) \times f_2(b, c) = f(a, b, c) \end{array}$$

Summing out a variable from a product of factors: move any constant factors outside the summation:

$$\Sigma_x f_1 \times \cdots \times f_k = f_1 \times \cdots \times f_i \Sigma_x f_{i+1} \times \cdots \times f_k = f_1 \times \cdots \times f_i \times f_{\bar{X}}$$

assuming f_1, \ldots, f_i do not depend on X

Variable elimination algorithm

```
 \begin{aligned} \textbf{function ELIMINATIONASK}(X, \mathbf{e}, bn) \ \textbf{returns} \ \textbf{a} \ distribution \ over \ X \\ \textbf{inputs:} \ X, \ \textbf{the query variable} \\ \textbf{e}, \ evidence \ specified \ as \ an \ event \\ bn, \ \textbf{a} \ belief \ network \ specifying \ joint \ distribution \ \mathbf{P}(X_1, \dots, X_n) \\ \textbf{if} \ X \in \textbf{e} \ \textbf{then \ return} \ observed \ point \ distribution \ for \ X \\ factors \leftarrow []; \ vars \leftarrow \text{Reverse}(\text{VARS}[bn]) \\ \textbf{for each } var \ \textbf{in } vars \ \textbf{do} \\ factors \leftarrow [MAKEFACTOR(var, \textbf{e})|factors] \\ \textbf{if } var \ \textbf{is } a \ \textbf{hidden variable then } factors \leftarrow \text{SUMOUT}(var, factors) \\ \textbf{return } \text{NORMALIZE}(\text{POINTWISEPRODUCT}(factors)) \end{aligned}
```

Complexity of exact inference

Singly connected networks (or polytrees):

- any two nodes are connected by at most one (undirected) path
- time and space cost of variable elimination are $O(d^k n)$

Multiply connected networks:

- can reduce 3SAT to exact inference \Rightarrow NP-hard
- equivalent to counting 3SAT models \Rightarrow #P-complete



Inference by stochastic simulation

Basic idea:

- 1) Draw N samples from a sampling distribution S
- 2) Compute an approximate posterior probability \hat{P}
- 3) Show this converges to the true probability P

Outline:

- Sampling from an empty network
- Rejection sampling: reject samples disagreeing with evidence
- Likelihood weighting: use evidence to weight samples
- MCMC: sample from a stochastic process whose stationary distribution is the true posterior

Sampling from an empty network

function PRIORSAMPLE(bn) returns an event sampled from $\mathbf{P}(X_1, \ldots, X_n)$ specified by bn $\mathbf{x} \leftarrow$ an event with n elements for i = 1 to n do $x_i \leftarrow$ a random sample from $\mathbf{P}(X_i \mid Parents(X_i))$ return \mathbf{x}



Sampling from an empty network contd.

Probability that PRIORSAMPLE generates a particular event $S_{PS}(x_1 \dots x_n) = \prod_{i=1}^n P(x_i | Parents(X_i)) = P(x_1 \dots x_n)$ i.e., the true prior probability

Let $N_{PS}(\mathbf{Y} = \mathbf{y})$ be the number of samples generated for which $\mathbf{Y} = \mathbf{y}$, for any set of variables \mathbf{Y} .

Then
$$\hat{P}(\mathbf{Y} = \mathbf{y}) = N_{PS}(\mathbf{Y} = \mathbf{y})/N$$
 and

$$\lim_{N \to \infty} \hat{P}(\mathbf{Y} = \mathbf{y}) = \Sigma_{\mathbf{h}} S_{PS}(\mathbf{Y} = \mathbf{y}, \mathbf{H} = \mathbf{h})$$

$$= \Sigma_{\mathbf{h}} P(\mathbf{Y} = \mathbf{y}, \mathbf{H} = \mathbf{h})$$

$$= P(\mathbf{Y} = \mathbf{y})$$

That is, estimates derived from **PRIORSAMPLE** are <u>consistent</u>

Rejection sampling

$\hat{\mathbf{P}}(X|\mathbf{e})$ estimated from samples agreeing with \mathbf{e}

function REJECTIONSAMPLING(X, e, bn, N) **returns** an approximation to P(X | e) $N[X] \leftarrow a$ vector of counts over X, initially zero **for** j = 1 to N **do** $\mathbf{x} \leftarrow \text{PRIORSAMPLE}(bn)$ **if** \mathbf{x} is consistent with **e then** $N[x] \leftarrow N[x]+1$ where x is the value of X in \mathbf{x} **return** NORMALIZE(N[X])

