

Chapter 17

Monte Carlo Methods

Monte Carlo Sampling

- To approximate sums or integrals (which are costly to evaluate or intractable) by drawing samples

$$s = \sum_{\mathbf{x}} p(\mathbf{x}) f(\mathbf{x}) \text{ or } s = \int p(\mathbf{x}) f(\mathbf{x}) d\mathbf{x}$$

- **Idea:** To view the sum/integral as an expectation under some distribution and to approximate it by an *average*

$$s = E_p[f(\mathbf{x})] \approx \hat{s}_n = \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}^{(i)})$$

where

$$\mathbf{x}^{(i)} \sim p(\mathbf{x})$$

- It is easy to verify that the estimator \hat{s}_n is unbiased

$$E[\hat{s}_n] = E_p[f(\mathbf{x})] = s$$

- If the samples $\mathbf{x}^{(i)}$ are independently and identically distributed (i.i.d.),

$$\text{Var}[\hat{s}_n] = \frac{\text{Var}[f(\mathbf{x})]}{n}$$

$$\hat{s}_n \sim \mathcal{N}(s, \text{Var}[\hat{s}_n]) \quad (\text{C.L.T.})$$

Importance Sampling

- To approximate the expectation based on a **proposal distribution** $q(\mathbf{x})$ that is easier to draw samples from than $p(\mathbf{x})$

$$s = \sum_{\mathbf{x}} p(\mathbf{x}) f(\mathbf{x}) = \sum_{\mathbf{x}} q(\mathbf{x}) \frac{p(\mathbf{x}) f(\mathbf{x})}{q(\mathbf{x})}$$

- Importance sampling estimator \hat{s}_q

$$\hat{s}_q = \frac{1}{n} \sum_{i=1}^n \frac{p(\mathbf{x}^{(i)}) f(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})} = \frac{1}{n} \sum_{i=1}^n \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})} f(\mathbf{x}^{(i)})$$

where

$$\mathbf{x}^{(i)} \sim q(\mathbf{x})$$

- $p(\mathbf{x}^{(i)})/q(\mathbf{x}^{(i)})$ are known as *importance weights*

- It is readily seen that \hat{s}_q is unbiased irrespective of the choice of $q(\mathbf{x})$

$$E_q[\hat{s}_q] = E_q\left[\frac{p(\mathbf{x})f(\mathbf{x})}{q(\mathbf{x})}\right] = E_p[f(\mathbf{x})] = s$$

- The variance of \hat{s}_q is however highly sensitive to the choice of $q(\mathbf{x})$

$$\text{Var}[\hat{s}_q] = \text{Var}\left[\frac{p(\mathbf{x})f(\mathbf{x})}{q(\mathbf{x})}\right]/n$$

Biased Importance Sampling

- Oftentimes $p(\mathbf{x})$ can only be evaluated up to a normalization constant

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

That is, $\tilde{p}(\mathbf{x})$ is easy to evaluate and Z_p is unknown (or intractable)

- We may also wish to use a $q(\mathbf{x})$ with the same property

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

- The importance sampling estimator is then given by

$$\begin{aligned}\hat{s}_q &= \frac{1}{n} \sum_{i=1}^n \frac{p(\mathbf{x}^{(i)})}{q(\mathbf{x}^{(i)})} f(\mathbf{x}^{(i)}) \\ &= \frac{Z_q}{Z_p} \frac{1}{n} \sum_{i=1}^n \frac{\tilde{p}(\mathbf{x}^{(i)})}{\tilde{q}(\mathbf{x}^{(i)})} f(\mathbf{x}^{(i)})\end{aligned}$$

$$= \frac{Z_q}{Z_p} \frac{1}{n} \sum_{i=1}^n \tilde{r}_i f(\mathbf{x}^{(i)})$$

where

$$\tilde{r}_i = \frac{\tilde{p}(\mathbf{x}^{(i)})}{\tilde{q}(\mathbf{x}^{(i)})} \text{ and } \mathbf{x}^{(i)} \sim q(\mathbf{x})$$

