Machine Learning Department
School of Computer Science
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Computational Complexity of Inference

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Monte Carlo Methods

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Lecture 12
Mar. 10, 2021

Reminders

- Homework 2: Exact inference and supervised learning (CRF+RNN)
  – Out: Wed, Feb. 24
  – Due: Wed, Mar. 10 at 11:59pm
- Project Team Formation Office Hours
  – Fri, Mar 12 at 3:10pm in Gather.Town
- Quiz 1: Mon, Mar. 15
- Homework 3: Structured SVM
  – Out: Wed, Mar. 10
  – Due: Wed, Mar. 24 at 11:59pm

COMPUTATIONAL COMPLEXITY OF INFERENCE

Proving Computational Complexity

Question:

In order to prove that a decision problem is NP-Hard, we must…

A. …reduce our decision problem to a known NP-Hard problem.
B. …reduce a known NP-Hard problem to our decision problem.

Answer:

Complexity Classes

- An algorithm runs in **polynomial time** if its runtime is a polynomial function of the input size (e.g. $O(n^k)$ for some fixed constant k)
- The **class P** consists of all problems that can be solved in polynomial time

- A problem for which the answer is binary (e.g. yes/no) is called a **decision problem**
- The **class NP** contains all decision problems where 'yes' answers can be verified (proved) in polynomial time
- A problem is **NP-Hard** if given an O(1) oracle to solve it, every problem in NP can be solved in polynomial time (e.g. by reduction)
- A problem is **NP-Complete** if it belongs to both the classes NP and NP-Hard

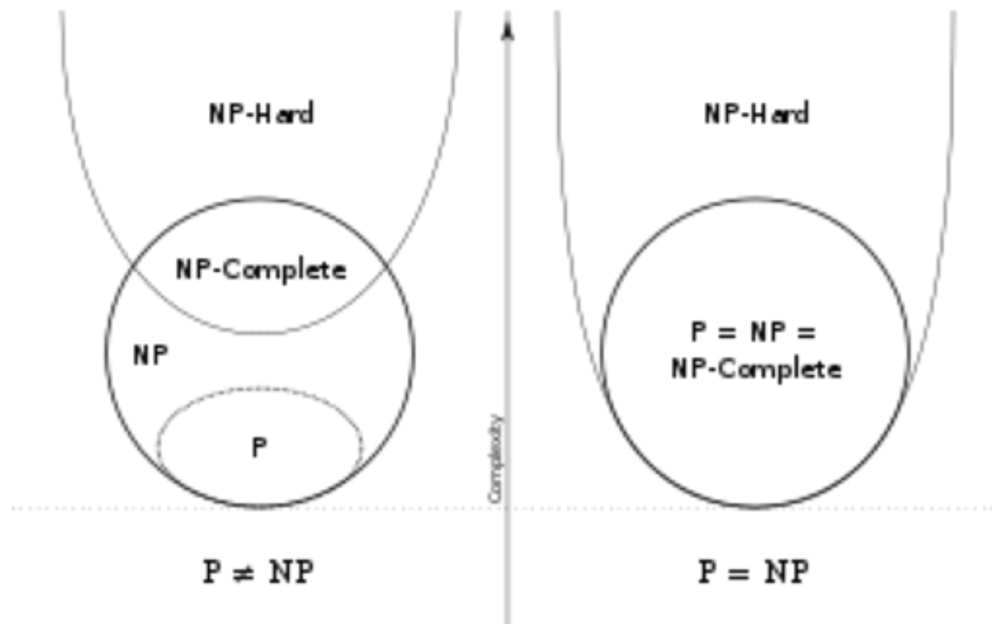


Figure from https://en.wikipedia.org/wiki/NP-completeness

Complexity Classes

Recall...

- A problem for which the answer is a nonnegative integer is called a **counting problem**
- The **class #P** contains the counting problems that align to decision problems in NP
  - really this is the class of problems that count the number of accepting paths in a Turing machine that is nondeterministic and runs in polynomial time
- A problem is **#P-Hard** if given an O(1) oracle to solve it, every problem in #P can be solved in polynomial time (e.g. by reduction)
- A problem is **#P-Complete** if it belongs to both the classes #P and #P-Hard
- There are no known polytime algorithms for solving #P-Complete problems. If we found one it would imply that P = NP.

Examples of #P-Hard problems

- #SAT, i.e. how many satisfying solutions for a given SAT problem?
- How many solutions for a given DNF formula?
- How many solutions for a 2-SAT problem?
- How many perfect matchings for a bipartite graph?
- How many graph colorings (with k colors) for a given graph G?

Examples from https://en.wikipedia.org/wiki/%E2%99%AFP-complete

Recall...

