Rao-Blackwellized Stochastic Gradients for Discrete Distributions

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Abstract

We wish to compute the gradient of an expectation over a finite or countably infinite sample space having $K \leq \infty$ categories, with distribution $q_\eta(z)$ parametrized by a real vector $\eta$ and differentiable in $\eta$. We aim to minimize

$$\mathcal{L}(\eta) := \mathbb{E}_{z \sim q_\eta(z)} [f_\eta(z)] = \sum_{k=1}^{K} q_\eta(z = k) f_\eta(k), \quad (1)$$

where the real-valued integrand $f_\eta$ also depends differentiably on $\eta$. If $K$ is finite and small enough, we can compute the exact gradient as

$$\nabla_\eta \mathbb{E}_{q_\eta(z)} [f_\eta(z)] = \sum_{z=1}^{K} \left\{ \nabla_\eta q_\eta(z) f_\eta(z) + q_\eta(z) \nabla_\eta f_\eta(z) \right\}, \quad (2)$$

provided $f_\eta$ is sufficiently regular to permit differentiation under the integral (which we assume throughout). On the other hand, $K$ may be infinite, or large relative to the cost of evaluating $q_\eta \cdot f_\eta$. In either of these cases, which are the focus of this paper, the exact gradient is computationally intractable. Thus, in order to optimize $\mathcal{L}(\eta)$, we seek low-variance stochastic approximations of the gradient.

The recently popularized reparametrization trick [1] provides efficient stochastic gradients when $q_\eta$ is a continuous distribution, but it does not apply in the setting of discrete $z$. Two well-known possibilities in the discrete case are continuous relaxation [2,3] and REINFORCE [4] (also known as the score function estimator). The former requires $O(K)$ computation, making it unsuitable for the setting of this paper, and is biased. The latter is known for its high variance.

Control variates are a popular mechanism for reducing the variance of REINFORCE, REBAR [5] and RELAX [6], however, combine continuous relaxations with control variates, so they too require $O(K)$ computation and are ruled out in our setting. Other approaches use control variates that can be computed in constant time [7,8], but these do not reduce the variance enough for many applications.

We propose here a meta-procedure that can be applied to any discrete-distribution stochastic-gradient procedure (e.g., REINFORCE, REINFORCE with control variate) to reduce its variance without changing its bias. In particular, an unbiased stochastic gradient remains unbiased after application of our technique. Further, our method is “anytime” in the sense that it can reduce stochastic-gradient variances given any computational budget, and the larger the budget, the greater the variance reduction. Hence it is well suited to our chosen setting, where $K$ is infinite or very large, and/or $q_\eta \cdot f_\eta$ is expensive to evaluate.

We show that our variance-reduction meta-procedure is an instance of a general statistical method called Rao-Blackwellization [9]. In previous work [10], Rao-Blackwellization was also proposed to reduce the variance of the score function estimator, but in a setting with a different focus from ours.

The rest of the paper is organized as follows. Section 2 presents our variance-reduction meta-procedure. Section 3 makes the connection to Rao-
Blackwellization, proves that the technique necessarily reduces stochastic-gradient variances, and proves that any computational budget is better spent on our technique than on simple stochastic-gradient minibatching. In Section 4, we exhibit the benefits of our procedure on synthetic data as well as on an attention mechanism \cite{11, 12} for galaxy detection in astronomical images. Section 5 closes.

2 Method

We consider the situation where the number of categories $K$ is infinite, or very large in the sense that computing the exact gradient in Equation (2) is intractable. One possible stochastic estimator for the gradient is the REINFORCE estimator,

$$f(z)\nabla_{\eta} \log q(z) + \nabla_{\eta} f(z) \ z \sim q(z), \quad (3)$$

which one can check is unbiased for the true gradient in Equation \cite{2}.

In practice, the REINFORCE estimator often has variance too large to be useful. Control variates have been proposed to decrease the variance of the REINFORCE estimator. The key observation is that the score function $\nabla_{\eta} \log q(z)$ has zero expectation under $q(z)$, so

$$[f(z) - C] \nabla_{\eta} \log q(z) + \nabla_{\eta} f(z) \ z \sim q(z) \quad (4)$$

is still unbiased for the true gradient. Several proposals have been put forth for choosing $C$ to reduce the variance \cite{2, 3}.

