Coupled Gradient Estimators for Discrete Latent Variables

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Abstract

Training models with discrete latent variables is challenging due to the high variance of unbiased gradient estimators. While low-variance reparameterization gradients of a continuous relaxation can provide an effective solution, a continuous relaxation is not always available or tractable. Dong et al. (2020) and Yin et al. (2020) introduced a performant estimator that does not rely on continuous relaxations; however, it is limited to binary random variables. We introduce a novel derivation of their estimator based on importance sampling and statistical couplings, which we extend to the categorical setting. Motivated by the construction of a stick-breaking coupling, we introduce gradient estimators based on reparameterizing categorical variables as sequences of binary variables and Rao-Blackwellization. In systematic experiments, we show that our proposed categorical gradient estimators provide state-of-the-art performance, whereas even with additional Rao-Blackwellization previous estimators (Yin et al., 2019) underperform a simpler REINFORCE with a leave-one-out-baseline estimator (Kool et al., 2019).

1 Introduction

Optimizing an expectation of a cost function of discrete variables with respect to the parameters of their distribution is a frequently encountered problem in machine learning. This problem is challenging because the gradient of the objective, like the objective itself, is an expectation over an exponentially large space of joint configurations of the variables. As the number of variables increases, these expectations quickly become intractable and thus are typically approximated using Monte Carlo sampling, trading a reduction in computation time for variance in the estimates. When such stochastic gradient estimates are used for learning, their variance determines the largest learning rate that can be used without making training unstable. Thus finding estimators with lower variance leads directly to faster training by allowing higher learning rates. For example, the use of the reparameterization trick to yield low-variance gradient estimates has been essential to the success of variational autoencoders (Kingma and Welling, 2014; Rezende et al., 2014). However, this estimator, also known as the pathwise derivative estimator (Glasserman, 2013), can only be applied to continuous random variables.

For discrete random variables, there are two common strategies for stochastic gradient estimation. The first one involves replacing discrete variables with continuous ones that approximate them as closely as possible (Maddison et al., 2017; Jang et al., 2017) and training the resulting relaxed system with the reparameterization trick. However, as after training, the system is evaluated with discrete variables, this approach is not guaranteed to perform well and requires a careful choice of the continuous relaxation. Moreover, evaluating the cost function at the relaxed values instead of the discrete ones is not always desirable or even possible. The second strategy, involves using the REINFORCE estimator (Williams, 1992), also known as the score-function (Rubinstein and Shapiro, 1990) or likelihood-ratio

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(Glynn, 1990) estimator, which, having fewer requirements than the reparameterization trick, also works with discrete random variables. As the simplest versions of this estimator tend to exhibit high variance, they are typically combined with variance reduction techniques. Some of the most effective such estimators (Tucker et al., 2017; Grathwohl et al., 2018), incorporate the gradient information provided by the continuous relaxation, while keeping the estimator unbiased w.r.t. the original discrete system.

The recently introduced Augment-REINFORCE-Merge (ARM) (Yin and Zhou, 2019) estimator for binary variables and Augment-REINFORCE-Swap (ARS) and Augment-REINFORCE-Swap-Merge (ARSM) estimators (Yin et al., 2019) for categorical variables provide a promising alternative to relaxation-based estimators. However, when compared to a simpler baseline approach (REINFORCE with a leave-one-out-baseline (RLOO; Kool et al., 2019)), ARM underperforms in the binary setting (Dong et al., 2020), and we similarly demonstrate that ARS and ARSM underperform in the categorical setting. Dong et al. (2020) and Yin et al. (2020) independently developed an estimator that improves ARM and outperforms RLOO, providing state-of-the-art performance in the binary setting.

In this paper, we explore how to devise a performant estimator in the categorical setting. As we show, it is straightforward if more challenging to apply the ideas of Dong et al. (2020) to ARS and ARSM. However, empirically, we find that this is insufficient to close the gap between ARS/ARSM and RLOO. Instead, we develop a novel derivation of DisARM/U2G (Dong et al., 2020; Yin et al., 2020) using importance sampling which is simpler and more direct while providing a natural extension to the categorical case. This estimator requires constructing a *coupling* on categorical variables, which we do using a stick-breaking process and antithetic Bernoulli variables. Motivated by this construction, we also consider estimators based on reparameterizing the problem with a sequence of binary variables. We systematically evaluate these estimators and their underlying design choices and find that they outperform RLOO across a range of problems without requiring more computation.

2 Background

We consider the problem of optimizing

$$\mathbb{E}_{q_\theta(z)}\left[f_\theta(z)\right], \tag{1}$$

with respect to the parameters θ of a factorial categorical distribution $q_\theta(z) = \prod_k \mathrm{Cat}(z_k; \alpha_{\theta,k})$ where k indexes dimension and $\alpha_{\theta,k}$ is the vector of logits of the categorical distribution with C choices.[1] This situation covers many problems with discrete latent variables, for example, in variational inference $f_\theta(z)$ could be the instantaneous ELBO (Jordan et al., 1999) and $q_\theta(z)$ the variational posterior.

The gradient with respect to θ is

$$\nabla_\theta \mathbb{E}_{q_\theta(z)}\left[f_\theta(z)\right] = \mathbb{E}_{q_\theta(z)}\left[f_\theta(z)\nabla_\theta \log q_\theta(z) + \nabla_\theta f_\theta(z)\right]. \tag{2}$$

It typically suffices to estimate the second term with a single Monte Carlo sample, so for notational clarity, we omit the dependence of f on θ in the following sections. Monte Carlo estimates of the first term can have large variance. Low-variance, unbiased estimators of the first term will be our focus.

