STA 414/2104: Probabilistic Machine Learning

Week 3: Exact/Approximate Inference

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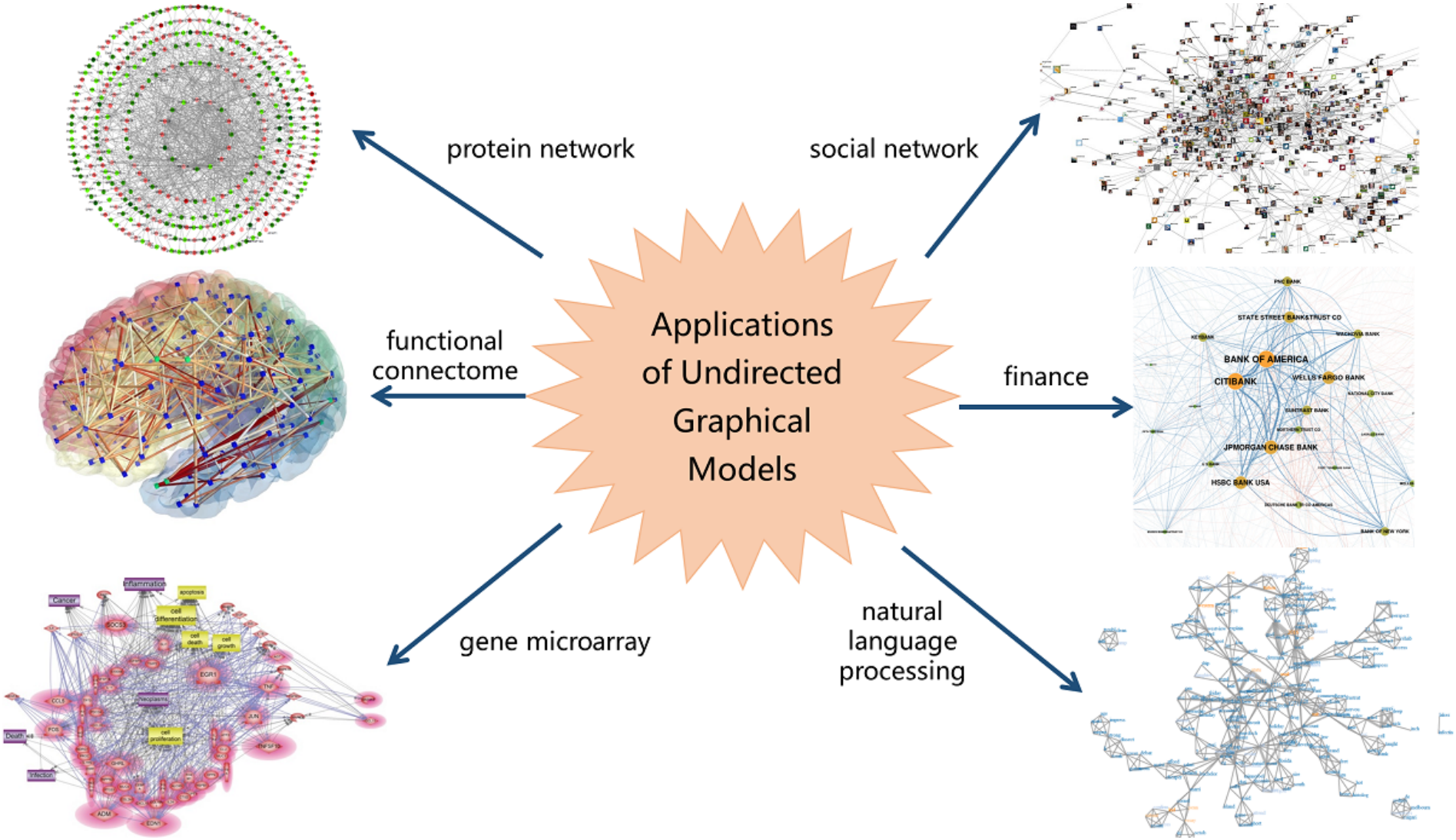
Today's lecture

Summary of the content:

- Exact inference on graphical models
- Variable elimination
- Intro to approximate inference

Some announcements:

- Assignment 1 is released this week.
- TA office hours next week.


protein network
social network
functional connectome
Applications of Undirected Graphical Models
finance
gene microarray
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Example

- This describes a probability distribution over 8 variables.
- In general, we are only interested in the conditional distribution of few.
- For example, ..