5. Inference

Three Tasks:

1. Marginal Inference (#P-Hard)
Compute marginals of variables and cliques

$$p(x_i) = \sum_{\boldsymbol{x}' : x'_i = x_i} p(\boldsymbol{x}' \mid \boldsymbol{\theta}) \quad \Bigg| \quad p(\boldsymbol{x}_C) = \sum_{\boldsymbol{x}' : \boldsymbol{x}'_C = \boldsymbol{x}_C} p(\boldsymbol{x}' \mid \boldsymbol{\theta})$$

2. Partition Function (#P-Hard)
Compute the normalization constant

$$Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C)$$

3. MAP Inference (NP-Hard)
Compute variable assignment with highest probability

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{argmax}}\ p(\boldsymbol{x} \mid \boldsymbol{\theta})$$

3-SAT

Background:

- Formulas
  - *Def:* a **literal** is a binary variable or its negation, e.g. x_1 is a positive literal and $\neg x_1$ is a negative literal, where $x_1 \in \{0, 1\}$
  - *Def*: a **clause** is a disjunction of literals, e.g. $(\neg x_1 \lor x_2 \lor \neg x_3)$
  - *Def*: a formula is in **conjunctive normal form (CNF)** if it is a conjunction of clauses, e.g.
    $(\neg x_1 \lor x_2 \lor \neg x_3) \land (x_2 \lor x_4 \lor \neg x_6) \land (x_1 \lor \neg x_3 \lor \neg x_5)$
- The 3-SAT Problem
  - **Given**: a CNF formula where each clause has at most 3 literals
  - **Goal**: report the satisfiability of the formula, i.e. whether there is a satisfying assignment to the variables that makes the entire formula true

Computational Complexity of MAP Inference

- **Claim**: MAP inference is NP-Hard
- **Proof Sketch**:
  Overview: we reduce 3-SAT (known to be NP-Hard) to the MAP Inference problem
  1. Construct a factor graph as follows:
     a. add a variable x_i to the factor graph for each variable in 3-SAT
     b. add a variable c_l to the factor graph for each clause in 3-SAT
     c. add a factor $\Psi(c_l, x_i, x_j, x_k)$ for each clause $c_l(x_i, x_j, x_k)$
     d. let the factor $\Psi(c_l, x_i, x_j, x_k) = 1$ if $c_l(x_i, x_j, x_k) =$ true and $\Psi(x_i, x_j, x_k) = 0$ otherwise
  2. Run MAP inference to obtain the most probable assignment
  3. Return true if all the clause variables are true; and false otherwise

#-SAT

Background:

- The 3-SAT Problem
  - **Given:** a CNF formula where each clause has at most 3 literals
  - **Goal**: report the satisfiability of the formula, i.e. whether there is a satisfying assignment to the variables that makes the entire formula true

- The #-SAT Problem
  - **Given:** a CNF formula where each clause has at most 3 literals
  - **Goal**: report the number of satisfying assignments of the formula

Computational Complexity of Marginal Inference

- **Claim:** Marginal inference is #P-Hard
- **Proof Sketch:**
  Overview: we reduce #-SAT (known to be #P-Hard) to the marginal inference problem
  1. Construct a factor graph as follows:
     a. …left as an exercise…
  2. Run marginal inference
  3. Return the number of satisfying assigments by…
     a. …left as an exercise…

Outline

- **Monte Carlo Methods**
- **MCMC (Basic Methods)**
  - Metropolis algorithm
  - Metropolis-Hastings (M-H) algorithm
  - Gibbs Sampling
- **Markov Chains**
  - Transition probabilities
  - Invariant distribution
  - Equilibrium distribution
  - Markov chain as a WFSM
  - Constructing Markov chains
  - Why does M-H work?
- **MCMC (Auxiliary Variable Methods)**
  - Slice Sampling
  - Hamiltonian Monte Carlo

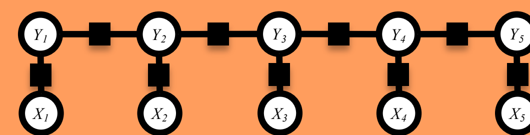
APPROXIMATE MARGINAL INFERENCE

1. Data

$$\mathcal{D} = \{\boldsymbol{x}^{(n)}\}_{n=1}^{N}$$

2. Model

$$p(\boldsymbol{x} \mid \boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C)$$



3. Objective

$$\ell(\theta; \mathcal{D}) = \sum_{n=1}^{N} \log p(\boldsymbol{x}^{(n)} \mid \boldsymbol{\theta})$$

5. Inference

1. Marginal Inference

$$p(\boldsymbol{x}_C) = \sum_{\boldsymbol{x}' : \boldsymbol{x}'_C = \boldsymbol{x}_C} p(\boldsymbol{x}' \mid \boldsymbol{\theta})$$

2. Partition Function

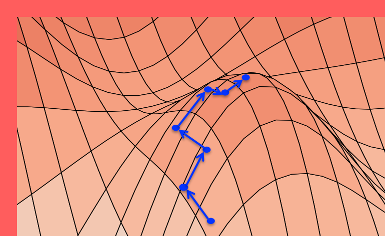
$$Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C)$$

3. MAP Inference

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{argmax}}\ p(\boldsymbol{x} \mid \boldsymbol{\theta})$$

4. Learning

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, \ell(\boldsymbol{\theta}; \mathcal{D})$$



