Probabilistic Reasoning

Bùi Tiến Lên

2022



Contents



- 1. Exact inference by enumeration
- 2. Exact inference by variable elimination
- 3. Approximate inference by stochastic simulation
- 4. Approximate inference by Markov chain Monte Carlo (MCMC)
- 5. Sampling for Continous Variables

Random Number
Direct Sampling
Rejection Sampling
Likelihood Weighti

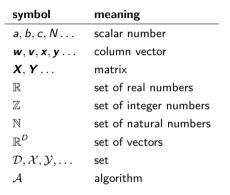
Approximate inference by Markov chair Monte Carlo (MCMC)

Gibbs Sampling MCMC for Baye Network

Sampling for Continuous Variables

Reject Sampling Metropolis-Hastings

Notation



symbol	meaning
<i>X</i> , <i>Y</i>	random variable
$\boldsymbol{X},\boldsymbol{Y}\dots$	multivariate random variable
$x, y \dots$	value
x , y	vector
p, pr, P, Pr	probability

Random Number
Direct Sampling
Rejection Sampling
Likelihood Weighti

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesi
Network

Sampling for Continuous Variables

Reject Sampling Metropolis-Hastings

Inference tasks



Simple queries:

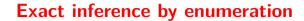
$$P(X \mid E = e) \tag{1}$$

Conjunctive queries:

$$P(X \mid E = e) \tag{2}$$

 Optimal decisions: decision networks include utility information; probabilistic inference required for

- 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?"





Random Number
Direct Sampling
Rejection Sampling

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesi Network

Sampling for Continuous Variables

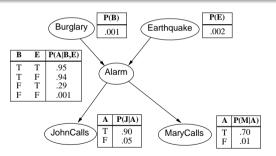
Reject Sampling
Metropolis-Hastings

Inference by enumeration



ldea

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



Inference by enumeration (cont.)

Simple query on the burglary network:

$$P(B | j, m) = P(B, j, m)/P(j, m)$$

$$= \alpha P(B, j, m)$$

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

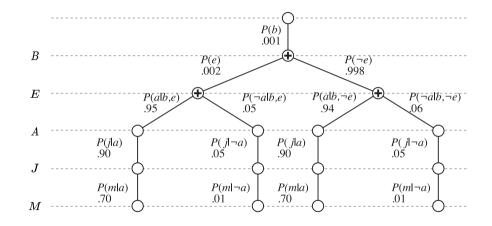
• Rewrite full joint entries using product of CPT entries:

$$\begin{array}{l} P(B \mid j, m) \\ = \alpha \; \sum_{e} \sum_{a} P(B) P(e) P(a \mid B, e) P(j \mid a) P(m \mid a) \\ = \alpha \; P(B) \sum_{e} P(e) \sum_{a} P(a \mid B, e) P(j \mid a) P(m \mid a) \\ = \alpha \; \langle 0.00059224, 0.0014919 \rangle \\ = \langle 0.284, 0.716 \rangle \end{array}$$

Metropolis-Hastings

Evaluation tree





• Enumeration is inefficient: repeated computation; e.g., computes $P(i \mid a)P(m \mid a)$ for each value of e