- The same set of data $\mathbf{x}^{(i)}$ can be used to approximate the ratio Z_p/Z_q

$$\begin{aligned} \frac{Z_p}{Z_q} &= \frac{\sum_{\mathbf{x}} \tilde{p}(\mathbf{x})}{Z_q} \\ &= \sum_{\mathbf{x}} \tilde{p}(\mathbf{x}) \frac{1}{Z_q} \\ &= \sum_{\mathbf{x}} \tilde{p}(\mathbf{x}) \frac{q(\mathbf{x})}{\tilde{q}(\mathbf{x})} \\ &= \sum_{\mathbf{x}} \frac{\tilde{p}(\mathbf{x})}{\tilde{q}(\mathbf{x})} q(\mathbf{x}) \end{aligned}$$

$$\begin{aligned} &\simeq \frac{1}{n} \sum_i \frac{\tilde{p}(\mathbf{x}^{(i)})}{\tilde{q}(\mathbf{x}^{(i)})} \\ &= \frac{1}{n} \sum_i \tilde{r}_i \end{aligned}$$

- We then arrive at a *biased importance estimator*

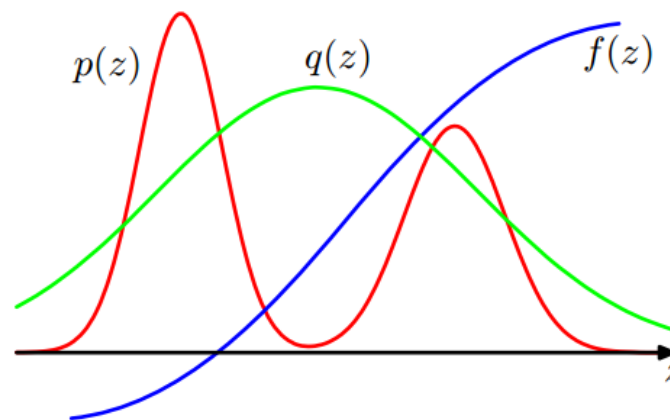
$$\hat{s}_{BIS} = \frac{\sum_{i=1}^n \tilde{r}_i f(\mathbf{x}^{(i)})}{\sum_{i=1}^n \tilde{r}_i} = \sum_{i=1}^n \tilde{w}_i f(\mathbf{x}^{(i)})$$

where

$$\tilde{w}_i = \frac{\tilde{r}_i}{\sum_{i=1}^n \tilde{r}_i}$$

- \hat{s}_{BIS} is asymptotically unbiased; that is, as $n \rightarrow \infty$, $E[\hat{s}_{BIS}] = s$

- The success of importance sampling depends crucially on how well $q(\mathbf{x})$ matches the desired distribution $p(\mathbf{x})$
- When $p(\mathbf{x})f(\mathbf{x})$ is strongly varying and has its mass concentrated over small regions of \mathbf{x} space, most samples collected may be useless since they contribute little to the final estimate due to the fact $q(\mathbf{x}^{(i)}) \gg p(\mathbf{x}^{(i)})|f(\mathbf{x}^{(i)})|$
- As such, underestimation of $E_p[f(\mathbf{x})]$ is typical, especially when \mathbf{x} is high dimensional



Markov Chain Monte Carlo Methods

- Methods that involve drawing samples from Markov chains to perform Monte Carlo estimation
- Drawing samples from a Markov Chain
 1. Start with an initial state $\mathbf{x}^{(1)}$
 2. Sample repeatedly from transition distributions $p(\mathbf{x}^{(\tau+1)}|\mathbf{x}^{(\tau)})$

$$\text{Sample } \mathbf{x}^{(\tau+1)} \sim p(\mathbf{x}^{(\tau+1)}|\mathbf{x}^{(\tau)}), \tau = 1, \dots, t-1$$

- Given a desired distribution $p^*(\mathbf{x})$, we choose transition distributions such that $\mathbf{x}^{(t)}$ eventually becomes a fair sample of $p^*(\mathbf{x})$

First-Order Markov Chains

- A sequence of discrete-valued random variables $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(M)}$ with the conditional independence property

$$p(\mathbf{x}^{(m+1)} | \mathbf{x}^{(m)}, \dots, \mathbf{x}^{(1)}) = p(\mathbf{x}^{(m+1)} | \mathbf{x}^{(m)}),$$

for $m \in \{1, \dots, M - 1\}$

- The joint distribution of $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(M)}$ is characterized by $p(\mathbf{x}^{(1)})$ together with the transition probabilities $p(\mathbf{x}^{(m+1)} | \mathbf{x}^{(m)})$

$$p(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(M)}) = p(\mathbf{x}^{(1)}) \prod_{i=1}^{M-1} p(\mathbf{x}^{(i+1)} | \mathbf{x}^{(i)})$$