2.1 DisARM/U2G

Dong et al. (2020) and Yin et al. (2020) derived a Rao-Blackwellized estimator for *binary* variables based on the coupled estimator of Yin and Zhou (2019). In particular, if $q_\theta(b) \sim \prod_k \mathrm{Bernoulli}(\alpha_{\theta,k})$ with θ parameterizing the logits α_{θ_k} of the Bernoulli distribution, and b and $\tilde{b}$ are antithetic samples from $q_\theta(b)$ (independent across dimension k), then the estimator

$$\frac{1}{2}\left(f(b) - f(\tilde{b})\right)\left((-1)^{\tilde{b}_k}\mathbb{1}_{b_k \neq \tilde{b}_k}\sigma(|(\alpha_{\theta,k}|)\right)$$

is an unbiased estimator of the gradient $\nabla_{\alpha_{\theta,k}}\mathbb{E}_{q_\theta(b)}\left[f(b)\right]$. This estimator has been shown to outperform RLOO, but is limited to the binary variable case.

[1] To simplify notation, we omit the subscripted θ on α when it is clear from context.

2.2 Augment-REINFORCE-Swap (ARS) & Augment-REINFORCE-Swap-Merge (ARSM)

Yin et al. (2019) use the fact that the discrete distribution can be reparameterized by an underlying continuous augmentation: if $\pi \sim \prod_k \text{Dirichlet}(1_C)$ and $z_k := \arg\min_i \pi_{k,i} e^{-\alpha_{k,i}}$, then $z_k \sim \text{Cat}(\alpha_k)$; and show that $\nabla_{\alpha_{k,c}} \mathbb{E}_{q_\theta(z)}[f(z)] = \mathbb{E}_\pi[f(z)(1 - C\pi_{k,c})]$. Furthermore, they define a swapped probability matrix $\pi_k^{i \leftrightharpoons j}$ by swapping the entries at indices i and j in π_k

$$\pi_{k,c}^{i \leftrightharpoons j} := \begin{cases} \pi_{k,i} & c = j \\ \pi_{k,j} & c = i \\ \pi_{k,c} & \text{o.w.} \end{cases},$$

and $z_k^{i \leftrightharpoons j} := \arg\min_c \pi_{k,c}^{i \leftrightharpoons j} e^{-\alpha_{k,c}}$. Using these constructions, they show an important identity

$$\nabla_{\alpha_{k,c}} \mathbb{E}_{q_\theta(z)}[f(z)] = \mathbb{E}_\pi \left[g_{\text{ARS}\,k,c} := \left[f(z^{c \leftrightharpoons j}) - \frac{1}{C} \sum_{m=1}^{C} f(z^{m \leftrightharpoons j}) \right] (1 - C\pi_{k,j}) \right],$$

which shows that $g_{\text{ARS}\,k,c}$ is an unbiased estimator. To further improve the estimator, Yin et al. (2019) average over the choice of the reference j, resulting in the ARSM estimator

$$g_{\text{ARSM}\,k,c} := \frac{1}{C} \sum_{j=1}^{C} \left[f(z^{c \leftrightharpoons j}) - \frac{1}{C} \sum_{m=1}^{C} f(z^{m \leftrightharpoons j}) \right] (1 - C\pi_{k,j}).$$

Notably, both ARS and ARSM only evaluate f at discrete values, and thus do not rely on a continuous relaxation.

3 Methods

First, we provide a novel derivation of DisARM (Dong et al., 2020) / U2G (Yin et al., 2020) from an importance-sampling perspective, which naturally extends to the categorical case. Starting with the (2-sample) REINFORCE LOO estimator (Kool et al., 2019) and applying importance sampling, we have

$$\begin{aligned} \nabla_{\theta_k} \mathbb{E}_{q_\theta(z)}[f(z)] &= \frac{1}{2} \mathbb{E}_{q_\theta(z) q_\theta(\tilde{z})} \left[(f(z) - f(\tilde{z})) \left(\nabla_{\theta_k} \log q_\theta(z_k) - \nabla_{\theta_k} \log q_\theta(\tilde{z}_k) \right) \right] \\ &= \frac{1}{2} \mathbb{E}_{p_\theta(z,\tilde{z})} \left[\frac{q_\theta(z) q_\theta(\tilde{z})}{p_\theta(z,\tilde{z})} (f(z) - f(\tilde{z})) \left(\nabla_{\theta_k} \log q_\theta(z_k) - \nabla_{\theta_k} \log q_\theta(\tilde{z}_k) \right) \right]. \end{aligned}$$

To reduce the variance of the estimator, we can use the joint distribution $p_\theta(z, \tilde{z})$ to emphasize terms that have high magnitude. However, controlling the weights can be challenging for high dimensional z. We can sidestep this issue by taking advantage of the structure of the integrand and requiring that p_θ be a properly supported[2] *coupling* that is independent across dimensions (i.e., a joint distribution $p(z, \tilde{z}) = \prod_k p(z_k, \tilde{z}_k)$ such that the marginals are maintained $p(z_k) = p(\tilde{z}_k) = q(z_k)$). Then with $(z, \tilde{z}) \sim p$, the following will be an unbiased estimator of the gradient (see Appendix A.3 for the derivation)

$$g_{\text{DisARM-IW}\,k} = \frac{1}{2} \frac{q_\theta(z_k) q_\theta(\tilde{z}_k)}{p_\theta(z_k, \tilde{z}_k)} (f(z) - f(\tilde{z})) \left(\nabla_{\theta_k} \log q_\theta(z_k) - \nabla_{\theta_k} \log q_\theta(\tilde{z}_k) \right). \tag{3}$$

Critically, because the coupling maintains the marginal distributions, we only need to importance weight a single dimension at a time, which ensures the weights are reasonable. The estimator is unbiased, so the coupling can be designed to reduce variance. In the binary case, with an antithetic Bernoulli coupling, it is straightforward to see that this precisely recovers DisARM/U2G. Conveniently, this estimator is also valid in the categorical case, however, the choice of coupling affects the performance of the estimator.