E.g., estimate $\mathbf{P}(Rain|Sprinkler = true)$ using 100 samples 27 samples have Sprinkler = trueOf these, 8 have Rain = true and 19 have Rain = false.

 $\hat{\mathbf{P}}(Rain|Sprinkler = true) = NORMALIZE(\langle 8, 19 \rangle) = \langle 0.296, 0.704 \rangle$

Similar to a basic real-world empirical estimation procedure

Analysis of rejection sampling

$$\hat{\mathbf{P}}(X|\mathbf{e}) = \alpha \mathbf{N}_{PS}(X, \mathbf{e})$$
 (algorithm defn.)

$$= \mathbf{N}_{PS}(X, \mathbf{e}) / N_{PS}(\mathbf{e})$$
 (normalized by $N_{PS}(\mathbf{e})$)

$$\approx \mathbf{P}(X, \mathbf{e}) / P(\mathbf{e})$$
 (property of PRIORSAMPLE)

$$= \mathbf{P}(X|\mathbf{e})$$
 (defn. of conditional probability)

Hence rejection sampling returns consistent posterior estimates

Problem: hopelessly expensive if $P(\mathbf{e})$ is small

Likelihood weighting

Idea: fix evidence variables, sample only nonevidence variables, and weight each sample by the likelihood it accords the evidence

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function WEIGHTEDSAMPLE(bn, e) returns an event and a weight

\mathbf{x} \leftarrow an event with n elements; w \leftarrow 1

for i = 1 to n do

if X_i has a value x_i in \mathbf{e}

then w \leftarrow w \times P(X_i = x_i \mid Parents(X_i))

else x_i \leftarrow a random sample from \mathbf{P}(X_i \mid Parents(X_i))

return \mathbf{x}, w

function LIKELIHOODWEIGHTING(X, \mathbf{e}, bn, N) returns an approximation to P(X \mid \mathbf{e})

\mathbf{W}[X] \leftarrow a vector of weighted counts over X, initially zero

for j = 1 to N do

\mathbf{x}, w \leftarrow \text{WEIGHTEDSAMPLE}(bn)

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

return NORMALIZE(\mathbf{W}[X])
```

Likelihood weighting example

Estimate $\mathbf{P}(Rain|Sprinkler = true, WetGrass = true)$



LW example contd.

Sample generation process:

- 1. $w \leftarrow 1.0$
- 2. Sample $\mathbf{P}(Cloudy) = \langle 0.5, 0.5 \rangle$; say *true*
- 3. Sprinkler has value true, so $w \leftarrow w \times P(Sprinkler = true | Cloudy = true) = 0.1$
- 4. Sample $\mathbf{P}(Rain|Cloudy = true) = \langle 0.8, 0.2 \rangle$; say true
- 5. WetGrass has value true, so $w \leftarrow w \times P(WetGrass = true | Sprinkler = true, Rain = true) = 0.099$

Likelihood weighting analysis

Sampling probability for WEIGHTEDSAMPLE is $S_{WS}(\mathbf{y}, \mathbf{e}) = \prod_{i=1}^{l} P(y_i | Parents(Y_i))$ Note: pays attention to evidence in *ancestors* only \Rightarrow somewhere "in between" prior and posterior distribution

Weight for a given sample \mathbf{y}, \mathbf{e} is $w(\mathbf{y}, \mathbf{e}) = \prod_{i=1}^{m} P(e_i | Parents(E_i))$

Weighted sampling probability is

$$S_{WS}(\mathbf{y}, \mathbf{e})w(\mathbf{y}, \mathbf{e}) = \prod_{i=1}^{l} P(y_i | Parents(Y_i)) \quad \prod_{i=1}^{m} P(e_i | Parents(E_i)) = P(\mathbf{y}, \mathbf{e}) \text{ (by standard global semantics of network)}$$

Hence likelihood weighting returns consistent estimates but performance still degrades with many evidence variables

Approximate inference using MCMC

"State" of network = current assignment to all variables

Generate next state by sampling one variable given Markov blanket Sample each variable in turn, keeping evidence fixed

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function MCMC-Ask(X, \mathbf{e}, bn, N) returns an approximation to P(X|\mathbf{e})
local variables: \mathbf{N}[X], a vector of counts over X, initially zero
\mathbf{Y}, the nonevidence variables in bn
\mathbf{x}, the current state of the network, initially copied from \mathbf{e}
initialize \mathbf{x} with random values for the variables in \mathbf{Y}
for j = 1 to N do
\mathbf{N}[x] \leftarrow \mathbf{N}[x] + 1 where x is the value of X in \mathbf{x}
for each Y_i in \mathbf{Y} do
sample the value of Y_i in \mathbf{x} from \mathbf{P}(Y_i|MB(Y_i)) given the values of MB(Y_i) in \mathbf{x}
return NORMALIZE(\mathbf{N}[X])
```

