DM825 Introduction to Machine Learning

> Lecture 12 Bayesian Networks

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Outline

Conditional Independence Inference in BN

1. Conditional Independence

2. Inference in BN

Exact inference by enumeration Exact inference by variable elimination Exact inference by message passing Approximate inference by stochastic simulation Approximate inference by Markov chain Monte Carlo

Factorization

BN encode local conditional independences

 $\Pr(X_i \mid X_{-i}) = \Pr(X_i \mid \operatorname{pa}(X_i))$

Joint probability factorization (the global semantics simplifies to):

$$Pr(X_1, \dots, X_n) = \prod_{i=1}^n Pr(X_i \mid X_1, \dots, X_{i-1}) \text{ (chain rule)}$$
$$= \prod_{i=1}^n Pr(X_i \mid pa(X_i)) \text{ (by construction)}$$

When working with Bayesian Networks, the following probability theory rules are worth remembering:

- Product rule
- Sum rule (marginalization)
- Bayes rule
- Factorization

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Three Examples



$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

$$p(a, b) = \sum_{c} p(a, b, c) = \sum_{c} p(a|c)p(b|c)p(c)$$

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

$$p(a, b, c) = p(a)p(c|a)p(b|c)$$

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

Example

$$p(G = 1|B = 1, F = 1) = 0.8$$

$$p(G = 1|B = 1, F = 0) = 0.2$$

$$p(B = 1) = 0.9$$

$$p(G = 1|B = 0, F = 1) = 0.2$$

$$p(F = 1) = 0.9$$

$$p(G = 1|B = 0, F = 0) = 0.1$$



 $\begin{array}{l} p(F=0 \mid G=0) = ?\\ p(F=0 \mid G=0) \geq p(F=0)\\ p(F=0 \mid G=0, B=0) = ?\\ p(F=0 \mid G=0, B=0) \leq p(F=0 \mid G=0) \text{ (not conditional independent)}\\ B \text{ explains away } F \end{array}$

d-separation

Definition (d-separation)

Two distinct variables A and B in a causal network are d-separated ("d" for "directed graph") if for all paths between A and B, there is an intermediate variable C (distinct from A and B) such that either

- 1. the connection is tail-to-tail or head-to-tail and ${\it C}$ is instantiated or
- 2. the connection is head-to-head, and neither C nor any of C's descendants have received evidence.

If A and B are not d-separated, we call them d-connected.

If (1) then A indep. of B given CIf (2) then A indep. of B



Markov Blanket

Each node is conditionally independent of all others given its Markov blanket: parents + children + co-parents

$$p(\mathbf{x}_i \mid \mathbf{x}_{j \neq i}) = \frac{p(\mathbf{x}_1, \dots, \mathbf{x}_D)}{\sum_{\mathbf{x}_i} p(\mathbf{x}_1, \dots, \mathbf{x}_D)}$$
$$= \frac{\prod_k p(\mathbf{x}_k \mid \mathrm{pa}_k)}{\sum_{\mathbf{x}_i} \prod_k (\mathbf{x}_k \mid \mathrm{pa}_k)}$$



Algebra of Potentials

- General algebra of multiplication and marginalization on tables.
- ► For each outcome a variable has a corresponding state. States are mutually exclusive and exhaustive. The set of states associated with a variable A is denoted by sp(A) = (a₁, a₂, ..., a_n).
- ▶ Potential $\phi : sp(\mathcal{X}) \to \mathbb{R}$
- $\operatorname{dom}(\phi(A, B|C)) = \{A, B, C\}$ domain
- multiplication: $\phi_1\phi_2 : \operatorname{dom}(\phi_1\phi_2) = \operatorname{dom}(\phi_1) \cup \operatorname{dom}(\phi_2)$
- marginalization: $\sum_{A} \phi$ has domain $\operatorname{dom}(\phi) \setminus \{A\}$
- unit potential property: $\sum_{A} P(A \mid \mathcal{V}) = 1$
- ▶ projection for marginalization. Eg: if A and B are marginalized out of $\phi(A, B, C)$, we say ϕ is projected down to C

Moralization



Converting a directed graph into an undirected graph: On the undirected:

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{C} \psi_C(\mathbf{x}_c)$$

On the directed:

$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4 \mid x_1, x_2, x_3)$$

we introduce and edge for every arc and we marry parents

1. Conditional Independence

2. Inference in BN

Exact inference by enumeration Exact inference by variable elimination Exact inference by message passing Approximate inference by stochastic simulation Approximate inference by Markov chain Monte Carlo