[2] As is standard for importance sampling, to ensure unbiasedness, we require that either $q(z, \tilde{z}) = 0$ or the integrand is 0 whenever $p(z, \tilde{z}) = 0$.

Stick-breaking Coupling

The ideal variance-reducing coupling would take into account the magnitude of $(f(z) - f(\tilde{z}))\left(\nabla_{\theta_k} \log q_\theta(z_k) - \nabla_{\theta_k} \log q_\theta(\tilde{z}_k)\right)$ which we do not know a priori. However, we do know that when $z_k = \tilde{z}_k$, the last multiplicative term of Eq. 3 vanishes, so moving mass away from this configuration will reduce variance. Furthermore, for the estimator to be valid, the coupling must put non-zero mass on all $z_k \neq \tilde{z}_k$ configurations.[3]

In the binary case, there is a natural construction of an antithetic coupling which minimizes the probability of $z_k = \tilde{z}_k$. We can extend this construction using formulations of categorical variables as a function of a sequence of binary decisions. The stick-breaking construction for categorical variables (Khan et al., 2012) provides such an approach. Suppose we have a categorical distribution $q(z_k)$ and we construct a sequence of independent binary variables $b_{k,1}, \ldots, b_{k,C}$ with $b_{k,i} \sim \mathrm{Bernoulli}(q(z_k = i)/\sum_{j=i}^{C} q(z_k = j))$ and define $z_k \coloneqq \mathrm{SB}(b_{k,1}, \ldots, b_{k,C}) \coloneqq \min i$ s.t. $b_{k,i} = 1$; then $z_k \sim q(z_k)$. Given each of $b_{k,1}, \ldots, b_{k,C}$, we can independently sample antithetic Bernoulli variables $\tilde{b}_{k,1}, \ldots, \tilde{b}_{k,C}$ and let $\tilde{z} \coloneqq \mathrm{SB}(\tilde{b}_{k,1}, \ldots, \tilde{b}_{k,C})$. This process defines a joint distribution on $(z_k, \tilde{z}_k)$, which we call the *stick-breaking coupling*. By construction, the joint distribution preserves the marginal distributions. Note that the stick-breaking coupling depends on the an arbitrary ordering of the categories.

Without reordering the categories, the coupling arising from the default ordering may not put non-zero mass on all $z_k \neq \tilde{z}_k$ configurations. When $p(b_{k,i}) > 0.5$, then $p(b_{k,i} = 0, \tilde{b}_{k,i} = 0) = 0$, which implies that $p(z_k > i, \tilde{z}_k > i) = 0$ by definition. So if $p(b_{k,i}) > 0.5$ for $i < C$, this violates the condition that the coupling put mass on all $z_k \neq \tilde{z}_k$ configurations. We can avoid this situation by relabeling the categories in ascending order of probability (as this guarantees that $q(z_k = i)/\sum_{j=i}^{C} q(z_k = j) \leq 0.5$). With this ordering, computing the required importance weights with the stick-breaking coupling is straightforward when $z_k \neq \tilde{z}_k$

$$\frac{q_\theta(z_k) q_\theta(\tilde{z}_k)}{p_\theta(z_k, \tilde{z}_k)} = \prod_{i=1}^{\min(z_k, \tilde{z}_k)-1} \frac{\sigma(-\alpha_{k,i})^2}{1 - 2\sigma(\alpha_{k,i})} \sigma\left(-\alpha_{\min(z_k, \tilde{z}_k)}\right),$$

where $\alpha_{k,i} = \mathrm{logit}\, \frac{q(z_k = i)}{\sum_{j=i+1}^{C} q(z_k = j)}$ (see Appendix A.4 for details). Note that due to the ascending ordering, the $\sigma(\alpha_{k,i})$ term in the product is always $\leq \frac{1}{3}$, ensuring that the weights are bounded.

Finally, we note that a mixture of couplings is also a coupling, so we can take any coupling and mix it with the independent coupling to ensure the support condition is met. Because the estimator is unbiased for any choice of nonzero mixing coefficient, the mixing coefficients can be optimized following the control variate tuning process described in (Ruiz et al., 2016; Tucker et al., 2017; Grathwohl et al., 2018). This also ensures that the performance of the estimator will be at least as strong as RLOO. Exploring this idea could be an interesting future direction.

3.1 Binary Reparameterization

Motivated by the stick-breaking construction, we can eschew importance sampling and directly reparameterize the problem in terms of the binary variables and apply DisARM/U2G. In particular, if we have binary variables $b_{k,1} \sim \mathrm{Bernoulli}(\sigma(\alpha_{k,1})), \ldots, b_{k,C} \sim \mathrm{Bernoulli}(\sigma(\alpha_{k,C}))$ such that $z_k \coloneqq h(b_{k,1}, \ldots, b_{k,C}) \sim q_\theta(z_k)$ where h is a deterministic function that does not depend on θ, then we can rewrite the gradient as

$$\begin{aligned}\nabla_{\alpha_{k,c}} \mathbb{E}_{q_\theta(z)}[f(h(b))] &= \nabla_{\alpha_{k,c}} \mathbb{E}_b[f(h(b))] = \mathbb{E}_b[f(h(b)) \nabla_{\alpha_{k,c}} \log q_\theta(b)] \\ &= \mathbb{E}_b[f(h(b)) \nabla_{\alpha_{k,c}} \log q_\theta(b_{k,c})],\end{aligned}$$

which is an expression that DisARM/U2G can be applied to.