What is the probability of a getting a job given you have 3.1 GPA?

Inference as Conditional Distribution

- We explore inference in probabilistic graphical models (PGMs).
  - x_E = The observed evidence
  - x_F = The unobserved variable we want to infer
  - $x_R = \boldsymbol{x} - \{x_F, x_E\}$ = Remaining variables, extraneous to query.

- Focus on computing the conditional probability distribution

$$p(x_F|x_E) = \frac{p(x_F, x_E)}{p(x_E)} = \frac{p(x_F, x_E)}{\sum_{x_F} p(x_F, x_E)}$$

- for which, we marginalize out these extraneous variables, focussing on the joint distribution over evidence and subject of inference:

$$p(x_F, x_E) = \sum_{x_R} p(x_F, x_E, x_R)$$

Variable elimination

Order in which we marginalize affects the computational cost!

Our main tool is **variable elimination**:

- A simple and general **exact inference** algorithm in any probabilistic graphical model (DAGMs or MRFs).
- Computational complexity depends on the graph structure.
- Dynamic programming avoids enumerating all variable assignments.

Example: Simple chain

- Lets start with the example of a simple chain

$$A \to B \to C \to D$$

  where we want to compute $p(D)$, with no evidence variables.
- We have

$$x_F = \{D\},\ x_E = \{\},\ x_R = \{A, B, C\}$$

- We saw last lecture that this graphical model describes the factorization of the joint distribution as:

$$p(A, B, C, D) = p(A)p(B|A)p(C|B)p(D|C)$$

- Assume each variable can take on k different values.

Example: Simple chain

- The goal is to compute the marginal $p(D)$:

$$p(D) = \sum_{A,B,C} p(A, B, C, D)$$

- However, if we do this sum naively, cost is exponential $O(k^{n=4})$:

$$\begin{aligned} p(D) &= \sum_{A,B,C} p(A, B, C, D) \\ &= \sum_{C} \sum_{B} \sum_{A} p(A)p(B|A)p(C|B)p(D|C) \end{aligned}$$

- Instead, choose an **elimination ordering**:

$$\begin{aligned} p(D) &= \sum_{C,B,A} p(A, B, C, D) \\ &= \sum_{C} p(D|C) \left(\sum_{B} p(C|B) \Big(\sum_{A} p(A)p(B|A) \Big) \right). \end{aligned}$$

Example: Simple chain

- This reduces the complexity by first computing terms that appear across the other sums.

$$p(D) = \sum_C p(D|C) \sum_B p(C|B) \sum_A p(A)p(B|A)$$

-

$$\begin{aligned} p(D) &= \sum_C p(D|C) \sum_B p(C|B) \sum_A p(A)p(B|A) \\ &= \sum_C p(D|C) \sum_B p(C|B)p(B) \\ &= \sum_C p(D|C)p(C) \end{aligned}$$

- The cost of performing inference on the chain in this manner is $\mathcal{O}(nk^2)$. In comparison, generating the full joint distribution and marginalizing over it has complexity $\mathcal{O}(k^n)$!