- The marginal distribution $p(\mathbf{x}^{(m+1)})$ can be expressed as

$$p(\mathbf{x}^{(m+1)}) = \sum_{\mathbf{x}^{(m)}} p(\mathbf{x}^{(m+1)} | \mathbf{x}^{(m)}) p(\mathbf{x}^{(m)})$$

- In matrix form, we have

$$\mathbf{v}^{(m+1)} = \mathbf{A}^{(m)} \mathbf{v}^{(m)}$$

where

$$v_i^{(m+1)} = p(\mathbf{x}^{(m+1)} = \mathbf{s}_i), \quad \text{Prob. of } \mathbf{x}^{(m+1)} \text{ in state } \mathbf{s}_i$$

$$v_j^{(m)} = p(\mathbf{x}^{(m)} = \mathbf{s}_j), \quad \text{Prob. of } \mathbf{x}^{(m)} \text{ in state } \mathbf{s}_j$$

$$A_{i,j}^{(m)} = p(\mathbf{x}^{(m+1)} = \mathbf{s}_i | \mathbf{x}^{(m)} = \mathbf{s}_j), \quad \text{Transition probabilities}$$

- A Markov chain is said to be **homogeneous** if the transition probability $p(\mathbf{x}^{(m+1)} | \mathbf{x}^{(m)})$ does not depend on m

- In this case, we see that $\mathbf{A}^{(m)} = \mathbf{A}$ is a constant matrix and that over time, all the eigenvalues are exponentiated

$$\mathbf{v}^{(t)} = \mathbf{A}^{t-1} \mathbf{v}^{(1)} = \mathbf{U} \mathbf{\Lambda}^{t-1} \mathbf{U}^{-1} \mathbf{v}^{(1)}$$

- Under some conditions (e.g. non-zero transition probabilities), \mathbf{A} has only one eigenvector \mathbf{v} with the largest eigenvalue 1
- $\mathbf{v}^{(t)}$ eventually converges to that eigenvector \mathbf{v} , which denotes the **equilibrium distribution**, regardless of the choice of initial state $\mathbf{v}^{(1)}$

$$\mathbf{A}\mathbf{v} = \mathbf{v}$$

- We hope that by choosing transition probabilities correctly, \mathbf{v} will be equal to the distribution we wish to sample from

- Running the Markov chain until it reaches its equilibrium is called **burning in** and the time required is called the **mixing time**
- Unfortunately, we only know that the chain will converge under some mild conditions, but not how much time it will take
- Most properties of discrete-valued Markov chains as presented here can carry over to the continuous-valued case

Gibbs Sampling

- To build a Markov chain that samples from a distribution $p_{\text{model}}(\mathbf{x})$

$$p_{\text{model}}(\mathbf{x}) = p_{\text{model}}(x_1, x_2, \dots, x_M)$$

- Procedure

1. Start with an initial state $x_i^{(1)}, i = 1, 2, \dots, M$

2. For $\tau = 1, \dots, t - 1$

- Sample $x_1^{(\tau+1)} \sim p_{\text{model}}(x_1 | x_2^{(\tau)}, x_3^{(\tau)}, \dots, x_M^{(\tau)})$
- Sample $x_2^{(\tau+1)} \sim p_{\text{model}}(x_2 | x_1^{(\tau+1)}, x_3^{(\tau)}, \dots, x_M^{(\tau)})$

⋮

- Sample $x_j^{(\tau+1)} \sim p_{\text{model}}(x_j | x_1^{(\tau+1)}, \dots, x_{j-1}^{(\tau+1)}, x_{j+1}^{(\tau)}, \dots, x_M^{(\tau)})$

⋮

- Sample $x_M^{(\tau+1)} \sim p_{\text{model}}(x_M | x_1^{(\tau+1)}, x_2^{(\tau+1)}, \dots, x_{M-1}^{(\tau+1)})$

- In words, each step replaces one variable x_i by drawing a sample from the distribution $p_{\text{model}}(x_i | \mathbf{x}_{-i})$ of x_i conditioned on the values of the remaining variables \mathbf{x}_{-i}
- This procedure eventually yields samples of $p_{\text{model}}(\mathbf{x})$ because
 - The resulting Markov chain will converge to an equilibrium distribution, if none of the transition probabilities is zero anywhere
 - $p_{\text{model}}(\mathbf{x})$ is **invariant** w.r.t. this Markov chain
- A distribution $p^*(\mathbf{x})$ is said to be invariant w.r.t. a Markov chain if each step in the chain leaves that distribution invariant, i.e.