Metropolis-Hastings

Enumeration algorithm



• 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 Bayes net with variables \{X\} \cup \boldsymbol{E} \cup \boldsymbol{Y} \# \boldsymbol{Y}: hidden variables
  Q(X) \leftarrow a distribution over X, initially empty
  for each value x_i of X do
    Q(x_i) \leftarrow \text{Enumerate-All}(bn.vars, e_{x_i})
        where e_{x_i} is e extended with X = x_i
return Normalize (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 v in e
  then return P(y \mid parents(Y)) \times \text{ENUMERATE-ALL}(\text{REST}(vars), e)
  else return \sum vP(v \mid parents(Y)) \times Enumerate-All(Rest(vars), e_v)
                   where e_v is e extended with Y = v
```





Exact inference by variable elimination

Approximate inference by stochastic

Random Number
Direct Sampling
Rejection Sampling

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesian Network

Sampling fo Continous Variables

Reject Sampling
Metropolis-Hastings

Inference by variable elimination



Idea

Carry out summations right-to-left, storing intermediate results (**factors**) to avoid recomputation

$$\begin{split} P(B \mid j, m) &= \alpha \underbrace{P(B)}_{B} \sum_{e} \underbrace{P(e)}_{E} \sum_{a} \underbrace{P(a \mid B, e)}_{A} \underbrace{P(j \mid a)}_{J} \underbrace{P(m \mid a)}_{M} \\ &= \alpha P(B) \sum_{e} P(e) \sum_{a} P(a \mid B, e) P(j \mid a) f_{M}(a) \\ &= \alpha P(B) \sum_{e} P(e) \sum_{a} P(a \mid B, e) f_{J}(a) f_{M}(a) \\ &= \alpha P(B) \sum_{e} P(e) \sum_{a} f_{A}(a, b, e) f_{J}(a) f_{M}(a) \\ &= \alpha P(B) \sum_{e} P(e) f_{\bar{A}JM}(b, e) \text{ (sum out A)} \\ &= \alpha P(B) f_{\bar{E}\bar{A}JM}(b) \text{ (sum out E)} \\ &= \alpha f_{B}(b) \times f_{\bar{E}\bar{A}JM}(b) \end{split}$$

Variable elimination: Basic operations



- **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

$$\sum_{x} f_{1} \times \cdots \times f_{k} = f_{1} \times \cdots \times f_{i} \sum_{x} f_{i+1} \times \cdots \times f_{k}$$

$$= f_{1} \times \cdots \times f_{i} \times f_{\bar{X}}$$
(3)

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

• **Pointwise product** of factors f_1 and f_2 :

$$f_1(x_1, ..., x_j, y_1, ..., y_k) \times f_2(y_1, ..., y_k, z_1, ..., z_l) = f(x_1, ..., x_j, y_1, ..., y_k, z_1, ..., z_l)$$
(4)

Exact inference by variable elimination

Approximate inference by stochastic

Random Numbe

Rejection Sampling

Approximate inforces by

inference by Markov chain Monte Carlo (MCMC)

MCMC for Bayesian Network

Sampling for Continuous Variables

Reject Sampling
Metropolis-Hastings

Variable elimination algorithm



```
function ELIMINATION-ASK(X, e, bn)
returns a distribution over X
inputs: X, the query variable
         e, observed values for variables E
         bn, a Bayesian network specifying
              joint distribution P(X_1, \ldots, X_n)
  factors \leftarrow \emptyset
  for each var in ORDER(bn.VARS) do
    factors \leftarrow [Make-Factor(var, e) \mid factors]
    if var is a hidden variable then
       factors \leftarrow Sum-Out(var, factors)
return Normalize(Pointwise-Product(factors))
```

Exact inference by variable elimination

Approximate inference by stochastic

Random Number
Direct Sampling
Rejection Sampling
Likelihood Weighti

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesian Network

Sampling for Continous Variables

Reject Sampling Metropolis-Hastings

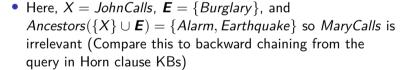
Irrelevant variables



• Consider the query $P(JohnCalls \mid Burglary = true)$

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

Sum over m is identically 1; M is *irrelevant* to the query



Theorem 1

Y is irrelevant unless $Y \in Ancestors(\{X\} \cup \mathbf{E})$

Exact inference by variable elimination

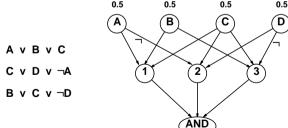
Metropolis-Hastings

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

 P-complete



- 2. C v D v ¬A
- 3. B v C v ¬D

Approximate inference by stochastic simulation

- Random Number
- Direct Sampling
- Rejection Sampling
- Likelihood Weighting



Random Number

Direct Sampling
Rejection Sampling
Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesia Network

Sampling for Continous Variables

Reject Sampling Metropolis-Hastings

Uniform Random Numbers



- The basis of all of these simulation methods is in the generation of random numbers
- The simplest method is the linear congruential generator to generate uniformly distributed random numbers

$$x_{n+1} = (ax_n + c) \bmod m \tag{5}$$

where a,c, and m are parameters that have to be chosen carefully, the initial input x_0 is known as the **seed**

ullet For example, we can use $\emph{m}=2^{32}$, $\emph{a}=1,664,525$ and $\emph{c}=1,013,904,223$

Random Number

Direct Sampling
Rejection Sampling
Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesi
Network

Sampling for Continuous Variables

Reject Sampling Metropolis-Hasti

Gaussian Random Numbers



The Box–Muller algorithm

- **1.** Pick two uniformly distributed random numbers $0 \le U_1, U_2 \le 1$
- 2. Set $\theta = 2\pi U_1$ and $r = \sqrt{-2\ln(U_2)}$
- 3. Then $x = r\cos(\theta)$ and $y = r\sin(\theta)$ are independent Gaussian-distributed variables with zero mean $(\mu = 0)$ and unit variance $(\sigma = 1)$

Approximate inference by stochastic simulation

Random Number

Direct Sampling
Rejection Sampling
Likelihood Weightin

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesian Network

Continuous Variables

Reject Sampling Metropolis-Hastings

Sampling for Single Categorical Variable



Want to sample values of a random variable X whose domain is {true, false},
 with probability distribution

true	false
0.4	0.6

Simple approach