We can additionally leverage the structure of the stick-breaking construction to further improve the estimator. Intuitively, by the definition of z_k in terms of $\mathrm{SB}(\cdots)$, if we know that $b_{k,c} = 1$, then the values of $b_{k,c'}$ for $c' > c$ do not change the value of z_k, which implies the gradient terms vanishing.

[3] Technically, the coupling can put zero mass on configurations as long as the expectation is zero across those configurations, however, this is hard to ensure for a general f.

In particular, given antithetically coupled Bernoulli samples, the following is an unbiased estimator (see Appendix A.4 for details):

$$g_{\text{DisARM-SB}\,k,c} = \begin{cases} \frac{1}{2}\left(f(z) - f(\tilde{z})\right)\left((-1)^{\tilde{b}_{k,c}}\mathbb{1}_{b_{k,c}\neq\tilde{b}_{k,c}}\sigma(|(\alpha_{k,c}|)\right) & c \leq \min(z_k, \tilde{z}_k) \\ \frac{1}{2}\left(f(\tilde{z}) - f(z)\right)\nabla_{\alpha_{k,c}}\log q_\theta(\tilde{b}_{k,c}) & z_k < c \leq \tilde{z}_k \\ \frac{1}{2}\left(f(z) - f(\tilde{z})\right)\nabla_{\alpha_{k,c}}\log q_\theta(b_{k,c}) & \tilde{z}_k < c \leq z_k \\ 0 & c > \max(z_k, \tilde{z}_k) \end{cases}. \tag{4}$$

In contrast to the previous section, *any* choice of ordering for the stick-breaking construction results in an unbiased estimator, and we experimentally evaluated several choices.

Alternatively, we can use a sequence of independent Bernoulli variables arranged as a binary tree to construct categorical variables, with each leaf node representing a category (Ghahramani et al., 2010). For simplicity, we only consider balanced binary trees (i.e., C a power of 2). The binary variables encode the internal routing decisions through the tree, defining a deterministic mapping from the binary variables to the categorical variable $z \coloneqq T(b_1, \ldots, b_{C-1})$. It is straightforward to derive the Bernoulli probabilities from $q_\theta(z)$ so that $z \sim q_\theta(z)$, so we defer the details to Appendix A.5.

As above, we can additionally leverage the structure of the tree construction to further improve the estimator. Given binary variables $b_1, \ldots, b_{C-1}$, let $I(b_1, \ldots, b_{C-1})$ be the set of variables used in routing decisions ($|I(b_1, \ldots, b_{C-1})| = \log_2 C$). By the definition of z_k in terms of $T(\ldots)$, we know that z_k is unaffected by binary decisions that occur outside $I(b_\cdot)$, which implies the gradient terms vanishing. With a pair of antithetically sampled binary sequences, the following is an unbiased estimator (see Appendix A.5 for details):

$$g_{\text{DisARM-Tree}\,k,c} = \begin{cases} \frac{1}{2}\left(f(z) - f(\tilde{z})\right)\left((-1)^{\tilde{b}_{k,c}}\mathbb{1}_{b_{k,c}\neq\tilde{b}_{k,c}}\sigma(|(\alpha_{k,c}|)\right) & c \in I(b_{k,\cdot}) \cap I(\tilde{b}_{k,\cdot}) \\ \frac{1}{2}\left(f(\tilde{z}) - f(z)\right)\nabla_{\alpha_{k,c}}\log q_\theta(\tilde{b}_{k,c}) & c \in I(\tilde{b}_{k,\cdot}) - I(b_{k,\cdot}) \\ \frac{1}{2}\left(f(z) - f(\tilde{z})\right)\nabla_{\alpha_{k,c}}\log q_\theta(b_{k,c}) & c \in I(b_{k,\cdot}) - I(\tilde{b}_{k,\cdot}) \\ 0 & c \notin I(b_{k,\cdot}) \cup I(\tilde{b}_{k,\cdot}) \end{cases}. \tag{5}$$

Again, the choice of ordering affects the coupling, however, we leave investigating the optimal choice to future work.

Notably both estimators include terms that are reminiscent of the LOO estimator, however, they use *dependent* $z, \tilde{z}$ and are still unbiased due to careful construction.

3.2 Rao-Blackwellized ARS & ARSM

Motivated by the approach of Dong et al. (2020), we can derive improved versions of ARS and ARSM by integrating out the extra randomness due to the continuous variables. ARS and ARSM heavily rely on a continuous reparameterization of the problem, yet the original problem only depends on the discrete values. Ideally, we would integrate out $\pi|z^{1\leftrightharpoons j}, ..., z^{C\leftrightharpoons j}$, however, unlike in the binary case, computing the expectation analytically appears infeasible. Instead, we analytically integrate out two dimensions of π and use Monte Carlo sampling to deal with the rest. This is a straightforward albeit tedious calculation, so we defer details to Appendix A.6. Furthermore, we note that conditional on $\mathbb{1}_{z_k^{1\leftrightharpoons j}=\cdots=z_k^{C\leftrightharpoons j}}$, both $g_{\text{ARS}\,k,c}$ and $g_{\text{ARSM}\,k,c}$ vanish in expectation, so we can zero out these terms explicitly. Combining these ideas results in a reduced variance version of ARS and ARSM, which we call ARS+ and ARSM+ in the experiments.

4 Related Work

Almost all unbiased gradient estimators for discrete random variables (RVs), including our proposed estimators, belong to the REINFORCE / score function / likelihood-ratio estimator family (Williams, 1992; Rubinstein and Shapiro, 1990; Glynn, 1990). The primary difference between such estimators is the variance reduction (VR) techniques they incorporate, trading additional computation for lower variance of the estimate. Averaging over multiple independent samples is the simplest but relatively inefficient VR technique, as the variance of the estimate is inversely proportional to the number of samples and thus decreases slowly. REINFORCE with the leave-out-out baseline (RLOO; Kool et al., 2019) provides a much more effective way of utilizing multiple independent samples, by using the average over all the other samples as the baseline for each sample.