Approaches <u>stationary distribution</u>: long-run fraction of time spent in each state is exactly proportional to its posterior probability

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MCMC example contd.

Random initial state: Cloudy = true and Rain = false

- 1. $\mathbf{P}(Cloudy|MB(Cloudy)) = \mathbf{P}(Cloudy|Sprinkler, \neg Rain)$ sample $\rightarrow false$
- 2. $\mathbf{P}(Rain|MB(Rain)) = \mathbf{P}(Rain|\neg Cloudy, Sprinkler, WetGrass)$ sample $\rightarrow true$

Visit 100 states

31 have Rain = true, 69 have Rain = false

$$\hat{\mathbf{P}}(Rain|Sprinkler = true, WetGrass = true) = NORMALIZE(\langle 31, 69 \rangle) = \langle 0.31, 0.69 \rangle$$

MCMC analysis: Outline

Transition probability $q(\mathbf{y} \rightarrow \mathbf{y}')$

Occupancy probability $\pi_t(\mathbf{y})$ at time t

Equilibrium condition on π_t defines stationary distribution $\pi(\mathbf{y})$ Note: stationary distribution depends on choice of $q(\mathbf{y} \rightarrow \mathbf{y}')$

Pairwise <u>detailed balance</u> on states guarantees equilibrium

Gibbs sampling transition probability:

sample each variable given current values of all others \Rightarrow detailed balance with the true posterior

For Bayesian networks, Gibbs sampling reduces to sampling conditioned on each variable's Markov blanket

Stationary distribution

 $\pi_t(\mathbf{y}) = \text{probability in state } \mathbf{y} \text{ at time } t$ $\pi_{t+1}(\mathbf{y}') = \text{probability in state } \mathbf{y}' \text{ at time } t+1$

 π_{t+1} in terms of π_t and $q(\mathbf{y} \to \mathbf{y}')$

$$\pi_{t+1}(\mathbf{y}') = \Sigma_{\mathbf{y}} \pi_t(\mathbf{y}) q(\mathbf{y} \to \mathbf{y}')$$

Stationary distribution: $\pi_t = \pi_{t+1} = \pi$

$$\pi(\mathbf{y}') = \Sigma_{\mathbf{y}} \pi(\mathbf{y}) q(\mathbf{y} \to \mathbf{y}') \qquad \text{for all } \mathbf{y}'$$

If π exists, it is unique (specific to $q(\mathbf{y} \rightarrow \mathbf{y}')$)

In equilibrium, expected "outflow" = expected "inflow"