In this paper, we present a meta-procedure that can be applied to any stochastic estimator for the gradient of a discrete expectation. Let $g(z)$ be any such estimator which is unbiased, i.e., satisfies $\mathbb{E}_{q(z)}[g(z)] = \mathbb{E}_{\eta} \mathbb{E}_{q(z)}[f(z)]$. An example is the REINFORCE estimator. We decompose the expectation $\mathbb{E}_{q(z)}[g(z)]$ into two components: one containing the high-probability atoms of $q$, and one containing the remaining atoms. We compute the exact contribution of the high-probability component to the expectation, and we use a stochastic estimator just for the other component. The idea comes from observing that in many applications, $q(z)$ only puts significant mass on a few categories. If $g(z)$ is reasonably well behaved over $z$, then $q(z)g(z)$ is large when $q(z)$ attains its largest values and smaller elsewhere. By computing the high-probability component of the expectation exactly, we obtain a value already close to correct. A stochastic estimator is then added to correct, on average, for what small error remains.

Formally, let $C_k$ be the set of $z$ such that $q(z)$ assumes one of its $k$ largest values. Ties may be broken arbitrarily. Let $\bar{C}_k$ denote the complement of $C_k$. Then

$$\nabla_{\eta} \mathbb{E}_{q(z)}[f(z)] = \mathbb{E}_{q(z)}[g(z)]$$

$$= \mathbb{E}_{q(z)}[g(z)] 1\{z \in C_k\} + g(z) 1\{z \in \bar{C}_k\} \quad (5)$$

$$= \sum_{z \in \bar{C}_k} q(z)g(z) + \mathbb{E}_{q(z)}[g(z)] 1\{z \in \bar{C}_k\}. \quad (6)$$

It remains to approximate the expectation in the second term. We use an importance-sampling approximation based on a single draw from an importance distribution. We choose a simple importance distribution: the conditional distribution of $q(z)$ on the event $\bar{C}_k$. We denote this importance distribution by $q(z|\bar{C}_k)$. By construction, the importance weighting function is identically equal to $q(z|\bar{C}_k)$, regardless of which $z \sim q(z|\bar{C}_k)$ we draw. (Note that the indicator inside the second term of (7) always equals one, because we are only sampling from $z \in \bar{C}_k$.)

Our estimator assumes that, given $k$, the set $C_k$ can be identified at little cost. While often true, a detailed exploration of the issue is outside the scope of this paper.

In summary, we estimate the gradient as

$$g_k'(v) = \sum_{z \in \bar{C}_k} q(z)g(z) + q(z|\bar{C}_k)g(v) \quad (8)$$

$$v \sim q(z|\bar{C}_k)$$

which also satisfies $\mathbb{E}_v[g_k'(v)] = \nabla_{\eta} \mathbb{E}_{q(z)}[f(z)]$.

We see that the first term of this estimator is deterministic and the second term is random, but scaled by $q(z|\bar{C}_k)$, which is small when $q(z)$ is concentrated on a small number of atoms. Intuitively, we expect this estimator to have smaller variance than the original estimator, $g(z)$.

In the next section, we confirm this intuition by interpreting the construction of the estimator $g_k'(v)$ as Rao-Blackwellization (which always reduces variance). Hence, we call $g_k'(v)$ the Rao-Blackwellized gradient estimator.

3 Theory

We begin by describing how a suitable augmentation of the original discrete variable $z$ allows us to interpret our estimator as an instance of Rao-Blackwellization. Let $q(z|\bar{C}_k)$ denote the distribution $q(z)$ restricted to $\bar{C}_k$. Consider the three independent random variables

$$u \sim q(z|\bar{C}_k), \quad (9)$$

$$v \sim q(z|\bar{C}_k), \quad (10)$$

and $b \sim \text{Bernoulli} \left( q(z|\bar{C}_k) \right)$. \quad (11)
The triplet \((u, v, b)\) provides an augmented representation of \(z\):
\[
T(u, v, b) \overset{d}{=} z,
\]
where
\[
T(u, v, b) := u^{1-b}v^b.
\]

The estimator in Equation (5) can then be written as
\[
g'(v) = E\left[g(T(u, v, b))\right|v],
\]
where \(g(z)\) is the original unbiased gradient estimator. To see this, break the right-hand side of (14) into two terms according to the value of \(b\), then simplify. Equation (14) demonstrates directly that our estimator is an instance of Rao-Blackwellization. As such, it has the same expectation as the original estimator \(g(z)\), a fact about Rao-Blackwellization that follows from a standard result about Rao-Blackwellization.

