CSC 412/2506: Probabilistic Learning and Reasoning

Week 4 - 2/2: Sampling

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Overview

- Ancestral Sampling
- Simple Monte Carlo
- Importance Sampling
- Rejection Sampling

Sampling

- A sample from a distribution $p(x)$ is a single realization x whose probability distribution is $p(x)$. Here, x can be high-dimensional or simply real valued.
- We assume the density from which we wish to draw samples, $p(x)$, can be evaluated to within a multiplicative constant. That is, we can evaluate a function $\tilde{p}(x)$ such that

$$p(x) = \frac{\tilde{p}(x)}{Z}.$$

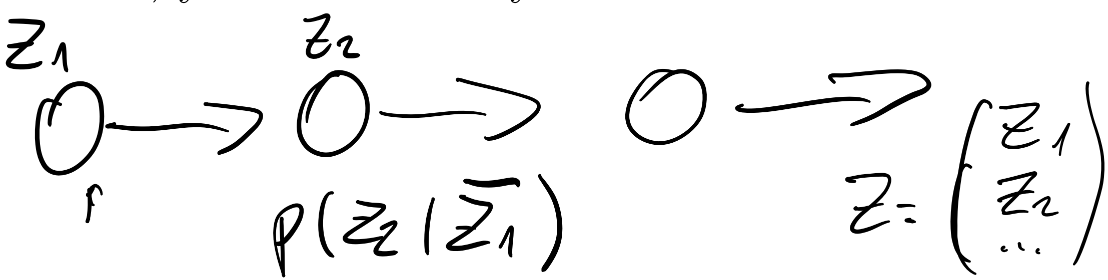
$Z = \int \dots \, dx$

Ancestral Sampling

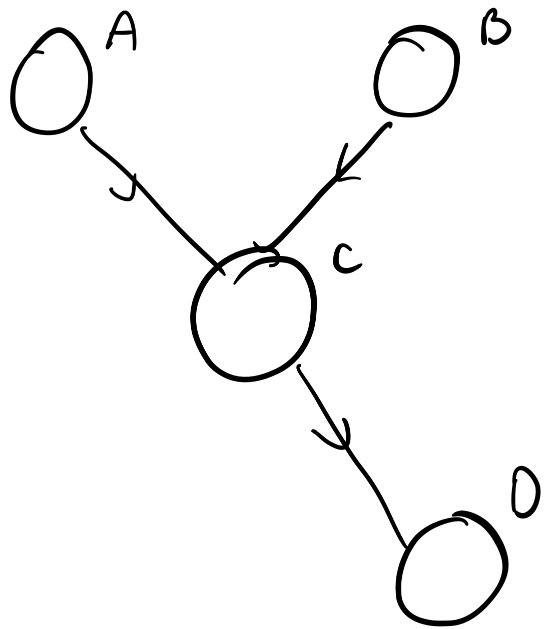
Given a DAG, and the ability to sample from each of its factors given its parents, we can sample from the joint distribution over all the nodes by **ancestral sampling**, which simply means sampling in a topoplogical order.

- at each step, sample from any conditional distribution that you haven't visited yet, whose parents have all been sampled.

Example: In a chain you would always start with z_1 and move to the right. In a tree, you would always start from the root.



Ancestral Sampling Example



$A = 0$ if $u < 0.2$

$ 1$ if $u \geq 0.2$

0.1

A	0	1
P(A)	0.2	0.8

0.2

B	0	1
	0.3	0.7

(A,B) \ C	0	1
(0,0)	1	0
(0,1)	0.5	0.5
(1,0)	0.5	0.5
(1,1)	0	1

$A = 0$

$B = 0$

$C = 0$

$D = 1$

$$x = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

0.4

C \ D	0	1
0	0.3	0.7
1	0.7	0.3

Main objectives of sampling

We will be using Monte Carlo methods to solve one or both of the following problems.

- **Problem 1**: To generate samples $\{x^{(r)}\}_{r=1}^{R}$ from a given probability distribution $p(x)$.
- **Problem 2**: To estimate expectations of functions, $\phi(x)$, under this distribution $p(x)$

$$\Phi = \mathop{\mathbb{E}}_{x \sim p(x)}[\phi(x)] = \int \phi(x)p(x)dx$$

$\phi(x) = x^2$

ϕ is called a test function.

