ARM: Augment-REINFORCE-Merge Gradient for Discrete Latent Variable Models

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Abstract

To backpropagate the gradients through discrete stochastic layers, we encode the true gradients into a multiplication between random noises and the difference of the same function of two different sets of discrete latent variables, which are correlated with these random noises. The expectations of that multiplication over iterations are zeros combined with spikes from time to time. To modulate the frequencies, amplitudes, and signs of the spikes to capture the temporal evolution of the true gradients, we propose the augment-REINFORCE-merge (ARM) estimator that combines data augmentation, the score-function estimator, permutation of the indices of latent variables, and variance reduction for Monte Carlo integration using common random numbers. The ARM estimator provides low-variance and unbiased gradient estimates for the parameters of discrete distributions, leading to state-of-the-art performance in both auto-encoding variational Bayes and maximum likelihood inference, for discrete latent variable models with one or multiple discrete stochastic layers.

1 Introduction

Given a function $f(\boldsymbol{z})$ of a random variable $\boldsymbol{z}$, which follows a distribution $q_{\boldsymbol{\phi}}(\boldsymbol{z})$ parameterized by $\boldsymbol{\phi}$, there has been significant recent interest in estimating $\boldsymbol{\phi}$ to maximize (or minimize) the expectation of $f(\boldsymbol{z})$ with respect to $\boldsymbol{z} \sim q_{\boldsymbol{\phi}}(\boldsymbol{z})$, expressed as

$$\mathcal{E}(\boldsymbol{\phi}) = \int f(\boldsymbol{z}) q_{\boldsymbol{\phi}}(\boldsymbol{z}) d\boldsymbol{z} = \mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\boldsymbol{z})}[f(\boldsymbol{z})]. \tag{1}$$

In particular, maximizing the marginal likelihood of a hierarchal Bayesian model [Bishop, 1995] and maximizing the evidence lower bound (ELBO) for variational inference [Blei et al., 2017, Jordan et al., 1999], two fundamental problems in statistical inference, both boil down to maximizing an expectation as in (1). To maximize (1), if $\nabla_{\boldsymbol{z}} f(\boldsymbol{z})$ is tractable to compute and $\boldsymbol{z} \sim q_{\boldsymbol{\phi}}(\boldsymbol{z})$ can be generated via reparameterization as $\boldsymbol{z} = \mathcal{T}_{\boldsymbol{\phi}}(\boldsymbol{\epsilon}),\ \boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$, where $\boldsymbol{\epsilon}$ are

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random noises and $\mathcal{T}_{\boldsymbol{\phi}}(\cdot)$ denotes a deterministic transform parameterized by $\boldsymbol{\phi}$, then one may apply the reparameterization trick [Kingma and Welling, 2013, Rezende et al., 2014] to compute the gradient as

$$\nabla_{\boldsymbol{\phi}}\mathcal{E}(\boldsymbol{\phi}) = \nabla_{\boldsymbol{\phi}}\mathbb{E}_{\boldsymbol{\epsilon}\sim p(\boldsymbol{\epsilon})}[f(\mathcal{T}_{\boldsymbol{\phi}}(\boldsymbol{\epsilon}))] = \mathbb{E}_{\boldsymbol{\epsilon}\sim p(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\phi}}f(\mathcal{T}_{\boldsymbol{\phi}}(\boldsymbol{\epsilon}))]. \tag{2}$$

Unfortunately, the reparameterization trick is not directly applicable to discrete random variables, which are widely used to construct discrete latent variable models such as the sigmoid belief net [Neal, 1992, Saul et al., 1996].

To maximize (1) for discrete $\boldsymbol{z}$, using the score function $\nabla_{\boldsymbol{\phi}}\log q_{\boldsymbol{\phi}}(\boldsymbol{z}) = \nabla_{\boldsymbol{\phi}}q_{\boldsymbol{\phi}}(\boldsymbol{z})/q_{\boldsymbol{\phi}}(\boldsymbol{z})$, one may compute $\nabla_{\boldsymbol{\phi}}\mathcal{E}(\boldsymbol{\phi})$ via REINFORCE [Williams, 1992] as

$$\nabla_{\boldsymbol{\phi}}\mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\boldsymbol{z})}[f(\boldsymbol{z})\nabla_{\boldsymbol{\phi}}\log q_{\boldsymbol{\phi}}(\boldsymbol{z})] \approx \frac{1}{K}\sum\nolimits_{k=1}^{K} f(\boldsymbol{z}^{(k)})\nabla_{\boldsymbol{\phi}}\log q_{\boldsymbol{\phi}}(\boldsymbol{z}^{(k)}), \tag{3}$$

where $\boldsymbol{z}^{(k)} \overset{iid}{\sim} q_{\boldsymbol{\phi}}(\boldsymbol{z})$ are independent, and identically distributed (*iid*). This estimator is also known as (a.k.a.) the score-function [Fu, 2006] or likelihood-ratio estimator [Glynn, 1990]. While it is very general in that it only requires drawing *iid* random samples from $q_{\boldsymbol{\phi}}(\boldsymbol{z})$ and computing $\nabla_{\boldsymbol{\phi}}\log q_{\boldsymbol{\phi}}(\boldsymbol{z}^{(k)})$, the high variance of Monte Carlo integration often limits its use in practice. Note that if $f(\boldsymbol{z})$ depends on $\boldsymbol{\phi}$, then we assume it is true that $\mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\boldsymbol{z})}[\nabla_{\boldsymbol{\phi}}f(\boldsymbol{z})] = 0$. For example, in variational inference, we need to maximize the ELBO as $\mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\boldsymbol{z})}[f(\boldsymbol{z})]$, where $f(\boldsymbol{z}) = \log[p(\boldsymbol{x}\,|\,\boldsymbol{z})p(\boldsymbol{z})/q_{\boldsymbol{\phi}}(\boldsymbol{z})]$. In this case, although $f(\boldsymbol{z})$ depends on $\boldsymbol{\phi}$, since $\mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\boldsymbol{z})}[\nabla_{\boldsymbol{\phi}}\log q_{\boldsymbol{\phi}}(\boldsymbol{z})] = 0$, we have $\mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\boldsymbol{z})}[\nabla_{\boldsymbol{\phi}}f(\boldsymbol{z})] = 0$.

To address the high-variance issue, one may introduce appropriate control variates (a.k.a. baselines) to reduce the variance of REINFORCE [Gu et al., 2016, Kucukelbir et al., 2017, Mnih and Gregor, 2014, Mnih and Rezende, 2016, Naesseth et al., 2017, Paisley et al., 2012, Ranganath et al., 2014, Ruiz et al., 2016]. Alternatively, one may first relax the discrete random variables with continuous ones and then apply the reparameterization trick to estimate the gradients, which reduces the variance of Monte Carlo integration at the expense of introducing bias [Jang et al., 2017, Maddison et al., 2017]. Combining both REINFORCE and the continuous relaxation of discrete random variables, several recently proposed algorithms are able to produce low-variance and unbiased gradient estimates, but need to introduce control variates that are updated for each mini-batch, increasing both the computational complexity and risk of overfitting the training data [Grathwohl et al., 2018, Tucker et al., 2017]. Another interesting variance-control idea applicable to discrete latent variables is using local expectation gradients, which estimates the gradients based on REINFORCE, by performing Monte Carlo integration using a single global sample together with many local samples for each latent dimension [Titsias and Lázaro-Gredilla, 2015].

Intuitively speaking, our strategy of variance control, which allows using a single random sample for Monte Carlo integration, is to encourage the expectation of the estimated gradient of a discrete distribution parameter to be exactly zero with high probability at each iteration, while allowing that expectation to be a random spike from time to time. The spike frequency, amplitude, and sign are modulated by the estimator to track the temporal evolution of the true gradient. Our intuition for why this strategy is effective for training a better model is that random spikes, whose temporal averages track the true gradients, provide large gradient-estimate-to-noise ratios, which could help move a parameter towards the right direction, even if its true gradient becomes so small that it is easily buried in noise caused by both mini-batch based stochastic update and Monte-Carlo estimation error.

Formally, we propose the augment-REINFORCE-merge (ARM) estimator, a novel low-variance and unbiased stochastic gradient estimator that estimates the gradients of discrete distribution parameters in an augmented space. More specifically, for a univariate discrete latent variable, we rewrite the expectation with respect to it as one with respect to augmented exponential random variables, express the gradient as an expectation via REINFORCE, re-express that expectation as an expectation with respect to standard exponential distributions, swap the index of each standard exponential random variable with that of its reference category, and then let different expectations to share common random numbers to effectively control the variance of Monte Carlo integration. The ARM estimator for univariate discrete latent variables is further generalized to one for multivariate discrete latent variables.

Our experimental results on both auto-encoding variational Bayes and maximum likelihood inference for discrete latent variable models, with one or multiple discrete stochastic layers, show that the ARM estimator has low computational complexity and provides state-of-the-art out-of-sample prediction performance, suggesting the effectiveness of using ARM spikes for gradient backpropagation through discrete stochastic layers.

2 ARM: Augment-REINFORCE-merge estimator

For simplicity, we will first present the ARM estimator for a univariate categorical/binary latent variable, and then generalize it to a multivariate one (*i.e.*, a vector of discrete latent variables). Let us denote $z \sim \text{Discrete}(\sigma(\boldsymbol{\phi}))$ as a categorical random variable such that

$$P(z = i \,|\, \boldsymbol{\phi}) = \sigma(\boldsymbol{\phi})_i = \frac{e^{\phi_i}}{\sum_{i=1}^M e^{\phi_i}},$$

where $\boldsymbol{\phi} = (\phi_1, \dots, \phi_M)'$ and $\sigma(\boldsymbol{\phi}) = (e^{\phi_1}, \dots, e^{\phi_M})' / \sum_{i=1}^M e^{\phi_i}$ is the softmax function. For an expectation of the function $f(\boldsymbol{z})$ with respect to $z \sim \text{Discrete}(\sigma(\boldsymbol{\phi}))$, expressed as $\mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{z \sim \text{Discrete}(\sigma(\boldsymbol{\phi}))}[f(z)]$, we need to evaluate its gradient with respect to $\boldsymbol{\phi}$. Without loss of generality, we assume $\mathbb{E}_{z \sim \text{Discrete}(\sigma(\boldsymbol{\phi}))}[\nabla_{\boldsymbol{\phi}} f(z)] = 0$.

We first present the ARM estimator for a univariate categorical latent variable in the following Theorem. We denote $\mathbf{1}_M$ as a vector of M ones, and $(m \leftrightharpoons M)$ as a vector of indices constructed by swapping the m-th and M-th elements of vector $(1, \dots, M)$, which means $(m \leftrightharpoons M)_M = m$, $(m \leftrightharpoons M)_m = M$, and $(m \leftrightharpoons M)_i = i$ for $i \notin \{m, M\}$. The ARM estimator can be further simplified for a univariate binary latent variable, where $M = 2$, as summarized in Corollary 2. The ARM gradient is generalized to mutivariate latent categorical and binary random variables in Corollary 3 4. The detailed derivations are provided in Sections 2.1–2.4.