$$p(\mathbf{x}') = \sum_{\mathbf{x}} p(\mathbf{x}' | \mathbf{x}) p^*(\mathbf{x}) = p^*(\mathbf{x}')$$

- In the present case, we have

$$\mathbf{x} = (x_i^{old}, \mathbf{x}_{-i}^{old}) \sim p_{\text{model}}(\mathbf{x})$$

$$\mathbf{x}' = (x_i^{new}, \mathbf{x}_{-i}^{old}) \text{ with } x_i^{new} \sim p_{\text{model}}(x_i | \mathbf{x}_{-i}^{old})$$

- It can be shown that $p(\mathbf{x}') = p_{\text{model}}(\mathbf{x}')$; that is, $p_{\text{model}}(\mathbf{x})$ is invariant

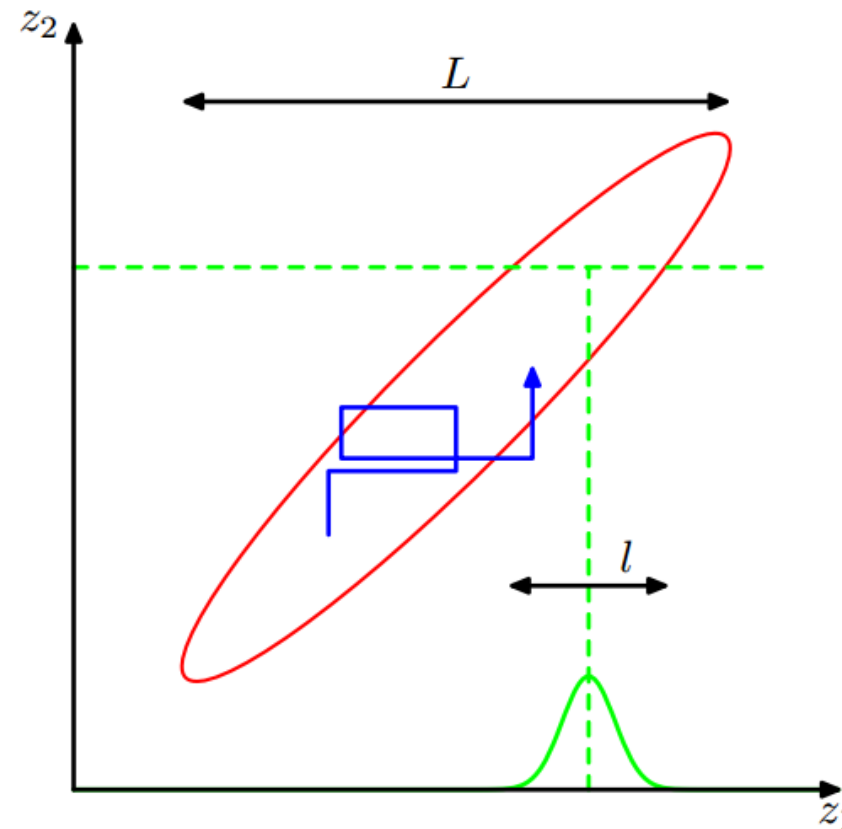
$$\begin{aligned} p(\mathbf{x}') &= p(x_i^{new}, \mathbf{x}_{-i}^{old}) \\ &= p(\mathbf{x}_{-i}^{old}) p(x_i^{new} | \mathbf{x}_{-i}^{old}) \\ &= p_{\text{model}}(\mathbf{x}_{-i}^{old}) p_{\text{model}}(x_i^{new} | \mathbf{x}_{-i}^{old}) \\ &= p_{\text{model}}(x_i^{new}, \mathbf{x}_{-i}^{old}) \\ &= p_{\text{model}}(\mathbf{x}') \end{aligned}$$

- **Block Gibbs sampling:** In some cases, it is possible to sample many variables simultaneously; for example, in RBM, $p(\mathbf{h}|\mathbf{v})$ and $p(\mathbf{v}|\mathbf{h})$ are factorial, suggesting that the elements of \mathbf{h} and of \mathbf{v} can be sampled simultaneously

