Deep Learning - Foundations and Concepts

Chapter 14. Sampling

nonlineark@github

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Outline

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.

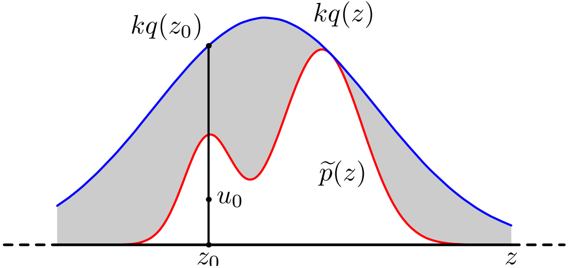
Rejection sampling

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 $Z|0 \leq U \leq \tilde{p}(Z)$:

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

We see that the random variable $Z|0 \leq U \leq \tilde{p}(Z)$ 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 $\tilde{p}(z)$.

Adaptive rejection sampling

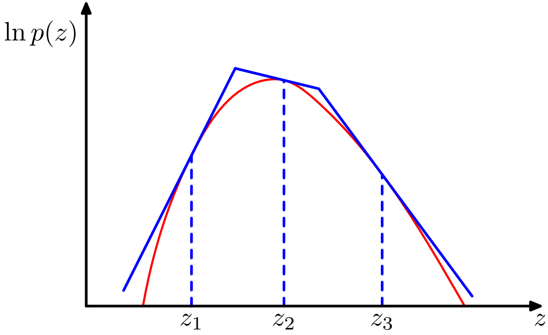
- In many instances, it can be difficult to determine a suitable analytic form for the envelope distribution $q(z)$.
- An alternative approach is to construct the envelope function on the fly based on measured values of the distribution $p(z)$.
- Constructing an envelope function is particularly straightforward when $p(z)$ is log concave.

Adaptive rejection sampling

- Evaluate the function $\log p(z)$ and its gradient at some initial set of grid points.
- The intersections of the resulting tangent lines are used to construct the envelope function.
- Draw a sample value from the envelope distribution. This is straightforward because the envelope function comprises a piecewise exponential distribution.
- If the sample is accepted, then it will be a draw from the desired distribution.
- If the sample is rejected, then it is incorporated into the set of grid points, a new tangent line is computed, and the envelope function is thereby refined.

Adaptive rejection sampling

Figure: Illustration of the construction of an envelope function for adaptive rejection sampling



Importance sampling

The technique of importance sampling provides a framework for approximating expectations directly but does not itself provide a mechanism for drawing samples from a distribution $p(z)$.

Suppose we wish to calculate the expectation of a function $f(z)$ with respect to a distribution $p(z)$:

- The distribution $p(z)$ can be evaluated only up to a normalization constant, so that $p(z) = \frac{\tilde{p}(z)}{Z_p}$, where Z_p is unknown.
- Because it is difficult to draw samples directly from $p(z)$, we rely on a proposal distribution $q(z)$ from which it is easy to draw samples.
- The distribution $q(z)$ also has an unknown normalization constant Z_q, so that $q(z) = \frac{\tilde{q}(z)}{Z_q}$.

Importance sampling

Let's calculate the expectation of $f(z)$ with respect to $p(z)$:

$$
\begin{aligned}
E(f) &= \int f(z)p(z)\mathrm{d}z = \int f(z)\frac{p(z)}{q(z)}q(z)\mathrm{d}z \\
&\approx \frac{1}{L}\sum_{l=1}^{L} f(z^{(l)})\frac{p(z^{(l)})}{q(z^{(l)})} = \frac{Z_q}{Z_p}\frac{1}{L}\sum_{l=1}^{L} f(z^{(l)})\frac{\tilde{p}(z^{(l)})}{\tilde{q}(z^{(l)})} \\
\frac{Z_p}{Z_q} &= \frac{1}{Z_q}\int \tilde{p}(z)\mathrm{d}z = \frac{1}{Z_q}\int \frac{\tilde{p}(z)}{q(z)}q(z)\mathrm{d}z \\
&\approx \frac{1}{Z_q}\frac{1}{L}\sum_{l=1}^{L}\frac{\tilde{p}(z^{(l)})}{q(z^{(l)})} = \frac{1}{L}\sum_{l=1}^{L}\frac{\tilde{p}(z^{(l)})}{\tilde{q}(z^{(l)})}
\end{aligned}
$$

where the samples $\{z^{(l)}\}$ are drawn from $q(z)$.

Importance sampling

Let:

$$\tilde{r}_l = \frac{\tilde{p}(z^{(l)})}{\tilde{q}(z^{(l)})}$$

$$w_l = \frac{\tilde{r}_l}{\sum_{l'} \tilde{r}_{l'}}$$

we see that:

$$E(f) \approx \frac{\sum_{l=1}^{L} f(z^{(l)})\tilde{r}_l}{\sum_{l=1}^{L} \tilde{r}_l} = \sum_{l=1}^{L} w_l f(z^{(l)})$$

Sampling-importance-resampling

- Draw L samples $z^{(1)}, \ldots, z^{(L)}$ from $q(z)$.
- Construct weights $w_1, \ldots, w_L$ using $w_l = \frac{\tilde{r}_l}{\sum_{l'} \tilde{r}_{l'}} = \frac{\tilde{p}(z^{(l)})/q(z^{(l)})}{\sum_{l'} \tilde{p}(z^{(l')})/q(z^{(l')})}$.
- Draw L samples from the discrete distribution $(z^{(1)}, \ldots, z^{(L)})$ with probabilities given by the weights $(w_1, \ldots, w_L)$.