```
r = uniform_random([0, 1])
if r < 0.4:
    sample = true
else:
    sample = false</pre>
```

Approximate inference by stochastic simulation

Random Number

Direct Sampling
Rejection Sampling
Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Baye
Network

Continous

Reject Sampling Metropolis-Hastings

Inference by stochastic simulation



Basic idea

- 1. Draw N samples from a sampling distribution S (sampling is a lot like repeated simulation)
- 2. Compute an approximate posterior probability \hat{P}
- **3.** Show this converges to the true probability *P*

Experiment



Stochastic simulation



ct inference

Exact inferer by variable elimination

Approximate inference by stochastic simulation

Random Number

Direct Sampling
Rejection Sampling
Likelihood Weightin

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesia Network

Sampling for Continous Variables

Reject Sampling Metropolis-Hastings

Inference by stochastic simulation (cont.)



Why sample?

- Learning: get samples from a distribution you don't know
- **Inference**: getting a sample is faster than computing the right answer (e.g. with variable elimination)

Approaches:

- 1. Sampling from an empty network
- 2. Rejection sampling: reject samples disagreeing with evidence
- 3. Likelihood weighting: use evidence to weight samples
- 4. Markov chain Monte Carlo (MCMC): sample from a stochastic process whose stationary distribution is the true posterior

Approximate inference by stochastic simulation

Random Numbe

Direct Sampling

Likelihood Weightin

Approximate inference by Markov chain Monte Carlo

Gibbs Sampling
MCMC for Bayesian

Sampling for Continuous Variables

Reject Sampling Metropolis-Hastings

Sampling from an empty network



xact inference enumeration

Exact inference by variable elimination

Approximate inference by stochastic

Random Numbe

Direct Sampling

Rejection Samplin

Approximate inference by Markov chain Monte Carlo

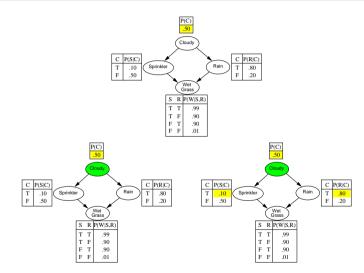
Gibbs Sampling
MCMC for Bayesian
Network

Sampling for Continuous Variables

Reject Sampling
Metropolis-Hastings

Example





Approximate inference by stochastic

Random Numbe

Direct Sampling

Rejection Sampling

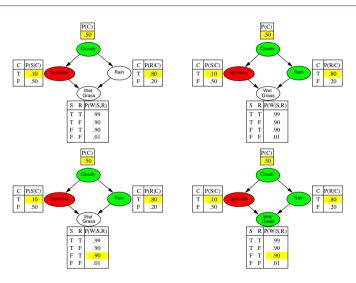
Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayes Network

Sampling for Continuous Variables

Reject Sampling
Metropolis-Hastings

Example (cont.)





Direct Sampling

Metropolis-Hastings

Example (cont.)



• **Estimate** P(Cloudy, Sprinkler, Rain, WetGrass) using 100 samples

#	Cloudy	Sprinkler	Rain	Wet Grass
1	Т	F	Т	Т
2	Т	Т	Т	T
3	F	Т	Т	F
4	Т	F	Т	Т
5	F	F	F	Т
			•••	
100	Т	F	Т	F

Approximate inference by stochastic simulation

Random Number

Direct Sampling

Rejection Sampling Likelihood Weighti

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayes Network

Sampling fo Continous Variables

Reject Sampling Metropolis-Hastings

Analysis



 \bullet Probability that $\operatorname{PRIORSample}$ generates a particular event

$$S_{PS}(x_1 \dots x_n) = \prod_{i=1}^n P(x_i \mid Parents(x_i)) = P(x_1 \dots x_n)$$

- Let $N_{PS}(x_1 \ldots x_n)$ be the number of samples generated for event x_1, \ldots, x_n
- Then we have

$$\lim_{N\to\infty} \hat{P}(x_1,\ldots,x_n) = \lim_{N\to\infty} N_{PS}(x_1,\ldots,x_n)/N$$
$$= S_{PS}(x_1,\ldots,x_n) = P(x_1\ldots x_n)$$

That is, estimates derived from PRIORSAMPLE are consistent

Approximate inference by stochastic

Random Numbe

Rejection Sampling

Likelihood Weighti

Approximate inference by Markov chain Monte Carlo

Gibbs Sampling
MCMC for Bayes
Network

Sampling fo Continous Variables

Reject Sampling Metropolis-Hastings

Rejection sampling



• $\hat{P}(X \mid e)$ estimated from samples agreeing with e