Example

Examples of test functions $\phi(x)$:

- the mean of a function f under $p(x)$ by finding the expectation of the function $\phi_1(x) = f(x)$.
- the variance of f under $p(x)$ by finding the expectations of the functions $\phi_1(x) = f(x)$ and $\phi_2(x) = f(x)^2$

$$\phi_1(x) = f(x) \Rightarrow \Phi_1 = \mathop{\mathbb{E}}_{x \sim p(x)}[\phi_1(x)]$$

$$\phi_2(x) = f(x)^2 \Rightarrow \Phi_2 = \mathop{\mathbb{E}}_{x \sim p(x)}[\phi_2(x)]$$

$$\Rightarrow \mathrm{var}(f(x)) = \Phi_2 - (\Phi_1)^2$$

Estimation problem

We start with the estimation problem using simple Monte Carlo:

- **Simple Monte Carlo**: Given $\{x^{(r)}\}_{r=1}^{R} \sim p(x)$ we can estimate the expectation $\mathop{\mathbb{E}}_{x \sim p(x)}[\phi(x)]$ using the estimator $\hat{\Phi}$:

$$\Phi = \mathop{\mathbb{E}}_{x \sim p(x)}[\phi(x)] \approx \frac{1}{R} \sum_{r=1}^{R} \phi(x^{(r)}) = \hat{\Phi}$$

$x^1 = 0$

$x^2 = 1$

$x^3 = 2$

- The fact that $\hat{\Phi}$ is a consistent estimator of Φ follows from the Law of Large Numbers (LLN).

$$\frac{1}{3} \sum_{r=1}^{3} (x^r)^2$$

$\phi(x) = x^2$

- **Unbiasedness:** If the vectors $\{x^{(r)}\}_{r=1}^{R}$ are generated independently from $p(x)$, then the expectation of $\hat{\Phi}$ is Φ.

$p(x)$

$$
\begin{aligned}
\mathbb{E}[\hat{\Phi}] &= \mathbb{E}\left[\frac{1}{R}\sum_{r=1}^{R}\phi(x^{(r)})\right] = \frac{1}{R}\sum_{r=1}^{R}\underbrace{\mathbb{E}\left[\phi(x^{(r)})\right]}\\
&= \frac{1}{R}\sum_{r=1}^{R}\mathop{\mathbb{E}}_{x\sim p(x)}\left[\phi(x)\right] = \frac{R}{R}\boxed{\mathop{\mathbb{E}}_{x\sim p(x)}\left[\phi(x)\right]} = \Phi\\
&= \Phi
\end{aligned}
$$

Simple properties of Monte Carlo estimation

- **Variance:** As the number of samples of R increases, the variance of $\hat{\Phi}$ will decrease with rate $\frac{1}{R}$

$$
\begin{aligned}
\mathrm{var}[\hat{\Phi}] &= \mathrm{var}\left[\frac{1}{R}\sum_{r=1}^{R}\phi(x^{(r)})\right] \\
&= \frac{1}{R^2}\mathrm{var}\left[\sum_{r=1}^{R}\phi(x^{(r)})\right] \\
&= \frac{1}{R^2}\sum_{r=1}^{R}\mathrm{var}\left[\phi(x^{(r)})\right] \\
&= \frac{R}{R^2}\mathrm{var}[\phi(x)] \\
&= \frac{1}{R}\underbrace{\mathrm{var}[\phi(x)]}
\end{aligned}
$$

$p(x)$

Accuracy of the Monte Carlo estimate depends on the variance of ϕ.