Proposition 1 further quantifies this variance reduction, showing the variance of \(g'(v)\) must be less than the variance of \(g(v)\) by the multiplicative factor \(q_\eta(\tilde{C}_k)\).

**Proposition 1.** Let \(g(z)\) be an unbiased gradient estimator and \(g'_k(v)\) denote the Rao-Blackwellized estimator defined in Equation (5). Then
\[
\mathbb{V}[g'_k(v)] \leq q_\eta(\tilde{C}_k)\mathbb{V}[g(z)].
\]

**Proof.** We apply the conditional variance decomposition. Let \(\epsilon = q_\eta(\tilde{C}_k)\) and recall the Bernoulli random variable \(b\) defined in Equation (11). First,
\[
\mathbb{V}[g(z)] = \mathbb{E}[\mathbb{V}[g(z)|b]] + \mathbb{V}[\mathbb{E}[g(z)|b]]
\geq \mathbb{E}[\mathbb{V}[g(z)|b]].
\]

Now,
\[
\mathbb{E}[\mathbb{V}[g(z)|b]] = \epsilon\mathbb{V}[g(z)|z \in C_k] + (1 - \epsilon)\mathbb{V}[g(z)|z \in \tilde{C}_k]
\geq \epsilon\mathbb{V}[g(z)|z \in C_k].
\]

But \(\mathbb{V}[g'_k(v)] = \epsilon^2\mathbb{V}[g(z)|z \in C_k]\), which in combination with the above yields the result.

The multiplicative factor of variance reduction guaranteed by Rao-Blackwellization can be significant if the probability mass of \(q_\eta(z)\) is concentrated on just a few categories. But while Rao-Blackwellization reduces the variance of \(g(z)\), this comes at the cost of evaluating \(f_\eta\) a total \(k+1\) times (cf. Equation (5)). An initial stochastic gradient \(g(z)\) such as REINFORCE will only require a single evaluation of \(f_\eta\).

There is an alternative approach to reducing the variance of an initial estimator \(g(z)\) via multiple evaluations of \(f_\eta\): minibatching, i.e., simple Monte-Carlo averaging over independent draws of \(z\). Thus, the question arises: given a budget of \(N < K\) evaluations of \(f_\eta\), is it better to Rao-Blackwellize or minibatch? The next proposition shows constructively that there is a choice of \(k \leq N\) for which Rao-Blackwellization reduces variance at least as much as minibatching.

**Proposition 2.** Suppose we have a budget of \(N\) evaluations of \(g\). Consider the estimators
\[
g'_{N,k}(v) = \sum_{u \in C_k} q_\eta(u)g(u) + \frac{q_{\eta}(\tilde{C}_k)}{N - k} \sum_{j=1}^{N-k} g(v_j),
\]
and
\[
g_N(z) = \frac{1}{N} \sum_{j=1}^{N} g(z_j), \quad z_1, ..., z_N \overset{iid}{\sim} q_\eta.
\]

If we choose
\[
\hat{k} = \arg\min_{k \in \{0, ..., N\}} \frac{q_\eta(\tilde{C}_k)}{N - k}
\]
then
\[
\mathbb{V}[g'_{N,\hat{k}}(v)] \leq \mathbb{V}[g_N(z)].
\]

**Proof.** Let \(V_1 = \mathbb{V}[q_1(z)]\). Then \(\mathbb{V}[g_N(z)] = (1/N)V_1\), while Proposition 1 shows that \(\mathbb{V}[g_{N,k}(v)] \leq \frac{q_\eta(\tilde{C}_k)}{N - k}V_1\). Since \(\frac{q_\eta(\tilde{C}_k)}{N - \hat{k}} = \frac{1}{N}\) when \(k = 0\), the result follows.

