CSC412/2506 Winter 2020: Probabilistic Learning and Reasoning

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1 Introduction

2 Probabilistic Models

Definition 2.1. Given an i.i.d. dataset $\mathcal{D}$, the log-likelihood of θ is defined as

$$\ell(\theta; \mathcal{D}) = \sum_{i=1}^{N} \log p(x^{(i)}|\theta) \tag{2.1}$$

Definition 2.2. A **statistic** is a deterministic function of a set of random variables.

Definition 2.3. $T(X)$ is a **sufficient statistic** for random variable X if

$$T(x^{(1)}) = T(x^{(2)}) \implies L(\theta; x^{(1)}) = L(\theta; x^{(2)}) \quad \forall\theta \tag{2.2}$$

equivalently,

$$P(\theta|T(X)) = P(\theta|X) \tag{2.3}$$

3 Directed Graphical Models

3.1 Decision Theory

3.2 Latent Variables

Complete data case Let $\mathcal{D} = \{x^{(i)}, y^{(i)}\}_{i=1}^{N}$ denote the dataset, then

$$\ell(\theta; \mathcal{D}) = \sum_{i=1}^{N} \log p\left(x^{(i)}, y^{(i)}|\theta\right) \tag{3.1}$$

Partially observed dataset Let

$$\mathcal{D}^c = \{(x^{(i)}, y^{(i)}) : i \in \mathcal{C}\} \subseteq \mathcal{D} \tag{3.2}$$

denote the part of dataset with observed labels, and let

$$\mathcal{D}^m = \{(x^{(i)}) : i \in \mathcal{M}\} \subseteq \mathcal{D} \tag{3.3}$$

denote the set of observations without labels. Note that $\mathcal{C} \cup \mathcal{M} = \{1, 2, \cdots, N\}$.
Then the log likelihood is

$$\begin{aligned} \ell(\theta; \mathcal{D}) &= \sum_{c\in\mathcal{C}} \log p\left(x^c, y^c|\theta\right) + \sum_{m\in\mathcal{M}} \log p\left(x^m|\theta\right) && (3.4) \\ &= \sum_{c\in\mathcal{C}} \log p\left(x^c, y^c|\theta\right) + \sum_{m\in\mathcal{M}} \log \sum_{y} p\left(x^m, y|\theta\right) && (3.5) \end{aligned}$$

Inference with Latent Variables Let z denote the latent variable, then

$$p(y|x) = \sum_{z} p(y|x, z)p(z) \tag{3.6}$$

3.3 Mixture Models

Inference using mixture models Let $\Theta = \{\theta_z\} \cup \{\theta_1, \theta_2, \cdots, \theta_K\}$. Where θ_z quantifies the distribution of z, and θ_k for each $k \in \{1, 2, \cdots, K\}$ denote the set of parameters describing $p(x|z = k)$.

$$\begin{aligned} p(x|\Theta) &= \sum_{k=1}^{K} p(x, z = k|\Theta) && (3.7) \\ &= \sum_{k=1}^{K} p(z = k|\Theta) p(x|z = k, \Theta) && (3.8) \\ &= \sum_{k=1}^{K} p\left(z = k|\theta_z\right) p\left(x|z = k, \theta_k\right) && (3.9) \end{aligned}$$

Posterior probabilities / responsibilities

$$\begin{aligned} p\left(z = k|x, \theta_z\right) &= \frac{p\left(x|z = k, \theta_k\right) p\left(z = k|\theta_z\right)}{p(x|\Theta)} && (3.10) \\ &= \frac{p\left(x|z = k, \theta_k\right) p\left(z = k|\theta_z\right)}{\sum_j p(x, z = j|\Theta)} && (3.11) \\ &= \frac{p\left(x|z = k, \theta_k\right) p\left(z = k|\theta_z\right)}{\sum_j p\left(z = j|\theta_z\right) p\left(x|z = j, \theta_j\right)} && (3.12) \end{aligned}$$

Gaussian mixture models

$$\begin{aligned} p(x|\theta) &= \sum_k \alpha_k \mathcal{N}\left(x|\mu_k, \Sigma_k\right) && (3.13) \\ \log\left(x_1, x_2, \ldots, x_N\right)|\theta) &= \sum_n \log \sum_k \alpha_k \mathcal{N}(x^{(n)}|\mu_k, \Sigma_k) && (3.14) \\ p(z = k|x, \theta) &= \frac{\alpha_k \mathcal{N}\left(x|\mu_k, \Sigma_k\right)}{\sum_j \alpha_j \mathcal{N}\left(x|\mu_j, \Sigma_j\right)} && (3.15) \end{aligned}$$