Table 1: Mean variational lower bounds and the standard error of the mean computed based on 5 runs of 5×10^5-steps training from different random initializations. The best performing method (up to the standard error) for each task is in bold. Top: comparing the performance of the proposed estimators and the RLOO baseline on three datasets. Bottom: comparing the effect of arranging the categories in the ascending or descending order to the default ordering for DisARM-SB.

Estimator Comparison with Train ELBO				
	DisARM-IW	DisARM-Tree	DisARM-SB	RLOO
Dynamic MNIST	-103.41 ± 0.23	$\mathbf{-103.10 \pm 0.25}$	-103.35 ± 0.17	-104.03 ± 0.23
Fashion MNIST	-240.08 ± 0.17	$\mathbf{-239.83 \pm 0.29}$	$\mathbf{-239.66 \pm 0.20}$	-240.89 ± 0.49
Omniglot	$\mathbf{-122.25 \pm 0.35}$	-123.08 ± 0.43	$\mathbf{-121.99 \pm 0.17}$	$\mathbf{-122.70 \pm 0.80}$

Ordering Comparison with Train ELBO			
	Ascending	Descending	Default
Dynamic MNIST	$\mathbf{-103.35 \pm 0.17}$	$\mathbf{-103.56 \pm 0.28}$	$\mathbf{-103.46 \pm 0.17}$
Fashion MNIST	$\mathbf{-239.66 \pm 0.20}$	-240.04 ± 0.24	-239.99 ± 0.20
Omniglot	$\mathbf{-121.99 \pm 0.17}$	-122.79 ± 0.12	-122.75 ± 0.15

The estimators we develop use a technique called *coupling* (Owen, 2013) to make better use of multiple samples by making them dependent. Recently, this kind of approach has been applied to binary RVs, resulting in the Augment-REINFORCE-Merge (ARM; Yin and Zhou, 2019) and DisARM (Dong et al., 2020) / U2G (Yin et al., 2020) estimators. ARM is constructed by reparameterizing Bernoulli RVs in terms of Logistic variables and applying antithetic sampling, which is the simplest kind of coupling, to the resulting REINFORCE estimator. DisARM / U2G is obtained by Rao-Blackwellizing ARM to eliminate the dependence on the values of the underlying Logistic variables, reducing its variance. We show how to employ DisARM with categorical RVs by representing them as sequences of binary decisions and applying DisARM to the resulting system. By considering the sequences obtained through stick-breaking and tree-structured decisions, we obtain the DisARM-SB and DisARM-Tree estimators respectively. We obtain DisARM-IW by generalizing the two-sample version of RLOO to allow the two samples to be coupled and using an importance-weighting correction to keep the estimator unbiased. DisARM-IW reduces to DisARM in the case of Bernoulli RVs and antithetic coupling, and thus can be seen as a generalization.

Augment-REINFORCE-Swap estimator (ARS; Yin et al., 2019) is a generalization of ARM to categorical RVs; it reparameterizes the categorical variables in terms of Dirichlet RVs and applies REINFORCE to them, using a coupling based on a swapping operation. Augment-REINFORCE-Swap-Merge (ARSM; Yin et al., 2019) goes one step further by averaging over all possible choices of the pivot dimension that ARS chooses arbitrarily. Our Rao-Blackwellized ARS and ARSM estimators are obtained by analytically integrating out the randomness introduced by the augmenting Dirichlet dimensions from the ARS and ARSM estimators respectively, following the strategy that was used to derive DisARM from ARM.

5 Experiments

Our goal was to derive unbiased, low-variance gradient estimators for the categorical setting which do not rely on continuous relaxation, so we compare to the best-performing existing methods in this category: ARS and ARSM (Yin et al., 2019) and the REINFORCE estimator with a leave-one-out baseline (RLOO, Kool et al., 2019). RLOO is a simple but effective method that has rarely been used as a baseline in prior work. As in prior work (Yin et al., 2019), we benchmark the estimators by training variational auto-encoders (Kingma and Welling, 2014; Rezende et al., 2014) (VAE) with *categorical* latent variables on three datasets: binarized MNIST[4] (LeCun et al., 2010), FashionMNIST[5] (Xiao et al., 2017), and Omniglot[6] (Lake et al., 2015). As we sought to evaluate optimization performance, we use dynamic binarization to avoid overfitting and largely find that

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[5]MIT license

[6]MIT license

Table 2: Evaluating the estimators and the effect of ordering on FashionMNIST with different model sizes. Mean variational lower bounds and the standard error of the mean computed based on 5 runs of 5×10^5-steps training from different random initializations. We consider three combinations of the number of categories (C) and the number of latent variables (V). The best performing method (up to the standard error) for each task is in bold. Top: evaluating the performance of the proposed estimators and the RLOO baseline. Bottom: comparing the effect of arranging the categories in the ascending or descending order to the default ordering for DisARM-SB.