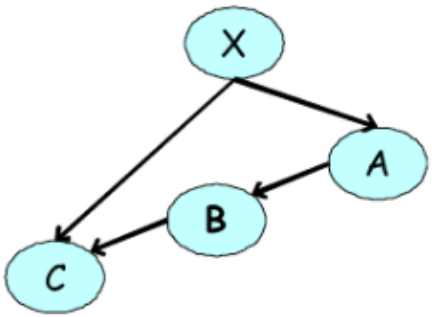
Best Elimination Ordering

- The complexity of variable elimination depends on the elimination ordering!
- Unfortunately, finding the best elimination ordering is NP-hard.

Intermediate Factors

The same algorithm both for DAGMs and MRFs:

- Introduce nonnegative **factors** ϕ (like for MRFs).
- e.g. in a simple DAG model:



$$
\begin{aligned}
p(A,B,C) &= \sum_X p(X)p(A|X)p(B|A)p(C|B,X) \\
&= \sum_X \phi_1(X)\phi_2(A,X)\phi_3(A,B)\phi_4(X,B,C) \\
&= \phi_3(A,B)\sum_X \phi_1(X)\phi_2(A,X)\phi_4(X,B,C) \\
&= \phi_3(A,B)\tau(A,B,C)
\end{aligned}
$$

- Marginalizing over X we introduce a new factor, denoted by τ.

Sum-Product Inference

- Abstractly, computing $p(x_F|x_E)$ is given by the **sum-product** algorithm:

$$p(x_F|x_E) \propto \tau(x_F, x_E) = \sum_{x_R} \prod_{C \in \mathcal{F}} \psi_C(x_C)$$

  where $\mathcal{F}$ is a set of potentials or factors.
- For DAGMs, $\mathcal{F}$ is given by the the sets of the form

$$\{i\} \cup \text{parents}(i) \qquad \text{for all nodes } i.$$

- For MRFs, $\mathcal{F}$ is given by the set of maximal cliques.

Example

- This describes a factorization:

$$p(C, D, I, G, S, L, H, J) = p(C)p(D|C)p(I) \times p(G|D, I)p(L|G)p(S|I)p(J|S, L)p(H|J, G)$$

We have

$$\mathcal{F} = \{\{C\}, \{C, D\}, \{I\}, \{G, D, I\}, \{L, G\}, \{S, I\}, \{J, S, L\}, \{H, J, G)\}\}$$

We are interested in the probability of getting a job, $p(J)$.

We perform exact inference as follows.

Example $\left(\mathcal{F} = \{\{C\}, \{C, D\}, \{I\}, \{G, D, I\}, \{L, G\}, \{S, I\}, \{J, S, L\}, \{H, J, G)\}\}\right)$

Elimination Ordering $\prec \{C, D, I, H, G, S, L\}$

$$p(J) = \sum_L \sum_S \psi(J, L, S) \sum_G \psi(L, G) \sum_H \psi(H, G, J) \sum_I \psi(S, I)\psi(I) \sum_D \psi(G, D, I) \underbrace{\sum_C \psi(C)\psi(C, D)}_{\tau(D)}$$

$$= \sum_L \sum_S \psi(J, L, S) \sum_G \psi(L, G) \sum_H \psi(H, G, J) \sum_I \psi(S, I)\psi(I) \underbrace{\sum_D \psi(G, D, I)\tau(D)}_{\tau(G,I)}$$

$$= \sum_L \sum_S \psi(J, L, S) \sum_G \psi(L, G) \sum_H \psi(H, G, J) \underbrace{\sum_I \psi(S, I)\psi(I)\tau(G, I)}_{\tau(S,G)}$$

$$= \sum_L \sum_S \psi(J, L, S) \sum_G \psi(L, G)\tau(S, G) \underbrace{\sum_H \psi(H, G, J)}_{\tau(G,J)}$$

$$= \sum_L \sum_S \psi(J, L, S) \underbrace{\sum_G \psi(L, G)\tau(S, G)\tau(G, J)}_{\tau(J,L,S)}$$

$$= \sum_L \underbrace{\sum_S \psi(J, L, S)\tau(J, L, S)}_{\tau(J,L)}$$

$$= \underbrace{\sum_L \tau(J, L)}_{\tau(J)}$$

$$= \tau(J)$$

Do we need to normalize the final τ?