Theorem 1 (ARM for univariate categorical)**.** *For a categorical random variable z, the gradient of $\mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{z \sim \text{Discrete}(\sigma(\boldsymbol{\phi}))}[f(z)] = \mathbb{E}_{z \sim \text{Discrete}(\sigma([\tilde{\boldsymbol{\phi}}', 0]'))}[f(z)]$ with respect to $\tilde{\boldsymbol{\phi}} =$*

$(\tilde{\phi}_1, \ldots, \tilde{\phi}_{M-1})'$, where $\tilde{\phi}_m = \phi_m - \phi_M$, can be expressed as

$$\begin{aligned}
&\nabla_{\tilde{\phi}_m} \mathcal{E}(\boldsymbol{\phi}) = \nabla_{\tilde{\phi}_m} \mathcal{E}([\tilde{\boldsymbol{\phi}}', 0]') = \mathbb{E}_{\boldsymbol{\pi} \sim \text{Dirichlet}(\mathbf{1}_M)}[f_\Delta(\boldsymbol{\pi}, \boldsymbol{\phi}, m)(1 - M\pi_M)], \quad \textit{where} \\
&f_\Delta(\boldsymbol{\pi}, \boldsymbol{\phi}, m) = \frac{1}{M} \sum\nolimits_{j \neq m} \big(f(z_{(m)}) - f(z_{(j)})\big) = f(z_{(m)}) - \frac{1}{M} \sum_{j=1}^{M} f(z_{(j)}), \\
&\qquad z_{(j)} = \underset{i \in \{1,\ldots,M\}}{\arg\min}\ \pi_{(j \leftrightharpoons M)_i} e^{-\phi_i} \ \textit{for } j = 1, \ldots, M.
\end{aligned} \tag{4}$$

Corollary 2 (ARM for univariate binary)**.** *For a binary random variable, the gradient of $\mathbb{E}_{z \sim \text{Bernoulli}(\sigma(\phi))}[f(z)]$ with respect to ϕ, the logit of the Bernoulli probability parameter, can be expressed as*

$$\begin{aligned}
&\nabla_\phi \mathcal{E}(\phi) = \mathbb{E}_{u \sim \text{Uniform}(0,1)}[f_\Delta(u, \phi)(u - 1/2)], \quad \textit{where} \\
&f_\Delta(u, \phi) = f(z_{(1)}) - f(z_{(2)}), \quad z_{(1)} = \mathbf{1}[u > \sigma(-\phi)], \quad z_{(2)} = \mathbf{1}[u < \sigma(\phi)].
\end{aligned} \tag{5}$$

We refer to both $\hat{\nabla}_{\tilde{\phi}_m} \mathcal{E}(\boldsymbol{\phi}) = f_\Delta(\boldsymbol{\pi}, \boldsymbol{\phi}, m)(1 - M\pi_M)$ in (4) and $\hat{\nabla}_\phi \mathcal{E}(\phi) = f_\Delta(u, \phi)(u - 1/2)$ in (5) as spike gradients, which are the unbiased estimates of the corresponding true gradients using a single Monte Carlo sample. Let "$\overset{whp}{=}$" represent "equal with high probability." For a categorical random variable, if there exists k such that ϕ_k is dominant: $\phi_k \gg \phi_i$ for $i \neq k$, then $\arg\min_i \pi_{(j \leftrightharpoons M)_i} e^{-\phi_i} \overset{whp}{=} k$ for all $j \in \{1, \ldots, M\}$, and consequently, $f_\Delta(\boldsymbol{\pi}, \boldsymbol{\phi}, m) \overset{whp}{=} 0$ and the spike gradient $\hat{\nabla}_{\tilde{\phi}_m} \mathcal{E}(\boldsymbol{\phi}) \overset{whp}{=} 0$. For a binary random variable, when $\sigma(\phi)$ is close to either one or zero, then $f_\Delta(u, \phi) \overset{whp}{=} 0$ and hence the spike gradient $\hat{\nabla}_\phi \mathcal{E}(\phi) \overset{whp}{=} 0$.

The ARM estimator for a univariate discrete latent variable, however, may be of little use in practice, as it is often easy to first analytically solve the expectation and then compute its gradient. We provide in the following two Corollaries on how to generalize the ARM estimator for multivariate discrete latent variables, for which it is often impractical to analytically compute the expectation, and defer detailed derivations to Section 2.5.

Corollary 3 (ARM for multivariate categorical)**.** *Denote $\mathbf{\Pi} = (\boldsymbol{\pi}_1, \ldots, \boldsymbol{\pi}_V) \in \mathbb{R}^{M \times V}$ and $\mathbf{\Phi} = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_V) \in \mathbb{R}^{M \times V}$, where $\boldsymbol{\pi}_v = (\pi_{1v}, \ldots, \pi_{Mv})'$ and $\boldsymbol{\phi}_v = (\phi_{1v}, \ldots, \phi_{Mv})'$, and $\boldsymbol{z} = (z_1, \ldots, z_V)'$ as a V dimensional vector of M-way categorical random variables $z_v \in \{1, \ldots, M\}$. The gradient of*

$$\mathcal{E}(\mathbf{\Phi}) = \mathbb{E}_{\boldsymbol{z} \sim \prod_{v=1}^V \text{Discrete}(z_v; \sigma(\boldsymbol{\phi}_v))}[f(\boldsymbol{z})] = \mathbb{E}_{\boldsymbol{z} \sim \prod_{v=1}^V \text{Discrete}(z_v; \sigma([\tilde{\boldsymbol{\phi}}_v', 0]'))}[f(\boldsymbol{z})] \tag{6}$$

with respect to $\tilde{\phi}_{mv} = \phi_{mv} - \phi_{Mv}$, can be expressed as

$$\begin{aligned}
&\nabla_{\tilde{\phi}_{mv}} \mathcal{E}(\mathbf{\Phi}) = \mathbb{E}_{\mathbf{\Pi} \sim \prod_{v=1}^V \text{Dirichlet}(\boldsymbol{\pi}_v; \mathbf{1}_M)}[f_\Delta(\mathbf{\Pi}, \mathbf{\Phi}, m)(1 - M\pi_{Mv})], \quad \textit{where} \\
&f_\Delta(\mathbf{\Pi}, \mathbf{\Phi}, m) = \frac{1}{M} \sum\nolimits_{j \neq m} \big[f\big(\boldsymbol{z}_{(m)}\big) - f\big(\boldsymbol{z}_{(j)}\big)\big] = f\big(\boldsymbol{z}_{(m)}\big) - \frac{1}{M} \sum\nolimits_{j=1}^{M} f\big(\boldsymbol{z}_{(j)}\big), \\
&\boldsymbol{z}_{(j)} = (z_{(j)1}, \ldots, z_{(j)V})' \ \textit{for } j = 1, \ldots, M, \quad z_{(j)v} = \underset{i \in \{1,\ldots,M\}}{\arg\min}\ \pi_{(j \leftrightharpoons M)_i v} e^{-\phi_{iv}}.
\end{aligned} \tag{7}$$

Corollary 4 (ARM for multivariate binary)**.** *For a vector of V binary random variables $\boldsymbol{z} = (z_1, \ldots, z_V)'$, the gradient of*

$$\mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{\boldsymbol{z} \sim \prod_{v=1}^V \text{Bernoulli}(z_v; \sigma(\phi_v))}[f(\boldsymbol{z})] \tag{8}$$

with respect to $\boldsymbol{\phi} = (\phi_1, \dots, \phi_V)'$*, the logits of the Bernoulli probability parameters, can be expressed as*

$$\begin{aligned}&\nabla_{\boldsymbol{\phi}} \mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{\boldsymbol{u} \sim \prod_{v=1}^V \text{Uniform}(u_v; 0,1)}[f_\Delta(\boldsymbol{u}, \boldsymbol{\phi})(\boldsymbol{u} - 1/2)], \quad \textit{where}\\ &f_\Delta(\boldsymbol{u}, \boldsymbol{\phi}) = f(\boldsymbol{z}_{(1)}) - f(\boldsymbol{z}_{(2)}), \quad \boldsymbol{z}_{(1)} = \mathbf{1}[\boldsymbol{u} > \sigma(-\boldsymbol{\phi})], \quad \boldsymbol{z}_{(2)} = \mathbf{1}[\boldsymbol{u} < \sigma(\boldsymbol{\phi})],\end{aligned} \tag{9}$$

where $\mathbf{1}[\boldsymbol{u} > \sigma(-\boldsymbol{\phi})] := \big(\mathbf{1}[u_1 > \sigma(-\phi_1)], \dots, \mathbf{1}[u_V > \sigma(-\phi_V)]\big)'$.

We refer to both

$$\hat{\nabla}_{\tilde{\boldsymbol{\phi}}_{mv}} \mathcal{E}(\boldsymbol{\Phi}) = f_\Delta(\boldsymbol{\Pi}, \boldsymbol{\Phi}, m)(1 - M\pi_{Mv})$$

in (4) and

$$\hat{\nabla}_{\phi_v} \mathcal{E}(\boldsymbol{\phi}) = f_\Delta(\boldsymbol{u}, \boldsymbol{\phi})(u_v - 1/2)$$

in (5) as spike gradients, which are the unbiased estimates of the corresponding true gradients using a single Monte Carlo sample as $\boldsymbol{\Pi} \sim \prod_{v=1}^V \text{Dirichlet}(\boldsymbol{\pi}_v; \mathbf{1}_M)$ or $\boldsymbol{u} \sim \prod_{v=1}^V \text{Uniform}(u_v; 0, 1)$.

Let us denote $(\boldsymbol{\cdot})_{\backslash v}$ as a vector/matrix whose vth element/column is removed and $z_{(j)v}$ as the vth element of $\boldsymbol{z}_{(j)}$. For the vth element of a V dimensional M-way categorical random variable, suppose there is a ϕ_{kv} whose value is dominant, which means $\phi_{kv} \gg \phi_{iv}$ for $i \neq k$, then $\arg\min_i \pi_{(j \leftrightharpoons M)_i v} e^{-\phi_{iv}} \overset{whp}{=} k$ for all $j \in \{1, \dots, M\}$ and hence

$$\begin{aligned}&\mathbb{E}[\hat{\nabla}_{\tilde{\boldsymbol{\phi}}_{mv}} \mathcal{E}(\boldsymbol{\Phi}) \,|\, \exists k \text{ such that } \phi_{kv} \gg \phi_{iv} \text{ for } i \neq k]\\ &\overset{whp}{=} \mathbb{E}_{\boldsymbol{\Pi}_{\backslash v} \sim \prod_{\nu \neq v} \text{Dirichlet}(\boldsymbol{\pi}_\nu; \mathbf{1}_M)}[f_\Delta(\boldsymbol{\Pi}, \boldsymbol{\Phi}, m) \,|\, z_{(j)v} = k \ \forall\ j] \times \mathbb{E}_{\boldsymbol{\pi}_v \sim \text{Dirichlet}(\mathbf{1}_M)}[(1 - M\pi_{Mv})] = 0.\end{aligned}$$

In other words, ARM gradient estimate $\hat{\nabla}_{\tilde{\boldsymbol{\phi}}_{mv}} \mathcal{E}(\boldsymbol{\Phi})$ has zero expectation with high probability if it is likely that all $z_{(j)v}$ for $j \in \{1, \dots, M\}$ will take the same value from $\{1, \dots, M\}$.