A Few Problems for a Factor Graph

Suppose we already have the parameters of a Factor Graph…

1. How do we compute the probability of a specific assignment to the variables?
   P(T=t, H=h, A=a, C=c)

2. How do we draw a sample from the joint distribution?
   t,h,a,c ~ P(T, H, A, C)

3. How do we compute marginal probabilities?
   P(A) = …

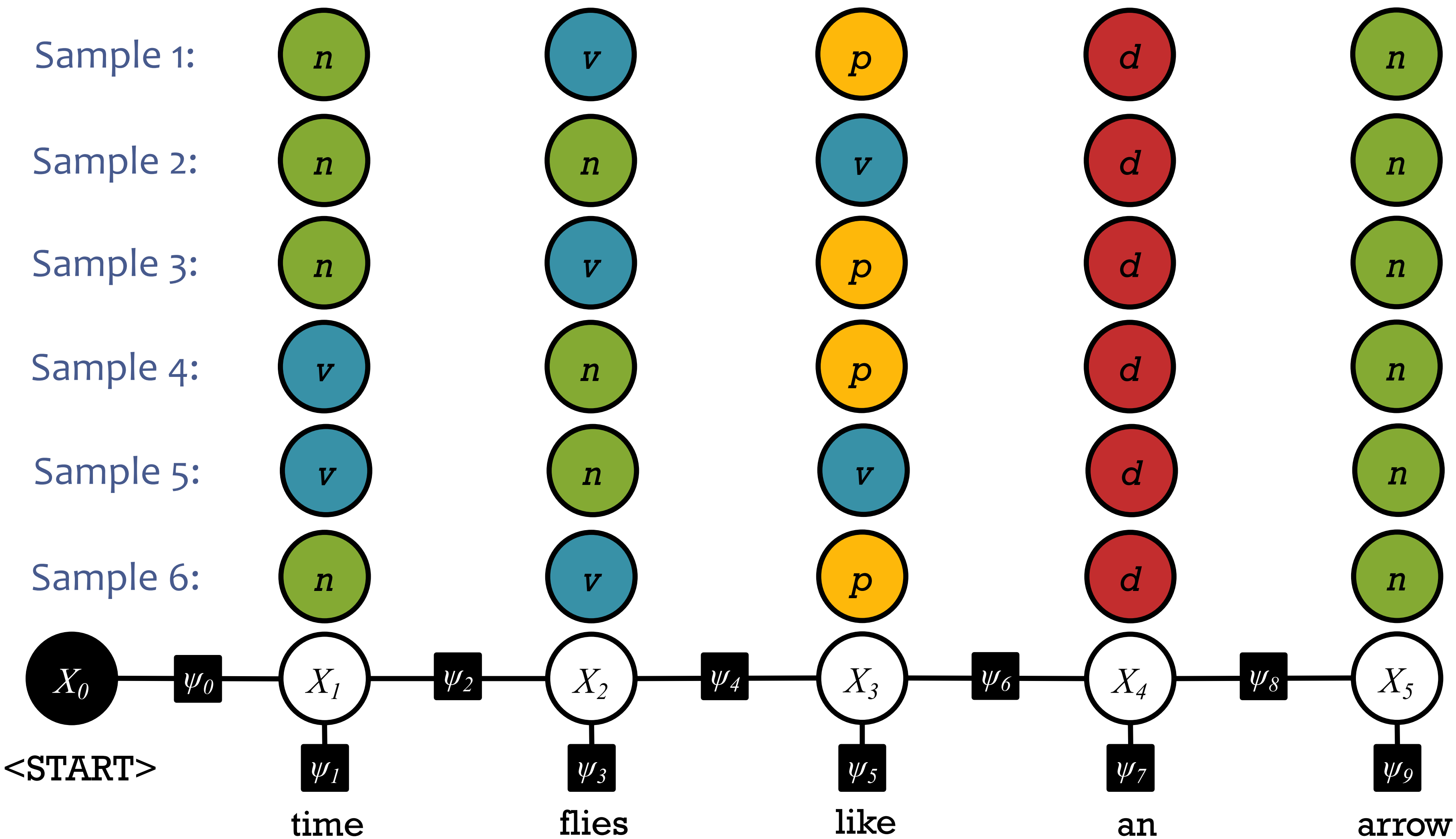
4. How do we draw samples from a conditional distribution?
   t,h,a ~ P(T, H, A | C = c)

5. How do we compute conditional marginal probabilities?
   P(H | C = c) = …

Can we use samples ?