Complexity of Variable Elimination Ordering

- We discussed previously that variable elimination ordering determines the computational complexity. This is due to how many variables appear inside each sum.
- Different elimination orderings will involve different number of variables appearing inside each sum.
- The complexity of the VE algorithm is (roughly)

$$O(mk^{N_{\max}})$$

where

  - m is the number of initial factors.
  - k is the number of states each random variable takes (assumed to be equal here).
  - N_i is the number of random variables inside each sum $\sum_i$.
  - $N_{\max} = \max_i N_i$ is the number of variables inside the largest sum.

Example

Elimination Ordering $\prec \{C, D, I, H, G, S, L\}$

- Here are all the initial factors:

$$\mathcal{F} = \{\{C\}, \{C, D\}, \{I\}, \{G, D, I\}, \{L, G\}, \{S, I\}, \{J, S, L\}, \{H, J, G)\}\}$$

$$\implies m = |\Phi| = 8$$

- Here are the sums, and the number of variables that appear in them

$$\underbrace{\sum_{C} \psi(C)\psi(C, D)}_{N_C=2} \quad \underbrace{\sum_{D} \psi(G, D, I)\tau(D)}_{N_D=3} \quad \underbrace{\sum_{I} \psi(S, I)\psi(I)\tau(G, I)}_{N_I=3}$$

$$\underbrace{\sum_{H} \psi(H, G, J)}_{N_H=3} \quad \underbrace{\sum_{G} \psi(L, G)\tau(S, G)\tau(G, J)}_{N_G=4} \quad \underbrace{\sum_{S} \psi(J, L, S)\tau(J, L, S)}_{N_S=3}$$

$$\underbrace{\sum_{L} \tau(J, L)}_{N_L=2} \implies \text{the largest sum is } N_G = 4.$$

- For simplicity, assume all variables take on k states. So the complexity of the variable elimination under this ordering is $O(8 \cdot k^4)$.

Summary

Variable elimination:

- Variable elimination can be used for exact inference in PGMs.
- The ordering in variable elimination can significantly reduce the computational complexity.
- The overall complexity of the variable elimination algorithm can be computed.

Approximate Inference: Overview

- In general, we do not have access to any (or some) of the (conditional) distributions, say $p(x)$.
- For this reason, we need tools to approximate them with $\hat{p}(x)$ when performing inference!
- Two common approaches:
  - Generate samples $x_i \sim p(x)$ and use them for estimation.
  - Directly approximate $\hat{p}(x)$, e.g. with neural networks.

Sampling approach

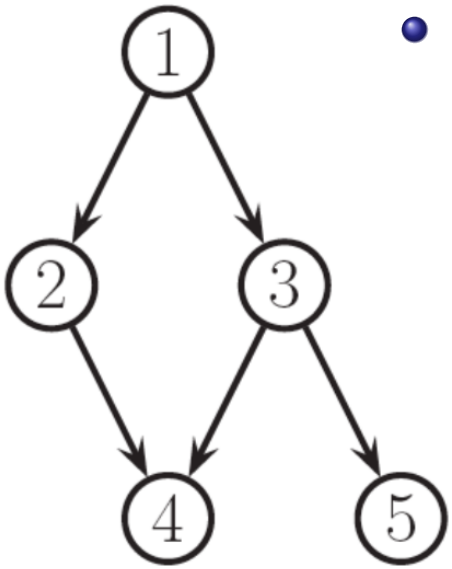
- A sample from a distribution $p(x)$ is a single realization x whose probability distribution is $p(x)$. Here, x can be high-dimensional or simply real valued.
- We assume the density from which we wish to draw samples, $p(x)$, can be evaluated to within a multiplicative constant. That is, we can evaluate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

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

Warm up: Ancestral Sampling

- Given a DAGM, 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.
- For this algorithm, we assume that we can sample from conditional distributions.