Sampling problem

- Assume we know the density $p(x)$ up to a multiplicative constant

$$p(x) = \frac{\tilde{p}(x)}{Z}$$

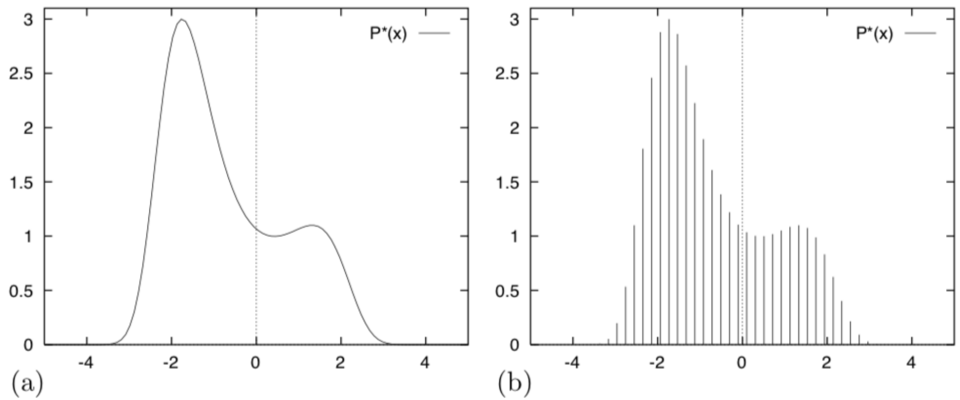
- There are two difficulties:
  - We do not generally know the normalizing constant, Z. The main diffuculty is computing it

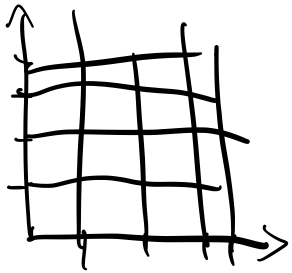
$$Z = \int \tilde{p}(x) dx$$

    which requires computing a high-dimensional integral.
  - Even if we did know Z, the problem of drawing samples from $p(x)$ is still a challenging one, especially in high-dimensional spaces.

Bad Idea: Lattice Discretization

Imagine that we wish to draw samples from the density $p(x) = \frac{\tilde{p}(x)}{Z}$ given in figure (a).



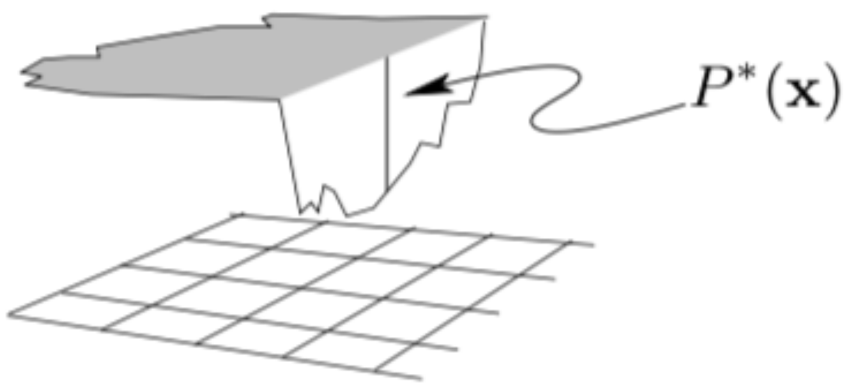


- How to compute Z?
- We could discretize the variable x and sample from the discrete distribution (figure (b)).
- In figure (b) there are 50 uniformly spaced points in one dimension. If our system had, $D = 1000$ dimensions say, then the corresponding number of points would be $50^D = 50^{1000}$. Thus, the cost is exponential in dimension!

An analogy

Imagine the tasks of drawing random water samples from a lake and finding the average plankton concentration. Let

- $\tilde{p}(\mathbf{x})$ = the depth of the lake at $\mathbf{x} = (x, y)$
- $\phi(\mathbf{x})$ = the plankton concentration as a function of $\mathbf{x}$
- Z = the volume of the lake = $\int \tilde{p}(\mathbf{x}) d\mathbf{x}$



