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

$$p(x_1, \dots, x_n) = \frac{1}{Z} \prod_C \psi_C(x_C)$$

- Idea: if we could generate i.i.d. 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

$$x^t = (x_1^t, \dots, x_n^t)$$

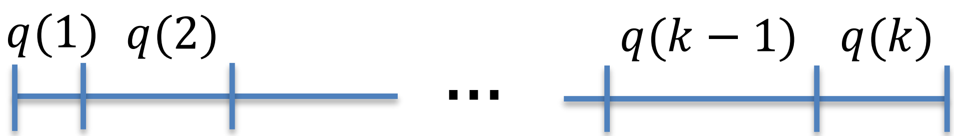
Sampling: The Basics

$$p(x_1, \dots, x_n) = \frac{1}{Z} \prod_C \psi_C(x_C)$$

- Given T i.i.d. samples $x^1, \dots, x^T$ 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 $y \in \{1, \dots, k\}$
  - Sampling algorithm:
    - Divide the unit interval into k pieces corresponding to the probabilities $q(1), \dots, q(k)$



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

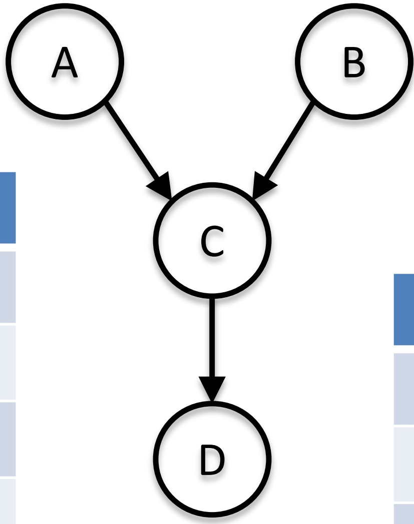
Sampling: Bayesian Networks

- 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

A	$P(A)$
0	.3
1	.7

B	$P(B)$
0	.4
1	.6



A	B	C	$P(C\|A,B)$
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

C	D	$P(D\|C)$
0	0	.3
0	1	.7
1	0	.4
1	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

$$\hat{f} = \sum_t \frac{f(x^t)}{T}$$

Monte Carlo Methods

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

$$\sum_t \frac{f(x^t)}{T} \to E_p[f(x)]$$

- $\hat{f}$ is an **unbiased estimator** of $E_p[f(x)]$

- $\mathrm{var}(\hat{f}) = \mathrm{var}\left(\sum_t \frac{f(x^t)}{T}\right) = \frac{\mathrm{var}(f(x))}{T}$

  – 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

$$p(y) = \sum_{x',y'} \delta(y' = y) \cdot p(x', y')$$

  - We can then use the previous sampling strategy to estimate this expectation

Rejection Sampling

- **Rejection sampling:**
  - To estimate $p(y)$, first draw samples from $p(x', y')$ 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^{th} sample from $p(x', y')$ was accepted
    - $E[\sum_{t=1}^{T} z^t] = T \cdot p(y)$

Importance Sampling

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

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

UTD

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 $p(y)$

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

Sampling: Bayesian Networks

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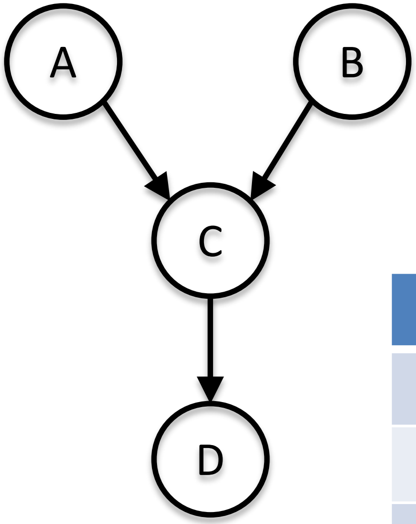
1	.6



A	B	C	$P(C\|A,B)$
0	0	0	.1
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1	0	0	0
1	0	1	1
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C	D	$P(D\|C)$
0	0	.3
0	1	.7
1	0	.4
1	1	.6

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 $p(x|y)$
  - 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?

$$p(x|y) = \frac{\sum_z p(x, y, z)}{p(y)}$$

  – 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

$$p(x|y) = \frac{\sum_{x',z} \delta(x' = x) p(x', y, z)}{\sum_{x',z} p(x', y, z)}$$

- 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?

$q(x|x')$ where x' is the previous sample and x is the new assignment to be sampled