Similarly, for a latent vector of V binary random variables, with probability $P(\boldsymbol{z}_{(1)v} = \boldsymbol{z}_{(2)v}) = \sigma(|\phi_v|) - \sigma(-|\phi_v|)$, we have

$$\begin{aligned}&\mathbb{E}_{\boldsymbol{u} \sim \prod_{v=1}^V \text{Uniform}(u_v; 0,1)}[\hat{\nabla}_{\phi_v} \mathcal{E}(\boldsymbol{\phi})]\\ &= \mathbb{E}_{\boldsymbol{u}_{\backslash v} \sim \prod_{\nu \neq v} \text{Uniform}(u_\nu; 0,1)}[f_\Delta(\boldsymbol{u}, \boldsymbol{\phi}) \,|\, \boldsymbol{z}_{(1)v} = \boldsymbol{z}_{(2)v}] \times \mathbb{E}_{u_v \sim \text{Uniform}(0,1)}[u_v - 1/2] = 0,\end{aligned}$$

which means that when $\sigma(|\phi_v|) \to 1$, the estimated gradient has zero expectation with probability $P(\boldsymbol{z}_{(1)v} = \boldsymbol{z}_{(2)v}) \to 1$ if there is little ambiguity about whether $\boldsymbol{z}_{(1)v} = \boldsymbol{z}_{(2)v}$.

In the remainder of the section, we provide detailed derivations for Theorem 1 and Corollaries 2 to 4.

2.1 Augmentation of a categorical random variable

Let us denote $\tau \sim \text{Exp}(\lambda)$ as the exponential distribution, with probability density function $p(\tau \,|\, \lambda) = \lambda e^{-\lambda \tau}$, where $\lambda > 0$ and $\tau > 0$. Its mean and variance are $\mathbb{E}[\tau] = \lambda^{-1}$ and $\text{var}[\tau] = \lambda^{-2}$, respectively. It is well known that, e.g. in Ross [2006], if $\tau_i \sim \text{Exp}(\lambda_i)$ are independent exponential random variables for $i = 1, \dots, M$, then the probability that τ_z, where $z \in \{1, \dots, M\}$, is the smallest can be expressed as

$$P\big(z = \arg\min_{i \in \{1,\dots,M\}} \tau_i\big) = P\left(\tau_z < \tau_i, \ \forall\ i \neq z\right) = \frac{\lambda_z}{\sum_{i=1}^M \lambda_i} \ . \tag{10}$$

Note this property is closely related to the Gumbel distribution (a.k.a. Type-I extreme-value distribution) based latent-utility-maximization representation of multinomial logistic regression [McFadden, 1974, Train, 2009], as well as the Gumbel-softmax trick [Jang et al., 2017, Maddison et al., 2017]. This is because the exponential random variable $\tau \sim \text{Exp}(\lambda)$ can be reparameterized as $\tau = \epsilon/\lambda,\ \epsilon \sim \text{Exp}(1)$, where $\epsilon \sim \text{Exp}(1)$ can be equivalently generated as $\epsilon = -\log u,\ u \sim \text{Uniform}(0,1)$, and hence we have

$$\arg\min_i \tau_i \overset{d}{=} \arg\min_i\{-\log u_i/\lambda_i\} = \arg\max_i\{\log\lambda_i - \log(-\log u_i)\},$$

where $\tau_i \sim \text{Exp}(\lambda_i)$, "$\overset{d}{=}$" denotes "equal in distribution," and $u_i \overset{iid}{\sim} \text{Uniform}(0,1)$; note that if $u \sim \text{Uniform}(0,1)$, then $-\log(-\log u)$ follows the Gumbel distribution [Train, 2009].

From (10) we know that if

$$z = \arg\min_{i\in\{1,\dots,M\}} \tau_i \text{ , where } \tau_i \sim \text{Exp}(e^{\phi_i}), \tag{11}$$

then $P(z \,|\, \boldsymbol{\phi}) = e^{\phi_z}/\sum_{i=1}^M e^{\phi_i}$, and hence (11) is an augmented representation of the categorical distribution $z \sim \text{Discrete}(\sigma(\boldsymbol{\phi}))$; one may consider $\tau_i \sim \text{Exp}(e^{\phi_i})$ as augmented latent variables, the marginalization of which from $z = \arg\min_{i\in\{1,\dots,M\}} \tau_i$ leads to $P(z \,|\, \boldsymbol{\phi})$. Consequently, the expectation with respect to the categorical random variable of M categories can be rewritten as one with respect to M augmented exponential random variables as

$$\mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{z\sim\text{Discrete}(\sigma(\boldsymbol{\phi}))}[f(z)] = \mathbb{E}_{\tau_1\sim\text{Exp}(e^{\phi_1}),\dots,\tau_M\sim\text{Exp}(e^{\phi_M})}[f(\arg\min_i \tau_i)]. \tag{12}$$

Since the exponential random variable $\tau \sim \text{Exp}(e^{\phi})$ can be reparameterized as $\tau = \epsilon e^{-\phi},\ \epsilon \sim \text{Exp}(1)$, by the law of the unconscious statistician (LOTUS) [Ross, 1976], we also have

$$\mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{\epsilon_1,\dots,\epsilon_M \overset{iid}{\sim} \text{Exp}(1)}[f(\arg\min_i \epsilon_i e^{-\phi_i})]. \tag{13}$$

Note as the arg min operator is non-differentiable, the reparameterization trick in (2) is not applicable to computing the gradient of $\mathcal{E}(\boldsymbol{\phi})$ via the reparameterized representation in (13).

2.2 REINFORCE estimator in the augmented space

Using REINFORCE on (12), we have $\nabla_{\boldsymbol{\phi}}\mathcal{E}(\boldsymbol{\phi}) = [\nabla_{\phi_1}\mathcal{E}(\boldsymbol{\phi}),\dots,\nabla_{\phi_M}\mathcal{E}(\boldsymbol{\phi})]'$, where

$$\begin{aligned}\nabla_{\phi_m}\mathcal{E}(\boldsymbol{\phi}) &= \mathbb{E}_{\tau_1\sim\text{Exp}(e^{\phi_1}),\dots,\tau_M\sim\text{Exp}(e^{\phi_M})}\Big[f(\arg\min_i \tau_i)\nabla_{\phi_m}\log\prod\nolimits_{i=1}^M \text{Exp}(\tau_i; e^{\phi_i})\Big]\\ &= \mathbb{E}_{\tau_1\sim\text{Exp}(e^{\phi_1}),\dots,\tau_M\sim\text{Exp}(e^{\phi_M})}[f(\arg\min_i \tau_i)\nabla_{\phi_m}\log\text{Exp}(\tau_m; e^{\phi_m})]\\ &= \mathbb{E}_{\tau_1\sim\text{Exp}(e^{\phi_1}),\dots,\tau_M\sim\text{Exp}(e^{\phi_M})}[f(\arg\min_i \tau_i)(1-\tau_m e^{\phi_m})]. \end{aligned}\tag{14}$$

As $\sigma(\boldsymbol{\phi} - \phi_M\mathbf{1}_M) = \sigma(\boldsymbol{\phi})$ is always true, one may choose category M for reference and only update $\tilde{\phi}_m = \phi_m - \phi_M$ for $m \le M-1$. Denoting $\tilde{\boldsymbol{\phi}} = (\tilde{\phi}_1,\dots,\tilde{\phi}_{M-1})' = \mathbf{A}\boldsymbol{\phi}$, where $\mathbf{A} = [\text{diag}(\mathbf{1}_{M-1}), -\mathbf{1}_{M-1}]$, we have $\mathcal{E}([\tilde{\boldsymbol{\phi}}', 0]') = \mathcal{E}(\boldsymbol{\phi})$ and hence

$$\nabla_{\boldsymbol{\phi}}\mathcal{E}(\boldsymbol{\phi})' = \nabla_{\tilde{\boldsymbol{\phi}}}\mathcal{E}([\tilde{\boldsymbol{\phi}}', 0]')'\frac{\partial\tilde{\boldsymbol{\phi}}}{\partial\boldsymbol{\phi}} = \nabla_{\tilde{\boldsymbol{\phi}}}\mathcal{E}([\tilde{\boldsymbol{\phi}}', 0]')'\mathbf{A}. \tag{15}$$

Therefore, we have a solution as $\nabla_{\tilde{\boldsymbol{\phi}}}\mathcal{E}([\tilde{\boldsymbol{\phi}}', 0]')' = \nabla_{\boldsymbol{\phi}}\mathcal{E}(\boldsymbol{\phi})'\mathbf{A}'(\mathbf{A}\mathbf{A}')^{-1}$, where $\mathbf{A}'(\mathbf{A}\mathbf{A}')^{-1} = [\text{diag}(\mathbf{1}_{M-1}), \mathbf{0}_{M-1}]' - \frac{1}{M}\mathbf{1}_{M\times(M-1)}$, and hence

$$\begin{aligned}\nabla_{\tilde{\phi}_m}\mathcal{E}([\tilde{\boldsymbol{\phi}}', 0]') &= \frac{1}{M}\sum\nolimits_{j\neq m}(\nabla_{\phi_m}\mathcal{E}(\boldsymbol{\phi}) - \nabla_{\phi_j}\mathcal{E}(\boldsymbol{\phi})) \\ &= \nabla_{\phi_m}\mathcal{E}(\boldsymbol{\phi}) - \frac{1}{M}\sum\nolimits_{j=1}^{M}\nabla_{\phi_j}\mathcal{E}(\boldsymbol{\phi}).\end{aligned} \tag{16}$$

Below we show how to merge $\nabla_{\phi_m}\mathcal{E}(\boldsymbol{\phi})$ and $-\nabla_{\phi_j}\mathcal{E}(\boldsymbol{\phi})$, by first re-expressing (14) into an expectation with respect to *iid* exponential random variables, swapping the indices of these random variables, and then sharing common random numbers [Owen, 2013] to well control the variance of Monte-Carlo integration.