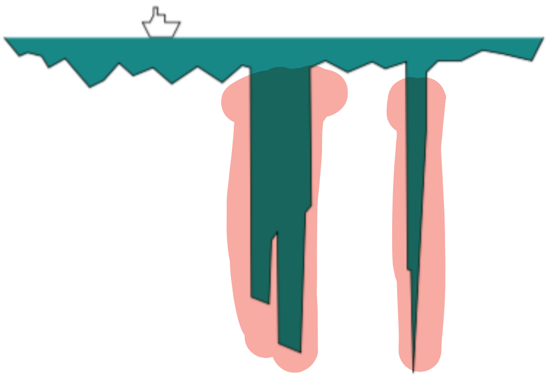
The average concentration of plankton is therefore

$$\Phi = \frac{1}{Z} \int \phi(\mathbf{x}) \tilde{p}(\mathbf{x}) d\mathbf{x}.$$

An analogy

You can take the boat to any desired location $\mathbf{x}$ on the lake, and can measure the depth, $\tilde{p}(\mathbf{x})$, and plankton concentration, $\phi(\mathbf{x})$, at that point. Therefore,

- **Problem 1** is to draw water samples at random such that each sample is equally likely to come from any point within the lake.
- **Problem 2** is to find the average plankton concentration.

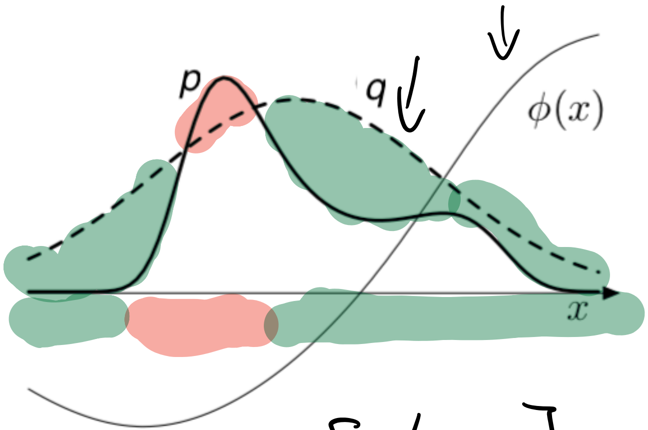


A slice through a lake that includes some canyons.

- We don't know the depth $\tilde{p}(\mathbf{x})$.
- To correctly estimate Φ, our method must implicitly discover the canyons and find their volume relative to the rest of the lake.

Estimation tool: Importance Sampling

Importance sampling is a method for estimating the expectation of a function $\phi(x)$.



$$\mathbb{E}_{x \sim p(x)}\left[\phi(x)\right]$$

$q > p$

- The density from which we wish to draw samples, $p(x)$, can be evaluated up to normalizing constant, $\tilde{p}(x)$

$$p(x) = \frac{\tilde{p}(x)}{Z_p}$$

- There is a simpler density, $q(x)$ from which it is easy to sample from and easy to evaluate up to normalizing constant (i.e. $\tilde{q}(x)$)

$$q(x) = \frac{\tilde{q}(x)}{Z_q}$$

Estimation tool: Importance Sampling

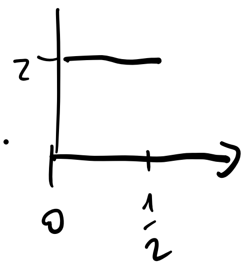
- In importance sampling, we generate R samples from $q(x)$

$$\{x^{(r)}\}_{r=1}^{R} \sim q(x)$$

- If these points were samples from $p(x)$ then we could estimate Φ by

$$\Phi = \mathop{\mathbb{E}}_{x \sim p(x)}[\phi(x)] \approx \frac{1}{R}\sum_{r=1}^{R} \phi(x^{(r)}) = \hat{\Phi}$$

  That is, we could use a simple Monte Carlo estimator.