Inference tasks

- \vec{e} assignment of values to some variables **E** (instantiation, evidence)
 - ▶ Probability of Evidence $Pr(\vec{e})$ Example: probability that an individual will come out positive on both tests Pr(T1 = +ve, T2 = +ve)overall reliability of the system Pr(S = avail)related: node marginals query: probability $Pr(x \mid e)$ for each X and for each of $x \in X$.
 - ▶ Most Probable Explanation (MPE) $\arg \max_{\vec{q} \in \mathbf{Q}} \Pr(\vec{q} \mid \vec{e}), \mathbf{Q} = \overline{\mathbf{E}}$ Example: find the most likely group, dissected by sex and condition, that will yield negative results for both tests ($\vec{e} = \{T_1 = -\text{ve}; T2 = -\text{ve}\}$ and $Q = \{S, C\}$)
 - ► Maximum a Posteriori Hypothesis (MAP) arg max_{q∈Q} Pr(q | e), Q ⊆ E Example: find most likely configuration of the two fans given that the system is unavailable (e = {S = unavail}, Q = {F1, F2}).

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Inference by enumeration

Sum out variables from the joint without actually constructing its explicit representation

Simple query on the burglary network:

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



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Rewrite full joint entries using product of CPT entries:

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

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

Enumeration algorithm

```
function Enumeration-Ask(X, e, bn) returns a distribution over X
   inputs: X, the query variable
             e, observed values for variables E
             bn, a Bayesian network with variables \{X\} \cup \mathbf{E} \cup \mathbf{Y}
    \mathbf{Q}(X) \leftarrow a distribution over X, initially empty
    for each value x_i of X do
         \mathbf{Q}(x_i) \leftarrow \mathsf{Enumerate-All}(bn.\mathsf{Vars}, \mathbf{e} \cup \{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 y in e
         then return P(y \mid parent(Y)) \times \text{Enumerate-All(Rest(vars), e)}
   else return \sum_{y} P(y \mid parent(Y)) \times \text{Enumerate-All(Rest(vars), e} \cup \{Y =
y
```

Evaluation tree



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

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Inference by variable elimination

Variable elimination: carry out summations right-to-left, storing intermediate results (factors) to avoid recomputation $\Pr(B \mid j, m)$

$$= \alpha \Pr(B) \sum_{B} \sum_{e} \Pr(e) \sum_{E} \sum_{a} \Pr(a \mid B, e) \Pr(j \mid a) \Pr(m \mid a)$$

$$= \alpha \Pr(B) \sum_{e} P(e) \sum_{a} \Pr(a \mid B, e) P(j \mid a) f_M(a)$$

$$= \alpha \Pr(B) \sum_{e} P(e) \sum_{a} \Pr(a \mid B, e) f_J(a) f_M(a)$$

$$= \alpha \Pr(B) \sum_{e} P(e) \sum_{a} f_A(a, b, e) f_J(a) f_M(a)$$

$$= \alpha \Pr(B) \sum_{e} P(e) f_{\bar{A}JM}(b, e) \text{ (sum out } A)$$

$$= \alpha \Pr(B) f_{\bar{E}\bar{A}JM}(b) \text{ (sum out } E)$$

$$= \alpha f_B(b) \times f_{\bar{E}\bar{A}JM}(b)$$

Variable elimination: Basic operations

Conditional Independence Inference in BN

Summing out a variable from a product of factors:

1. move any constant factors outside the summation:

2. add up submatrices in pointwise product of remaining factors:

Variable elimination: Basic operations

Summing out a variable from a product of factors:

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$$\sum_{f_1 \times \cdots \times f_k} f_1 \times \cdots \times f_k = f_1 \times \cdots \times f_i \sum_x f_{i+1} \times \cdots \times f_k = f_1 \times \cdots \times f_i \times f_{\bar{X}}$$
assuming f_1, \ldots, f_i do not depend on X

2. add up submatrices in pointwise product of remaining factors:

Variable elimination: Basic operations

Summing out a variable from a product of factors:

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

2. add up submatrices in pointwise product of remaining factors:

Eg: pointwise product of f_1 and f_2 : $f_1(x_1, ..., x_j, y_1, ..., y_k) \times f_2(y_1, ..., y_k, z_1, ..., z_l)$ $= f(x_1, ..., x_j, y_1, ..., y_k, z_1, ..., z_l)$ E.g., $f_1(a, b) \times f_2(b, c) = f(a, b, c)$

Irrelevant variables



Irrelevant variables contd.