Mixtures of experts

$$\begin{aligned} p(y|x, \theta) &= \sum_{k=1}^{K} p\left(z = k|x, \theta_z\right) p\left(y|z = k, x, \theta_K\right) && (3.16) \\ &= \sum_{k=1}^{K} \alpha_k\left(x|\theta_z\right) p_k\left(y|x, \theta_k\right) && (3.17) \end{aligned}$$

4 Exact Inference

Notation 4.1. Let X denote the set of all random variables in the model, and

1. $X_E =$ The observed evidence;
2. $X_F =$ The unobserved variable we want to infer;
3. $X_R = X - \{X_F, X_E\} =$ Remaining variables, extraneous to query.

The model defines the joint distribution of all random variables:

$$p(X_E, X_F, X_R) \tag{4.1}$$

Definition 4.1. The joint distribution over evidence and subject of inference is

$$p\left(X_F, X_E\right) = \sum_{X_R} p\left(X_F, X_E, X_R\right) \tag{4.2}$$

Definition 4.2. The conditional probability distribution for inference given evidence is

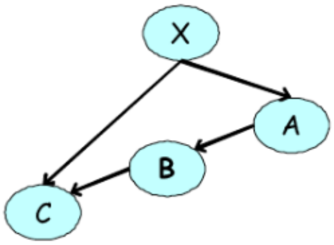
$$p\left(X_F | X_E\right) = \frac{p\left(X_F, X_E\right)}{p\left(X_E\right)} = \frac{p\left(X_F, X_E\right)}{\sum_{X_F} p\left(X_F, X_E\right)} \tag{4.3}$$

Definition 4.3. The distribution of evidence can be computed as

$$p\left(X_E\right) = \sum_{X_F, X_R} p\left(X_F, X_E, X_R\right) \tag{4.4}$$

4.1 Variable Elimination

4.2 Intermediate Factors



$$\begin{aligned} p(A, B, C) &= \sum_X p(X) p(A|X) p(B|A) p(C|B, X) \qquad (4.5) \\ &= p(B|A) \underbrace{\sum_X p(X) p(A|X) p(C|B, X)}_{\text{unnormalized}} \qquad (4.6) \end{aligned}$$

Definition 4.4. A **factor** ϕ describes the local relation between random variables, meanwhile, $\int d\phi$ is <u>not</u> necessarily one.

Remark 4.1. Let $X_\ell \subseteq X$ be a group of local random variables, then $p(X_\ell)$ is automatically a factor $\phi(X_\ell)$.

$$
\begin{aligned}
p(A,B,C) &= \sum_X \underbrace{p(X)p(A|X)p(B|A)p(C|B,X)}_{\text{from graphical representation}} && (4.7)\\
&= \sum_X \underbrace{\phi(X)\phi(A,X)\phi(A,B)\phi(X,B,C)}_{\text{factor representation}} && (4.8)\\
&= \phi(A,B)\sum_X \phi(X)\phi(A,X)\phi(X,B,C) && (4.9)\\
&= \phi(A,B)\ \underbrace{\tau(A,B,C)}_{\text{another factor}} && (4.10)
\end{aligned}
$$

4.3 Sum-Product Inference

Theorem 4.1. Consider a graphical model with random variables $X = Y \cup Z$. For an random variable Y in a directed or undirected model, $P(Y)$ can be computed using the **sum-product**

$$\tau(Y) = \sum_z \prod_{\phi \in \Phi} \phi(Scope[\phi] \cap Z, Scope[\phi] \cap Y) \tag{4.11}$$

where Φ is a set of factors.

Remark 4.2. For directed models,

$$\Phi = \{\phi_{x_i}\}_{i=1}^N = \{p\left(x_i \middle| \text{ parents } \left(x_i\right)\right)\}_{i=1}^N \tag{4.12}$$

4.4 Complexity of Variable Elimination Ordering

Theorem 4.2. The complexity of the variable elimination algorithm is

$$\mathcal{O}(mk^{N_{max}}) \tag{4.13}$$

where

(i) m is the number of initial factors $|\Phi|$;

(ii) k is the number of states each random variable takes, assumed to be equal;

(iii) N_i is the number of random variables within each summation;

(iv) $N_{max} = \max_i N_i$.