- But we sampled from q. We need to correct this!
- Values of x where $q(x)$ is greater than $p(x)$ will be over-represented in this estimator, and points where $q(x)$ is less than $p(x)$ will be under-represented. Thus, we introduce weights.

$$p(x) = \frac{\tilde{p}(x)}{Z_p}$$

- Introduce weights: $\tilde{w}_r = \frac{\tilde{p}(x^{(r)})}{\tilde{q}(x^{(r)})}$ and notice that

$$\underbrace{\frac{1}{R}\sum_{r=1}^{R} \tilde{w}_r}\approx \mathop{\mathbb{E}}_{x\sim q(x)}\left[\frac{\tilde{p}(x)}{\tilde{q}(x)}\right] = \int \frac{\tilde{p}(x)}{\tilde{q}(x)} q(x)dx = \frac{Z_p}{Z_q}$$

- Finally, we rewrite our estimator under q

$$\Phi = \int \phi(x)p(x)dx = \int \phi(x)\cdot\frac{p(x)}{q(x)}\cdot q(x)dx \approx \frac{1}{R}\sum_{r=1}^{R}\phi(x^{(r)})\frac{p(x^{(r)})}{q(x^{(r)})} = (*)$$

- However, the estimator relies on p. It can only rely on $\tilde{p}$ and $\tilde{q}$.

$$(*) = \frac{Z_q}{Z_p}\frac{1}{R}\sum_{r=1}^{R}\phi(x^{(r)})\cdot\frac{\tilde{p}(x^{(r)})}{\tilde{q}(x^{(r)})} = \frac{Z_q}{Z_p}\frac{1}{R}\sum_{r=1}^{R}\phi(x^{(r)})\cdot\boxed{\tilde{w}_r}$$

$$\approx \frac{\frac{1}{R}\sum_{r=1}^{R}\phi(x^{(r)})\cdot\tilde{w}_r}{\frac{1}{R}\sum_{r=1}^{R}\tilde{w}_r} = \underbrace{\frac{1}{R}\sum_{r=1}^{R}\phi(x^{(r)})}\cdot w_r = \boxed{\hat{\Phi}_{iw}}$$

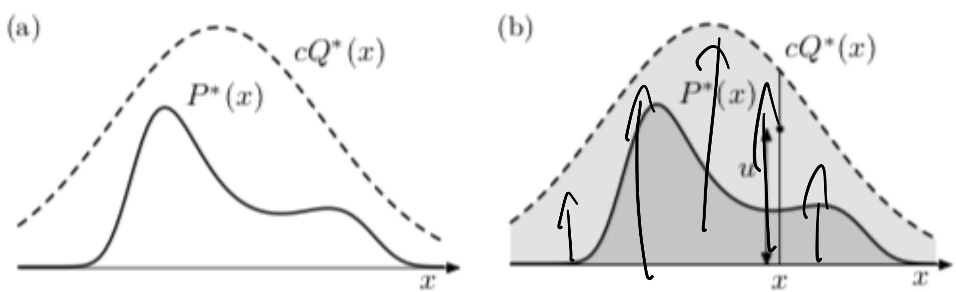
where $w_r = \frac{\tilde{w}_r}{\sum_{r=1}^{R}\tilde{w}_r}$ and $\hat{\Phi}_{iw}$ is our importance weighted estimator.

Sampling tool: Rejection sampling

$\tilde{p}$ $\tilde{q}$

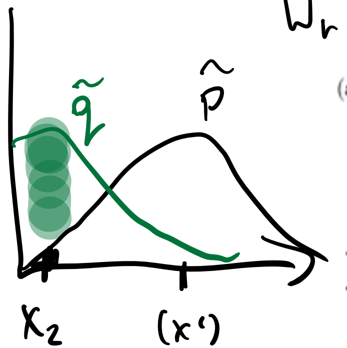
- We want expectations under $p(x) = \tilde{p}(x)/Z$ which is a very complicated one-dimensional density.
- Assume that we have a simpler proposal density $q(x)$ which we can evaluate (within a multiplicative factor Z_q, as before), and from which we can generate samples.
- Further assume that we know the value of a constant c such that