```
function REJECTION-SAMPLING (X, e, bn, N)
returns an estimate of P(X \mid e)
inputs: X, the query variable
        e. observed values for variables E
        bn, a Bayesian network
        N, the total number of samples to be generated
local variables: N, a vector of counts for each value of X,
                      initially zero
 for i = 1 to N do
    x \leftarrow PRIOR-SAMPLE(hn)
    if x is consistent with e then
       N[x] \leftarrow N[x] + 1 where x is the value of X in x
  return NORMALIZE(N)
```

Rejection Sampling

Metropolis-Hastings

Exampe



- Estimate $P(Rain \mid Sprinkler = true)$ using 100 samples
- Results 27 samples have Sprinkler = true; of these, 8 have Rain = true and 19 have Rain = false.

#	Cloudy	Sprinkler	Rain	Wet Grass
1	T	F	Т	Т
2	Т	Т	T	Т
3	F	Т	Т	F
4	Т	F	Т	Т
5	F	F	F	Т
100	Т	F	Т	F

	#	Sprinkler	Rain
	1	Т	Т
	2	Т	Т
,	3	Т	Т
\rightarrow	2 3 4 5	Т	F
	5	Т	Т
	27	Т	F

Approximate inference by stochastic simulation

Random Numbe

Rejection Sampling Likelihood Weightin

Approximate inference by Markov chain Monte Carlo

Gibbs Sampling
MCMC for Bayesian
Network

Sampling for Continous Variables

Reject Sampling Metropolis-Hastings

Analysis of rejection sampling



$$\hat{P}(X \mid e) = \alpha N_{PS}(X, e)$$
 (algorithm defn.)
 $= N_{PS}(X, e)/N_{PS}(e)$ (normalized by $N_{PS}(e)$)
 $\approx P(X, e)/P(e)$ (property of PRIORSAMPLE)
 $= P(X \mid e)$ (defn. of conditional probability)

- Hence rejection sampling returns consistent posterior estimates
- Problem: hopelessly expensive if P(e) is small. P(e) drops off exponentially with number of evidence variables!

Random Numbe Direct Sampling

Rejection Samplin

Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesian Network

Sampling f Continous Variables

Reject Sampling
Metropolis-Hastings

Likelihood weighting



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