Challenges

- Successive samples are preferably independent and different regions in x space should be visited proportional to their probability
- In reality, successive samples are highly correlated even though they have identical distributions
- Independent samples may be obtained by retaining every M samples for sufficiently large M , or by running multiple chains in parallel

- Moreover, Gibbs sampling may mix slowly when the variables of $p_{\text{model}}(\mathbf{x})$ are highly correlated



Sampling a correlated Gaussian of two variables

- Mixing between modes may be difficult if they are widely separated by regions of low probability
 - Toy problem: Consider the following energy model

$$\tilde{p}(a, b) = \exp(-E(a, b)), \quad a, b \in \{-1, 1\}$$

where

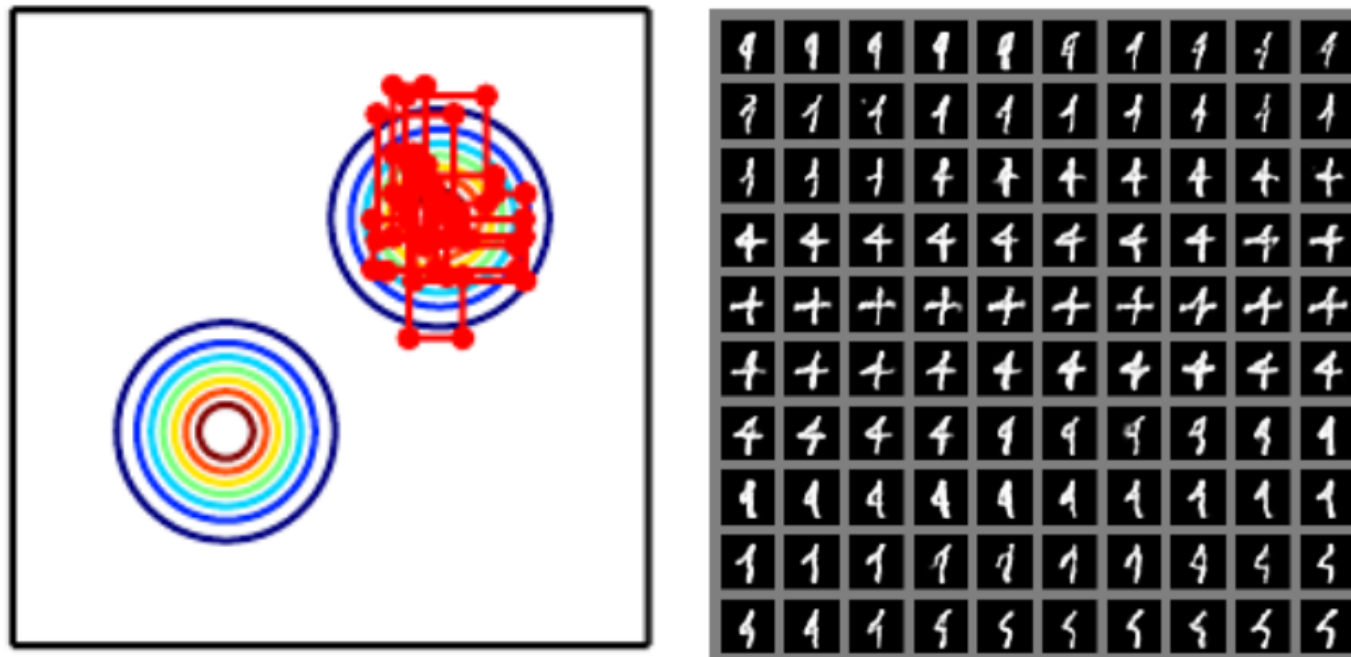
$$E(a, b) = -wab$$

- It is seen that

$$p(b = 1|a = 1) = \sigma(w)$$

- When w is extremely large, Gibbs sampling will only rarely flip the signs of a, b even if $p(b = 1, a = 1) = p(b = -1, a = -1)$

— More examples:



Confronting The Partition Function

- Many undirected graphical models are defined by an unnormalized distribution $\tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})$ with an intractable partition function $Z(\boldsymbol{\theta})$

$$p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) = \frac{\tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})}{Z(\boldsymbol{\theta})}$$

where

$$Z(\boldsymbol{\theta}) = \sum_{\mathbf{x}} \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) \text{ or } Z(\boldsymbol{\theta}) = \int_{\mathbf{x}} \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) d\mathbf{x}$$

