Deep Learning - Foundations and Concepts

Chapter 14. Sampling

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Outline

1 Basic Sampling Algorithms

Expectations

For some applications the goal is to evaluate expectations with respect to the distribution. Suppose we wish to find the expectation of a function $f(z)$ with respect to a probability distribution $p(z)$:

$$E(f) = \int f(z)p(z)\mathrm{d}z$$

The general idea behind sampling methods is to obtain a set of samples $z^{(l)}$ drawn independently from the distribution $p(z)$. This allows the expectation to be approximated by a finite sum:

$$\bar{f} = \frac{1}{L}\sum_{l=1}^{L} f(z^{(l)})$$

Expectations

Let's calculate the expectation and variance of $\bar{f}$:

$$E(\bar{f}) = E(\frac{1}{L}\sum_{l=1}^{L} f(z^{(l)})) = E(f)$$

$$E(\bar{f}^2) = E(\frac{1}{L^2}\sum_{l,l'} f(z^{(l)})f(z^{(l')})) = (E(f))^2 + \frac{1}{L}\mathrm{var}(f)$$

$$\mathrm{var}(\bar{f}) = E(\bar{f}^2) - (E(\bar{f}))^2 = \frac{1}{L}\mathrm{var}(f)$$

Which shows that:

- $\bar{f}$ is an unbiased estimator of $E(f)$.
- Due to the linear decrease of the variance with increasing L, in principle, high accuracy may be achievable with a relatively small number of samples $z^{(l)}$.

Standard distributions

Problem

Suppose that z is uniformly distributed over the interval $(0, 1)$. Given a probability density function p, find a function g such that the random variable $y = g(z)$ has p as its probability density function.

Standard distributions

Let U be the probability density function of the uniform distribution over the interval $(0, 1)$, we have:

$$\begin{aligned} p(y)\mathrm{d}y &= U(z)\mathrm{d}z \\ f(y_0) &= \int_{-\infty}^{y_0} p(y)\mathrm{d}y = \int_{-\infty}^{z_0} U(z)\mathrm{d}z = z_0 \\ y_0 &= f^{-1}(z_0) \end{aligned}$$

So we have to transform the uniformly distributed random numbers using a function that is the inverse of the cumulative distribution function of the desired probability density function.

Standard distributions

Some examples:

- Exponential distribution $p(y) = \lambda \exp(-\lambda y)$:
  - $z = f(y) = \int_0^y p(t)\mathrm{d}t = 1 - \exp(-\lambda y)$.
  - $y = -\frac{1}{\lambda} \log(1 - z)$.
- Cauchy distribution $p(y) = \frac{1}{\pi} \frac{1}{1+y^2}$:
  - $z = f(y) = \int_{-\infty}^y p(t)\mathrm{d}t = \frac{1}{\pi} \arctan y + \frac{1}{2}$.
  - $y = \tan(\pi(z - \frac{1}{2}))$.

Standard distributions

The generalization to multiple variables involves the Jacobian of the change of variables, so that:

$$p_Y(y_1, \ldots, y_M) = p_Z(z_1, \ldots, z_M) \left| \frac{\partial(z_1, \ldots, z_M)}{\partial(y_1, \ldots, y_M)} \right|$$

Standard distributions

The Box-Muller method for generating samples from a Gaussian distribution. First, suppose we generate pairs of uniformly distributed random numbers $z_1, z_2 \in (-1, 1)$. Next, we discard each pair unless it satisfies $z_1^2 + z_2^2 \leq 1$. This leads to a uniform distribution of points inside the unit circle with $p_Z(z_1, z_2) = \frac{1}{\pi}$. Then, for each pair z_1, z_2 we evaluate the quantities:

$$y = z\frac{\sqrt{-4\log ||z||}}{||z||}$$

The joint distribution of y_1 and y_2 is given by:

$$p_Y(y_1, y_2) = p_Z(z_1, z_2)|\frac{\partial(z_1, z_2)}{\partial(y_1, y_2)}| = (\frac{1}{\sqrt{2\pi}}\exp(-\frac{y_1^2}{2}))(\frac{1}{\sqrt{2\pi}}\exp(-\frac{y_2^2}{2}))$$

So y_1 and y_2 are independent and each has a Gaussian distribution with zero mean and unit variance.

Rejection sampling

Suppose that:

- We wish to sample from a distribution $p(z)$, and sampling directly from $p(z)$ is difficult.
- We are easily able to evaluate $p(z)$ for any given value of z, up to some normalizing constant Z_p, so that $p(z) = \frac{1}{Z_p}\tilde{p}(z)$, where $\tilde{p}(z)$ can readily be evaluated, but Z_p is unknown.

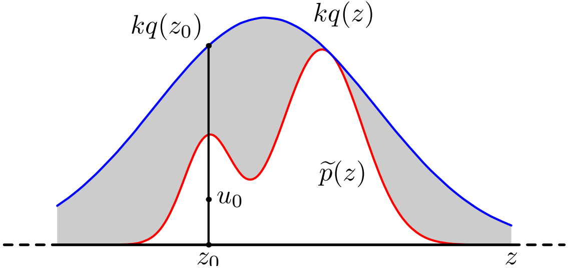
Rejection sampling

To apply rejection sampling:

- Find a simpler distribution $q(z)$, called a proposal distribution, from which we can readily draw samples.
- Introduce a constant k whose value is chosen such that $kq(z) \geq \tilde{p}(z)$ for all values of z.
- Generate a number z_0 from the distribution $q(z)$.
- Generate a number u_0 from the uniform distribution over $[0, kq(z_0)]$.
- If $u_0 > \tilde{p}(z_0)$ then the sample is rejected, otherwise u_0 is retained.
- The corresponding z values in the remaining pairs are distributed according to $p(z)$.

Rejection sampling

Figure: Illustration of the rejection sampling method



Rejection sampling

Let's verify the correctness of the rejection sampling method. Suppose that random variable Z is distributed according to $q(z)$, and random variable U is uniformly distributed over $[0, kq(Z)]$. We want to calculate the probability density function of the random variable $Z|0 \le U \le \tilde{p}(Z)$:

$$\begin{aligned} P(Z \in E|0 \le U \le \tilde{p}(Z)) &= \frac{P(Z \in E, 0 \le U \le \tilde{p}(Z))}{P(0 \le U \le \tilde{p}(Z))} \\ &= \frac{\int_E q(z) \frac{\tilde{p}(z)}{kq(z)} \mathrm{d}z}{\int_{\mathbb{R}} q(z) \frac{\tilde{p}(z)}{kq(z)} \mathrm{d}z} \\ &= \int_E p(z) \mathrm{d}z \end{aligned}$$

We see that the random variable $Z|0 \le U \le \tilde{p}(Z)$ is indeed distributed according to $p(z)$.

Rejection sampling

Let's calculate the probability that a sample will be accepted:

$$P_{\text{accept}} = \int_{\mathbb{R}} q(z) \frac{\tilde{p}(z)}{kq(z)} \mathrm{d}z = \frac{Z_p}{k}$$

We see that the constant k should be as small as possible subject to the limitation that $kq(z)$ must be nowhere less than $\tilde{p}(z)$.