5 Message passing, Hidden Markov Models, and Sampling

5.1 Message Passing (Computing All Marginals)

Notation 5.1. Let T denote the set of edges in a tree. For a node i, let $N(i)$ denote the set of its neighbours.

The factor of all random variables can be computed following

$$P\left(X_{1:n}\right)=\frac{1}{Z}\underbrace{\left[\prod_{i=1}^{n}\phi\left(x_i\right)\right]}_{\text{prior factors}}\underbrace{\prod_{(i,j)\in T}\phi_{i,j}\left(x_i,x_j\right)}_{\text{local factors}} \tag{5.1}$$

Definition 5.1. The **message** sent from variable j to $i\in N(j)$ is

$$m_{j\to i}\left(x_i\right)=\sum_{x_j}\left[\phi_j\left(x_j\right)\phi_{ij}\left(x_i,x_j\right)\prod_{k\in N(j)\neq i}m_{k\to j}\left(x_j\right)\right] \tag{5.2}$$

Algorithm 5.1 (Belief Propagation Algorithm)**.** Given a tree, inference on an arbitrary node $p(x_i)$ can be computed following:

1. Choose root r arbitrarily;
2. Pass messages from leaves to r;
3. Pass messages from r to leaves;
4. Compute inference

$$p\left(x_i\right)\propto\phi_i\left(x_i\right)\prod_{j\in N(i)}m_{j\to i}\left(x_i\right) \tag{5.3}$$

5.2 Markov Chains

Using chain rule of probability:

$$p\left(x_{1:T}\right)=\prod_{t=1}^{T}p\left(x_t|x_{t-1},\dots,x_1\right) \tag{5.4}$$

Definition 5.2. A Markov chain is said to be **first-order** if

$$p\left(x_t|x_{1:t-1}\right)=p\left(x_t|x_{t-1}\right) \tag{5.5}$$

Simplification Therefore, for all first-order Markov chains, the full joint distribution can be reduced to

$$p\left(x_{1:T}\right)=\prod_{t=1}^{T}p\left(x_t|x_{t-1}\right) \tag{5.6}$$

Definition 5.3. A Markov chain is at m-order if

$$p\left(x_t|x_{1:t-1}\right)=p\left(x_t|x_{t-m:t-1}\right) \tag{5.7}$$

Definition 5.4. A Markov chain is said to be **homogenous** (i.e., stationary) if

$$p\left(x_t|x_{t-1}\right)=p\left(x_{t+k}|x_{t-1+k}\right)\quad\forall t,k \tag{5.8}$$

Parameterization Assume the random variable X_t takes k states, further suppose the chain is time homogenous. Then characterizing the transition probability

$$p(x_t|x_{t-1}, x_{t-2}, \cdots, x_{t-m}) \tag{5.9}$$

requires $(k-1)k^m$ parameters.

5.3 Hidden Markov Models

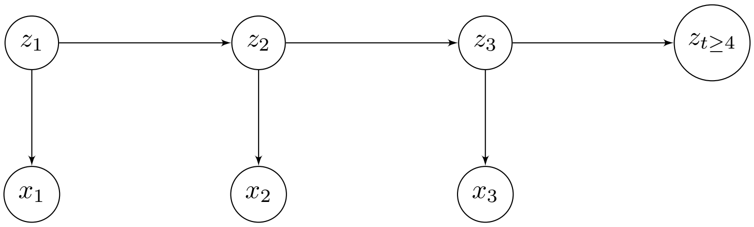


Figure 5.1: Hidden Markov Model

Joint distribution Following the conventional expansion

$$p(x_{1:T}, z_{1:T}) = p(z_1) \prod_{t=2}^{T} p(z_t|z_{t-1}) \prod_{t=1}^{T} p(x_t|z_t) \tag{5.10}$$

Parameterization Assuming the HMM is homogenous with order 1, then the set of parameters Φ consists of

(i) Initial distribution of $p(z_1)$: $k-1$ parameters;

(ii) Transition distribution of $p(z_{t+1}|z_t)$: $(k-1)k$ parameters;

(iii) Emission distribution of $p(x_t|z_t)$: $(k-1)k$ parameters.

