Monte Carlo Estimation of the KL Divergence

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This is a summary of the note by John Schulman's on how to approximate the KL divergence between two probability distributions [Sch20].

1 Preliminary

- Given two probability distributions p and q on $\mathbb{R}^d$, the **Kullback–Liebler divergence (KL divergence)** between them is defined by

$$\mathrm{KL}(p \,\|\, q) = E_{x \sim p}\bigg[\log \frac{p(x)}{q(x)} \bigg].$$

- It is a non-negative number, and it measures how different the probability distributions are. You can read more about it in my note on information theory [Khu19].
- We are interested in estimating the KL divergence via Monte Carlo integration. The simplest estimator is as follows.
  - Sample $x_1, x_2, \dots x_N$ independently according to p.
  - Compute

$$A = \frac{1}{N} \sum_{i=1}^{N} \log \frac{p(x_i)}{q(x_i)}.$$

  We have that A is an unbiased estimator of $\mathrm{KL}(p \,\|\, q)$. In other words, $E[A] = \mathrm{KL}(p \,\|\, q)$.
- The problem with this is that A might have high variance. This can result in an unintuitive result where the actual value of A is less than 0 while the KL-divergence is always positive.

2 Schulman's Unbiased Estimator

- Schulman proposes using the following estimator instead.
  - Sample $x_1, x_2, \dots x_N$ independently according to p.
  - Compute

$$B = \frac{1}{N} \sum_{i=1}^{N} \bigg(\frac{q(x_i)}{p(x_i)} - 1 - \log \frac{q(x_i)}{p(x_i)} \bigg).$$

- First, we note that B is an unbiased estimator of $\mathrm{KL}(p\,\|\,q)$. It is the Monte Carlo integration of the expectation

$$\begin{aligned}
E_{x\sim p}\bigg[\frac{q(x)}{p(x)} - 1 - \log\frac{q(x)}{p(x)}\bigg] &= E_{x\sim p}\bigg[\frac{q(x)}{p(x)} - 1\bigg] - E_{x\sim p}\bigg[\log\frac{q(x)}{p(x)}\bigg] \\
&= \int p(x)\bigg(\frac{q(x)}{p(x)} - 1\bigg)\,\mathrm{d}x + E_{x\sim p}\bigg[\log\frac{p(x)}{q(x)}\bigg] \\
&= \int q(x)\,\mathrm{d}x - \int p(x)\,\mathrm{d}x + E_{x\sim p}\bigg[\log\frac{p(x)}{q(x)}\bigg] \\
&= E_{x\sim p}\bigg[\log\frac{p(x)}{q(x)}\bigg] \\
&= \mathrm{KL}(p\,\|\,q).
\end{aligned}$$

- Second, it is the case that B is non-negative. This is because, if we let $r_i = q(x_i)/p(x_i)$, then we have that

$$B = \frac{1}{N}\sum_{i=1}^{N}(r_i - 1 - \log r_i).$$

Now, we know that $\log x \le x - 1$ for all $x > 0$. So, $B \ge 0$.

- Unfortunately, we cannot show that B has lower variance than A, but there are things that we know about it. Let X be a random variable whose distribution is p. Let

$$\begin{aligned}
V &= -\log\frac{q(X)}{p(X)}, \\
U &= \exp(V) - 1 = \frac{q(X)}{p(X)} - 1
\end{aligned}$$

We have that

$$\begin{aligned}
\mathrm{Var}(B) &= \frac{1}{N}\mathrm{Var}(U+V) \\
&= \frac{1}{N}\big[\mathrm{Var}(U) + \mathrm{Var}(V) + 2\mathrm{Cov}(U,V)\big] \\
&= \frac{\mathrm{Var}(V)}{N} + \frac{\mathrm{Var}(U) + 2\mathrm{Cov}(U,V)}{N} \\
&= \mathrm{Var}(A) + \frac{\mathrm{Var}(U) + 2\mathrm{Cov}(U,V)}{N}.
\end{aligned}$$

We note that U and V are negatively correlated, so $\mathrm{Var}(U) + 2\mathrm{Cov}(U,V)$ has a potential to be negative.

References

[Khu19] Pramook Khungurn. A primer on information theory. `https://pkhungurn.github.io/notes/notes/math/info-theory-primer/info-theory-primer.pdf`, 2019.

[Sch20] John Schulman. Approximating kl divergence. `http://joschu.net/blog/kl-approx.html`, 2020.