Ancestral Sampling Example



- The graph factorizes according to the local conditional probabilities

$$p(x_{1,\ldots,N}) = \prod_{i}^{N} p(x_i|\text{parents}(x_i))$$
$$= p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_4|x_2,x_3)p(x_5|x_3)$$

- Start by sampling from $p(x_1)$.
- Then sample from $p(x_2|x_1)$ and $p(x_3|x_1)$.
- Then sample from $p(x_4|x_2,x_3)$.
- Finally, sample from $p(x_5|x_3)$.

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 $p(x)$

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

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 $\phi_2(x) = f(x)^2$

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

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

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

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 $\underset{x\sim p(x)}{\mathbb{E}}[\phi(x)]$ using the estimator $\hat{\Phi}$:

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

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

Basic properties of Monte Carlo estimation

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

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

Simple properties of Monte Carlo estimation

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

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

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

Normalizing constant

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

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

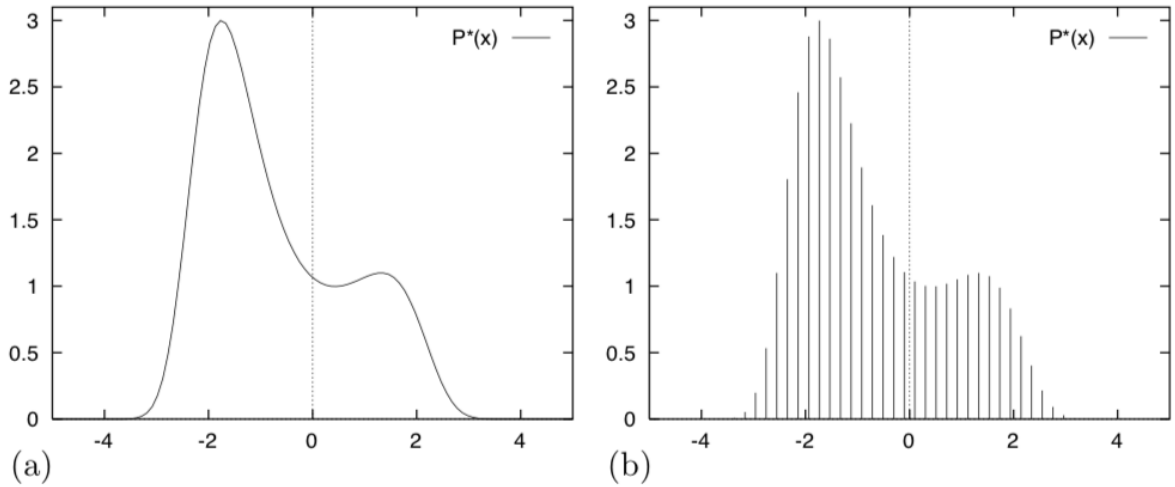
- There are two difficulties:
  - We do not generally know the normalizing constant, Z. The main diffuculty is computing it

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

    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).