Estimator Comparison with Train ELBO				
	DisARM-IW	DisARM-Tree	DisARM-SB	RLOO
C64 / V5	$\mathbf{-244.75 \pm 0.53}$	$\mathbf{-244.29 \pm 0.30}$	$\mathbf{-244.81 \pm 0.64}$	-245.27 ± 0.30
C64 / V32	-240.08 ± 0.17	$\mathbf{-239.83 \pm 0.29}$	$\mathbf{-239.66 \pm 0.20}$	-240.89 ± 0.49
C16 / V32	$\mathbf{-239.94 \pm 0.14}$	-240.52 ± 0.22	-240.43 ± 0.13	-240.99 ± 0.25

Ordering Comparison with Train ELBO			
	Ascending	Descending	Default
C64 / V5	$\mathbf{-244.81 \pm 0.64}$	$\mathbf{-244.95 \pm 0.36}$	$\mathbf{-244.61 \pm 0.38}$
C64 / V32	$\mathbf{-239.66 \pm 0.20}$	-240.04 ± 0.24	-239.99 ± 0.20
C16 / V32	$\mathbf{-240.43 \pm 0.13}$	$\mathbf{-240.39 \pm 0.21}$	$\mathbf{-240.50 \pm 0.13}$

training performance mirrors test performance. We use the standard split into train, validation, and test sets.

To allow direct comparison, we use the same model structure as in (Yin et al., 2019). Briefly, the model has a single layer of categorical latent variables which are then represented as one-hot vectors and decoded to Bernoulli logits for the observation through either a linear transformation or an MLP with two hidden layers of 256 and 512 of LeakyReLU units (Xu et al., 2015). The encoder mirrors the structure, with two hidden layers of 512 and 256 LeakyReLU units and outputs producing the softmax logits. For most experiments, we used 32 latent variables with 64 categories unless specified otherwise. See Appendix A.2 for more details.

5.1 Evaluating DisARM-IW, DisARM-SB & DisARM-Tree

First, we evaluated the importance-weighted estimator (DisARM-IW), and DisARM estimators with the stick breaking construction (DisARM-SB) and the tree structured construction (DisARM-Tree). These estimators require only 2 expensive function evaluations regardless of the number of categories (C), unlike ARS/ARSM which require up to $O(C)/O(C^2)$ evaluations, so we use the 2-independent sample RLOO estimator as a baseline.

In the case of nonlinear models (Figure 1), all three proposed estimators perform similarly, with lower gradient variance and better performance than the baseline estimator (RLOO) across all datasets. While for DisARM-IW, we have to use the ascending order for the stick-breaking construction to ensure unbiasedness, for DisARM-SB any ordering results in an unbiased estimator. We experimented with ordering the categories in the ascending and descending order by probability as well as using the default ordering (Figure 2). We found that the estimator with the ascending order consistently outperforms the other ordering schemes, though the gain is dataset-dependent. However, when we varied the number of categories and variables (Figure 3), we found that no ordering dominates. Given that ordering introduces an additional complexity, we recommend no ordering in practice.

In the case of linear models, we found that all estimators performed similarly (Appendix A.1). Dong et al. (2020) found that for multi-layer linear models in the binary case, DisARM showed increasing improvement over RLOO for models with deeper hierarchies. As nonlinear models are more common and expressive, we leave exploring whether this trend holds in the categorical case to future work.

We further verified that the observed improvements of the proposed estimators w.r.t. the RLOO baseline are consistent for models with different sizes of the latent space. As shown in Figure 3, we find that the best choice of the proposed estimators depends on the model size, however all three estimators outperform RLOO in all cases.

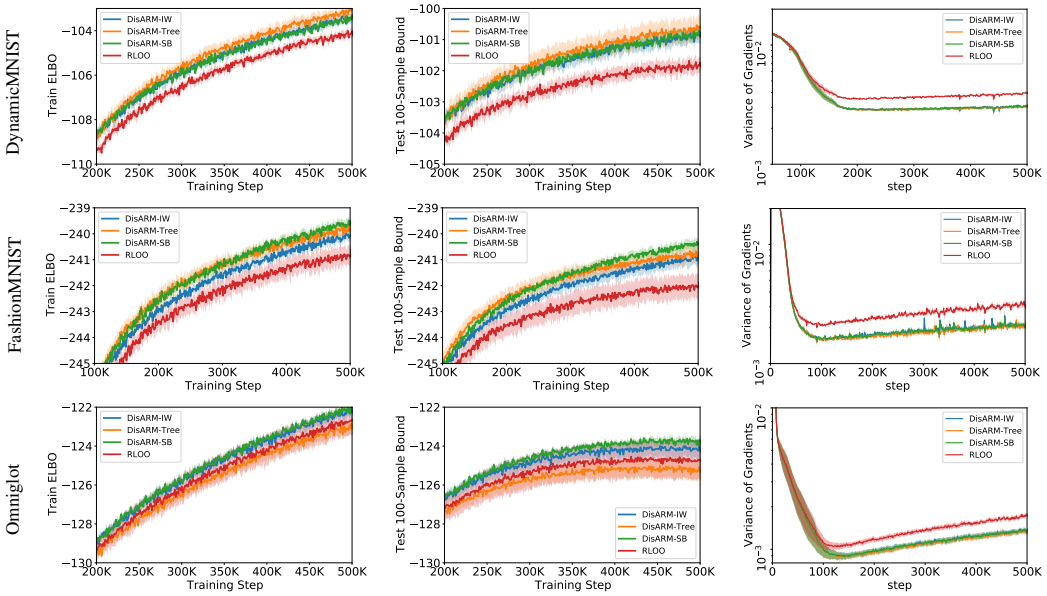
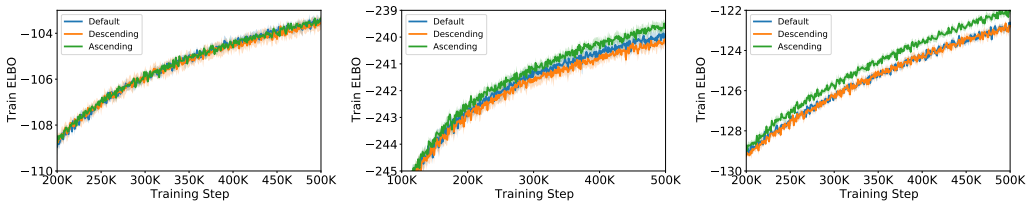


Figure 1: Training a non-linear categorical VAE with 32 latent variables with 64 categories on dynamically binarized MNIST, FashionMNIST, Omniglot datasets by maximizing the ELBO. We plot the train ELBO (left column), test 100-sample bound (middle column), and the variance of gradient estimator (right column). For a fair comparison, the variance of all the gradient estimators was computing along the training trajectory of the RLOO estimator. We plot the mean and one standard error based on 5 runs from different random initializations.