2.3 Merge of REINFORCE gradients

A key observation of the paper is we can use LOTUS to re-express the expectation in (14) as

$$\nabla_{\phi_m}\mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{\epsilon_1,\ldots,\epsilon_M \overset{iid}{\sim} \text{Exp}(1)}[f(\arg\min\nolimits_i \epsilon_i e^{-\phi_i})(1-\epsilon_m)]. \tag{17}$$

Denote $\tilde{\boldsymbol{\epsilon}} = (\tilde{\epsilon}_1, \ldots, \tilde{\epsilon}_M)$ as an arbitrary permutation of $\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_M)$; since letting $\tilde{\boldsymbol{\epsilon}} \sim \prod_{i=1}^M \text{Exp}(\tilde{\epsilon}_i; 1)$ is the same in distribution as letting $\boldsymbol{\epsilon} \sim \prod_{i=1}^M \text{Exp}(\epsilon_i; 1)$ and permuting $\tilde{\boldsymbol{\epsilon}}$ from $\boldsymbol{\epsilon}$, another key observation is the expectation in (17) can be equivalently expressed as

$$\begin{aligned}\nabla_{\phi_m}\mathcal{E}(\boldsymbol{\phi}) &= \mathbb{E}_{\tilde{\epsilon}_1,\ldots,\tilde{\epsilon}_M \overset{iid}{\sim} \text{Exp}(1)}[f(\arg\min\nolimits_i \tilde{\epsilon}_i e^{-\phi_i})(1-\tilde{\epsilon}_m)] \\ &= \mathbb{E}_{\epsilon_1,\ldots,\epsilon_M \overset{iid}{\sim} \text{Exp}(1)}[f(\arg\min\nolimits_i \tilde{\epsilon}_i e^{-\phi_i})(1-\tilde{\epsilon}_m)].\end{aligned} \tag{18}$$

Therefore, choosing a specific permutation as $\tilde{\epsilon}_i = \epsilon_{(m \leftrightharpoons M)_i}$, which means swapping the mth and the last element of $\boldsymbol{\epsilon}$ to construct $\tilde{\boldsymbol{\epsilon}}$, we have

$$\nabla_{\phi_m}\mathcal{E}(\boldsymbol{\phi}) = \mathbb{E}_{\epsilon_1,\ldots,\epsilon_M \overset{iid}{\sim} \text{Exp}(1)}[f(\arg\min\nolimits_i \epsilon_{(m \leftrightharpoons M)_i} e^{-\phi_i})(1-\epsilon_M)]. \tag{19}$$

Using (19) on (16), we introduce the ARM estimator as

$$\nabla_{\tilde{\phi}_m}\mathcal{E}([\tilde{\boldsymbol{\phi}}', 0]') = \mathbb{E}_{\epsilon_1,\ldots,\epsilon_M \overset{iid}{\sim} \text{Exp}(1)}[f_\Delta(\boldsymbol{\epsilon}, \boldsymbol{\phi}, m)(1-\epsilon_M)], \tag{20}$$

in which we share common random numbers to compute different expectations, with

$$\begin{aligned}f_\Delta(\boldsymbol{\epsilon}, \boldsymbol{\phi}, m) &= \frac{1}{M}\sum\nolimits_{j\neq m}[f(\arg\min\nolimits_i \epsilon_{(m \leftrightharpoons M)_i} e^{-\phi_i}) - f(\arg\min\nolimits_i \epsilon_{(j \leftrightharpoons M)_i} e^{-\phi_i})] \\ &= f(\arg\min\nolimits_i \epsilon_{(m \leftrightharpoons M)_i} e^{-\phi_i}) - \frac{1}{M}\sum\nolimits_{j=1}^{M} f(\arg\min\nolimits_i \epsilon_{(j \leftrightharpoons M)_i} e^{-\phi_i}).\end{aligned} \tag{21}$$

Distinct from a usual REINFORCE estimator, an attractive property of the ARM estimator in (20) is that inside the expectation, $1 - \epsilon_M$, which is equal in distribution to the score function $\nabla_{\phi_M}\log\prod_{m=1}^M \text{Exp}(\tau_m; e^{\phi_m})$, is multiplied by a function with zero expectation as

$$\mathbb{E}_{\epsilon_1,\ldots,\epsilon_M \overset{iid}{\sim} \text{Exp}(1)}[f_\Delta(\boldsymbol{\epsilon}, \boldsymbol{\phi}, m)] = 0.$$

Having zero expectation for the term that is multiplied by the score function, regardless of the current value of $\boldsymbol{\phi}$, is a desirable property for ARM to control the variance of Monte Carlo integration. Moreover, if $f_\Delta(\boldsymbol{\epsilon}, \boldsymbol{\phi}, m) \overset{whp}{=} 0$, then it is likely that the gradients estimated by a single Monte Carlo sample will be zeros during most iterations, while becoming spikes from time to time. In other words, rather than making an estimated gradient be as close as possible to the true gradient at each iteration, the ARM estimator for a univariate categorical latent variable makes it only moves as frequently as necessary, using its time-averaged values to approximate the true time-varying gradients.

Furthermore, noting that $\text{Exp}(1) \overset{d}{=} \text{Gamma}(1,1)$, letting $\epsilon_1, \ldots, \epsilon_M \overset{iid}{\sim} \text{Exp}(1)$ is the same (e.g., as proved in Lemma IV.3 of Zhou and Carin [2012]) in distribution as letting

$$\epsilon_i = \pi_i \epsilon, \quad \text{for } i = 1, \ldots, M, \text{ where } \boldsymbol{\pi} \sim \text{Dirichlet }(\mathbf{1}_M),\ \epsilon \sim \text{Gamma}(M, 1),$$

and $\arg\min_i \pi_{(m \rightleftharpoons M)_i} e^{-\phi_i} = \arg\min_i \epsilon \pi_{(m \rightleftharpoons M)_i} e^{-\phi_i}$, we can re-express the gradient in (19) as

$$\begin{aligned}\nabla_{\phi_m} \mathcal{E}(\boldsymbol{\phi}) &= \mathbb{E}_{\epsilon \sim \text{Gamma}(M,1),\ \boldsymbol{\pi} \sim \text{Dirichlet}(\mathbf{1}_M)} [f(\arg\min_i \pi_{(m \rightleftharpoons M)_i} e^{-\phi_i})(1 - \epsilon \pi_M)] \\ &= \mathbb{E}_{\boldsymbol{\pi} \sim \text{Dirichlet}(\mathbf{1}_M)} [f(\arg\min_i \pi_{(m \rightleftharpoons M)_i} e^{-\phi_i})(1 - M \pi_M)]. \end{aligned} \tag{22}$$

Thus, plugging (22) into (16), we have now concluded the proof for Theorem 1.

2.4 ARM for a binary random variable

Note in distribution, drawing $(u_1, u_2) \sim \text{Dirichlet}(1, 1)$ is the same as drawing $u \sim \text{Uniform}[0, 1]$ and letting $u_1 = u$ and $u_2 = 1 - u$. Denoting $\phi = \phi_1 - \phi_2$, for the expectation as

$$\mathcal{E}([\phi_1, \phi_2]') = \mathbb{E}_{[z, 1-z] \sim \text{Discrete}(\sigma([\phi_1, \phi_2]))}[f(z)] = \mathbb{E}_{z \sim \text{Bernoulli}(e^{\phi_1}/(e^{\phi_1} + e^{\phi_2}))}[f(z)],$$

we can deduce Corollary 2 from Theorem 1. Furthermore, the following Theorem, whose proof is provided in Appendix, shows that the ARM spike gradient for a binary random variable, expressed as $f_\Delta(u, \phi)(u - 1/2)$, concentrates around 0, is unbiased, and achieves low variance.

Theorem 5. *Assume $f \geq 0$ (or $f \leq 0$) is a function of Bernoulli random variable z. Using a single Monte Carlo sample, the ARM spike gradient is expressed as $g_A(u, \phi) = f_\Delta(u, \phi)(u - 1/2)$, where f_Δ is defined as in (5) and $u \sim \text{Uniform}(0, 1)$, and the REINFORCE gradient is expressed as $g_R(z, \phi) = f(z) \nabla_\phi \log \text{Bernoulli}(z; \sigma(\phi)) = f(z)(z - \sigma(\phi))$, where $z \sim \text{Bernoulli}(\sigma(\phi))$. We have the following properties:*

(i) $f_\Delta(u, \phi) = 0$ with probability $\sigma(|\phi|) - \sigma(-|\phi|)$, $f_\Delta(u, \phi) = f(1) - f(0)$ with probability $1 - \sigma(|\phi|)$, and $f_\Delta(u, \phi) = f(0) - f(1)$ with probability $\sigma(-|\phi|)$.

(ii) $g_A(u, \boldsymbol{\phi})$ is unbiased with $\mathbb{E}_{u \sim \text{Uniform}(0,1)}[g_A(u, \boldsymbol{\phi})] = \mathbb{E}_{z \sim \text{Bernoulli}(\sigma(\phi))}[g_R(z, \boldsymbol{\phi})]$.

(iii) $g_A(u, \boldsymbol{\phi})$ reaches its largest variance at $0.039788[f(1) - f(0)]^2$ when $\frac{P(f_\Delta = 0)}{P(f_\Delta \neq 0)}$ is equal to the golden ratio $\frac{\sqrt{5}+1}{2}$.

(iv) $\frac{\sup_\phi \text{Var}[g_A]}{\sup_\phi \text{Var}[g_R]} \leq \frac{16}{25}(1 - 2\frac{f(0)}{f(0)+f(1)})^2$ and $\sup_\phi \text{Var}[g_A] \leq \frac{1}{25}[f(1) - f(0)]^2$.

2.5 ARM for multivariate discrete latent variables

Below we show how to generalize Theorem 1 and Corollary 2 for univariate discrete latent variables to Corollaries 3 and 4 for multivariate discrete latent variables.

For the expectation in (6), since z_v are conditionally independent given $\boldsymbol{\phi}_v$, we have

$$\nabla_{\tilde{\phi}_{mv}} \mathcal{E}(\boldsymbol{\Phi}) = \mathbb{E}_{\boldsymbol{z}_{\setminus v} \sim \prod_{\nu \neq v} \text{Discrete}(z_\nu; \sigma(\boldsymbol{\phi}_\nu))} \big[\nabla_{\tilde{\phi}_{mv}} \mathbb{E}_{z_v \sim \text{Discrete}(\sigma(\boldsymbol{\phi}_v))} [f(\boldsymbol{z})] \big]. \tag{23}$$

Using Theorem 1 to compute the gradient in the above equation directly leads to

$$\nabla_{\tilde{\phi}_{mv}} \mathcal{E}(\boldsymbol{\Phi}) = \mathbb{E}_{\boldsymbol{z}_{\setminus v} \sim \prod_{\nu \neq v} \text{Discrete}(z_\nu; \sigma(\boldsymbol{\phi}_\nu))} \Big\{ \mathbb{E}_{\boldsymbol{\pi}_v \sim \text{Dirichlet}(\mathbf{1}_M)} \Big[(1 - M\pi_{Mv}) \frac{1}{M} \sum\nolimits_{j \neq m} \\ \big(f(\boldsymbol{z}_{\setminus v}, z_{(m)v}) - f(\boldsymbol{z}_{\setminus v}, z_{(j)v}) \big) \Big] \Big\}, \text{ where } z_{(j)v} = \underset{i \in \{1,\dots,M\}}{\arg\min}\ \pi_{(j \rightleftharpoons M)iv} e^{-\phi_{iv}} \text{ for } j = 1, \dots, M. \tag{24}$$