5.4 Forward-backward Algorithm

Smoothing compute posterior over past hidden state

$$p(z_\tau|x_{1:t}) \ s.t. \ 1 < \tau < t \tag{5.11}$$

Filtering compute posterior over current hidden state

$$p(z_t|x_{1:t}) \tag{5.12}$$

Prediction compute posterior over future hidden state

$$p(z_\tau|x_{1:t}) \ s.t. \ \tau > t \tag{5.13}$$

5.5 Procedure of Smoothing (Forward-backward Algorithm)

$$\begin{aligned}
p(z_t|x_{1:T}) &\propto p(x_{1:T}, z_t) && (5.14)\\
&= p(z_t, x_{1:t})p(x_{t+1:T}|z_t, x_{1:t}) && (5.15)\\
&= p(z_t, x_{1:t})p(x_{t+1:T}|z_t) && (5.16)\\
&= p(z_t|x_{1:t})p(x_{1:t})p(x_{t+1:T}|z_t) && (5.17)\\
&\propto p(z_t|x_{1:t})p(x_{t+1:T}|z_t) && (5.18)
\end{aligned}$$

Forward filtering (encoding) Define

$$\alpha_t(z_t) := p(z_t|x_{1:t}) \tag{5.19}$$

Then

$$\begin{aligned}
p(z_t|x_{1:t}) &\propto p(z_t, x_{1:t}) && (5.20)\\
&= \sum_{z_{t-1}=1}^{k} p(z_{t-1}, z_t, x_{1:t}) && (5.21)\\
&= \sum_{z_{t-1}=1}^{k} p(x_t|z_{t-1}, z_t, x_{1:t-1})p(z_t|z_{t-1}, x_{1:t-1})p(z_{t-1}, x_{1:t-1}) && (5.22)\\
&= \sum_{z_{t-1}=1}^{k} p(x_t|z_t)p(z_t|z_{t-1})p(z_{t-1}, x_{1:t-1}) && (5.23)\\
&= p(x_t|z_t) \sum_{z_{t-1}=1}^{k} p(z_t|z_{t-1})p(z_{t-1}, x_{1:t-1}) && (5.24)\\
& && (5.25)
\end{aligned}$$

Therefore, we have the forward recursion:

$$\begin{aligned}
\alpha_t(z_t) &= p(x_t|z_t) \sum_{z_{t-1}=1}^{k} p(z_t|z_{t-1})\alpha_{t-1}(z_{t-1}) && (5.26)\\
\alpha_1(z_1) &= p(x_1, z_1) && (5.27)
\end{aligned}$$

Backward filtering (decoding) Define

$$\beta_t(z_t) = p(x_{t+1:T}|z_t) \tag{5.28}$$

Then,

$$
\begin{aligned}
p(x_{t+1:T}|z_t) &= \sum_{z_{k+1}=1}^{k} p(x_{t+1:T}, z_{t+1}|z_t) && (5.29)\\
&= \sum_{z_{k+1}=1}^{k} p(x_{t+1}, x_{t+2:T}, z_{t+1}|z_t) && (5.30)\\
&= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}, z_{t+1}|z_t, x_{t+1})p(x_{t+1}|z_t) && (5.31)\\
&= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}, z_{t+1}|z_t, x_{t+1})p(x_{t+1}|z_t) && (5.32)\\
&= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}, z_{t+1}|z_t)p(x_{t+1}|z_t) && (5.33)\\
&= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}|z_t, z_{t+1})p(z_{t+1}|z_t)p(x_{t+1}|z_t) && (5.34)\\
&= \sum_{z_{k+1}=1}^{k} p(x_{t+2:T}|z_{t+1})p(z_{t+1}|z_t)p(x_{t+1}|z_t) && (5.35)\\
&= \sum_{z_{k+1}=1}^{k} \beta_{t+1}(z_{t+1})p(z_{t+1}|z_t)p(x_{t+1}|z_t) && (5.36)
\end{aligned}
$$

5.6 Sampling

Problem 1 Generate samples

$$\{x^{(r)}\}_{r=1}^{R} \sim p(x) \tag{5.37}$$

Problem 2 Estimate expectations of functions $f(x)$ taking random variable $x \sim p(x)$.

$$
\begin{aligned}
\mathbb{E}_{x\sim p(x)} f(x) &= \int f(x)p(x)\ dx && (5.38)\\
&\approx \hat{E} = \frac{1}{N}\sum_{i=1}^{N} f(x^{(i)}) && (5.39)
\end{aligned}
$$

Ancestral sampling sampling in a topological order. At each step, sample from any conditional distribution that you haven't visited yet, whose parents have all been sampled. This procedure will always start with the nodes that have no parents (i.e., a root).

