Probabilistic Artificial Intelligence
Problem Set 3

Oct 21, 2019

1. Markov chains and detailed balance

Assume that you are given a Markov chain with finite state space Ω and transition matrix T, which is defined for all $x, y \in \Omega$ and $t \geq 0$ as $T(x, y) := P(X_{t+1} = y \mid X_t = x)$. Furthermore, let π be the stationary distribution of the chain.

(i) Show that, if for some t the current state X_t is distributed according to the stationary distribution and additionally the chain satisfies the detailed balance equations

$$\pi(x)T(x,y) = \pi(y)T(y,x), \text{ for all } x, y \in \Omega,$$

then the following holds for all $k \geq 0$ and $x_0, \ldots, x_k \in \Omega$:

$$P(X_t = x_0, \ldots, X_{t+k} = x_k) = P(X_t = x_k, \ldots, X_{t+k} = x_0).$$

(This is why a chain that satisfies detailed balance is called *reversible*.)

(ii) Show that, if T is a symmetric matrix, then the chain satisfies detailed balance, and the uniform distribution on Ω is stationary for that chain.

2. Convergence of the Metropolis-Hastings algorithm

We use Markov Chain Monte Carlo (MCMC) methods to sample from a target distribution $P(x) = Q(x)/Z$ using a proposal distribution $R(x|x')$, without computing the normalization constant Z. A famous MCMC method is the Metropolis-Hastings algorithm, given below:

```
Algorithm 1 METROPOLIS-HASTINGS
Input: Unnormalized target distribution $Q(x)$, proposal distribution $R(x|x')$
Initialize: $x_1$ arbitrary
For $t = 1, 2, \ldots, T$:
    1. Sample proposal $x$ from the proposal distribution $R(x|x_t)$.
    2. Compute the acceptance probability $\alpha = \min\left(1, \frac{Q(x)R(x_t|x)}{Q(x_t)R(x|x_t)}\right)$.
    3. With probability $\alpha$, set $x_{t+1} = x$, else $x_{t+1} = x_t$.
```

The algorithm defines a Markov chain with transition kernel $T(x, x') = P(x_{t+1} = x'|x_t = x)$. In this exercise, we prove that the stationary distribution of this Markov chain is equal to the target distribution $P(x)$. *Remark:* While we show, that Metropolis-Hastings converges to the correct distribution, the proof doesn't tell us how fast it converges. In practice, we typically use samples only after a 'burn-in' period, which allows the chain to converge.

(i) Show that if a unnormalized distribution Q on Ω satisfies the detailed balance equations,

$$Q(x)T(x,y) = Q(y)T(y,x), \text{ for all } x, y \in \Omega, \tag{1}$$

then $\pi(x) = \frac{1}{Z}Q(x)$ is the stationary distribution of the Markov chain defined by the transition kernel $T(x, x')$.

(ii) Show that if Metropolis-Hastings transitions to a new state, i.e. $x_{t+1} \neq x_t$, then the transition probability $T(x_t, x_{t+1})$ can be written as

$$T(x_t, x_{t+1}) = \frac{1}{Q(x_t)} \min\left(Q(x_t)R(x_{t+1}|x_t), Q(x_{t+1})R(x_t|x_{t+1})\right). \tag{2}$$

Use this to show that the detailed balance equation for Q is satisfied if $x_{t+1} \neq x_t$.

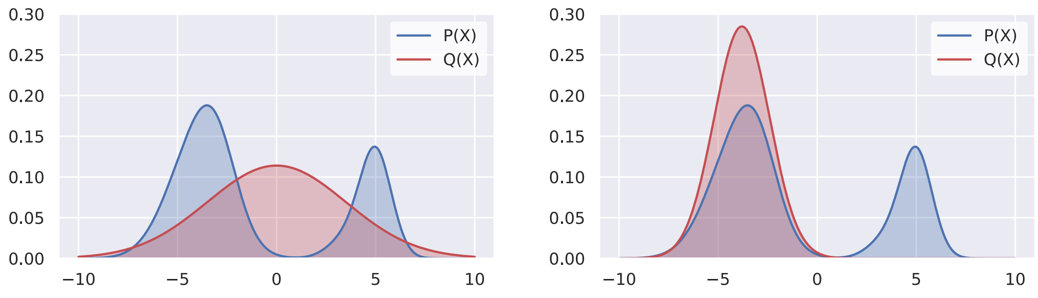
(iii) Finally, show that if $x_t = x_{t+1}$, the detailed balance condition is trivially satisfied. *Remark:* You can still compute the transition probability $T(x_t, x_{t+1})$ for this case, but the result follows independent of the exact transition probability.

3. Forward and Reverse KL for Variational Inference

In variational inference we seek to find a distribution Q in a class of distributions $\mathcal{Q}$, that minimizes the KL-distance to a target distribution P, i.e.

$$Q \in \arg\min_{Q \in \mathcal{Q}} \mathrm{KL}(Q \| P) . \tag{3}$$

The KL-distance (for finite support) is defined as $\mathrm{KL}(Q\|P) = \sum_x Q(x)\log(Q(x)/P(x))$. The KL-distance is not symmetric, so in general, $\mathrm{KL}(Q\|P) \neq \mathrm{KL}(P\|Q)$. We refer to $\mathrm{KL}(P\|Q)$ as *forward KL* and $\mathrm{KL}(Q\|P)$ as *reverse KL*. It is possible to use both, forward and reverse KL for variational inference, but the approximations will be different. In the plots below, we fit the true distribution $P(x)$ with a Gaussian $Q(x)$, using either forward or reverse KL. Explain which KL was used in either case!


0.30
0.25
0.20
0.15
0.10
0.05
0.00
−10
−5
0
5
10
P(X)
Q(X)
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−10
−5
0
5
10
P(X)
Q(X)