The term inside $[\cdot]$ of (24) can already be used to estimate the gradient, however, in the worst case scenario that all the elements of $\{z_{(j)v}\}_{j=1,M}$ are different, it needs to evaluate the function $f(\boldsymbol{z}_{\setminus v}, z_{(j)v})$ for $j = 1, \dots, M$, and hence M times for each v and MV times in total. To reduce computation and simplify implementation, exchanging the order of the two expectations in (24), we have

$$\nabla_{\tilde{\phi}_{mv}} \mathcal{E}(\boldsymbol{\Phi}) = \mathbb{E}_{\boldsymbol{\pi}_v \sim \text{Dirichlet}(\mathbf{1}_M)} \Big\{ (1 - M\pi_{Mv})\ \frac{1}{M} \sum\nolimits_{j \neq m} \Big(\\ \mathbb{E}_{\boldsymbol{z}_{\setminus v} \sim \prod_{\nu \neq v} \text{Discrete}(z_\nu; \sigma(\boldsymbol{\phi}_\nu))} \big[f(\boldsymbol{z}_{\setminus v}, z_{(m)v}) \big] - \mathbb{E}_{\boldsymbol{z}_{\setminus v} \sim \prod_{\nu \neq v} \text{Discrete}(z_\nu; \sigma(\boldsymbol{\phi}_\nu))} \big[f(\boldsymbol{z}_{\setminus v}, z_{(j)v}) \big] \Big) \Big\}. \tag{25}$$

Note that

$$\begin{aligned} &\mathbb{E}_{\boldsymbol{z}_{\setminus v} \sim \prod_{\nu \neq v} \text{Discrete}(z_\nu; \sigma(\boldsymbol{\phi}_\nu))} [f(\boldsymbol{z}_{\setminus v}, z_{(j)v})] \\ &= \mathbb{E}_{\boldsymbol{\epsilon}_{\setminus v} \sim \prod_{\nu \neq v} \prod_{i=1}^M \text{Exp}(\epsilon_{i\nu}; e^{\phi_{i\nu}})} \big[f\big((z_\nu = \arg\min\nolimits_{i \in \{1,\dots,M\}} \epsilon_{i\nu} e^{-\phi_{i\nu}})_{\nu \neq v},\ z_{(j)v} \big) \big] \\ &= \mathbb{E}_{\boldsymbol{\epsilon}_{\setminus v} \sim \prod_{\nu \neq v} \prod_{i=1}^M \text{Exp}(\epsilon_{i\nu}; e^{\phi_{i\nu}})} \big[f\big((z_\nu = \arg\min\nolimits_{i \in \{1,\dots,M\}} \epsilon_{(j \rightleftharpoons M)i\nu} e^{-\phi_{i\nu}})_{\nu \neq v},\ z_{(j)v} \big) \big] \\ &= \mathbb{E}_{\boldsymbol{\Pi}_{\setminus v} \sim \prod_{\nu \neq v} \text{Dirichlet}(\boldsymbol{\pi}_\nu; \mathbf{1}_M)} \big[f\big((z_\nu = \arg\min\nolimits_{i \in \{1,\dots,M\}} \pi_{(j \rightleftharpoons M)i\nu} e^{-\phi_{i\nu}})_{\nu \neq v},\ z_{(j)v} \big) \big]. \end{aligned}$$

Plugging the above equation into (25) leads to a simplified representation as (7) shown in Corollary 3, with which, regardless of the dimension V, we draw $\boldsymbol{\Pi} = (\boldsymbol{\pi}_1, \dots, \boldsymbol{\pi}_V)$ once to produce M correlated $\boldsymbol{z}$'s, that is $\{\boldsymbol{z}_{(j)}\}_{j=1,M}$, and evaluate the function $f(\boldsymbol{z})$ M times.

Similarly, for the expectation in (8), we have

$$\begin{aligned} \nabla_{\phi_v} \mathcal{E}(\boldsymbol{\phi}) &= \mathbb{E}_{\boldsymbol{z}_{\setminus v} \sim \prod_{\nu \neq v} \text{Bernoulli}(z_\nu; \sigma(\phi_\nu))} \{ \nabla_{\phi_v} \mathbb{E}_{z_v \sim \text{Bernoulli}(\sigma(\phi_v))} [f(\boldsymbol{z})] \} && (26) \\ &= \mathbb{E}_{\boldsymbol{z}_{\setminus v} \sim \prod_{\nu \neq v} \text{Bernoulli}(z_\nu; \sigma(\phi_\nu))} \big\{ \mathbb{E}_{u_v \sim \text{Uniform}(0,1)} \big[(u_v - 1/2) \\ &\qquad \times \big(f(\boldsymbol{z}_{\setminus v}, z_{(1)v} = \mathbf{1}[u_v > \sigma(-\phi_v)]) - f(\boldsymbol{z}_{\setminus v}, z_{(2)v} = \mathbf{1}[u_v < \sigma(\phi_v)]) \big) \big] \big\}, && (27) \end{aligned}$$

which can already be used to estimate the gradient. To further simplify computation and implementation, exchanging the order of the two expectations in (27), we have

$$\begin{aligned} \nabla_{\phi_v} \mathcal{E}(\boldsymbol{\phi}) &= \mathbb{E}_{u_v \sim \text{Uniform}(0,1)} \big\{ (u_v - 1/2)\ \mathbb{E}_{\boldsymbol{z}_{\setminus v} \sim \prod_{\nu \neq v} \text{Bernoulli}(z_\nu; \sigma(\phi_\nu))} \big[\\ &\qquad f(\boldsymbol{z}_{\setminus v}, z_{(1)v} = \mathbf{1}[u_v > \sigma(-\phi_v)]) - f(\boldsymbol{z}_{\setminus v}, z_{(2)v} = \mathbf{1}[u_v < \sigma(\phi_v)]) \big] \big\} \\ &= \mathbb{E}_{\boldsymbol{u} \sim \prod_{v=1}^V \text{Uniform}(u_v; 0,1)} \big[(u_v - 1/2) \big(f(\boldsymbol{z}_{(1)} = \mathbf{1}[\boldsymbol{u} > \sigma(-\boldsymbol{\phi})]) - f(\boldsymbol{z}_{(2)} = \mathbf{1}[\boldsymbol{u} < \sigma(\boldsymbol{\phi})]) \big) \big], && (28) \end{aligned}$$

which leads to a simplified representation as (9) shown in Corollary 4. Note inside the expectation in (28), the term multiplied with $u_v - 1/2$ is a scalar that is the same for all $v \in \{1, \dots, V\}$, whereas in (27), each $u_v - 1/2$ is multiplied by a term specific to itself.

In Appendix, we summarize ARM gradient ascent for multivariate categorical latent variables and that for multivariate binary latent variables in Algorithms 1 and 2, respectively.

2.5.1 Connections to local expectation gradients

By examining (23) and (24) for multivariate categorical and (26) and (27) for multivariate binary, we notice interesting connections between ARM and the local expectation gradients (LeGrad) method of Titsias and Lázaro-Gredilla [2015]. In particular, LeGrad will solve the local expectation gradient inside (23) analytically as

$$\nabla_{\tilde{\phi}_{mv}} \mathbb{E}_{z_v \sim \text{Discrete}(\sigma(\boldsymbol{\phi}_v))}[f(\boldsymbol{z})] = \nabla_{\tilde{\phi}_{mv}} \sum\nolimits_{i=1}^{M} \frac{e^{\phi_{iv}}}{\sum\nolimits_{i'=1}^{M} e^{\phi_{i'v}}} f(\boldsymbol{z}_{\setminus v}, z_v = i).$$

Thus, if the complexity of evaluating each function $f(\boldsymbol{z}_{\setminus v}, z_v = i)$ is $O(V)$, then LeGrad has a computation complexity of $O(MV)$ for each v and hence $O(MV^2)$ in total.

By contrast, plugging ARM into the LeGrad framework, one will re-express the local expectation gradient inside (23) as an location expectation in an augmented space, leading to (24), and solve that local expectation using a single Monte Carlo sample $\boldsymbol{\pi}_v \sim \text{Dirichlet}(\mathbf{1}_M)$, which is used to define M correlated categorical variables as $\{z_{(j)v}\}_{j=1:M}$; since $\{z_{(j)v}\}_{j=1:M}$ have at least one and at most M unique values, the best-case and worst-case computation complexities for ARM plugged LeGrad are $O(MV)$ and $O(MV^2)$, respectively.

Rather than naively plugging ARM into the LeGrad framework that separately treats the global expectation with respect to $\boldsymbol{z}_{\setminus v}$ and the local expectation with respect z_v for each dimension $v \in \{1, \dots, V\}$, in this paper, we generalize (24) or (27) by merging the global and local expectations for all dimensions. This leads to the ARM multivariate-discrete estimator (7) or (9) that only needs to draw a single global Monte Carlo sample to estimate the gradients for all V dimensions. Therefore, the proposed ARM estimator has a computation complexity of $O(MV)$, and hence scales linearly in V rather than quadratically as LeGrad does.

3 Backpropagation through discrete stochastic layers

A latent variable model with multiple stochastic hidden layers can be constructed as

$$\boldsymbol{x} \sim p_{\boldsymbol{\theta}_0}(\boldsymbol{x} \,|\, \boldsymbol{b}_1),\ \boldsymbol{b}_1 \sim p_{\boldsymbol{\theta}_1}(\boldsymbol{b}_1 \,|\, \boldsymbol{b}_2), \dots, \boldsymbol{b}_t \sim p_{\boldsymbol{\theta}_t}(\boldsymbol{b}_t \,|\, \boldsymbol{b}_{t+1}), \dots, \boldsymbol{b}_T \sim p_{\boldsymbol{\theta}_T}(\boldsymbol{b}_T), \tag{29}$$

whose joint likelihood given the distribution parameters $\boldsymbol{\theta}_{0:T} = \{\boldsymbol{\theta}_0, \dots, \boldsymbol{\theta}_T\}$ is expressed as

$$p(\boldsymbol{x}, \boldsymbol{b}_{1:T} \,|\, \boldsymbol{\theta}_{0:T}) = p_{\boldsymbol{\theta}_0}(\boldsymbol{x} \,|\, \boldsymbol{b}_1) \Big[\prod\nolimits_{t=1}^{T-1} p_{\boldsymbol{\theta}_t}(\boldsymbol{b}_t \,|\, \boldsymbol{b}_{t+1})\Big] p_{\boldsymbol{\theta}_T}(\boldsymbol{b}_T). \tag{30}$$

In comparison to deterministic feedforward neural networks, stochastic ones can represent complex distributions and show natural resistance to overfitting [Gu et al., 2016, Neal, 1992, Raiko et al., 2014, Saul et al., 1996, Tang and Salakhutdinov, 2013]. However, training such kind of networks, especially if different stochastic layers are linked through discrete latent variables, is often considerably more difficult [Tang and Salakhutdinov, 2013]. Below we show for both auto-encoding variational Bayes and maximum likelihood inference, how to apply the ARM estimator for gradient backpropagation in stochastic binary networks.