- For training, we maximize the log-likelihood w.r.t. training data

$$E_{\mathbf{x} \sim p_{\text{data}}} \log p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) = E_{\mathbf{x} \sim p_{\text{data}}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) - \log Z(\boldsymbol{\theta})$$

through gradient descent

$$\nabla_{\boldsymbol{\theta}} E_{\mathbf{x} \sim p_{\text{data}}} \log p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) = \underbrace{E_{\mathbf{x} \sim p_{\text{data}}} \nabla_{\boldsymbol{\theta}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})}_{\text{Positive phase}} - \underbrace{\nabla_{\boldsymbol{\theta}} \log Z(\boldsymbol{\theta})}_{\text{Negative phase}}$$

- For discrete-valued \mathbf{x} , the gradient of $\log Z$ can be evaluated as

$$\nabla_{\boldsymbol{\theta}} \log Z(\boldsymbol{\theta}) = \frac{\nabla_{\boldsymbol{\theta}} Z(\boldsymbol{\theta})}{Z(\boldsymbol{\theta})} = \frac{\nabla_{\boldsymbol{\theta}} \sum_{\mathbf{x}} \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})}{Z(\boldsymbol{\theta})} = \frac{\sum_{\mathbf{x}} \nabla_{\boldsymbol{\theta}} \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})}{Z(\boldsymbol{\theta})}$$

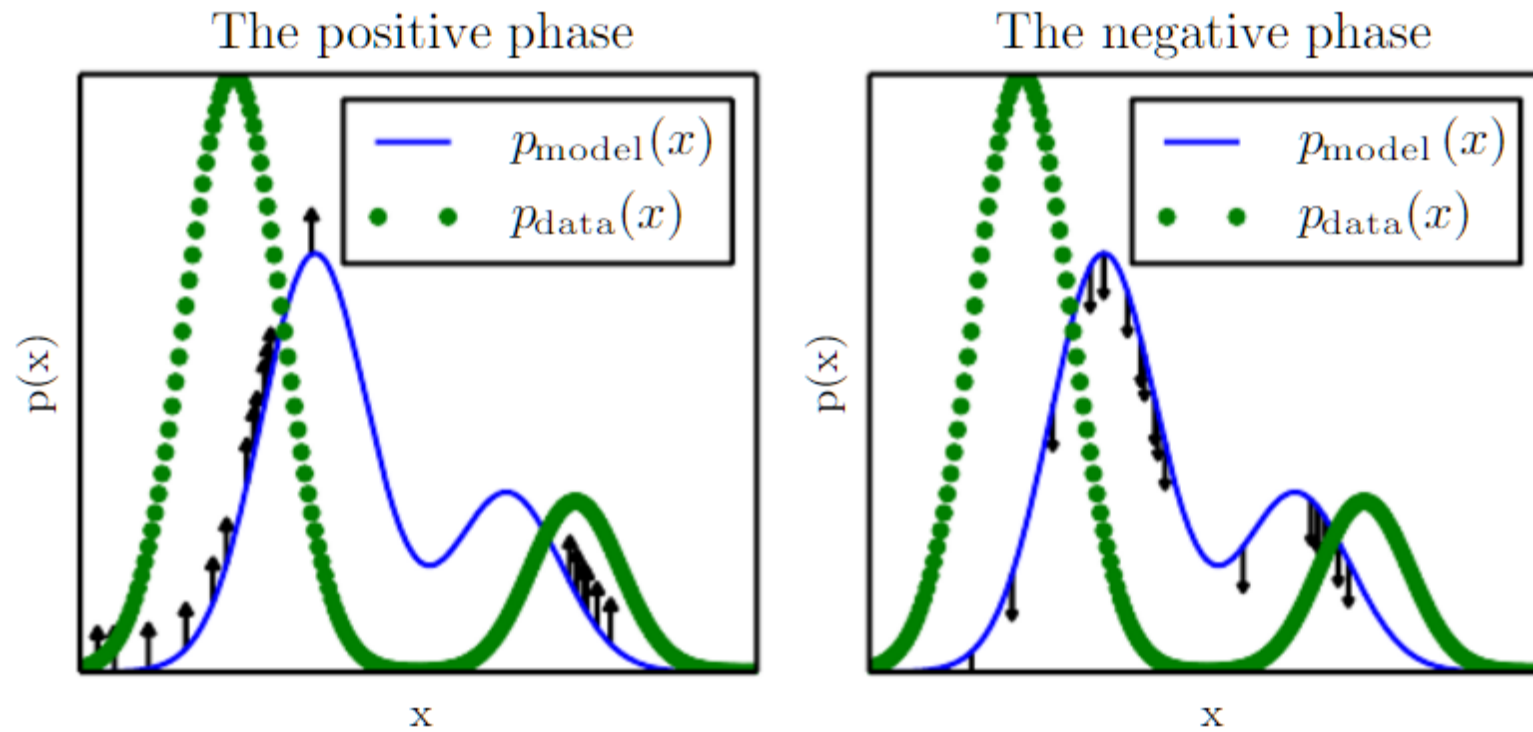
- Additionally, if $\tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) > 0$ for all \mathbf{x} (e.g. energy-based models),