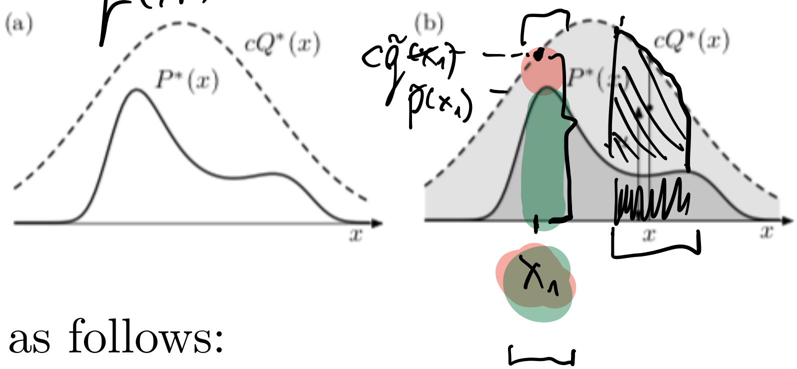
$$c\tilde{q}(x) > \tilde{p}(x) \quad \forall x$$



$$\tilde{w}_r = \frac{\tilde{p}(x_r)}{\tilde{q}(x_r)}$$

$x_r \sim \tilde{q}(x)$





$c = 20$

$c\tilde{q}(x) = 20 \cdot \tilde{q}(x)$

The procedure is as follows:

1. Generate two random numbers.
   1.1 The first, x, is generated from the proposal density $\tilde{q}(x)$.
   1.2 The second, u is generated uniformly from the interval $\underbrace{[0, c\tilde{q}(x)]}$ (see figure (b) above).
2. Evaluate $\tilde{p}(x)$ and accept or reject the sample x by comparing the value of u with the value of $\tilde{p}(x)$

   $\tilde{p}(x_r)$

   2.1 If $u > \tilde{p}(x)$, then x is rejected
   2.2 Otherwise x is accepted; x is added to our set of samples $\{x^{(r)}\}$ and the value of u discarded.

Why does rejection sampling work?

1. $x \sim \tilde{q}(x)$
2. $u|x \sim \text{Unif}[0, c\tilde{q}(x)]$ $\rightarrow$ $p(u|x) =$
3. x is accepted if $u \leq \tilde{p}(x)$.

For any set A

$$\mathbb{P}_{x\sim p}(x \in A) = \int_A p(x)dx = \int \mathbf{1}_{\{x\in A\}} p(x)dx = \mathbb{E}_{x\sim p}[\mathbf{1}_{\{x\in A\}}].$$

$$\mathbb{P}_{x\sim q}(x \in A | u \leq \tilde{p}(x)) = \mathbb{P}_{x\sim q}(x \in A, u \leq \tilde{p}(x)) / \mathbb{E}_{x\sim q}[\mathbb{P}(u \leq \tilde{p}(x)|x)]$$

$$= \mathbb{E}_{x\sim q}[\mathbf{1}_{\{x\in A\}} \mathbb{P}(u \leq \tilde{p}(x)|x)] / \underbrace{\mathbb{E}_{x\sim q}[\frac{\tilde{p}(x)}{c\tilde{q}(x)}]}_{\frac{1}{c}\frac{Z_p}{Z_q}}$$

$$= \mathbb{E}_{x\sim q}[\mathbf{1}_{\{x\in A\}} \frac{\tilde{p}(x)}{c\tilde{q}(x)}] / \frac{Z_p}{cZ_q}$$

$$= \mathbb{P}_{x\sim p}(x \in A) \cancel{\frac{Z_p}{cZ_q}} / \cancel{\frac{Z_p}{cZ_q}}$$

$$\boxed{= \mathbb{P}_{x\sim p}(x \in A)}$$

Rejection sampling in many dimensions

- In high-dimensional problems, the requirement that $c\tilde{q}(x) \geq \tilde{p}(x)$ will force c to be huge, so acceptances will be very rare.
- Finding such a value of c may be difficult too, since we don't know where the modes of $\tilde{p}$ are located nor how high they are.
- In general c grows exponentially with the dimensionality, so the acceptance rate is expected to be exponentially small in dimension

$$\boxed{\text{acceptance rate}} = \frac{\text{area under } \tilde{p}}{\text{area under } c\tilde{q}} = \frac{1}{Z}$$

Summary

- Estimating expectations is an important problem, which is in general hard. We learned ~~3~~ 4 sampling-based tools for this task:
  - Simple Monte Carlo
  - Importance Sampling
  - Rejection Sampling
  - Ancestral Sampling
- Next lecture, we will learn to generate samples from a particular distribution.