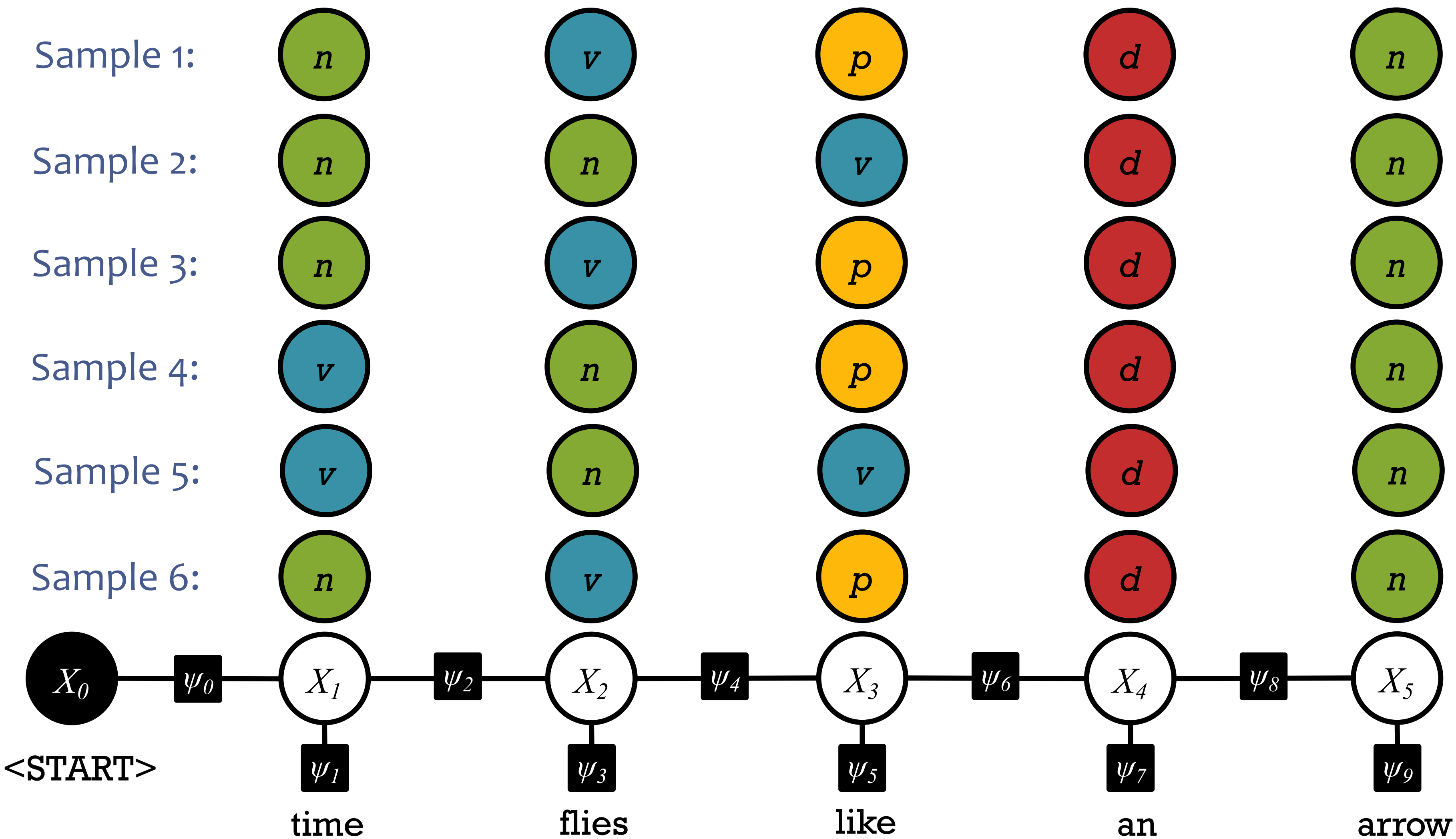
Marginals by Sampling on Factor Graph

Suppose we took many samples from the distribution over taggings: $p(\boldsymbol{x}) = \frac{1}{Z} \prod_{\alpha} \psi_{\alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}})$