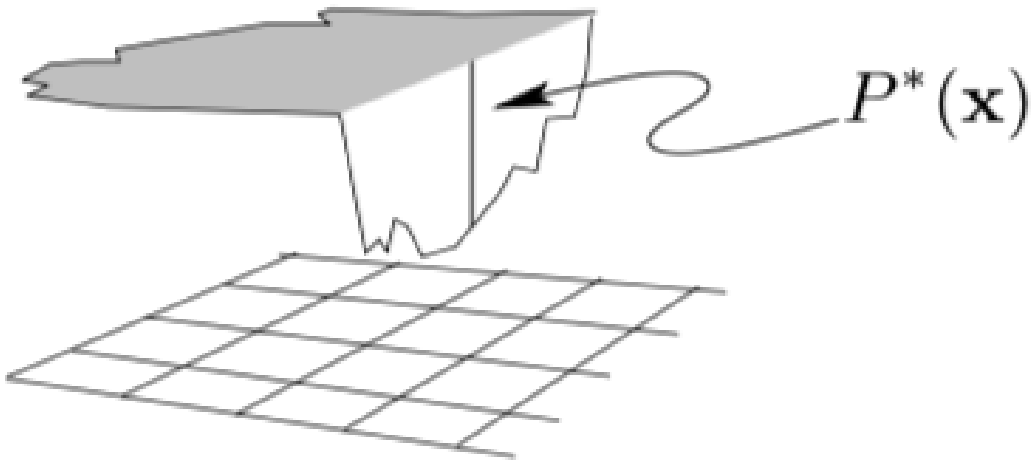


- How to compute Z?
- We could discretize the variable x and sample from the discrete distribution (figure (b)).
- In figure (b) there are 50 uniformly spaced points in one dimension. If our system had, $D = 1000$ dimensions say, then the corresponding number of points would be $50^D = 50^{1000}$. Thus,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

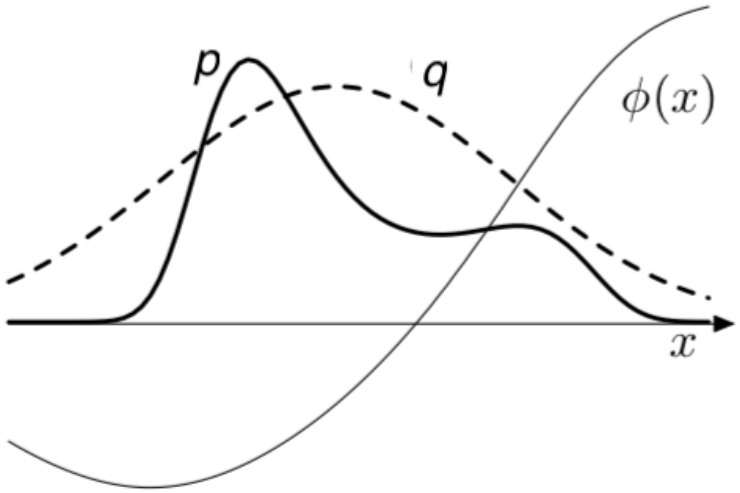
- **Problem 1** is to draw water samples at random such that each sample is equally likely to come from any point within the lake.
- **Problem 2** is to find the average plankton concentration.

A slice through a lake that includes some canyons.

- 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 $\phi(x)$.



- 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. It is also 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.

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

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

- 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 $\tilde{q}$.

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

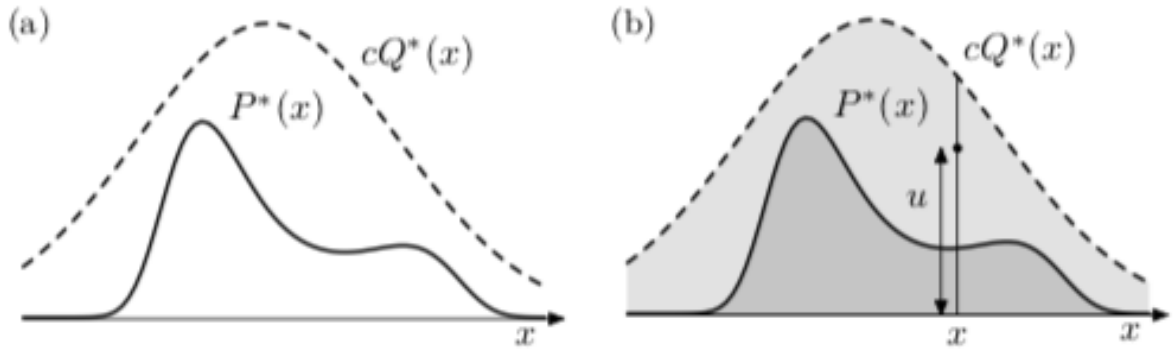
$$\approx \frac{\frac{1}{R}\sum_{r=1}^{R}\phi(x^{(r)})\cdot\tilde{w}_r}{\frac{1}{R}\sum_{r=1}^{R}\tilde{w}_r} = \sum_{r=1}^{R}\phi(x^{(r)})\cdot w_r = \hat{\Phi}_{iw}$$