Defn: moral graph of DAG Bayes net: marry all parents and drop arrows Defn: $\overline{\mathbf{A}}$ is m-separated from \mathbf{B} by \mathbf{C} iff separated by \mathbf{C} in the moral graph

Theorem

Y is irrelevant if m-separated from X by E

For $P(JohnCalls \mid Alarm = true)$, both Burglary and Earthquake are irrelevant



Singly connected networks (or polytrees):

- any two nodes are connected by at most one (undirected) path
- time and space cost (with variable elimination) are ${\cal O}(d^kn),\,k$ number of parents
 - hence time and space cost are linear in n and k bounded by a constant

Multiply connected networks:

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

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Exact inference by message passing

Approximate inference by stochastic simulation Approximate inference by Markov chain Monte Carlo If we want the posteriror of each variable then even if poly tree O(n)O(n)Join tree reduce the complexity to O(n)Idea: join individual nodes such that the resulting network is a polytree

Chains



We want to infer maringal of x_j with no evidence

Chains



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$$p(x_{n}) = \frac{1}{Z}$$

$$\underbrace{\left[\sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_{n}) \cdots \left[\sum_{x_{2}} \psi_{2,3}(x_{2}, x_{3}) \left[\sum_{x_{1}} \psi_{1,2}(x_{1}, x_{2})\right]\right] \cdots\right]}_{\mu_{\alpha}(x_{n})}_{\mu_{\alpha}(x_{n})}$$

$$\underbrace{\left[\sum_{x_{n+1}} \psi_{n,n+1}(x_{n}, x_{n+1}) \cdots \left[\sum_{x_{N}} \psi_{N-1,N}(x_{N-1}, x_{N})\right] \cdots\right]}_{\mu_{\beta}(x_{n})}.$$
(8.52)

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Conditional Independence Inference in BN

Basic idea:

- \blacktriangleright Draw N samples from a sampling distribution S
- Compute an approximate posterior probability \hat{P}
- 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
- Markov chain Monte Carlo (MCMC): sample from a stochastic process whose stationary distribution is the true posterior

Sampling from an empty network

```
function Prior-Sample(bn) returns an event sampled from bn

inputs: bn, a belief network specifying joint distribution

Pr(X_1, ..., X_n)

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

for i = 1 to n do

x_i \leftarrow a random sample from Pr(X_i \mid parents(X_i))

given the values of pa(X_i) in \mathbf{x}

return \mathbf{x}
```

Ancestor sampling

Conditional Independence Inference in BN

Example














Probability that PriorSample generates a particular event

 $S_{PS}(x_1 \dots x_n) = P(x_1 \dots x_n)$

i.e., the true prior probability

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Proof: Let $N_{PS}(x_1 \dots x_n)$ be the number of samples generated for event x_1, \dots, x_n . Then we have

$$\lim_{N \to \infty} \bar{P}(x_1, \dots, x_n) = \lim_{N \to \infty} N_{PS}(x_1, \dots, x_n) / N$$
$$= S_{PS}(x_1, \dots, x_n)$$
$$= \prod_{i=1}^n P(x_i | parents(X_i)) = P(x_1 \dots x_n)$$

Probability that PriorSample generates a particular event

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

 \sim That is, estimates derived from PriorSample are consistent Shorthand: $\hat{P}(x_1, \ldots, x_n) \approx P(x_1 \ldots x_n)$

Rejection sampling

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

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```
function Rejection-Sampling(X, e, bn, N) returns an estimate of P(X|e)
local variables: N, a vector of counts over X, initially zero
for j = 1 to N do
x \leftarrow Prior-Sample(bn)
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[X])
```

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```

E.g., estimate Pr(Rain|Sprinkler = true) using 100 samples 27 samples have Sprinkler = trueOf these, 8 have Rain = true and 19 have Rain = false.

 $\hat{\Pr}(Rain|Sprinkler = true) = \text{Normalize}(\langle 8, 19 \rangle) = \langle 0.296, 0.704 \rangle$ Similar to a basic real-world empirical estimation procedure Rejection sampling returns consistent posterior estimates

 $\begin{array}{ll} \mbox{Proof:} \\ \hat{\Pr}(X|\mathbf{e}) &= \alpha \mathbf{N}_{PS}(X,\mathbf{e}) & (\mbox{algorithm defn.}) \\ &= \mathbf{N}_{PS}(X,\mathbf{e})/N_{PS}(\mathbf{e}) & (\mbox{normalized by } N_{PS}(\mathbf{e})) \\ &\approx \Pr(X,\mathbf{e})/P(\mathbf{e}) & (\mbox{property of PriorSample}) \\ &= \Pr(X|\mathbf{e}) & (\mbox{defn. of conditional probability}) \end{array}$

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Problem: hopelessly expensive if $P(\mathbf{e})$ is small $P(\mathbf{e})$ drops off exponentially with number of evidence variables!

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 Likelihood-Weighting(X, e, bn, N) returns an estimate of P(X|e)
local variables: W, a vector of weighted counts over X, initially zero
```

```
for j = 1 to N do

\mathbf{x}, w \leftarrow \text{Weighted-Sample}(bn)

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

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

function Weighted-Sample(bn, e) returns an event and a weight