Together, Propositions 1 and 2 imply the following:

- Rao-Blackwellization leads to a significant variance reduction if the mass of \(q_\eta(z)\) is concentrated.
- Even when restricting minibatched versions of the initial and Rao-Blackwellized estimators to an equal number of evaluations of \(f_\eta\), Rao-Blackwellization yields the same or lower variance, for a computable choice of \(k\).
4 Experiments

In our experiments, we take $g(z)$ to be either the REINFORCE estimator,

$$g(z) = f_\eta(z) \nabla_\eta \log q_\eta(z) + \nabla_\eta f_\eta(z), \quad z \sim q_\eta(z),$$

or REINFORCE with a control variate $C$,

$$g(z) = [f_\eta(z) - C] \nabla_\eta \log q_\eta(z) + \nabla_\eta f_\eta(z).$$

We take as our control variate $C = f_\eta(z')$ for an independent draw $z' \sim q_\eta$.

Note that in both cases $g(z)$ is unbiased for the true gradient. (In the second case, $g(z)$ is unbiased conditional on $z'$, and hence unconditionally unbiased as well).

We abbreviate the second estimator as REINFORCE+CV.

4.1 Bernoulli latent variables

We fix a vector $p = [0.6, 0.51, 0.48]^\top$ and seek to minimize the loss function

$$\mathbb{E}_{b_1, b_2, b_3 \mid \text{Bern}(\sigma(\eta))} \left\{ \sum_{i=1}^{3} (b_i - p_i)^2 \right\}$$

over $\eta \in \mathbb{R}$, where $\sigma(\eta)$ is the sigmoid function. Here, the discrete random vector $b = [b_1, b_2, b_3]^\top$ is supported over $K = 2^3 = 8$ categories. The optimal value of $\sigma(\eta)$ is 1, approached as $\eta \to \infty$.

Figure 1 shows the performance of our Rao-Blackwellization of REINFORCE both with and without a control variate. Rao-Blackwellization improves the performance of both gradient estimators.

Figure 2 shows the variances of the gradient estimates at $\eta = 0$ and $\eta = -4$, as a function of $k$. As expected, the variance decreases as more categories are analytically summed. At $\eta = 0$, the corresponding $q_\eta$ distribution is uniform, i.e., maximally anti-concentrated, so the variance reduction of Rao-Blackwellization is not large. However, the gains are quite substantial at $\eta = -4$, where $q_\eta$ is concentrated around the point $b = (0, 0, 0)$. In this case, analytically summing out one category removes nearly all the variance.

4.2 Gaussian mixture model

For our next experiment, we draw $N = 200$ observations $(y_n)$ from a $d$-dimensional Gaussian mixture model with $K = 10$ components, taking $d = 2$:

$$z_n \overset{\text{iid}}{\sim} \text{Categorical}(\pi_{1:K}), \quad n = 1, \ldots, N,$$

We then seek to minimize $\text{KL}(q(\mu, z) \mid \mid p(\mu, z \mid y))$ over the variational parameters $\hat{\mu}$ and $\hat{\pi}$. This is equivalent
Figure 2: The distribution of gradient estimates from REINFORCE+CV in the Bernoulli experiments. We examine the gradients at $\eta = 0$ and $\eta = -4$, and as a function of $k$, the number of categories summed. (Note there is still random noise when we sum out all 8 categories here, because of the random control variate.)

Figure 3: Results for Gaussian mixture model experiment. (Top) Simulated data. (Bottom) Negative ELBO per iteration using REINFORCE+CV, for $k$ categories summed.

We initialized the optimization with K-means. Figure 3 shows that Rao-Blackwellization improves the convergence rate, particularly towards the end of the run.

4.3 Astronomical images

Locating and characterizing galaxies in telescope images is an import problem in astronomy. The deep generative model for galaxy images proposed in [14] achieves state-of-the-art results, but only for images cropped to have a single galaxy at their center. In this section, we use a hard-attention mechanism [11, 12] to remove the restriction that galaxies must be centered in images.

