Inference in belief networks

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Outline

- ♦ Exact inference by enumeration
- ♦ Exact inference by variable elimination
- ♦ Approximate inference by stochastic simulation
- ♦ Approximate inference by Markov chain Monte Carlo

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Inference tasks

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\frac{\text{Simple queries:}}{\text{e.g., }P(NoGas|Gauge=empty,Lights=on,Starts=false)}
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Conjunctive queries: $P(X_i, X_j | E = e) = P(X_i | E = e)P(X_j | X_i, E = e)$

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?

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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:

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\begin{aligned} \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 \sum_{e} \sum_{a} \mathbf{P}(B, e, a, J = true, M = true) \end{aligned}
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Rewrite full joint entries using product of CPT entries:

P(B = true | J = true, M = true) $= \alpha \sum_{e} \sum_{a} P(B = true) P(e) P(a | B = true, e) P(J = true | a) P(M = true | a)$

 $= \alpha P(B = true) \sum_{e} P(e) \sum_{a} P(a|B = true, e) P(J = true|a) P(M = true|a)$

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Enumeration algorithm

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

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ENUMERATION 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,\dots,X_n) \mathbf{Q}(x) \leftarrow \mathbf{a} \text{ distribution over } X for each value x_i of X do extend e with value x_i for X \mathbf{Q}(x_i) \leftarrow \mathbf{ENUMERATEALL}(\mathbf{VARS}[bn], \mathbf{e}) return Normalize(\mathbf{Q}(X)) \mathbf{ENUMERATEALL}(vars, \mathbf{e}) \text{ return } 1.0 else do Y \leftarrow \mathbf{FIRST}(vars) if Y has value y in e then return Y(y \mid Pa(Y)) \times \mathbf{ENUMERATEALL}(\mathbf{REST}(vars), \mathbf{e}) else return \sum_y P(y \mid Pa(Y)) \times \mathbf{ENUMERATEALL}(\mathbf{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

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

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Variable elimination: Basic operations

Pointwise product of factors f_1 and f_2 :

$$\begin{array}{l} f_1(x_1,\ldots,x_j,\,y_1,\ldots,y_k)\times f_2(y_1,\ldots,y_k,\,z_1,\ldots,z_l) \\ = f(x_1,\ldots,x_j,\,y_1,\ldots,y_k,\,z_1,\ldots,z_l) \\ \text{E.g., } f_1(a,b)\times f_2(b,c) = f(a,b,c) \end{array}$$

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, \dots, f_i do not depend on X

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Variable elimination algorithm

function ELIMINATIONASK(X,e,bn) returns a distribution over Xinputs: X, the query variable
 e, evidence specified as an event

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

if $X \in \mathbf{e}$ then return observed point distribution for X

 $factors \leftarrow [\]; \ vars \leftarrow Reverse(Vars[bn])$

 $\mathbf{for} \ \mathbf{each} \ \mathit{var} \ \mathbf{in} \ \mathit{vars} \ \mathbf{do}$

 $factors \leftarrow [MakeFactor(var, e)|factors]$

if var is a hidden variable then $factors \leftarrow \text{SumOut}(var, factors)$ return Normalize(PointwiseProduct(factors))

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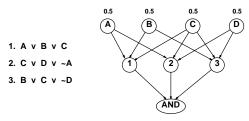
Complexity of exact inference

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 ⇒ NP-hard
- equivalent to $counting 3SAT models \Rightarrow$ #P-complete



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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

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Sampling from an empty network

$$\begin{aligned} & \textbf{function} \ \mathbf{PRIORSAMPLE}(bn) \ \mathbf{returns} \ \text{an event sampled from} \ \mathbf{P}(X_1, \dots, X_n) \ \text{specified by} \ bn \\ & \mathbf{X} \leftarrow \text{an event with} \ n \ \text{elements} \\ & \text{for} \ i = 1 \ \text{to} \ n \ \text{do} \\ & x_i \leftarrow \text{a random sample from} \ \mathbf{P}(X_i \mid Parents(X_i)) \\ & \mathbf{return} \ \mathbf{X} \end{aligned}$$

$$\begin{split} \mathbf{P}(Cloudy) &= \langle 0.5, 0.5 \rangle \\ &\text{sample} \rightarrow true \\ \mathbf{P}(Sprinkler|Cloudy) &= \langle 0.1, 0.9 \rangle \\ &\text{sample} \rightarrow false \\ \mathbf{P}(Rain|Cloudy) &= \langle 0.8, 0.2 \rangle \\ &\text{sample} \rightarrow true \\ \mathbf{P}(WetGrass|\neg Sprinkler, Rain) &= \langle 0.9, 0.1 \rangle \\ &\text{sample} \rightarrow true \end{split}$$

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 \boldsymbol{Y}

$$\begin{split} \text{Then } \hat{P}(\mathbf{Y} = \mathbf{y}) &= N_{PS}(\mathbf{Y} = \mathbf{y})/N \text{ and } \\ \lim_{N \to \infty} \hat{P}(\mathbf{Y} = \mathbf{y}) &= \sum_{\mathbf{h}} S_{PS}(\mathbf{Y} = \mathbf{y}, \mathbf{H} = \mathbf{h}) \\ &= \sum_{\mathbf{h}} P(\mathbf{Y} = \mathbf{y}, \mathbf{H} = \mathbf{h}) \\ &= P(\mathbf{Y} = \mathbf{y}) \end{split}$$