Generating marginal samples for nodes $Y \subseteq X$:

(i) Construct $p(X) = \prod_{x_i \in X} p(x_i|\text{parent}[x_i])$;

(ii) Sample $(x_1, x_2, \cdots, x_N) \sim p(X)$;

(iii) Ignore $x_i \notin Y$.

Generating conditional samples for nodes $Y \subseteq Xt$ conditioned on $Z \subseteq X$:

Definition 5.5. The **simple Monte Carlo** estimator $\hat{\Phi}$ is defined as

$$\frac{1}{R}\sum_{r=1}^{R} f\left(x^{(r)}\right) = \hat{E} \approx E = \mathop{\mathbb{E}}_{x\sim p(x)}[f(x)] \tag{5.40}$$

Proposition 5.1. If the sample $\{x^{(r)}\}_{r=1}^{R}$ are generated from $p(x)$, then $\hat{E}$ is an unbiased estimator of E.

Proof.

$$\begin{aligned}
\mathbb{E}[\hat{E}]_{x\sim p\left(\{x^{(i)}\}_{r=1}^{R}\right)} &= \mathbb{E}\left[\frac{1}{R}\sum_{r=1}^{R} f\left(x^{(r)}\right)\right] && (5.41)\\
&= \frac{1}{R}\sum_{r=1}^{R}\mathbb{E}\left[f(x^{(r)})\right] && (5.42)\\
&= \frac{1}{R}\sum_{r=1}^{R}\mathbb{E}_{x\sim p(x)}[f(x)] && (5.43)\\
&= \frac{R}{R}\mathbb{E}_{x\sim p(x)}[f(x)] && (5.44)\\
&= E && (5.45)
\end{aligned}$$

■

Proposition 5.2. As the number of samples of R increases, the variance of $\hat{E}$ will decrease proportional to $\frac{1}{R}$.

Proof.

$$\begin{aligned}
Var[\hat{E}] &= Var[\frac{1}{R}\sum_{r=1}^{R} f(x^{(r)})] && (5.46)\\
&= \frac{1}{R^2}Var[\sum_{r=1}^{R} f(x^{(r)})] && (5.47)\\
&= \frac{1}{R^2}\sum_{r=1}^{R} Var[f(x^{(r)})] && (5.48)\\
&= \frac{1}{R^2}RVar[f(x)] && (5.49)\\
&= \frac{1}{R}Var[f(x)] && (5.50)
\end{aligned}$$

■

6 True Skill

Let $z_i \in \mathbb{R}$ denote player's skill such that

$$z_i \sim \mathcal{N}(0, 1) \tag{6.1}$$

And skills of players are independent such that

$$p(z_{1:n}) = \prod_{i=1}^{n} p(z_i) \tag{6.2}$$

Therefore, the joint distribution of skills can be written as a multivariate Gaussian distribution.
Let X_j player A beats player B, then

$$p(\text{A beat B}|z_A, z_B) = \sigma(z_A - z_B) \tag{6.3}$$

where $\sigma = 1/(1 + \exp(z))$.
Then,

$$p(z_1, z_2|\text{A beat B}) \propto p(z_1, z_2)p(\text{A beat B}|z_1, z_2) \tag{6.4}$$

Question 1 What's the chance that player A is better than player B in game $\mathcal{G}$?

$$\begin{aligned} p(z_A > z_B|\mathcal{G}) &= \mathbb{E}_{p(z_A,z_B|\mathcal{G})}\mathbb{1}\{z_A > z_B\} &(6.5)\\ &\approx \frac{1}{K}\sum_{i=1}^{K}\mathbb{1}\{z_A > z_B\} \quad z_A, z_B \sim p(z_A, z_B|\text{data}) &(6.6)\end{aligned}$$