3.1 ARM variational auto-encoder

For auto-encoding variational Bayes inference [Kingma and Welling, 2013, Rezende et al., 2014], we construct a variational distribution as

$$q_{\boldsymbol{w}_{1:T}}(\boldsymbol{b}_{1:T}\,|\,\boldsymbol{x}) = q_{\boldsymbol{w}_1}(\boldsymbol{b}_1\,|\,\boldsymbol{x})\Big[\prod\nolimits_{t=1}^{T-1} q_{\boldsymbol{w}_{t+1}}(\boldsymbol{b}_{t+1}\,|\,\boldsymbol{b}_t)\Big], \tag{31}$$

with which the ELBO can be expressed as

$$\begin{aligned}&\mathcal{E}(\boldsymbol{w}_{1:T}) = \mathbb{E}_{\boldsymbol{b}_{1:T}\sim q_{\boldsymbol{w}_{1:T}}(\boldsymbol{b}_{1:T}\,|\,\boldsymbol{x})}\left[f(\boldsymbol{b}_{1:T})\right],\ \text{where}\\ &f(\boldsymbol{b}_{1:T}) = \log p_{\boldsymbol{\theta}_0}(\boldsymbol{x}\,|\,\boldsymbol{b}_1) + \log p_{\boldsymbol{\theta}_{1:T}}(\boldsymbol{b}_{1:T}) - \log q_{\boldsymbol{w}_{1:T}}(\boldsymbol{b}_{1:T}\,|\,\boldsymbol{x}).\end{aligned} \tag{32}$$

Theorem 6 (ARM backpropagation)**.** *For a stochastic binary network with T binary stochastic hidden layers, constructing a variational auto-encoder (VAE) defined with $\boldsymbol{b}_0 = \boldsymbol{x}$ and*

$$q_{\boldsymbol{w}_t}(\boldsymbol{b}_t\,|\,\boldsymbol{b}_{t-1}) = \text{Bernoulli}(\boldsymbol{b}_t; \sigma(\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}))) \tag{33}$$

for $t = 1,\dots,T$, the gradient of the ELBO with respect to $\boldsymbol{w}_t$ can be expressed as

$$\begin{aligned}&\nabla_{\boldsymbol{w}_t}\mathcal{E}(\boldsymbol{w}_{1:T}) = \mathbb{E}_{q(\boldsymbol{b}_{1:t-1})}\left[\mathbb{E}_{\boldsymbol{u}_t\sim\text{Uniform}(0,1)}[f_\Delta(\boldsymbol{u}_t,\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}),\boldsymbol{b}_{1:t-1})(\boldsymbol{u}_t - 1/2)]\nabla_{\boldsymbol{w}_t}\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1})\right],\\ &\textit{where } f_\Delta(\boldsymbol{u}_t,\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}),\boldsymbol{b}_{1:t-1}) = \mathbb{E}_{\boldsymbol{b}_{t+1:T}\sim q(\boldsymbol{b}_{t+1:T}\,|\,\boldsymbol{b}_t),\ \boldsymbol{b}_t=\mathbf{1}[\boldsymbol{u}_t>\sigma(-\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}))]}[f(\boldsymbol{b}_{1:T})]\\ &\qquad\qquad - \mathbb{E}_{\boldsymbol{b}_{t+1:T}\sim q(\boldsymbol{b}_{t+1:T}\,|\,\boldsymbol{b}_t),\ \boldsymbol{b}_t=\mathbf{1}[\boldsymbol{u}_t<\sigma(\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}))]}[f(\boldsymbol{b}_{1:T})],\end{aligned}$$

which can be estimated with a single Monte Carlo sample as

$$\hat{f}_\Delta(\boldsymbol{u}_t,\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}),\boldsymbol{b}_{1:t-1}) = \begin{cases}0, & \textit{if } \boldsymbol{b}_t^{(1)} = \boldsymbol{b}_t^{(2)}\\ f(\boldsymbol{b}_{1:t-1},\boldsymbol{b}_{t:T}^{(1)}) - f(\boldsymbol{b}_{1:t-1},\boldsymbol{b}_{t:T}^{(2)}), & \textit{otherwise}\end{cases}, \tag{34}$$

where $\boldsymbol{b}_t^{(1)} = \mathbf{1}[\boldsymbol{u}_t > \sigma(-\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}))]$, $\boldsymbol{b}_{t+1:T}^{(1)} \sim q(\boldsymbol{b}_{t+1:T}\,|\,\boldsymbol{b}_t^{(1)})$, $\boldsymbol{b}_t^{(2)} = \mathbf{1}[\boldsymbol{u}_t < \sigma(\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}))]$, and $\boldsymbol{b}_{t+1:T}^{(2)} \sim q(\boldsymbol{b}_{t+1:T}\,|\,\boldsymbol{b}_t^{(2)})$.

The proof of Theorem 6 is provided in the Appendix.

3.2 ARM maximum likelihood inference

For maximum likelihood inference, the log marginal likelihood can be expressed as

$$\begin{aligned}\log p_{\boldsymbol{\theta}_{0:T}}(\boldsymbol{x}) &= \log \mathbb{E}_{\boldsymbol{b}_{1:T}\sim p_{\boldsymbol{\theta}_{1:T}}(\boldsymbol{b}_{1:T})}[p_{\boldsymbol{\theta}_0}(\boldsymbol{x}\,|\,\boldsymbol{b}_1)]\\ &\geq \mathcal{E}(\boldsymbol{\theta}_{1:T}) = \mathbb{E}_{\boldsymbol{b}_{1:T}\sim p_{\boldsymbol{\theta}_{1:T}}(\boldsymbol{b}_{1:T})}[\log p_{\boldsymbol{\theta}_0}(\boldsymbol{x}\,|\,\boldsymbol{b}_1)].\end{aligned} \tag{35}$$

Generalizing Thoerem 6 leads to the following Corollary.

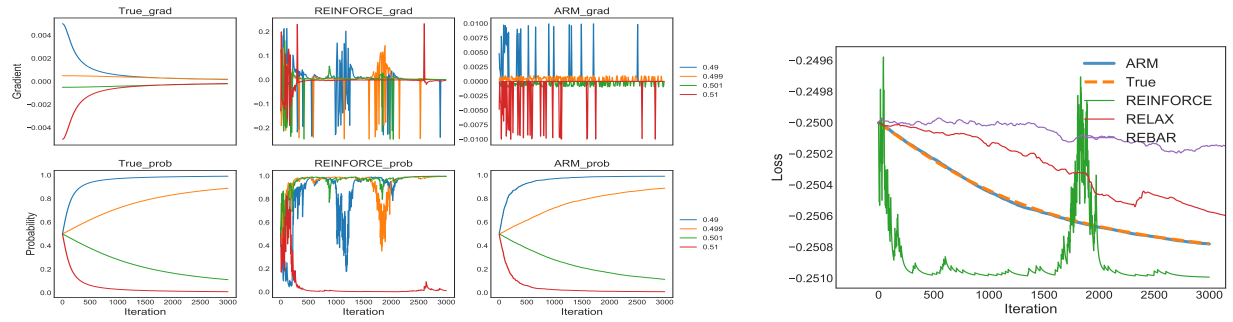


Figure 1: Left: Trace plots of the true/estimated gradients and estimated Bernoulli probability parameters for $p_0 \in \{0.49, 0.499, 0.501, 0.51\}$; Right: Trace plots of the loss functions for $p_0 = 0.499$.

Corollary 7. *For a stochastic binary network defined as*

$$p_{\boldsymbol{\theta}_t}(\boldsymbol{b}_t \mid \boldsymbol{b}_{t+1}) = \text{Bernoulli}(\boldsymbol{b}_t; \sigma(\mathcal{T}_{\boldsymbol{\theta}_t}(\boldsymbol{b}_{t+1}))), \tag{36}$$

the gradient of the lower bound in (35) *with respect to* $\boldsymbol{\theta}_t$ *can be expressed as*

$$\nabla_{\boldsymbol{\theta}_t}\mathcal{E}(\boldsymbol{\theta}_{1:T}) = \mathbb{E}_{p(\boldsymbol{b}_{t+1:T})}\left[\mathbb{E}_{\boldsymbol{u}_t\sim\text{Uniform}(0,1)}[f_\Delta(\boldsymbol{u}_t, \mathcal{T}_{\boldsymbol{\theta}_t}(\boldsymbol{b}_{t+1}), \boldsymbol{b}_{t+1:T})(\boldsymbol{u}_t - 1/2)]\nabla_{\boldsymbol{\theta}_t}\mathcal{T}_{\boldsymbol{\theta}_t}(\boldsymbol{b}_{t+1})\right],$$

$$\textit{where } f_\Delta(\boldsymbol{u}_t, \mathcal{T}_{\boldsymbol{\theta}_t}(\boldsymbol{b}_{t+1}), \boldsymbol{b}_{t+1:T}) = \mathbb{E}_{\boldsymbol{b}_{1:t-1}\sim p(\boldsymbol{b}_{1:t-1}\mid\boldsymbol{b}_t),\ \boldsymbol{b}_t=\mathbf{1}[\boldsymbol{u}_t>\sigma(-\mathcal{T}_{\boldsymbol{\theta}_t}(\boldsymbol{b}_{t+1}))]}[\log p_{\boldsymbol{\theta}_0}(\boldsymbol{x}\mid\boldsymbol{b}_1)]$$
$$- \mathbb{E}_{\boldsymbol{b}_{1:t-1}\sim p(\boldsymbol{b}_{1:t-1}\mid\boldsymbol{b}_t),\ \boldsymbol{b}_t=\mathbf{1}[\boldsymbol{u}_t<\sigma(\mathcal{T}_{\boldsymbol{\theta}_t}(\boldsymbol{b}_{t+1}))]}[\log p_{\boldsymbol{\theta}_0}(\boldsymbol{x}\mid\boldsymbol{b}_1)].$$

4 Experimental results

To illustrate the working mechanism of the ARM estimator, related to Tucker et al. [2017] and Grathwohl et al. [2018], we consider learning ϕ to maximize $\mathcal{E}(\phi) = \mathbb{E}_{z\sim\text{Bernoulli}(\sigma(\phi))}[(z-p_0)^2]$, where $p_0 \in \{0.49, 0.499, 0.501, 0.51\}$, or equivalently, minimize the loss as $-\mathcal{E}(\phi)$. The optimal solution is $\sigma(\phi) = \mathbf{1}(p_0 < 0.5)$. The closer p_0 is to 0.5, the more challenging the optimization becomes. We compare the ARM estimator to the true gradient as $g_\phi = (1-2p_0)\sigma(\phi)(1-\sigma(\phi))$ and three previously proposed unbiased estimators, including REINFORCE, REBAR [Tucker et al., 2017], and RELAX [Grathwohl et al., 2018]. Following Theorem 5, with a single random sample $u \sim \text{Uniform}(0,1)$ for Monte Carlo integration, the ARM spike gradient can be expressed as

$$g_{\phi,\text{ARM}} = \{[\mathbf{1}(u > \sigma(-\phi)) - p_0]^2 - [\mathbf{1}(u < \sigma(\phi)) - p_0]^2\}(u - 1/2),$$

while the REINFORCE gradient can be expressed as

$$g_{\phi,\text{REINFORCE}} = [\mathbf{1}(u < \sigma(\phi)) - p_0]^2[\mathbf{1}(u < \sigma(\phi)) - \sigma(\phi)].$$

See Tucker et al. [2017] and Grathwohl et al. [2018] for the details about REBAR and RELAX, respectively.