```
function Likelihood-Weighting (X, e, bn, N) returns an estimate of P(X \mid e)
inputs: X, the query variable
        e, observed values for variables E
        bn, a Bayesian network specifying joint distribution P(X_1, \ldots, X_n)
        N. the total number of samples to be generated
local variables: W. a vector of weighted counts for each value of X. initially zero
 for j = 1 to N do
    x, w \leftarrow \text{Weighted-Sample}(bn, e)
    W[x] \leftarrow W[x] + w where x is the value of X in x
  return NORMALIZE(W)
function WEIGHTED-SAMPLE(bn, e) returns an event and a weight
  w \leftarrow 1
  x \leftarrow an event with n elements initialized from e
  foreach variable X_i in X_1, \ldots, X_n do
    if X_i is an evidence variable with 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 P(X_i \mid parents(X_i))
  return x. w
```

Direct Sampling
Rejection Sampling

Likelihood Weighting

Approximate inference by Markov chain Monte Carlo

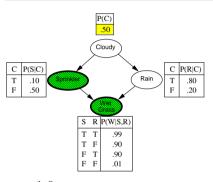
(MCMC)
Gibbs Sampling
MCMC for Baye

Sampling for Continuous

Reject Sampling
Metropolis-Hastings

Likelihood weighting example





$$w = 1.0$$

Random Number
Direct Sampling

Likelihood Weighting

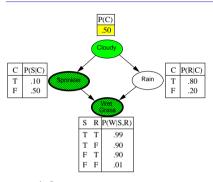
Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Baye Network

Sampling to Continous Variables

Reject Sampling
Metropolis-Hastings





$$w = 1.0$$

Random Number
Direct Sampling

Likelihood Weighting

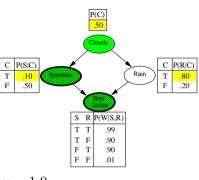
Approximate inference by Markov chair Monte Carlo (MCMC)

MCMC for Baye Network

Continous Variables

Metropolis-Hastings





$$w = 1.0$$

inference by stochastic simulation

Random Number
Direct Sampling
Rejection Samplin

Likelihood Weighting

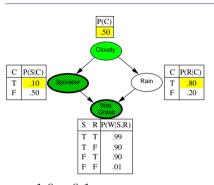
Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Baye Network

Sampling to Continous Variables

Reject Sampling
Metropolis-Hastings



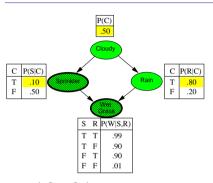


$$w = 1.0 \times 0.1$$

Likelihood Weighting

Metropolis-Hastings





$$w = 1.0 \times 0.1$$

Random Number Direct Sampling

Likelihood Weighting

Annyovimata

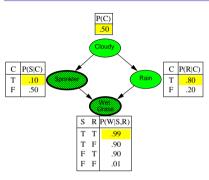
inference by Markov chair Monte Carlo (MCMC)

Gibbs Sampling MCMC for Baye Network

Sampling fo Continous Variables

Reject Sampling Metropolis-Hastings





$$w = 1.0 \times 0.1$$

Random Numbe Direct Sampling

Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

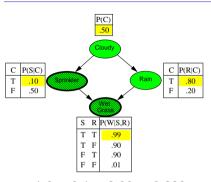
Gibbs Sampling MCMC for Baye Network

Sampling for Continuous Variables

Reject Sampling
Metropolis-Hastings

Likelihood weighting example (cont.)





$$w = 1.0 \times 0.1 \times 0.99 = 0.099$$

Random Number
Direct Sampling
Rejection Sampling

Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesi Network

Sampling for Continuous Variables

Reject Sampling Metropolis-Hastings

Likelihood weighting example (cont.)



• Estimate $P(Rain \mid Sprinkler = true, WetGrass = true)$ using 100 samples

#	Cloudy	Sprinkler	Rain	Wet Grass	weight w
1	Т	Т	Т	Т	0.099
2	F	Т	Т	Т	
3	Т	Т	Т	Т	
4	F	Т	Т	Т	
5	Т	Т	F	Т	
100	F	Т	T	Т	

Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesian Network

Sampling for Continuous Variables

Reject Sampling Metropolis-Hasti