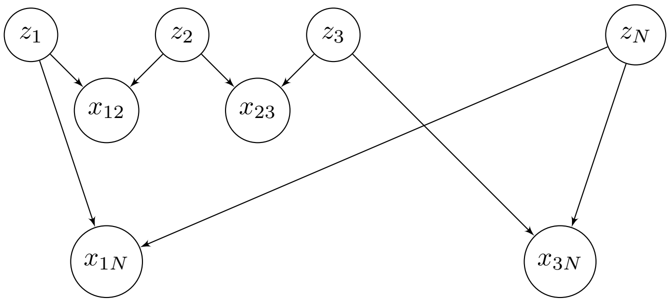


Figure 6.1: Structure of Games

Approximate Inferences We have $p(z), p(x|z)$ and x (data).
Wish to compute

$$q(z|x) \approx p(z|x) \tag{6.7}$$

Intractability

$$\begin{aligned} p(z_1|x) &= \int_{\mathbb{R}} p(z_1, z_2|x)\ dz_2 &(6.8)\\ &= \frac{\int_{\mathbb{R}} p(z_1, z_2, x)\ dz_2}{\iint_{\mathbb{R}^2} p(z_1, z_2, x)\ dz_2\ dz_1} &(6.9)\end{aligned}$$

6.1 Variational Inferences

General Idea of Variational Inferences

(i) Parameterize tractable $q_\varphi(z|x)$ using φ, such as

$$q_\varphi(z|x) = \mathcal{N}(z|\mu_\varphi, \Sigma_\varphi) \tag{6.10}$$

(ii) Define <u>distance</u> (not necessary distance metric) between $p(z|x)$ and $q(z|x)$.

(iii) Optimize φ to minimize distrance.

Kullback–Leibler Divergence

Definition 6.1. Let q and p be density functions of two distributions Q and P, then the **KL divergence** between Q and P is defined as

$$\begin{aligned} KL(q||p) &:= \mathbb{E}_q\left(\log\frac{q}{p}\right) &(6.11)\\ &= \int q(z)\left(\log q(z) - \log p(z)\right)\ dz &(6.12)\end{aligned}$$

Properties of KL divergence

$$\begin{aligned} &KL(q||p) \geq 0\ \forall p, q \in \Delta(\mathcal{X}) &(6.13)\\ &KL(q||p) = 0 \iff p = q &(6.14)\\ &KL(q||p) \neq KL(p||q) \text{ in general} &(6.15)\end{aligned}$$

Define

$$\begin{aligned} -KL(q_\varphi(z|x)||p(z|x)) &= -\mathbb{E}_{q_\varphi(z|x)}\left[\log q_\varphi(z|x) - \log p(z|x)\right] &(6.16)\\ &= -\mathbb{E}_{q_\varphi(z|x)}\left[\log q_\varphi(z|x) - \log\frac{p(z,x)}{p(x)}\right] &(6.17)\\ &= -\mathbb{E}_{q_\varphi(z|x)}\left[\log q_\varphi(z|x) - \log p(z,x) + \log p(x)\right] &(6.18)\\ &= -\mathbb{E}_{q_\varphi(z|x)}\left[\log q_\varphi(z|x) - \log p(z,x)\right] + \mathbb{E}_{q_\varphi(z|x)}\left[\log p(x)\right] &(6.19)\\ &= \underbrace{-\mathbb{E}_{q_\varphi(z|x)}\left[\log q_\varphi(z|x) - \log p(z,x)\right]}_{L(\varphi)} + \underbrace{\log p(x)}_{\perp\varphi} &(6.20)\end{aligned}$$

where $L(\varphi)$ is often referred to as the evidence/empirical lower bound (ELBO).