Sampling-importance-resampling

Let's verify the correctness of the sampling-importance-resampling method.

$$P(z \leq a) = \sum_{l=1}^{L} I(z^{(l)} \leq a) w_l = \frac{\sum_{l=1}^{L} I(z^{(l)} \leq a) \frac{\tilde{p}(z^{(l)})}{q(z^{(l)})}}{\sum_{l=1}^{L} \frac{\tilde{p}(z^{(l)})}{q(z^{(l)})}}$$

where I is the indicator function. Taking the limit $L \to \infty$:

$$P(z \leq a) = \frac{\int I(z \leq a) \frac{\tilde{p}(z)}{q(z)} q(z) \mathrm{d}z}{\int \frac{\tilde{p}(z)}{q(z)} q(z) \mathrm{d}z} = \frac{\int_{-\infty}^{a} \tilde{p}(z) \mathrm{d}z}{\int_{-\infty}^{\infty} \tilde{p}(z) \mathrm{d}z} = \int_{-\infty}^{a} p(z) \mathrm{d}z$$

Markov Chain Monte Carlo

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.
- We maintain a record of the current state $z^{(\tau)}$, and the proposal distribution $q(z|z^{(\tau)})$ is conditioned on this current state.
- At each cycle of the algorithm, we generate a candidate sample z^* from the proposal distribution and then accept the sample according to an appropriate criterion.

The Metropolis algorithm

In the basic Metropolis algorithm, we assume that the proposal distribution is symmetric, that is $q(z_A|z_B) = q(z_B|z_A)$ for all values of z_A and z_B. The candidate sample is then accepted with probability:

$$A(z^*, z^{(\tau)}) = \min(1, \frac{\tilde{p}(z^*)}{\tilde{p}(z^{(\tau)})})$$

As we will see, if $q(z_A|z_B)$ is positive for any values of z_A and z_B, the distribution of $z^{(\tau)}$ tends to $p(z)$ as $\tau \to \infty$.

The Metropolis algorithm

Algorithm 1: Metropolis sampling

$z_{\text{prev}} \leftarrow z^{(0)}$;

for $\tau \leftarrow 1$ **to** T **do**

    $z^* \sim q(z|z_{\text{prev}})$;

    $u \sim \mathcal{U}(0,1)$;

    if $\frac{\tilde{p}(z^*)}{\tilde{p}(z_{\text{prev}})} > u$ **then**

        $z_{\text{prev}} \leftarrow z^*$;

    end

end

return z_{prev};

Markov chains

For a first-order Markov chain $z^{(1)}, \ldots, z^{(M)}, \ldots$:

- The transition probability $T_m(z^{(m)}, z^{(m+1)})$ from $z^{(m)}$ to $z^{(m+1)}$ is defined as $p(z^{(m+1)}|z^{(m)})$.
- A Markov chain is called homogeneous if the transition probabilities are the same for all m.
- A distribution is said to be invariant with respect to a Markov chain if the marginal distributions $p(z^{(m)})$ are invariant.

Markov chains

A transition probability $T(z, z')$ is said to satisfy detailed balance with respect to a distribution $p(z)$ if:

$$p(z)T(z, z') = p(z')T(z', z)$$

It is easily seen that $p(z)$ is invariant:

$$\int p(z)T(z, z')\mathrm{d}z = \int p(z')T(z', z)\mathrm{d}z = p(z') \int p(z|z')\mathrm{d}z = p(z')$$

A Markov chain that respects detailed balance is said to be reversible.

Markov chains

Our goal is to use Markov chains to sample from a given distribution $p^*(z)$:

- We can achieve this if we set up a Markov chain such that $p^*(z)$ is invariant.
- We must also require that for $m \to \infty$, the distribution $p(z^{(m)})$ converges to $p^*(z)$, irrespective of the choice of initial distribution $p(z^{(0)})$. This property is called ergodicity, and the invariant distribution is then called the equilibrium distribution.

The Metropolis-Hastings algorithm

The Metropolis-Hastings algorithm, which is a generalization of the basic Metropolis algorithm, applies when the proposal distribution is no longer a symmetric function of its arguments. The candidate sample is accepted with probability:

$$A_k(z^*, z^{(\tau)}) = \min(1, \frac{\tilde{p}(z^*)q_k(z^{(\tau)}|z^*)}{\tilde{p}(z^{(\tau)})q_k(z^*|z^{(\tau)})})$$

Here k labels the members of the set of possible transitions being considered. For a symmetric proposal distribution, the Metropolis-Hastings criterion reduces to the standard Metropolis criterion.

The Metropolis-Hastings algorithm

Algorithm 2: Metropolis-Hastings sampling

$z_{\text{prev}} \leftarrow z^{(0)}$;
for $\tau \leftarrow 1$ **to** T **do**
    $k \leftarrow M(\tau)$;
    $z^* \sim q_k(z|z_{\text{prev}})$;
    $u \sim \mathcal{U}(0,1)$;
    if $\frac{\tilde{p}(z^*)q_k(z_{\text{prev}}|z^*)}{\tilde{p}(z_{\text{prev}})q_k(z^*|z_{\text{prev}})} > u$ **then**
        $z_{\text{prev}} \leftarrow z^*$;
    end
end
return z_{prev};

The Metropolis-Hastings algorithm

We can show that $p(z)$ is an invariant distribution of the Markov chain defined by the Metropolis-Hastings algorithm by showing that detailed balance is satisfied:

$$\begin{aligned}
p(z)T_k(z, z') &= p(z)q_k(z'|z)A_k(z', z) \\
&= \min(p(z)q_k(z'|z), p(z')q_k(z|z')) \\
&= \min(p(z')q_k(z|z'), p(z)q_k(z'|z)) \\
&= p(z')q_k(z|z')A_k(z, z') \\
&= p(z')T_k(z', z)
\end{aligned}$$