DynamicMNIST FashionMNIST Omniglot

Figure 2: Comparison of ordering on the performance of DisARM-SB. We sort the encoder logits in ascending and descending order and compare against the default ordering.

5.2 Evaluation Rao-Blackwellized ARS & ARSM

We train models with 10/5/3/2-category latent variables on dynamically binarized MNIST. For comparison, we train models with ARS, ARSM, and an n-sample RLOO. To match computation, RLOO uses C samples for comparing against ARS/ARS+, and uses $C(C-1)/2+1$ samples for ARSM/ARSM+, where C is the number of categories. Based on preliminary experiments with ARS+, we found that leveraging the symmetry (Appendix A.6.1) led to most of the performance improvement for ARS+. So, for ARSM, we reduce the variance only by leveraging the symmetry and call the resulting estimator ARSM+.

As shown in Figure 4 and Appendix Figure 7, the proposed estimators, ARS+/ARSM+, significantly outperform ARS/ARSM. Surprisingly, we find that both ARS and ARSM underperform the simpler RLOO baseline in all cases. For $C = 2$, ARS+ and ARSM+ reduce to DisARM/U2G and as expected, outperform REINFORCE LOO; however, for $C > 2$, REINFORCE LOO is superior and the gap increases as C does. This suggests that partially integrating out the randomness is insufficient to account for the variance introduced by the continuous augmentation.

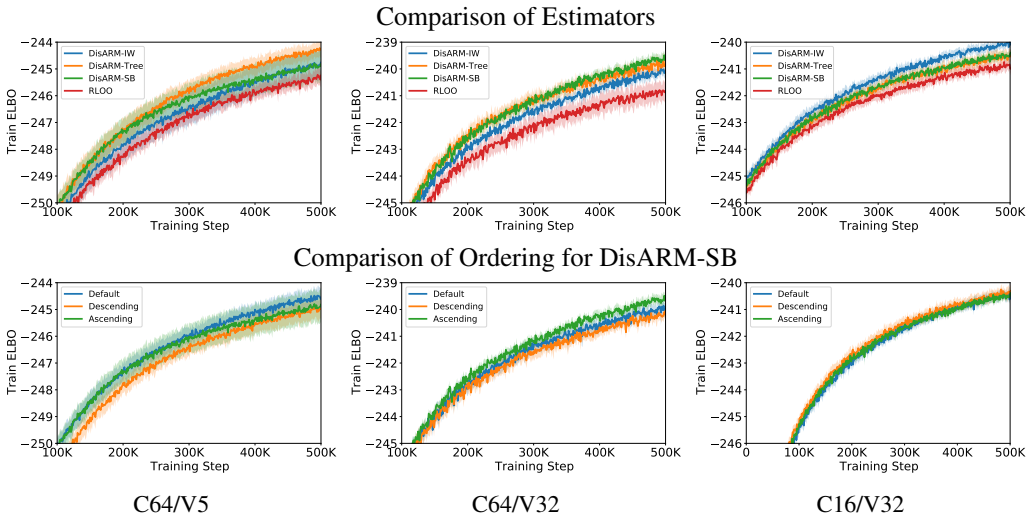


Figure 3: Training non-linear categorical VAEs with different model sizes on dynamically binarized FashionMNIST. Left: 5 latent variables of 64 categories. Middle: with 32 latent variables with 64 categories. Right: 32 latent variables with 16 categories.

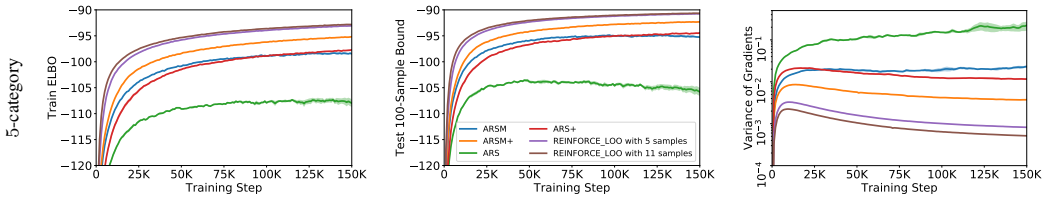


Figure 4: Training a non-linear categorical VAE with latent variables with 5 categories on dynamically binarized MNIST dataset by maximizing the ELBO. We plot the train ELBO (left column), test 100-sample bound (middle column), and the variance of gradient estimator (right column). We plot the mean and one standard error based on 5 runs from different random initializations.

6 Conclusion

We introduce a novel derivation of DisARM/U2G estimator based on importance sampling and statistical couplings, and naturally extend it to the categorical setting, calling the resulting estimator DisARM-IW. Motivated by the construction of a stick-breaking coupling, we introduce two estimators, DisARM-SB and DisARM-Tree, by reparameterizing the problem with a sequence of binary variables and performing Rao-Blackwellization.

With systematic experiments, we demonstrate that the proposed estimators provide state-of-the-art performance. We find that the proposed estimators usually perform similarly and all outperform RLOO, with the winner depending on the dataset and the model. As the importance sampling estimator DisARM-IW is simpler to implement, more natural to understand, and easier to generalize, we recommend it in practice. We expect that this estimator can be further improved through better couplings, which is something we intend to explore in the future.