Re-parameterization Tricks Want to compute

$$\begin{aligned} \nabla_\varphi \mathbb{E}_{q_\varphi(z)} f(z) &= \nabla_\varphi \int q_\varphi(z) f(z)\ dz &(6.21)\\ &= \int \nabla_\varphi q_\varphi(z) f(z)\ dz \text{ (†) assume continuity} &(6.22)\end{aligned}$$

But (†) is not an expectation, so we cannot use Monte Carlo.
So we need to re-parameterize such that the expectation does not depend on φ.
Find $p(\varepsilon)$ (i.e., re-parameterize using ε) and $T(\varepsilon, \varphi)$ such that

$$\begin{aligned} &t \sim p(\varepsilon) &(6.23)\\ &z = T(t, \varphi) &(6.24)\end{aligned}$$

then

$$z \sim q_\varphi(z) \tag{6.25}$$

Stochastic/Automatic Differentiation Variational Inference

$$\nabla_\varphi \mathbb{E}_{q_\varphi(z|x)} \left[\log p(x,z) - \log q_\varphi(z|x)\right] \tag{6.26}$$
$$= \nabla_\varphi \mathbb{E}_{p(\varepsilon)} \left[\log p(x, T(\varepsilon,\varphi)) - \log q_\varphi(T(\varepsilon,\varphi)|x)\right] \tag{6.27}$$
$$= \mathbb{E}_{p(\varepsilon)} \nabla_\varphi \left[\log p(x, T(\varepsilon,\varphi)) - \log q_\varphi(T(\varepsilon,\varphi)|x)\right] \tag{6.28}$$
$$\approx \frac{1}{K}\sum_{i=1}^{K} \nabla_\varphi \left[\log p(x, T(\varepsilon,\varphi)) - \log q_\varphi(T(\varepsilon,\varphi)|x)\right] \tag{6.29}$$

Reinforce / Score Function Estimation Another method to estimate $-\nabla_\varphi \mathbb{E}_{q_\varphi(z|x)} L(\varphi)$. Want

$$\nabla_\varphi \mathbb{E}_{q_\varphi(z)}[f(z)] \tag{6.30}$$
$$= \nabla_\varphi \int q_\varphi(z) f(z) \; dz \tag{6.31}$$
$$= \int \nabla_\varphi q_\varphi(z) f(z) \; dz \tag{6.32}$$
$$= \int f(z) \nabla_\varphi q_\varphi(z) \; dz \tag{6.33}$$

Note that

$$\nabla_\varphi \log q_\varphi(z) = \frac{\nabla_\varphi q_\varphi(z)}{q_\varphi(z)} \tag{6.34}$$

Therefore,

$$\int f(z) \nabla_\varphi q_\varphi(z) \; dz \tag{6.35}$$
$$= \int f(z) q_\varphi(z) \nabla_\varphi \log q_\varphi(z) \; dz \tag{6.36}$$
$$= \mathbb{E}_{q_\varphi(z)}[f(z) \nabla_\varphi \log q_\varphi(z)] \tag{6.37}$$

Mean-Field Variational Inference

$$q(z_1, \cdots, z_N|x) = \prod_{i=1}^{N} q(z_i|x) \tag{6.38}$$

Jensen's Inequality

Theorem 6.1. If f is convex, then

$$f(\mathbb{E}\left[X\right]) \leq \mathbb{E}\left[f(x)\right] \tag{6.39}$$

Using Jensen's inequality,

$$
\begin{aligned}
\log p_\theta(x) &= \log \int p_\theta(x,z)\ dz && (6.40)\\
&= \log \int p_\theta(x,z) \frac{q_\varphi(z|x)}{q_\varphi(z|x)}\ dz && (6.41)\\
&= \log \mathbb{E}_{q_\varphi(z|x)} \int \frac{p_\theta(x,z)}{q_\varphi(z|x)}\ dz && (6.42)\\
&\geq \mathbb{E}_{q_\varphi(z|x)} \int \log \frac{p_\theta(x,z)}{q_\varphi(z|x)}\ dz && (6.43)\\
&\equiv ELBO(\theta, \varphi) && (6.44)
\end{aligned}
$$

7 Markov Chain Monte Carlo

Problem Statement A target distribution

$$p(x) \tag{7.1}$$

and a function

$$f(x) \tag{7.2}$$

Wish to compute

$$\mathbb{E}_{x\sim p}[f] \equiv \int f(x)p(x)\ dx \tag{7.3}$$

Note that $\int_{p(x)}$ is rarely analytic, so we have to approximate it.