Likelihood weighting analysis



• Sampling probability for WEIGHTEDSAMPLE is

$$S_{WS}(z, e) = \prod_{i=1}^{l} P(z_i \mid parents(Z_i))$$

- Note: pays attention to evidence in ancestors only

 somewhere "in between" prior and posterior distribution
- Weight for a given sample z, e is

$$w(z, e) = \prod_{i=1}^{m} P(e_i \mid parents(E_i))$$

Random Number
Direct Sampling
Rejection Sampling

Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesian
Network

Continous Variables

Reject Sampling Metropolis-Hastings

Likelihood weighting analysis (cont.)

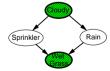


Weighted sampling probability is

$$S_{WS}(z, e)w(z, e)$$

= $\prod_{i=1}^{l} P(z_i \mid parents(Z_i)) \prod_{i=1}^{m} P(e_i \mid parents(E_i))$
= $P(z, e)$ (by standard global semantics of network)

 Hence likelihood weighting returns consistent estimates but performance still degrades with many evidence variables because a few samples have nearly all the total weight





- Gibbs Sampling
- MCMC for Bayesian Network



Random Number
Direct Sampling
Rejection Samplin
Likelihood Weight

Approximate inference by Markov chair Monte Carlo (MCMC)

Gibbs Sampling

MCMC for Bayesian Network

Continous
Variables

Reject Sampling Metropolis-Hastings

State



Concept 1

State x is current assignment to all variables.

Concept 2

- Transition probability $q(\mathbf{x} \to \mathbf{x}')$ is the probability to change from state \mathbf{x} to \mathbf{x}'
- Occupancy probability $\pi_t(x)$ is the probability in state x at time t

Gibbs Sampling

Stationary distribution



- $\pi_t(\mathbf{x}) = \text{probability in state } \mathbf{x} \text{ at time } t$
- $\pi_{t+1}(\mathbf{x}') = \text{probability in state } \mathbf{x}' \text{ at time } t+1$
- π_{t+1} in terms of π_t and $q(\mathbf{x} \to \mathbf{x'})$

$$\pi_{t+1}(q(\mathbf{x} \to \mathbf{x}')') = \sum_{\mathbf{x}} \pi_t(\mathbf{x}) q(\mathbf{x} \to \mathbf{x}')$$
 (6)

Concept 3

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

$$\pi(\mathbf{x}') = \sum_{\mathbf{x}} \pi(\mathbf{x}) q(\mathbf{x} \to \mathbf{x}') \text{ for all } \mathbf{x}'$$
 (7)

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

Random Number Direct Sampling

Rejection Sampling

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling

MCMC for Bayes Network

Continous
Variables

Reject Sampling Metropolis-Hastings

Detailed balance



Concept 4

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

$$\pi(\mathbf{x})q(\mathbf{x}\to\mathbf{x}') = \pi(\mathbf{x}')q(\mathbf{x}'\to\mathbf{x}) \text{ for all } \mathbf{x},\mathbf{x}'$$
 (8)

Theorem 2

Detailed balance \implies stationarity:

$$\sum_{\mathbf{x}} \pi(\mathbf{x}) q(\mathbf{x} \to \mathbf{x}') = \sum_{\mathbf{x}} \pi(\mathbf{x}') q(\mathbf{x}' \to \mathbf{x})$$
$$= \pi(\mathbf{x}') \sum_{\mathbf{x}} q(\mathbf{x}' \to \mathbf{x})$$
$$= \pi(\mathbf{x}')$$

Approximate inference by stochastic simulation

Random Number Direct Sampling Rejection Sampli Likelihood Weigh

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling

MCMC for Bayesia Network

Sampling for Continuous Variables

Reject Sampling Metropolis-Hastings

Gibbs sampling



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