$$\begin{aligned} \frac{\sum_{\mathbf{x}} \nabla_{\boldsymbol{\theta}} \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})}{Z(\boldsymbol{\theta})} &= \frac{\sum_{\mathbf{x}} \nabla_{\boldsymbol{\theta}} \exp(\log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}))}{Z(\boldsymbol{\theta})} \\ &= \frac{\sum_{\mathbf{x}} \exp(\log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})) \nabla_{\boldsymbol{\theta}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})}{Z(\boldsymbol{\theta})} \\ &= \frac{\sum_{\mathbf{x}} \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})}{Z(\boldsymbol{\theta})} \\ &= \sum_{\mathbf{x}} p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) \\ &= E_{\mathbf{x} \sim p_{\text{model}}} \nabla_{\boldsymbol{\theta}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) \end{aligned}$$

- To summarize, we see that

$$\begin{aligned} & \nabla_{\boldsymbol{\theta}} E_{\mathbf{x} \sim p_{\text{data}}} \log p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) \\ &= E_{\mathbf{x} \sim p_{\text{data}}} \nabla_{\boldsymbol{\theta}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) - E_{\mathbf{x} \sim p_{\text{model}}} \nabla_{\boldsymbol{\theta}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta}) \end{aligned}$$

- In the **positive phase**, we increase the log-likelihood by increasing $\log \tilde{p}(\mathbf{x}; \boldsymbol{\theta})$ with \mathbf{x} drawn from **training data** $p_{\text{data}}(\mathbf{x})$
- In the **negative phase**, we increase the log-likelihood by decreasing the partition function $Z(\boldsymbol{\theta})$, or equivalently, by decreasing $\log \tilde{p}(\mathbf{x}; \boldsymbol{\theta})$ with \mathbf{x} drawn from the **model distribution** $p_{\text{model}}(\mathbf{x})$
- When $p_{\text{model}}(\mathbf{x}) = p_{\text{data}}(\mathbf{x})$, there is no longer gradient



Contrastive Divergence and Its Variants

- To compute the gradient of the negative phase with Gibbs sampling

$$E_{\mathbf{x} \sim p_{\text{model}}} \nabla_{\boldsymbol{\theta}} \log \tilde{p}_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})$$

- There are different strategies for initializing the Markov chains
 - Contrastive divergence (CD) – from training data
 - Persistent contrastive divergence (PCD) – from previous step
 - (Study by yourself)

- Example: Contrastive Divergence (CD)

while not converged **do**

Sample a minibatch of m examples $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ from the training set.

$\mathbf{g} \leftarrow \frac{1}{m} \sum_{i=1}^m \nabla_{\boldsymbol{\theta}} \log \tilde{p}(\mathbf{x}^{(i)}; \boldsymbol{\theta}).$

for $i = 1$ to m **do**

$\tilde{\mathbf{x}}^{(i)} \leftarrow \mathbf{x}^{(i)}.$

end for

for $i = 1$ to k **do**

for $j = 1$ to m **do**

$\tilde{\mathbf{x}}^{(j)} \leftarrow \text{gibbs_update}(\tilde{\mathbf{x}}^{(j)}).$

end for

end for

$\mathbf{g} \leftarrow \mathbf{g} - \frac{1}{m} \sum_{i=1}^m \nabla_{\boldsymbol{\theta}} \log \tilde{p}(\tilde{\mathbf{x}}^{(i)}; \boldsymbol{\theta}).$

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \epsilon \mathbf{g}.$

end while

Review

- Why sampling?
- Importance sampling
- Gibbs sampling
- Issues with mixing of MCMC methods
- MCMC approach to learning with intractable partition functions