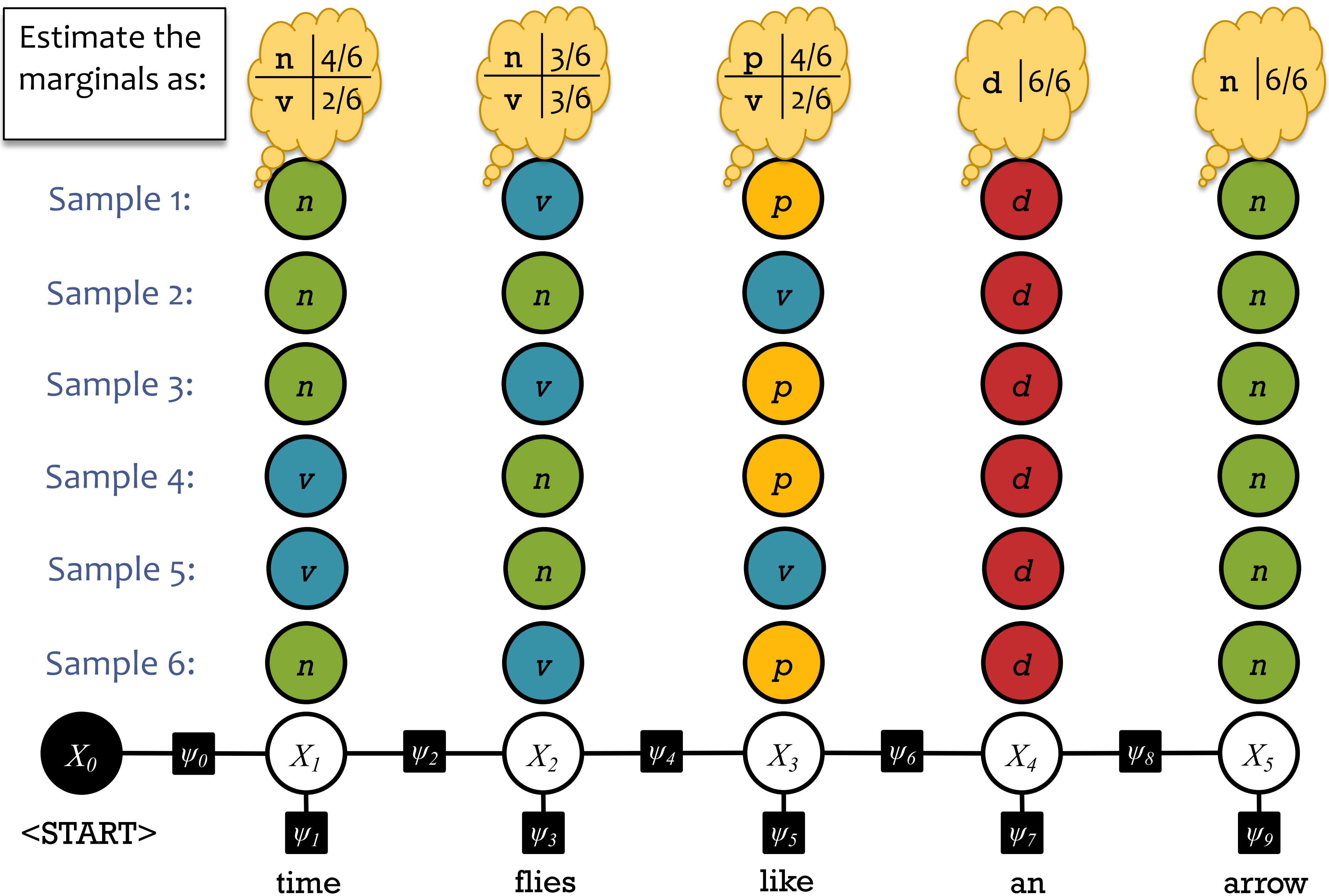


Marginals by Sampling on Factor Graph

The marginal $p(X_i = x_i)$ gives the probability that variable X_i takes value x_i in a random sample



Marginals by Sampling on Factor Graph



MONTE CARLO METHODS

Monte Carlo Methods

Whiteboard

- Problem 1: Generating samples from a distribution
- Problem 2: Estimating expectations
- Why is sampling from p(x) hard?
- Example: estimating plankton concentration in a lake
- Algorithm: Uniform Sampling
- Example: estimating partition function of high dimensional function

Properties of Monte Carlo

Estimator: $$\int f(x)P(x)\,\mathrm{d}x \;\approx\; \hat{f} \;\equiv\; \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)}), \quad x^{(s)} \sim P(x)$$

Estimator is unbiased:

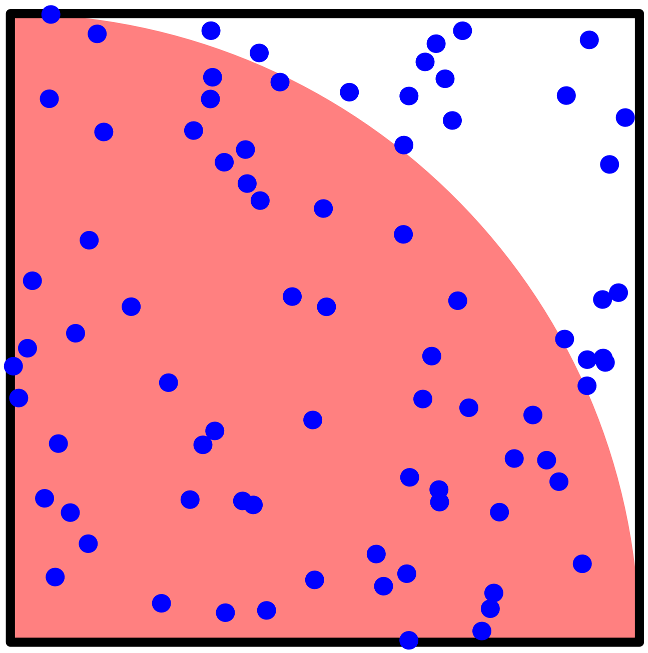
$$\mathbb{E}_{P(\{x^{(s)}\})}\left[\hat{f}\right] \;=\; \frac{1}{S}\sum_{s=1}^{S}\mathbb{E}_{P(x)}[f(x)] \;=\; \mathbb{E}_{P(x)}[f(x)]$$

Variance shrinks $\propto 1/S$:

$$\mathrm{var}_{P(\{x^{(s)}\})}\left[\hat{f}\right] \;=\; \frac{1}{S^2}\sum_{s=1}^{S}\mathrm{var}_{P(x)}[f(x)] \;=\; \mathrm{var}_{P(x)}[f(x)]\,/S$$

“Error bars” shrink like $\sqrt{S}$

A dumb approximation of π



$$P(x,y) = \begin{cases} 1 & 0 < x < 1 \text{ and } 0 < y < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\pi = 4 \iint \mathbb{I}\left((x^2+y^2) < 1\right) P(x,y)\, \mathrm{d}x\, \mathrm{d}y$$

```
octave:1> S=12; a=rand(S,2); 4*mean(sum(a.*a,2)<1)
ans = 3.3333
octave:2> S=1e7; a=rand(S,2); 4*mean(sum(a.*a,2)<1)
ans = 3.1418
```

Aside: don't always sample!