- 1. Generate next state by sampling one variable given all other variables
- 2. Sample each variable in turn, keeping evidence fixed

$$\mathbf{x}_0 \to \mathbf{x}_1 \to \mathbf{x}_2 \to \dots \to \mathbf{x}_n$$

Random Number Direct Sampling Rejection Sampling Likelihood Weightin

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling

MCMC for Bayesia Network

Continuous
Variables

Reject Sampling
Metropolis-Hastings

Gibbs sampling (cont.)



- Sampling X_i , let \bar{X}_i be all other nonevidence variables
- Current values are x_i and \bar{x}_i ; e is fixed
- Transition probability is given by

$$q(\mathbf{x} \to \mathbf{x}') = q(x_i, \bar{\mathbf{x}}_i \to x_i', \bar{\mathbf{x}}_i) = P(x_i' \mid \bar{\mathbf{x}}_i, \mathbf{e})$$

This gives detailed balance with true posterior $P(x \mid e)$:

$$\pi(\mathbf{x})q(\mathbf{x} \to \mathbf{x}') = P(\mathbf{x} \mid \mathbf{e})P(x_i' \mid \bar{\mathbf{x}}_i, \mathbf{e}) = P(x_i, \bar{\mathbf{x}}_i \mid \mathbf{e})P(x_i' \mid \bar{\mathbf{x}}_i, \mathbf{e})$$

$$= P(x_i \mid \bar{\mathbf{x}}_i, \mathbf{e})P(\bar{\mathbf{x}}_i \mid \mathbf{e})P(x_i' \mid \bar{\mathbf{x}}_i, \mathbf{e}) \text{ (chain rule)}$$

$$= P(x_i \mid \bar{\mathbf{x}}_i, \mathbf{e})P(x_i', \bar{\mathbf{x}}_i \mid \mathbf{e}) \text{ (chain rule backwards)}$$

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

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

Approximate inference by stochastic simulation

Random Number Direct Sampling Rejection Sampling Likelihood Weightin

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesian

Sampling for Continuous

Reject Sampling Metropolis-Hastings

Analysis



Theorem 3

Chain approaches **stationary distribution**: long-run fraction of time spent in each state is exactly proportional to its posterior probability

- **Gibbs sampling** transition probability: sample each variable given current values of all others ⇒ detailed balance with the true posterior
- For Bayesian networks, Gibbs sampling reduces to sampling conditioned on each variable's Markov blanket

Random Number
Direct Sampling
Rejection Sampling
Likelihood Weightin

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesian
Network

Sampling for Continous Variables

Reject Sampling Metropolis-Hastings

Performance of approximation algorithms



Absolute approximation:

$$|P(X \mid \boldsymbol{e}) - \hat{P}(X \mid \boldsymbol{e})| \leq \epsilon$$

• Relative approximation:

$$\frac{\mid P(X \mid \mathbf{e}) - \hat{P}(X \mid \mathbf{e}) \mid}{P(X \mid \mathbf{e})} \le \epsilon$$

Relative \implies 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 4 (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)

Direct Sampling Rejection Samplin Likelihood Weigh

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesian
Network

Sampling fo Continous Variables

Reject Sampling Metropolis-Hastings

Approximate inference using MCMC



Concept 5

"State" of network = current assignment to all variables.

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

Note: We can also choose a variable to sample at random each time

MCMC for Bayesian Network

Metropolis-Hastings

Approximate inference using MCMC (cont.)