7.1 Monte Carlo

Sample

$$\{x_i\}_{i=1}^R \sim p \tag{7.4}$$

Simple MC estimator

$$\mathbb{E}_p[f] \approx \hat{f} \equiv \frac{1}{R}\sum_{i=1}^R f(x_i) \tag{7.5}$$

Therefore, Monte Carlo turns estimation problem into a sampling problem.
Note that MC estimator is unbiased and variance shrinks proportional to $\frac{1}{R}$.
Further, the variance is independent of dimensionality.
Note that sampling from high dimensions is still hard. Why? So far, we've assumed

$$
\begin{aligned}
p(x) &= \frac{\tilde{p}(x)}{Z} = \frac{\tilde{p}(x)}{\int d\tilde{p}(x)} && (7.6)\\
p(x) &\propto \tilde{p}(x) && (7.7)
\end{aligned}
$$

Aside No that $\tilde{p}$ is the joint distribution of $q(pred; data)$. In this case, p could be the likelihood $q(pred|data) = \frac{q(pred,data)}{\int_{pred} dq(pred,data)}$.
$Z = p(data)$ is often referred to as the **evidence**.

Why is sampling $x \sim p$ hard? Want samples from volumes with high $p(x)$, can't do exactly without enumerating all possible x, which is challenging when x is in high dimensional spaces.

Lattice (Bad idea!) Using lattice to sample is a bad idea, if the lattice is too coarse, the estimated distribution is biased. If the lattice is too dense, then we're wasting computational resources.

Uniform Sampling

Importance Weight Sampler Sampling from p is hard, we sample x^r from a simpler distribution q (e.g., $p \sim \mathcal{N}$) instead. Weight each sample from q by $w_r = \frac{\tilde{p}(x^r)}{q(x^r)}$. Recall that we know how to evaluate the unnormalized density $\tilde{p}$.

Rejection Sampling Assume

$$\tilde{p}(x) = p(x)Z_p \ Z_p \in \mathbb{R} \tag{7.8}$$

$$\tilde{q}(x) = q(x)Z_q \ Z_q \in \mathbb{R} \tag{7.9}$$

and we can sample from q cheaply. Further, assume

$$\exists\ c\ s.t.\ c\tilde{q}(x) > \tilde{p}(x) \quad \forall x \tag{7.10}$$

Algorithm 7.1. (Rejection Sampling)

(i) Sample $x \sim q$;

(ii) Sample $u \sim [0, c\tilde{q}(x)]$;

(iii) Accept if $u < \tilde{p}(x)$ (i.e., append x to the sample list), reject otherwise.

Limitations The rejection sampling requires $p \approx q$. Otherwise, the C required is large. When p and q are on D dimensions, then $C \in \mathcal{O}(\exp(\sqrt{D}))$. The acceptance rate is $\frac{1}{C}$ in one dimension, and the rate reduces exponentially in dimension.

$$\mathbb{E}_p[f] = \int f(x)p(x)\ dx \tag{7.11}$$

Since integral is a linear operator, when integrant is large, the expectation is large as well.

Typical set Because expectation is a linear operator, all samples that contribute significantly to the $\mathbb{E}$ come from the typical set.

Check the definition of typical set.

Markov Chain Monte Carlo (MCMC) Stochastically explore the typical set. We need a Markov transition distribution, from which we can sample x_{t+1}:

$$x_{t+1} \sim T(x'|x_t) \tag{7.12}$$

Proposition 7.1. Properties of T 1) p is invariant under T:

$$p(x) = \int T(x|x')p(x')\ dx' \tag{7.13}$$

2) Ergodic: $p^{(t)} \to p(x)$.

Metropolis Given background distribution p, we only observe $\tilde{p}$ but not p. Define T as

(i) Proposal distribution q

$$x' \sim q(x'|x_t) \tag{7.14}$$

(ii) Accept x' as x_{t+1}?

$$a := \frac{\tilde{p}(x')q(x_t|x')}{\tilde{p}(x_t)q(x'|x_t)} \tag{7.15}$$

If $a \geq 1$, then accept it. If $a \in [0, 1)$, accept with probability a. If rejected, $x_{t+1} = x_t$.

Random Walk Metropolis

$$q(x'|x_t) = \mathcal{N}(x'|x_t, \sigma^2) \tag{7.16}$$

Hamiltonian Monte Carlo

$$x \to (x, v) \tag{7.17}$$

$$q(x) \to q(x, v) = q(x)q(v|x) \tag{7.18}$$

$$H(x, v) = -\log(q(x, v)) = -\overbrace{\log(q(x))}^{U:PE} - \overbrace{\log(q(v|x))}^{K:KE} \tag{7.19}$$