As shown in Figure 1 (a), the REINFORCE gradients have large variances. Consequently, a REINFORCE based gradient ascent algorithm may diverge. For example, when $p_0 = 0.501$, the optimal value for the Bernoulli probability $\sigma(\phi)$ is 0, but the algorithm infers it to be close

Table 1: The constructions of three differently structured discrete variational auto-encoders. The following symbols "$\rightarrow$", "]", ")", and "$\rightsquigarrow$" represent deterministic linear transform, leaky rectified linear units (LeakyReLU) [Maas et al., 2013] nonlinear activation, sigmoid nonlinear activation, and discrete stochastic activation, respectively, in the encoder (a.k.a., recognition network); their reversed versions are used in the decoder (a.k.a. generator).

	Nonlinear	Linear	Linear two layers
Encoder	784$\rightarrow$200]$\rightarrow$200]$\rightarrow$200)$\rightsquigarrow$200	784$\rightarrow$200)$\rightsquigarrow$200	784$\rightarrow$200)$\rightsquigarrow$200$\rightarrow$200)$\rightsquigarrow$200
Decoder	784$\leftsquigarrow$(784$\leftarrow$[200$\leftarrow$[200$\leftarrow$200	784$\leftsquigarrow$(784$\leftarrow$200	784$\leftsquigarrow$(784$\leftarrow$200$\leftsquigarrow$(200$\leftarrow$200

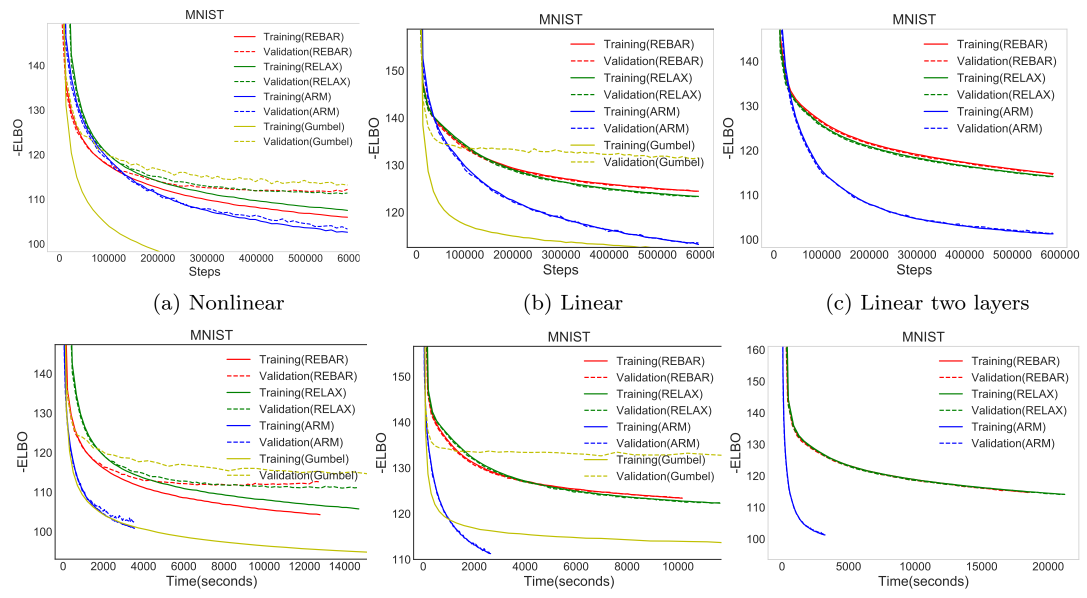
Table 2: Test negative ELBOs of discrete VAEs trained with four different stochastic gradient estimators.

			ARM	RELAX	REBAR	ST Gumbel-Softmax
Bernoulli	Nonlinear	MNIST	**101.3**	110.9	111.6	112.5
		OMNIGLOT	129.5	**128.2**	128.3	140.7
	Linear	MNIST	**110.3**	122.1	123.2	129.2
		OMNIGLOT	**124.2**	124.4	124.9	129.8
	Two layers	MNIST	**98.2**	114.0	113.7	NA
		OMNIGLOT	**118.3**	119.1	118.8	NA
Categorical	Nonlinear	MNIST	**105.8**	NA	NA	107.9
		OMNIGLOT	**121.9**	NA	NA	127.6

to 1 at the end of 3000 iterations of a random trial. By contrast, the ARM estimator well approximates the time-varying true gradients by adjusting the frequencies, amplitudes, and signs of its gradient estimates, with larger and more frequent spikes for larger true gradients. Even though the trace plots of the ARM gradients, characterized by random spikes, look very different from these of the true gradients, using them in gradient ascent leads to almost indistinguishable trace plots for the Bernoulli probability parameter $\sigma(\phi)$. As shown in Figure 1 (b), using the ARM estimator is indistinguishable from using the true gradient for updating ϕ to minimize the loss $-\mathbb{E}_{z\sim \text{Bernoulli}(\sigma(\phi))}[(z-0.499)^2]$, significantly outperforming not only REINFORCE, which has a large variance, but also both REBAR and RELAX, which improve on REINFORCE by introducing carefully constructed control variates for variance reduction. Updating ϕ using the true gradient, we further plot in Figure 5 of the Appendix the gradient estimated with multiple Monte Carlo samples against the true gradient at each iteration, showing that the ARM estimator has significantly lower variance than REINFORCE does given the same number of Monte Carlo samples.

4.1 Discrete variational auto-encoders

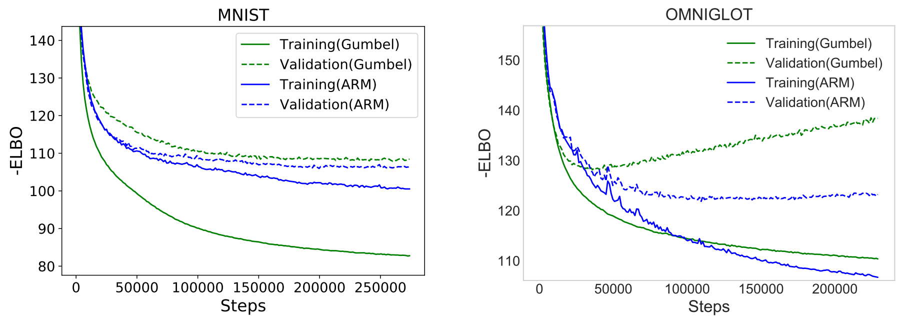
To optimize a variational auto-encoder (VAE) for a discrete latent variable model, existing solutions often rely on biased but low-variance stochastic gradient estimators [Bengio et al., 2013, Jang et al., 2017], unbiased but high-variance ones [Mnih and Gregor, 2014], or both unbiased and low-variance but computationally expensive ones [Grathwohl et al., 2018, Tucker et al., 2017]. Comparing to previously proposed ones for discrete latent variables, the ARM



(a) Nonlinear (b) Linear (c) Linear two layers

(d) Nonlinear (e) Linear (f) Linear two layers

Figure 2: Test negative ELBOs on MNIST with respect to training iterations, shown in the top row, and wall clock times on Tesla-K40 GPU, shown in the bottom row, for three differently structured Bernoulli VAEs.



(a) (b)

Figure 3: Comparison of the negative ELBOs for categorical variational auto-encoders trained by ARM and ST Gumbel-softmax on MNIST and OMNIGLOT, using the "Nonlinear" network.

estimator exhibits low variance and is unbiased, computationally efficient, and simple to implement.

For discrete VAEs, we compare ARM with Gumbel-Softmax [Jang et al., 2017, Maddison et al., 2017], REBAR [Grathwohl et al., 2018], and RELAX [Tucker et al., 2017], three representative stochastic gradient estimators for discrete latent variables. Following the settings in Tucker et al. [2017] and Grathwohl et al. [2018], for the encoder defined in (30) and decoder defined in (31), we consider three different network structures, including "Nonlinear" that has one stochastic but two LeaklyReLU deterministic hidden layers, "Linear" that has one stochastic hidden layer, and "Linear two layers" that has two stochastic hidden layers; we summarize the network structure in Table 1. We apply all four methods to both the MNIST and OMNIGLOT datasets.

We train a discrete VAE with either Bernoulli or Categorical latent variables. More

Table 3: For the MNIST conditional distribution estimation benchmark task, comparison of the test negative log-likelihood between various gradient estimators, with the best results in Gu et al. [2016], Jang et al. [2017] reported here.

Gradient estimator	ARM	ST	1/2	Annealed ST	ST Gumbel-S.	SF	MuProp
$-\log p(\boldsymbol{x}_l \,\vert\, \boldsymbol{x}_u)$	**54.8**	56.1	57.2	58.7	59.3	72.0	56.7

specifically, for each stochastic hidden layer, we use either 200 conditionally *iid* latent Bernoulli random variables or the concatenation of 20 conditionally *iid* categorical latent variables, each of which is represented as a 10 dimension one-hot vector. We maximize a single-Monte-Carlo-sample ELBO using Adam [Kingma and Ba, 2014], with the learning rate set as 10^{-4} and batch size as 25 for Bernoulli VAEs and 100 for Categorical VAEs. Using the standard training-validation-testing splitting, we train all methods on the training set, calculate ELBO on the validation set for every epoch, and report the negative ELBO on the test set when the validation negative ELBO reaches its minimum. Training and validation curves are shown in Figure 2 and all numerical results are summarized in Table 2. Note to make a fair comparison between different methods, we report the results produced by our own experiments with public available REBAR and RELAX code provided for [Grathwohl et al., 2018] and ST Gumbel-Softmax code provided for [Jang et al., 2017], sharing the same hyper-parameters and optimization procedure used in ARM. We also provide in Table 4 of the Appendix the comparison with the reported results of some additional algorithms, using the "Nonlinear" network structure on the MNIST dataset. The MNIST results show ARM outperforms the other competing methods in all tested network structures no matter at given steps or given times. On OMNIGLOT data, for nonlinear network, RELAX/REBAR achieve slightly higher ELBO but may be due to its severe overfitting caused by the auxiliary network used for variance reduction. For less overfitting linear and two-stochastic-layer networks, ARM performs on par with or better than RELAX/REBAR and converges significantly faster (about 6-8 times faster).