Discrete latent variables have particular applicability to interpretable models and sparse/conditional computation. Improving the foundational tools to train such models will make them more widely available. While interpretable systems are typically viewed as a positive, they only give a partial view of a complex system, and they can be misused to give a false sense of understanding. While sparse/conditional models can reduce the environmental cost of learned models (Patterson et al., 2021), the unintended implications of large models must also be considered (Bender et al., 2021).

References

Bender, E. M., Gebru, T., McMillan-Major, A., and Shmitchell, S. (2021). On the dangers of stochastic parrots: Can language models be too big?. In *Proceedings of the 2021 ACM Conference on Fairness, Accountability, and Transparency*, pages 610–623.

Dong, Z., Mnih, A., and Tucker, G. (2020). DisARM: An antithetic gradient estimator for binary latent variables. *arXiv preprint arXiv:2006.10680*.

Ghahramani, Z., Jordan, M., and Adams, R. P. (2010). Tree-structured stick breaking for hierarchical data. In *Advances in Neural Information Processing Systems*, volume 23.

Glasserman, P. (2013). *Monte Carlo Methods in Financial Engineering*. Springer Science & Business Media.

Glynn, P. W. (1990). Likelihood ratio gradient estimation for stochastic systems. *Communications of the ACM*, 33(10):75–84.

Grathwohl, W., Choi, D., Wu, Y., Roeder, G., and Duvenaud, D. (2018). Backpropagation through the void: Optimizing control variates for black-box gradient estimation. In *International Conference on Learning Representations*.

Jang, E., Gu, S., and Poole, B. (2017). Categorical reparameterization with gumbel-softmax. In *International Conference on Learning Representations*.

Jordan, M. I., Ghahramani, Z., Jaakkola, T. S., and Saul, L. K. (1999). An introduction to variational methods for graphical models. *Machine learning*, 37(2):183–233.

Khan, M., Mohamed, S., Marlin, B., and Murphy, K. (2012). A stick-breaking likelihood for categorical data analysis with latent gaussian models. In *Artificial Intelligence and Statistics*, pages 610–618. PMLR.

Kingma, D. P. and Welling, M. (2014). Auto-encoding variational Bayes. In *International Conference on Learning Representations*.

Kool, W., van Hoof, H., and Welling, M. (2019). Buy 4 reinforce samples, get a baseline for free! In *Deep RL Meets Structured Prediction ICLR Workshop*.

Lake, B. M., Salakhutdinov, R., and Tenenbaum, J. B. (2015). Human-level concept learning through probabilistic program induction. *Science*, 350(6266):1332–1338.

LeCun, Y., Cortes, C., and Burges, C. (2010). Mnist handwritten digit database. *ATT Labs [Online]. Available: http://yann.lecun.com/exdb/mnist*, 2.

Maddison, C. J., Mnih, A., and Teh, Y. W. (2017). The Concrete Distribution: A Continuous Relaxation of Discrete Random Variables. In *International Conference on Learning Representations*.

Owen, A. B. (2013). *Monte Carlo theory, methods and examples*.

Patterson, D., Gonzalez, J., Le, Q., Liang, C., Munguia, L.-M., Rothchild, D., So, D., Texier, M., and Dean, J. (2021). Carbon emissions and large neural network training. *arXiv preprint arXiv:2104.10350*.

Rezende, D. J., Mohamed, S., and Wierstra, D. (2014). Stochastic backpropagation and approximate inference in deep generative models. In *Proceedings of The 31st International Conference on Machine Learning*, pages 1278–1286.

Rubinstein, R. Y. and Shapiro, A. (1990). Optimization of static simulation models by the score function method. *Mathematics and Computers in Simulation*, 32(4):373–392.

Ruiz, F. J., Titsias, M. K., and Blei, D. M. (2016). Overdispersed black-box variational inference. In *Proceedings of the Thirty-Second Conference on Uncertainty in Artificial Intelligence*, pages 647–656. AUAI Press.

Tucker, G., Mnih, A., Maddison, C. J., Lawson, J., and Sohl-Dickstein, J. (2017). REBAR: Low-variance, unbiased gradient estimates for discrete latent variable models. In *Advances in Neural Information Processing Systems 30*.

Williams, R. J. (1992). Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine learning*, 8(3-4):229–256.

Xiao, H., Rasul, K., and Vollgraf, R. (2017). Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms.

Xu, B., Wang, N., Chen, T., and Li, M. (2015). Empirical evaluation of rectified activations in convolutional network. *arXiv preprint arXiv:1505.00853*.

Yin, M., Ho, N., Yan, B., Qian, X., and Zhou, M. (2020). Probabilistic Best Subset Selection by Gradient-Based Optimization. *arXiv e-prints*.

Yin, M., Yue, Y., and Zhou, M. (2019). ARSM: Augment-REINFORCE-swap-merge estimator for gradient backpropagation through categorical variables. In *Proceedings of the 36th International Conference on Machine Learning*.

Yin, M. and Zhou, M. (2019). ARM: Augment-REINFORCE-merge gradient for stochastic binary networks. In *International Conference on Learning Representations*.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See throughout and Section 6.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Section 6.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes] See Appendices A.3,A.4,A.5,A.6.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] Code and instructions are provided in the supplemental material.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Sections 5 and A.2.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] All figures and tables include standard error of the mean over random seeds.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Section A.2.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] See Section 5.
   (b) Did you mention the license of the assets? [Yes] See Section 5.
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]

(e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]

5. If you used crowdsourcing or conducted research with human subjects...

(a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

(b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]