```
 \begin{array}{l} \mathbf{x} \leftarrow \text{an event with } n \text{ elements; } w \leftarrow 1 \\ \text{for } i = 1 \text{ to } n \text{ do} \\ \text{ if } X_i \text{ has a value } x_i \text{ in e} \\ & \quad \text{then } w \leftarrow w \times \ P(X_i = \ x_i \mid parents(X_i)) \\ & \quad \text{else } x_i \leftarrow \text{a random sample from } \Pr(X_i \mid parents(X_i)) \\ \text{return } \mathbf{x}, \ w \end{array}
```



w = 1.0



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w = 1.0



 $w = 1.0 \times 0.1$



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 $w=1.0\ \times 0.1$



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

Likelihood weighting analysis

Likelihood weighting returns consistent estimates

Sampling probability for WeightedSample is

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

(pays attention to evidence in ancestors only) ${\sim}{\rightarrow}$ somewhere "in between" prior and posterior distribution

Weight for a given sample \mathbf{z}, \mathbf{e} is

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



Likelihood weighting analysis

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Weighted sampling probability is

$$S_{WS}(\mathbf{z}, \mathbf{e})w(\mathbf{z}, \mathbf{e}) = \prod_{i=1}^{l} P(z_i | parents(Z_i)) \prod_{i=1}^{m} P(e_i | parents(E_i)) = P(\mathbf{z}, \mathbf{e})$$



Likelihood weighting analysis

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Weight for a given sample \mathbf{z}, \mathbf{e} is

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



but performance still degrades with many evidence variables because a few samples have nearly all the total weight

Weighted sampling probability is

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Summary

Approximate inference by LW:

- LW does poorly when there is lots of (late-in-the-order) evidence
- LW generally insensitive to topology
- Convergence can be very slow with probabilities close to 1 or 0
- Can handle arbitrary combinations of discrete and continuous variables

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Approximate inference using MCMC

Conditional Independence Inference in BN

"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 estimate of P(X|e)
local variables: N[X], a vector of counts over X, initially zero
Z, nonevidence variables in bn, hidden + query
x, current state of the network, initially copied from e
initialize x with random values for the variables in Z
for j = 1 to N do
N[x] \leftarrow N[x] + 1 where x is the value of X in x
for each Z_i in Z do
sample the value of Z_i in x from Pr(Z_i|mb(Z_i))
given the values of MB(Z_i) in x
return Normalize(N[X])
```

Can also choose a variable to sample at random each time

The Markov chain

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



Wander about for a while, average what you see

The Markov chain

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Wander about for a while, average what you see

Probabilistic finite state machine

Estimate Pr(Rain|Sprinkler = true, WetGrass = true)

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Sample Cloudy or Rain given its Markov blanket, repeat.

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Sample *Cloudy* or *Rain* given its Markov blanket, repeat. Count number of times *Rain* is true and false in the samples.

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Sample *Cloudy* or *Rain* given its Markov blanket, repeat. Count number of times *Rain* is true and false in the samples.

E.g., visit 100 states 31 have Rain = true, 69 have Rain = false

 $\hat{\Pr}(Rain|Sprinkler = true, WetGrass = true) = \mathsf{Normalize}(\langle 31, 69 \rangle) = \langle 0.31, 0.5 \rangle$
MCMC example contd.

Estimate Pr(Rain|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.

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 $\hat{\Pr}(Rain|Sprinkler = true, WetGrass = true) = \mathsf{Normalize}(\langle 31, 69 \rangle) = \langle 0.31, 0.5 \rangle$

Theorem

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

Markov blanket sampling

Markov blanket of *Cloudy* is *Sprinkler* and *Rain*

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



Conditional Independence Inference in BN

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Probability given the Markov blanket is calculated as follows:

$$P(x'_i|mb(X_i)) = P(x'_i|parents(X_i)) \prod_{Z_j \in Children(X_i)} P(z_j|parents(Z_j))$$

Easily implemented in message-passing parallel systems

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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:

 $P(X_i|mb(X_i))$ won't change much (law of large numbers)

Local semantics and Markov Blanket

Conditional Independence Inference in BN

Local semantics: each node is conditionally independent of its nondescendants given its parents Each node is conditionally independent of all others given its Markov blanket: parents + children + children's parents





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

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- If π exists, it is unique (specific to $q(\mathbf{x} \to \mathbf{x}')$)
- In equilibrium, expected "outflow" = expected "inflow"

Detailed balance

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

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

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

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

Summary

Exact inference by variable elimination:

- polytime on polytrees, NP-hard on general graphs
- space = time, very sensitive to topology

Approximate inference by LW, MCMC:

- PriorSampling and RejectionSampling unusable as evidence grow
 - LW does poorly when there is lots of (late-in-the-order) evidence
 - LW, MCMC generally insensitive to topology
 - Convergence can be very slow with probabilities close to $1 \mbox{ or } 0$
 - Can handle arbitrary combinations of discrete and continuous variables