## CS 6347

## Lecture 10

## Sampling Methods

## Sampling vs. Variational Methods

- Sampling:
- Guaranteed to approach the correct answer in the limit
- Can be quite slow to converge
- Variational methods:
- Only approximate the true solution
- Possible to make them quite fast


## Sampling: The Basics

$$
p\left(x_{1}, \ldots, x_{n}\right)=\frac{1}{Z} \prod_{C} \psi_{C}\left(x_{C}\right)
$$

- Idea: if we could generate independent samples from $p$, we could use them to estimate the partition function, marginals, etc.
- A sample is an instantiation/assignment of a value for each of the random variables

$$
x^{t}=\left(x_{1}^{t}, \ldots, x_{n}^{t}\right)
$$

## Sampling: The Basics

$$
p\left(x_{1}, \ldots, x_{n}\right)=\frac{1}{Z} \prod_{C} \psi_{C}\left(x_{C}\right)
$$

- Given $T$ i.i.d. samples $x^{1}, \ldots, x^{T}$ drawn from the distribution $p$, we could estimate marginal probabilities
- But how do we generate samples from a distribution?


## Sampling: The Basics

- Let's begin with a simple example
- Suppose we want to sample from a univariate probability distribution, $q(y)$, where $y \in\{1, \ldots, k\}$
- Sampling algorithm:
- Divide the unit interval into $k$ pieces corresponding to the probabilities $q(1), \ldots, q(k)$

- Pick a random number $z$ in $[0,1]$
- If $z$ is in the $j^{t h}$ box, return $j$


## Sampling: Bayesian Networks

- We can use the same idea to sample from (discrete) Bayesian networks
- Sample the variables one at a time, in topological order
- Because of the graph structure, we only have to sample from univariate (conditional) distributions!


## Sampling: Bayesian Networks

|  |  |  | $P(A)$ |
| :---: | :---: | :---: | :---: |
|  |  |  | . 3 |
|  |  |  | . 7 |
| A | $B$ | C | $P(C \mid A, B)$ |
| 0 | 0 | 0 | . 1 |
| 0 | 0 | 1 | . 9 |
| 0 | 1 | 0 | . 2 |
| 0 | 1 | 1 | . 8 |
| 1 | 0 | 0 | 0 |
| 1 | 0 | 1 | 1 |
| 1 | 1 | 0 | . 25 |
| 1 | 1 | 1 | . 75 |


| $B$ | $P(B)$ |
| :---: | :---: |
| 0 | .4 |
| 1 | .6 |


random numbers: $0.8663,0.0253,0.1714,0.8309$

## Monte Carlo Methods

- Express the estimation problem as the expectation of a random variable

$$
E_{p}[f(x)]=\sum_{x} f(x) \cdot p(x)
$$

- To estimate this expectation, draw samples $x^{1}, \ldots, x^{T}$ i.i.d. from $p$ and approximate the expectation as

$$
\hat{f}=\sum_{t} \frac{f\left(x^{t}\right)}{T}
$$

## Monte Carlo Methods

- Law of Large Numbers: as $T \rightarrow \infty$,

$$
\sum_{t} \frac{f\left(x^{t}\right)}{T} \rightarrow E_{p}[f(x)]
$$

- $\hat{f}$ is an unbiased estimator of $E_{p}[f(x)]$
- $\operatorname{var}(\hat{f})=\operatorname{var}\left(\sum_{t} \frac{f\left(x^{t}\right)}{T}\right)=\frac{\operatorname{var}(f(x))}{T}$
- More samples means less variance


## Sampling from Marginal Distributions

- Suppose that we have a joint distribution $p(x, y)$ and we would like to estimate $p(y)$
- Express this as an expectation

$$
p(y)=\sum_{x^{\prime}, y^{\prime}} 1_{y^{\prime}=y} \cdot p\left(x^{\prime}, y^{\prime}\right)
$$

- We can then use the previous sampling strategy to estimate this expectation (known as rejection sampling)


## Rejection Sampling

- Rejection sampling:
- To estimate $p(y)$, first draw samples from $p\left(x^{\prime}, y^{\prime}\right)$ and discard those for which $\mathrm{y}^{\mathrm{t}} \neq y$
- This process can fail miserably if $p(y)$ is very small
- Let $z^{t}$ be a random variable that indicates whether or not the $t^{t h}$ sample from $p\left(x^{\prime}, y^{\prime}\right)$ was accepted
- $E\left[\sum_{t=1}^{T} z^{t}\right]=T \cdot p(y)$


## Importance Sampling

- Introduce a proposal distribution $q(x)$ such that $p(x, y)>0$ implies that $q(x)>0$

$$
\begin{aligned}
p(y) & =\sum_{x} p(x, y) \\
& =\sum_{x} p(x, y) \frac{q(x)}{q(x)} \\
& =\sum_{x} \frac{p(x, y)}{q(x)} q(x) \\
& =E_{q}\left[\frac{p(x, y)}{q(x)}\right]
\end{aligned}
$$

## Importance Sampling

- Draw samples from $q(x)$
- Note that we can never generate a sample that occurs with probability zero
- Use the samples from $q$ to approximate $p(y)$

$$
p(y) \approx \frac{1}{T} \sum_{t} \frac{p\left(x^{t}, y\right)}{q\left(x^{t}\right)}
$$

## Sampling: Bayesian Networks



Estimate $p(D=1)$ using $q(A, B, C)$ uniform over $A, B, C$

## Importance Sampling

- The proposal distribution should be close as possible to $p(x \mid y)$
- Often, this requires knowing an analytic form of the distribution $p$
- If we had that, we wouldn't need to sample!
- Picking good proposal distribution is more "art" than science


## Sampling from Conditional Distributions

- Can we use the same ideas to sample from conditional distributions?

$$
p(x \mid y)=\frac{\sum_{z} p(x, y, z)}{p(y)}
$$

- Using sampling to estimate the numerator and denominator can produce very bad estimates
- For example, if we over estimate the numerator and underestimate the denominator


## Normalized Importance Sampling

- Rewrite the conditional distribution as

$$
p(x \mid y)=\frac{\sum_{x^{\prime}, z} \delta\left(x^{\prime}=x\right) p\left(x^{\prime}, y, z\right)}{\sum_{x^{\prime}, z} p\left(x^{\prime}, y, z\right)}
$$

- Can use the same proposal distribution to sample from the numerator and the denominator
- Common random numbers reduce the variance


## Beyond Monte Carlo Methods

- All of the methods discussed so far can have serious limitations depending on the quantity being estimated
- Idea: instead of having a single proposal distribution, why not have an adaptive proposal distribution that depends on the previous sample?
$q\left(x \mid x^{\prime}\right)$ where $x^{\prime}$ is the previous sample and $x$ is the new assignment to be sampled
- We'll explore this class of proposals more next lecture...