That is, estimates derived from $\ensuremath{\mathrm{PRIORSAMPLE}}$ are consistent

Rejection sampling

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

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function REJECTIONSAMPLING(X, \mathbf{e}, bn, N) returns an approximation to P(X | \mathbf{e})
\mathbf{N}[X] \leftarrow \mathbf{a} \text{ vector of counts over } X, \text{ initially zero}
\mathbf{for } j = 1 \text{ to } N \text{ do}
\mathbf{x} \leftarrow \text{PRIORSAMPLE}(bn)
\mathbf{if } \mathbf{x} \text{ is consistent with } \mathbf{e} \text{ then}
\mathbf{N}[z] \leftarrow \mathbf{N}[x] + 1 \text{ where } z \text{ is the value of } X \text{ in } \mathbf{x}
\mathbf{return } \text{ Normalize}(\mathbf{N}[X])
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E.g., estimate $\mathbf{P}(Rain|Sprinkler = true)$ using 100 samples 27 samples have Sprinkler = true

Of these, 8 have Rain = true and 19 have Rain = false.

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

Similar to a basic real-world empirical estimation procedure

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Analysis of rejection sampling

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\begin{array}{ll} \hat{\mathbf{P}}(X|\mathbf{e}) = \alpha \mathbf{N}_{PS}(X,\mathbf{e}) & \text{(algorithm defn.)} \\ = \mathbf{N}_{PS}(X,\mathbf{e})/N_{PS}(\mathbf{e}) & \text{(normalized by } N_{PS}(\mathbf{e})) \\ \approx \mathbf{P}(X,\mathbf{e})/P(\mathbf{e}) & \text{(property of $P_{RIORSAMPLE}$)} \\ = \mathbf{P}(X|\mathbf{e}) & \text{(defn. of conditional probability)} \end{array}
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Hence rejection sampling returns consistent posterior estimates

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

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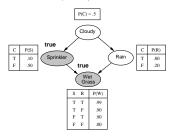
Likelihood weighting

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 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_e, bn, N) returns an approximation to P(X|e) \mathbf{W}[X] \leftarrow a vector of weighted counts over X, initially zero for j=1 to N do \mathbf{x}, w \leftarrow \mathbf{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])
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Likelihood weighting example

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



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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 $W{\ensuremath{\mathrm{EIGHTEDSAMPLE}}}$ 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

⇒ 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

 $S_{WS}(\mathbf{y}, \mathbf{e})w(\mathbf{y}, \mathbf{e})$ = $\prod_{i=1}^{l} P(u_i|Parents(Y_i))$

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

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

function MCMC-Ask(X, e, bn, N) returns an approximation to P(X|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 stationary distribution: 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(\lambda1, 69 \rangle) = \lambda 0.31, 0.69 \rangle

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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 $q(\mathbf{y} \to \mathbf{y}')$)

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

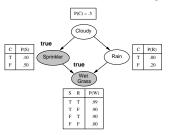
MCMC Example

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

Sample Cloudy then Rain, repeat.

Count number of times Rain is true and false in the samples.

Markov blanket of Cloudy is Sprinkler and Rain Markov blanket of Rain is Cloudy, Sprinkler, and WetGrass



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MCMC analysis: Outline

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

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 $q(\mathbf{y} \to \mathbf{y}')$

Pairwise detailed balance 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

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Detailed balance

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

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

Detailed balance \Rightarrow stationarity:

$$\Sigma_{\mathbf{y}}\pi(\mathbf{y})q(\mathbf{y}\to\mathbf{y}') = \Sigma_{\mathbf{y}}\pi(\mathbf{y}')q(\mathbf{y}'\to\mathbf{y})$$

$$= \pi(\mathbf{y}')\Sigma_{\mathbf{y}}q(\mathbf{y}'\to\mathbf{y})$$

$$= \pi(\mathbf{y}')$$

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 $Y_{i\cdot}$ let $\bar{\mathbf{Y}}_i$ be all other nonevidence variables Current values are y_i and $\bar{\mathbf{y}}_{i\cdot}$ 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 $P(\mathbf{y}|\mathbf{e})$: $\pi(\mathbf{y})q(\mathbf{y} \to \mathbf{y}') = P(\mathbf{y}|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i,\mathbf{e}) = P(y_i,\bar{\mathbf{y}}_i|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i,\mathbf{e}) \\ = P(y_i|\bar{\mathbf{y}}_i,\mathbf{e})P(\bar{\mathbf{y}}_i|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i,\mathbf{e}) \quad \text{(chain rule)} \\ = P(y_i|\bar{\mathbf{y}}_i,\mathbf{e})P(y_i',\bar{\mathbf{y}}_i|\mathbf{e}) \quad \text{(chain rule backwards)} \\ = q(\mathbf{y}' \to \mathbf{y})\pi(\mathbf{y}') = \pi(\mathbf{y}')q(\mathbf{y}' \to \mathbf{y})$

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Performance of approximation algorithms

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

Relative approximation: $\frac{|P(X|\mathbf{e}) - \hat{P}(X|\mathbf{e})|}{P(X|\mathbf{e})} \le \epsilon$

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)

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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: $P(y_i'|MB(Y_i)) = P(y_i'|Parents(Y_i)) \Pi_{Z_i \in Children(Y_i)} P(z_j|Parents(Z_j))$

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)

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