"Monte Carlo is an extremely bad method; it should be used only when all alternative methods are worse."

— Alan Sokal, 1996

Example: numerical solutions to (nice) 1D integrals are fast

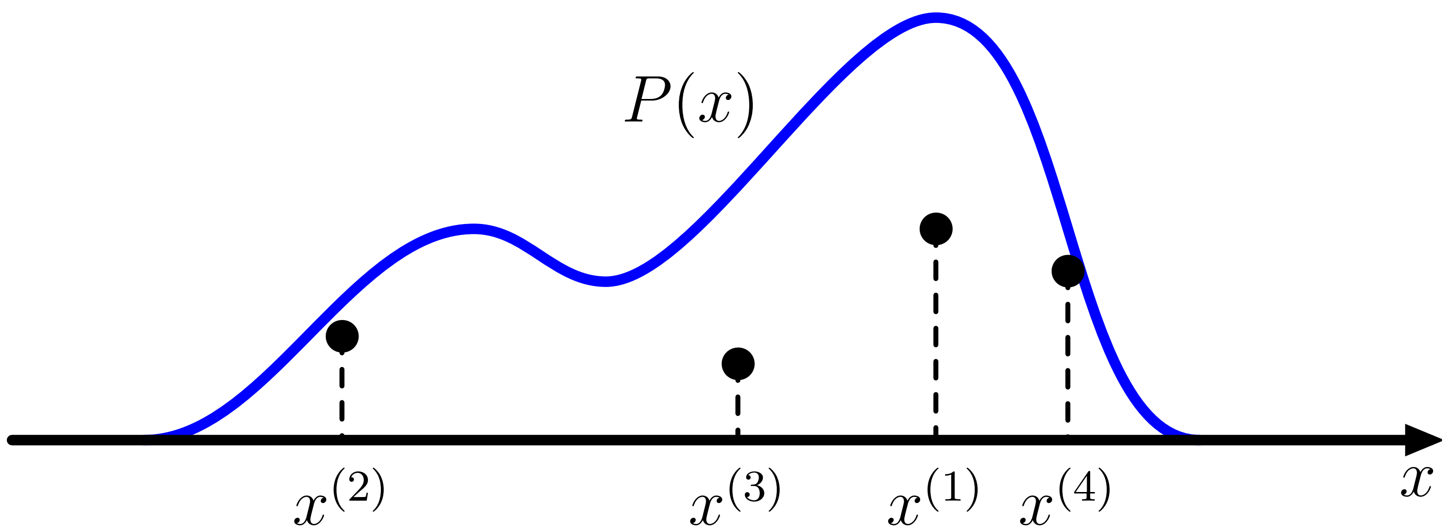
```
octave:1> 4 * quadl(@(x) sqrt(1-x.^2), 0, 1, tolerance)
```

Gives π to 6 dp's in 108 evaluations, machine precision in 2598.

(NB Matlab's `quadl` fails at zero tolerance)

Sampling from distributions

Draw points uniformly under the curve:



Probability mass to left of point $\sim$ Uniform[0,1]

Sampling from distributions

How to convert samples from a Uniform[0,1] generator:

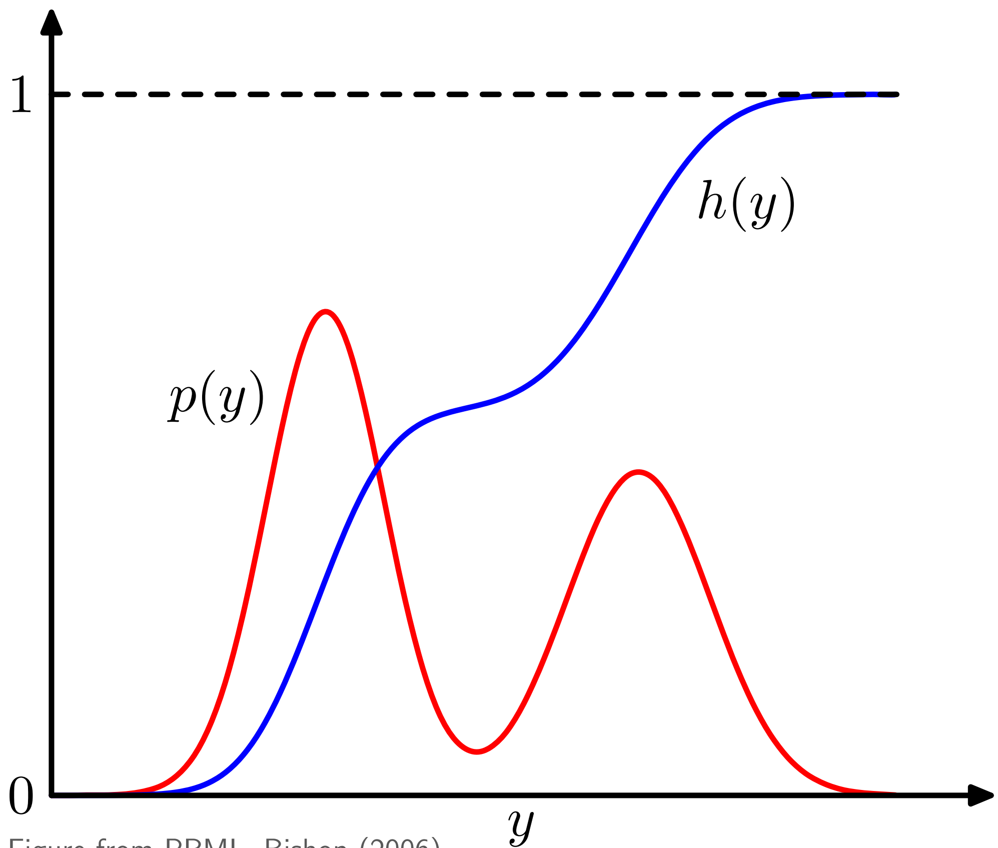


Figure from PRML, Bishop (2006)

$$h(y) = \int_{-\infty}^{y} p(y')\, \mathrm{d}y'$$

Draw mass to left of point:
$u \sim$ Uniform[0,1]

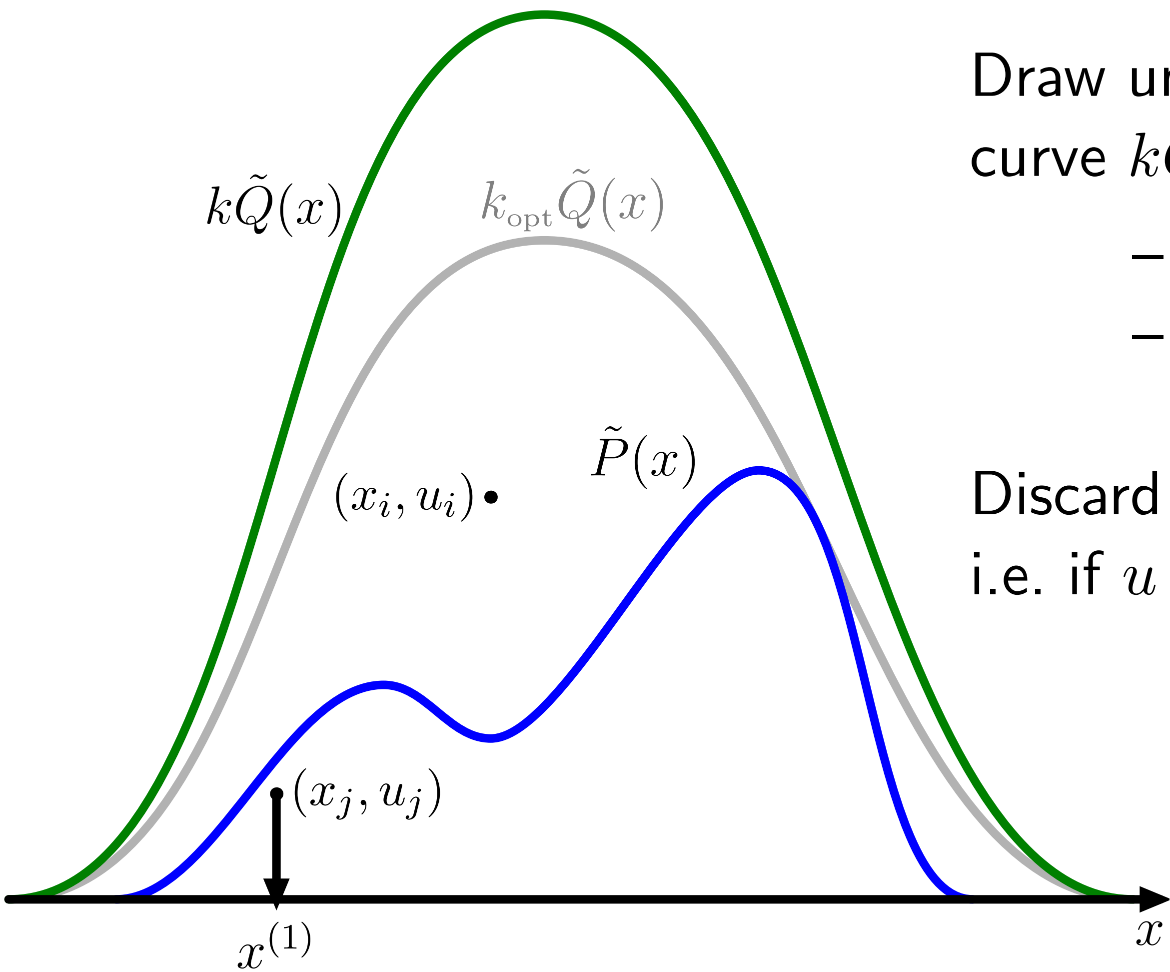
Sample, $y(u) = h^{-1}(u)$

Although we can't always compute and invert $h(y)$

$x^{(2)}$
$x^{(1)}$
x

Rejection sampling

Sampling underneath a $\tilde{P}(x) \propto P(x)$ curve is also valid



Draw underneath a simple curve $k\tilde{Q}(x) \geq \tilde{P}(x)$:

- Draw $x \sim Q(x)$
- height $u \sim$ Uniform$[0, k\tilde{Q}(x)]$

Discard the point if above $\tilde{P}$, i.e. if $u > \tilde{P}(x)$

Importance sampling

Computing $\tilde{P}(x)$ and $\tilde{Q}(x)$, then *throwing* x *away* seems wasteful
Instead rewrite the integral as an expectation under Q:

$$\int f(x)P(x)\,\mathrm{d}x \;=\; \int f(x)\frac{P(x)}{Q(x)}Q(x)\,\mathrm{d}x, \qquad (Q(x)>0 \text{ if } P(x)>0)$$

$$\approx \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)})\frac{P(x^{(s)})}{Q(x^{(s)})}, \quad x^{(s)} \sim Q(x)$$

This is just simple Monte Carlo again, so it is unbiased.

Importance sampling applies when the integral is not an expectation.
Divide and multiply any integrand by a convenient distribution.

Importance sampling (2)

Previous slide assumed we could evaluate $P(x) = \tilde{P}(x)/\mathcal{Z}_P$

$$\int f(x)P(x)\,\mathrm{d}x \;\approx\; \frac{\mathcal{Z}_Q}{\mathcal{Z}_P}\,\frac{1}{S}\sum_{s=1}^{S} f(x^{(s)})\underbrace{\frac{\tilde{P}(x^{(s)})}{\tilde{Q}(x^{(s)})}}_{\tilde{r}^{(s)}}, \quad x^{(s)} \sim Q(x)$$

$$\approx\; \frac{\cancel{1}}{\cancel{S}}\sum_{s=1}^{S} f(x^{(s)})\frac{\tilde{r}^{(s)}}{\frac{\cancel{1}}{\cancel{S}}\sum_{s'}\tilde{r}^{(s')}} \;\equiv\; \sum_{s=1}^{S} f(x^{(s)})w^{(s)}$$

This estimator is **consistent** but **biased**

Exercise: Prove that $\mathcal{Z}_P/\mathcal{Z}_Q \approx \frac{1}{S}\sum_s \tilde{r}^{(s)}$

Summary so far

- Sums and integrals, often expectations, occur frequently in statistics
- **Monte Carlo** approximates expectations with a sample average
- **Rejection sampling** draws samples from complex distributions
- **Importance sampling** applies Monte Carlo to 'any' sum/integral

Pitfalls of Monte Carlo

Rejection & importance sampling scale badly with dimensionality

Example:

$$P(x) = \mathcal{N}(0, \mathbb{I}), \quad Q(x) = \mathcal{N}(0, \sigma^2\mathbb{I})$$

Rejection sampling:

Requires $\sigma \geq 1$. Fraction of proposals accepted $= \sigma^{-D}$

Importance sampling:

Variance of importance weights $= \left(\frac{\sigma^2}{2-1/\sigma^2}\right)^{D/2} - 1$

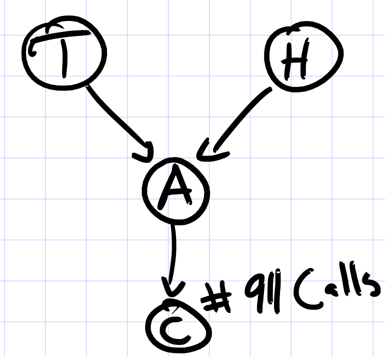
Infinite / undefined variance if $\sigma \leq 1/\sqrt{2}$

Metropolis, Metropolis-Hastings, Gibbs Sampling

MCMC (BASIC METHODS)

Sampling from a Joint Distribution

Ex: Tornado



$$T \sim \text{Bernoulli}(\tau) \qquad \tau = 1/2$$

$$H \sim \text{Bernoulli}(\eta) \qquad \eta = 1/3$$

$$A \sim \text{Bernoulli}(\alpha_{H,T}) \qquad \alpha = \begin{array}{c|cc} & T=0 & T=1 \\ \hline H=0 & 0 & 1/2 \\ H=1 & 1/2 & 1 \end{array}$$

$$C \sim \text{Unif}(\{1,\ldots,63\}) + A * \text{Unif}(\{1,\ldots,63\})$$

← integer

We can use these samples to estimate many different probabilities!

T	H	A	C

A Few Problems for a Factor Graph

Suppose we already have the parameters of a Factor Graph…

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   $P(T=t, H=h, A=a, C=c)$

2. How do we draw a sample from the joint distribution?
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3. How do we compute marginal probabilities?
   $P(A) = \dots$

4. How do we draw samples from a conditional distribution?
   $t,h,a \sim P(T, H, A \mid C = c)$

5. How do we compute conditional marginal probabilities?
   $P(H \mid C = c) = \dots$

Can we use samples ?

MCMC

- **Goal:** Draw approximate, correlated samples from a target distribution p(x)
- **MCMC:** Performs a biased random walk to explore the distribution