Detailed balance

"Outflow" = "inflow" for each pair of states:

$$\pi(\mathbf{y})q(\mathbf{y}\rightarrow\mathbf{y}')=\pi(\mathbf{y}')q(\mathbf{y}'\rightarrow\mathbf{y})\qquad\text{for all }\mathbf{y},\ \mathbf{y}'$$

Detailed balance \Rightarrow stationarity: $\Sigma_{\mathbf{y}} \pi(\mathbf{y}) q(\mathbf{y} \rightarrow \mathbf{y}') = \Sigma_{\mathbf{y}} \pi(\mathbf{y}') q(\mathbf{y}' \rightarrow \mathbf{y})$ $= \pi(\mathbf{y}') \Sigma_{\mathbf{y}} q(\mathbf{y}' \rightarrow \mathbf{y})$ $= \pi(\mathbf{y}')$

MCMC algorithms typically constructed by designing a transition probability q that is in detailed balance with desired π

Gibbs sampling

Sample each variable in turn, given *all other variables*

Sampling Y_i , let $\bar{\mathbf{Y}}_i$ be all other nonevidence variables Current values are y_i and $\bar{\mathbf{y}}_i$; e is fixed Transition probability is given by

$$q(\mathbf{y} \to \mathbf{y}') = q(y_i, \bar{\mathbf{y}}_i \to y'_i, \bar{\mathbf{y}}_i) = P(y'_i | \bar{\mathbf{y}}_i, \mathbf{e})$$

This gives detailed balance with true posterior $P(\mathbf{y}|\mathbf{e})$: $\pi(\mathbf{y})q(\mathbf{y} \rightarrow \mathbf{y}') = P(\mathbf{y}|\mathbf{e})P(y'_i|\bar{\mathbf{y}}_i, \mathbf{e}) = P(y_i, \bar{\mathbf{y}}_i|\mathbf{e})P(y'_i|\bar{\mathbf{y}}_i, \mathbf{e})$ $= P(y_i|\bar{\mathbf{y}}_i, \mathbf{e})P(\bar{\mathbf{y}}_i|\mathbf{e})P(y'_i|\bar{\mathbf{y}}_i, \mathbf{e})$ (chain rule) $= P(y_i|\bar{\mathbf{y}}_i, \mathbf{e})P(y'_i, \bar{\mathbf{y}}_i|\mathbf{e})$ (chain rule backwards) $= q(\mathbf{y}' \rightarrow \mathbf{y})\pi(\mathbf{y}') = \pi(\mathbf{y}')q(\mathbf{y}' \rightarrow \mathbf{y})$

Markov blanket sampling

A variable is independent of all others given its Markov blanket: $P(y'_i | \bar{\mathbf{y}}_i, \mathbf{e}) = P(y'_i | MB(Y_i))$

Probability given the Markov blanket is calculated as follows: $P(y'_i|MB(Y_i)) = P(y'_i|Parents(Y_i)) \prod_{Z_j \in Children(Y_i)} P(z_j|Parents(Z_j))$

Hence computing the sampling distribution over Y_i for each flip requires just cd multiplications if Y_i has c children and d values; can cache it if c not too large.

Main computational problems:

- 1) Difficult to tell if convergence has been achieved
- 2) Can be wasteful if Markov blanket is large:

 $P(Y_i|MB(Y_i))$ won't change much (law of large numbers)

Performance of approximation algorithms

<u>Absolute approximation</u>: $|P(X|\mathbf{e}) - \hat{P}(X|\mathbf{e})| \leq \epsilon$

<u>Relative approximation</u>: $\frac{|P(X|\mathbf{e}) - \hat{P}(X|\mathbf{e})|}{P(X|\mathbf{e})} \leq \epsilon$

Relative \Rightarrow absolute since $0 \le P \le 1$ (may be $O(2^{-n})$)

Randomized algorithms may fail with probability at most δ

Polytime approximation: $poly(n, \epsilon^{-1}, \log \delta^{-1})$

Theorem (Dagum and Luby, 1993): both absolute and relative approximation for either deterministic or randomized algorithms are NP-hard for any $\epsilon, \delta < 0.5$

(Absolute approximation polytime with no evidence—Chernoff bounds)