Our generative model is as follows. For each image, we sample a particular two-vector representing the pixel at the imaged galaxy’s center:

$$z \sim \text{Categorical}(H \times W).$$

Here $H$ and $W$ are respectively the height and width, in pixels, of the images. Next, as in [14], to represent the shape and brightness of the galaxy, we sample an eight-dimensional vector:

$$y \sim N(0, I).$$
Finally, for each pixel \((h, w) \in H \times W\), the pixel intensity is
\[
x_{h,w}|y, z \sim N(\mu(y)[h - z_0, w - z_1], \Sigma(y)[h - z_0, w - z_1]).
\]
(35)
Here \(\mu\) and \(\Sigma\) are neural networks that return a grid of, respectively, means and variances.

In this way, \(x \in \mathbb{R}^{H \times W}\) is a random sample of an image containing a single non-centered galaxy.

Hence, not only do we need to learn the generative model for a single galaxy, but we need to infer the pixel at which the galaxy is centered. Our two latent variables are \(z_n\) and \(y_n\). We find a variational approximation to the posterior using an approximating family of the form
\[
z_n | x_n \sim \text{Categorical}(\zeta(x_n))
\]
(36)
and
\[
y_n | x_n, z_n \sim \mathcal{N}(h_\mu(x_n, z_n), h_\Sigma(x_n, z_n)),
\]
(37)
where \(\zeta\), \(h_\mu\), and \(h_\Sigma\) are neural networks.

We minimize
\[
\text{KL}(q(y_n, z_n | x_n) \| p(y_n, z_n | x_n)),
\]
(38)
which is equivalent to maximizing the ELBO
\[
\mathbb{E}_{z_n \sim q(z_n)} \left[ \mathbb{E}_{y_n \sim q(y_n | z_n)} \left[ \log p(x_n | y_n, z_n) \
+ \log p(z_n) + \log (y_n)\right. \right.
\left. \left. - \log q(z_n | x_n) - \log q(y_n | z_n, x_n) \right] \right].
\]
(39)
Since \(y_n\) is a continuous random variable, we use the reparameterization trick for the inner expectation. We use the REINFORCE+CV estimator to compute the discrete expectation over \(z_n\). In this case, there are \(H \times W\) categories for \(z_n\), so procedures whose computational cost scales linearly with the number of categories would likely be intractable.

We again examine the gains of Rao-Blackwellizing the REINFORCE+CV gradient estimator. The negative ELBO per epoch is shown in Figure 4. We simulate new galaxy images at each epoch: an epoch consists of 200 batches, each batch having 64 images. Rao-Blackwellizing improves the convergence rate of the optimization.

Figure 5 compares Rao-Blackwellization to naïve minibatching. It shows the loss per epoch of summing out \(k = 3\) categories, thus evaluating the objective function four times, compared to averaging four independent samples of the REINFORCE+CV gradient estimate. Here too, Rao-Blackwellization provides an improvement.

Finally, we show the original image against the reconstructed image in Figure 6. Note that we simulated images of size \(31 \times 31\) pixels, for a total of 961 discrete categories. The experiment shows that summing out a few high-probability categories can lead to material speed-ups in the optimization, and Figure 6 shows that the optimization is ultimately successful.

5 Discussion

Efficient stochastic approximation of the gradient \(\nabla_z \mathbb{E}_{q(z)}[f(z)]\), where \(z\) is discrete, is a basic problem that arises in many probabilistic modeling tasks. We have presented a general method to reduce the variance of stochastic estimates of \(\nabla_z \mathbb{E}_{q(z)}[f(z)]\), grounded in the classical technique of Rao-Blackwellization. Our experiments on synthetic data and a large-scale galaxy modeling problem show the practical benefits of our variance-reduced estimators.
We have focused on the particular setting where $z$ is a univariate discrete random variable, which is relevant for many applications. In other situations, multiple discrete variables will naturally appear in the expectations being optimized. Treating these as a single discrete variable over the Cartesian product of the sample spaces may make such problems amenable to our Rao-Blackwellization approach. In addition, many multivariate discrete distributions arising in modeling applications will be structured (e.g., the discrete-space latent Markov chain of an HMM). High-dimensional expectations over these multivariate discrete distributions can be reduced to iterated low-dimensional expectations through appropriate conditioning on variable sets, in which case we expect our technique will still be applicable for variance reduction. This is an avenue of future research.

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