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

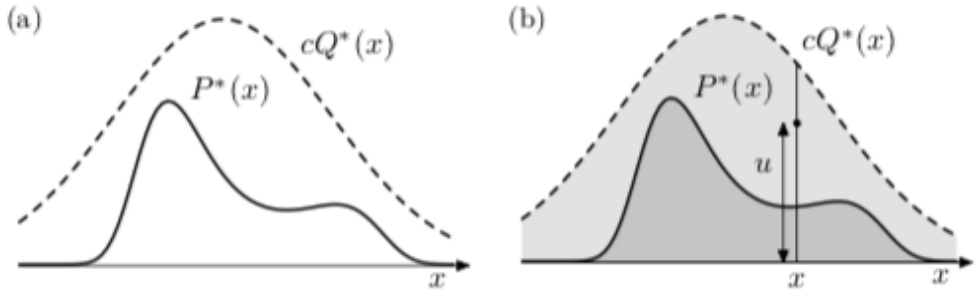
Sampling tool: Rejection sampling

- We want expectations under $p(x) = \tilde{p}(x)/Z_p$ 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, i.e. $\tilde{q}(x) = Z_q \cdot q(x)$.
- Further assume that we know the value of a constant c such that

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



Sampling tool: Rejection sampling



The procedure is as follows:

1. Generate two random numbers.
   - 1.1 The first, x, is generated from the proposal density $q(x)$.
   - 1.2 The second, u is generated uniformly from the interval $[0, c\tilde{q}(x)]$ (see figure (b) above: book's notation $P^* = \tilde{p}$, $Q^* = \tilde{q}$).
2. Accept or reject the sample x by comparing the value of u with the value of $\tilde{p}(x)$
   - 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. $x \sim q(x)$
2. $u|x \sim \text{Unif}[0, c\tilde{q}(x)]$
3. x is accepted if $u \leq \tilde{p}(x)$.

For any set A

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

$$\begin{aligned}
\mathbb{P}_{x\sim q}(x \in A|u \leq \tilde{p}(x)) =& \mathbb{P}_{x\sim q}(x \in A, u \leq \tilde{p}(x))/\mathbb{E}_{x\sim q}[\mathbb{P}(u \leq \tilde{p}(x)|x)] \\
=& \mathbb{E}_{x\sim q}[\mathbf{1}_{\{x\in A\}}\mathbb{P}(u \leq \tilde{p}(x)|x)]/\mathbb{E}_{x\sim q}[\frac{\tilde{p}(x)}{c\tilde{q}(x)}] \\
=& \mathbb{E}_{x\sim q}[\mathbf{1}_{\{x\in A\}}\frac{\tilde{p}(x)}{c\tilde{q}(x)}]/\frac{Z_p}{cZ_q} \\
=& \mathbb{P}_{x\sim p}(x \in A)\frac{Z_p}{cZ_q}/\frac{Z_p}{cZ_q} \\
=& \mathbb{P}_{x\sim p}(x \in A)
\end{aligned}$$

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

$$\text{acceptance rate} = \frac{\text{area under } \tilde{p}}{\text{area under } c\tilde{q}} = \frac{Z_p}{cZ_q}$$

Summary

- Estimating expectations is an important problem, which is in general hard. We learned 3 sampling-based tools for this task:
  - Simple Monte Carlo
  - Importance Sampling
  - Rejection Sampling
- Next lecture, message passing!