```
function McMc-Ask(X, e, bn, N)
returns an estimate of P(X \mid e)
local variables: N, a vector of counts for each value of X,
                     initially zero
                  Z, the nonevidence variables in bn
                  x, the current state of the network,
                     initially copied from e
  initialize x with random values for the variables in Z
 for i = 1 to N do
    for each Z_i in Z do
      set the value of Z_i in x by sampling from P(Z_i | 
mb(Z_i)
      N[x] \leftarrow N[x] + 1 where x is the value of X in x
  return NORMALIZE(N)
```

enumeration

Exact inferent by variable elimination

Approximate inference by stochastic

Random Number
Direct Sampling
Rejection Sampling

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesian
Network

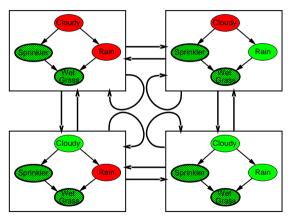
Sampling fo Continous

Reject Sampling
Metropolis-Hastings

The Markov chain



• With Sprinkler = true, WetGrass = true, there are four states:



• Wander about for a while, average what you see

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesian
Network

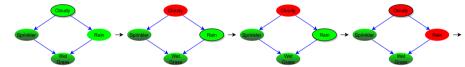
Sampling for Continuous Variables

Reject Sampling
Metropolis-Hastings

MCMC example



- **Estimate** $P(Rain \mid Sprinkler = true, WetGrass = true)$
 - Sample Cloudy or Rain given its Markov blanket, repeat.
 - Count number of times Rain is true and false in the samples.
 - **Result**: visit 100 states, 31 have Rain = true, 69 have Rain = false



#	Cloudy	Sprinkler	Rain	Wet Grass
1	Т	Т	Т	Т
2	F	Т	T	Т
3	F	Т	Т	Т
4	F	Т	F	Т
100	T	T	F	T

ct inference

Exact inferently by variable elimination

Approximate inference by stochastic simulation

Random Number
Direct Sampling
Rejection Sampling
Likelihood Weightin

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling
MCMC for Bayesian
Network

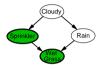
Sampling for Continous Variables

Reject Sampling Metropolis-Hastings

Markov blanket sampling



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



• Probability given the Markov blanket is calculated as follows:

$$P(x_i' \mid mb(X_i)) = P(x_i' \mid parents(X_i)) \prod_{Z_j \in children(X_i)} P(z_j \mid parents(Z_j))$$

- Easily implemented in message-passing parallel systems
- Main computational problems:
 - 1. Difficult to tell if convergence has been achieved
 - **2.** Can be wasteful if Markov blanket is large: $P(X_i \mid mb(X_i))$ won't change much (law of large numbers)

Sampling for Continous Variables

- Reject Sampling
- Metropolis-Hastings



act inference

Exact inferer by variable elimination

Approximate inference by stochastic simulation

Random Numbe

Rejection Sampling

Likelihood Weighting

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesi Network

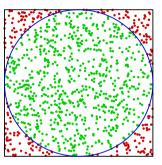
Sampling for Continuous Variables

Reject Sampling

Metropolis-Hastings

Reject Sampling





 $\pi \approx 4 \times \frac{\text{number of points inside circle}}{\text{number of points inside square}}$

Random Number Direct Sampling Rejection Sampl

Approximate inference by Markov chain Monte Carlo (MCMC)

Gibbs Sampling MCMC for Bayesi Network

Sampling fo Continous Variables

Reject Sampling

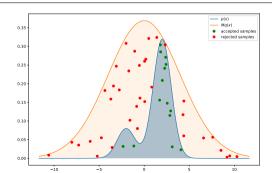
Metropolis-Hastings

Reject Sampling (cont.)



p(x) is a **target distribution**, q(x) is an an **easy-to-sample distribution** and M is a constant such that $\forall x \in \mathcal{X}, p(x) \leq Mq(x)$

- 1. Sample x from a known q(x)
- **2.** Sample *u* from a $\mathcal{U}[0, Mq(x)]$
- 3. If u < p(x) accept the sample x; otherwise reject the sample



Random Number
Direct Sampling
Rejection Sampling
Likelihood Weighti

Approximate inference by Markov chain Monte Carlo (MCMC)

Sampling for Continous

Reject Sampling
Metropolis-Hastings

Metropolis-Hastings algorithm



- **1.** Choose an initial value for a sample x_0
- **2.** Propose a new sample value x_{i+1} given x_i from $q(x \mid x_i)$
- **3.** Compute the probability of accepting a new parameter value by using the Metropolis-Hastings criteria:

$$\rho = \min\left(1, \frac{p(x_{i+1})}{p(x_i)}\right) \tag{9}$$

- **4.** Sample u from a $\mathcal{U}[0,1]$
- **5.** If $u < \rho$ we accept the new value x_{i+1} ; otherwise, we stay in the old value x_i

Random Number

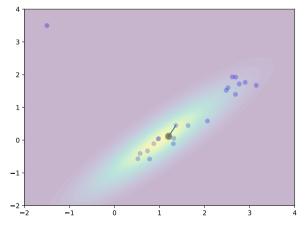
Gibbs Sampling MCMC for Bayesian Network

Reject Sampling

Metropolis-Hastings

Example





References



Goodfellow, I., Bengio, Y., and Courville, A. (2016). Deep learning. MIT press.

Lê, B. and Tô, V. (2014).
Cở sở trí tuệ nhân tạo.
Nhà xuất bản Khoa học và Kỹ thuật.

Russell, S. and Norvig, P. (2021).

Artificial intelligence: a modern approach.

Pearson Education Limited.