4.2 Maximum likelihood inference for a stochastic binary network

Denoting $\boldsymbol{x}_l, \boldsymbol{x}_u \in \mathbb{R}^{394}$ as the lower and upper halves of an MNIST digit, respectively, we consider a standard benchmark task of estimating the conditional distribution $p_{\boldsymbol{\theta}_{0:2}}(\boldsymbol{x}_l \,|\, \boldsymbol{x}_u)$ [Bengio et al., 2013, Gu et al., 2016, Jang et al., 2017, Raiko et al., 2014, Tucker et al., 2017], using a stochastic binary network with two stochastic binary hidden layers, expressed as

$$\boldsymbol{x}_l \sim \text{Bernoulli}(\sigma(\mathcal{T}_{\boldsymbol{\theta}_0}(\boldsymbol{b}_1))),\ \boldsymbol{b}_1 \sim \text{Bernoulli}(\sigma(\mathcal{T}_{\boldsymbol{\theta}_1}(\boldsymbol{b}_2))),\ \boldsymbol{b}_2 \sim \text{Bernoulli}(\sigma(\mathcal{T}_{\boldsymbol{\theta}_2}(\boldsymbol{x}_u))). \quad (37)$$

We set the network structure as $392 \leftrightsquigarrow (392 \leftarrow [300 \leftarrow 200 \leftrightsquigarrow (200 \leftarrow [300 \leftarrow 200 \leftrightsquigarrow (200 \leftarrow [300 \leftarrow 392$, which means both $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ are 200 dimensional binary vectors, and $\mathcal{T}_{\boldsymbol{\theta}_t}(\boldsymbol{b}_{t+1})$ can be represented as $\mathcal{T}_{\boldsymbol{\theta}_t}(\boldsymbol{b}_{t+1}) = \boldsymbol{\theta}_{t,1}\text{LeakyReLU}(\boldsymbol{\theta}_{t,2}\boldsymbol{b}_{t+1} + \boldsymbol{\theta}_{t,3}) + \boldsymbol{\theta}_{t,4}$.

We approximate $\log p_{\boldsymbol{\theta}_{0:2}}(\boldsymbol{x}_l \,|\, \boldsymbol{x}_u)$ with $\log \frac{1}{K}\sum_{k=1}^{K} \text{Bernoulli}(\boldsymbol{x}_l; \sigma(\mathcal{T}_{\boldsymbol{\theta}_0}(\boldsymbol{b}_1^{(k)})))$, where $\boldsymbol{b}_1^{(k)} \sim \text{Bernoulli}(\sigma(\mathcal{T}_{\boldsymbol{\theta}_1}(\boldsymbol{b}_2^{(k)})))$, $\boldsymbol{b}_2^{(k)} \sim \text{Bernoulli}(\sigma(\mathcal{T}_{\boldsymbol{\theta}_2}(\boldsymbol{x}_u)))$. We perform training with $K = 1$, which can also be considered as optimizing on a single-Monte-Carlo-sample estimate of the lower bound of the log likelihood shown in (35). We use Adam [Kingma and Ba, 2014], with the learning rate set as 10^{-4}, mini-batch size as 100, and number of epochs for training as 2000. Given the inferred point estimate of $\boldsymbol{\theta}_{0:2}$ after training, we evaluate the accuracy of conditional density estimation by estimating the negative log-likelihood as $-\log p_{\boldsymbol{\theta}_{0:2}}(\boldsymbol{x}_l \,|\, \boldsymbol{x}_u)$, averaging over the test set using $K = 1000$. We show example results of predicting $\boldsymbol{x}_l$ given $\boldsymbol{x}_u$ in Figure 3 of the Appendix.

As shown in Table 3, optimizing a stochastic binary network with the ARM estimator, which is unbiased and computationally efficient, achieves the lowest test negative log-likelihood, outperforming all previously proposed biased stochastic gradient estimators on similarly structured stochastic networks, including 1/2 [Gregor et al., 2013, Gu et al., 2016], straight through (ST) [Bengio et al., 2013], slope-annealed ST [Chung et al., 2016], and ST Gumbel-softmax [Jang et al., 2017], and unbiased ones, including score-function (SF) and MuProp [Gu et al., 2016].

5 Conclusions

To train a discrete latent variable model with one or multiple discrete stochastic layers, we propose the augment-REINFORCE-merge (ARM) estimator to provide unbiased and low-variance gradient estimates of the parameters of discrete distributions. With a single Monte Carlo sample, the estimated gradient is the multiplication between uniform/Dirichlet random noises and the difference of a function of two vectors of correlated binary/categorical latent variables. Without relying on learning control variates for variance reduction, it maintains efficient computation and avoids increasing the risk of overfitting. Applying the ARM gradient leads to state-of-the-art out-of-sample prediction performance on both auto-encoding variational and maximum likelihood inference for discrete stochastic feedforward neural networks.

Appendix

Proof of Theorem 5.

(i): Using the definition of $f_\Delta(u,\phi)$ in (5), when $\phi > 0$, we have

$$f_\Delta(u,\phi) = \begin{cases} 0 & \text{if } \sigma(-\phi) < u < \sigma(\phi) \\ f(1) - f(0) & \text{if } u > \sigma(\phi) \\ f(0) - f(1) & \text{if } u < \sigma(-\phi) \end{cases}$$

and when $\phi < 0$, we have

$$f_\Delta(u,\phi) = \begin{cases} 0 & \text{if } \sigma(\phi) < u < \sigma(-\phi) \\ f(1) - f(0) & \text{if } u > \sigma(-\phi) \\ f(0) - f(1) & \text{if } u < \sigma(\phi) \end{cases}$$

Algorithm 1: ARM gradient for V-dimensional M-way categorical latent vector

```
input  : Categorical distribution $\{q_{\phi_v}(z_v)\}_{v=1:V}$ with probability $\{\sigma(\phi_v)\}_{v=1:V}$, number of
         category $M$, target $f(z)$; $z = (z_1, \cdots, z_V)$, $\Phi = (\phi_1, \cdots, \phi_V)$
output : $\Phi$ and $\psi$ that maximize $\mathcal{E}(\Phi, \psi) = \mathbb{E}_{z \sim \prod_{v=1}^{V} q_{\phi_v}(z_v)}[f(z; \psi)]$
1  Initialize $\{\tilde{\phi}_v\}_{1,V}$, $\psi$ randomly;
2  while not converged do
3      Let $\phi_v = [\tilde{\phi}_v', 0]'$;
4      Sample $z_v \sim \text{Categorical}(\sigma(\phi_v))$ for $v = 1, \cdots, V$ ;
5      Sample $\pi_v \sim \text{Dirichlet}(\mathbf{1}_M)$ for $v = 1, \cdots, V$, stacking row-wisely as $\Pi = (\pi_1, \ldots, \pi_V)$ ;
6      $g_\psi = \nabla_\psi f(z; \psi)$ ;
7      $z_{(j)} = \arg\min_{\text{column-wise}} \Pi_{(j \rightleftharpoons M)} \odot e^{-\Phi}$;
8      $\bar{f} = \frac{1}{M} \sum_{j=1}^{M} f(z_{(j)})$;
9      for $m = 1$ to $M - 1$ do
10         $f_\Delta(\Pi, \phi, m) = f(z_{(m)}) - \bar{f}$ ;
11         for $v = 1$ to $V$ do
12             $(g_{\tilde{\phi}})_{mv} = f_\Delta(\Pi, \phi, m)(1 - M\Pi_{Mv})$
13         end
14     end
15     $(\tilde{\phi}_v)_{v=1:V} = (\tilde{\phi}_v)_{v=1:V} + \rho_t g_{\tilde{\phi}}$,    $\psi = \psi + \eta_t g_\psi$    with step-size $\rho_t$, $\eta_t$
16 end
17 *Here we define $\Pi_{(m \rightleftharpoons M)}$ as a matrix constructed by swapping the $m$th and $M$th rows of $\Pi$,
   $\odot$ as hardmard (element-wise) product, and $\arg\min_{\text{column-wise}}(\mathbf{X})$ as an operation that finds
   the argument of the minimum of each column of $\mathbf{X}$.
```

These two cases can be summarized as

$$f_\Delta(u, \phi) = \begin{cases} 0 & \text{if } \sigma(-|\phi|) < u < \sigma(|\phi|) \\ f(1) - f(0) & \text{if } u > \sigma(|\phi|) \\ f(0) - f(1) & \text{if } u < \sigma(-|\phi|) \end{cases} \tag{38}$$

(ii): With Eq.(38), we have

$$\begin{aligned} &\mathbb{E}_{u \sim \text{Uniform}(0,1)}[g_A(u, \phi)] = \mathbb{E}_{u \sim \text{Uniform}(0,1)}[f_\Delta(u, \phi)(u - 1/2)] \\ =& \int_{\sigma(|\phi|)}^{1} (f(1) - f(0))(u - 1/2)du + \int_{0}^{\sigma(-|\phi|)} (f(0) - f(1))(u - 1/2)du \\ =& \left[\sigma(|\phi|)(1 - \sigma(|\phi|))/2 + \sigma(-|\phi|)(1 - \sigma(-|\phi|))/2\right][f(1) - f(0)] \\ =& \sigma(|\phi|)(1 - \sigma(|\phi|))[f(1) - f(0)] \\ =& \sigma(\phi)(1 - \sigma(\phi))[f(1) - f(0)]. \end{aligned}$$

Algorithm 2: ARM gradient for V-dimensional binary latent vector

```
input  : Bernoulli distribution $\{q_{\phi_v}(z_v)\}_{v=1:V}$ with probability $\{\sigma(\phi_v)\}_{v=1:V}$, target $f(\boldsymbol{z})$;
         $\boldsymbol{z} = (z_1, \cdots, z_V)$, $\boldsymbol{\phi} = (\phi_1, \cdots, \phi_V)$
output : $\boldsymbol{\phi}$ and $\boldsymbol{\psi}$ that maximize $\mathcal{E}(\boldsymbol{\phi}, \boldsymbol{\psi}) = \mathbb{E}_{\boldsymbol{z} \sim \prod_{v=1}^{V} q_{\phi_v}(z_v)}[f(\boldsymbol{z}; \boldsymbol{\psi})]$
1 Initialize $\boldsymbol{\phi}$, $\boldsymbol{\psi}$ randomly;
2 while not converged do
3     Sample $z_v \sim \text{Bernoulli}(\sigma(\phi_v))$ for $v = 1, \cdots, V$ ;
4     sample $u_v \sim \text{Uniform}(0,1)$ for $v = 1, \cdots, V$, $\boldsymbol{u} = (u_1, \cdots, u_V)$ ;
5     $g_{\boldsymbol{\psi}} = \nabla_{\boldsymbol{\psi}} f(\boldsymbol{z}; \boldsymbol{\psi})$ ;
6     $f_\Delta(\boldsymbol{u}, \boldsymbol{\phi}) = f\big(\mathbf{1}[\boldsymbol{u} > \sigma(-\boldsymbol{\phi})]\big) - f\big(\mathbf{1}[\boldsymbol{u} < \sigma(\boldsymbol{\phi})]\big)$ ;
7     $g_{\boldsymbol{\phi}} = f_\Delta(\boldsymbol{u}, \boldsymbol{\phi})(\boldsymbol{u} - \frac{1}{2})$
8     $\boldsymbol{\phi} = \boldsymbol{\phi} + \rho_t g_{\boldsymbol{\phi}}$,   $\boldsymbol{\psi} = \boldsymbol{\psi} + \eta_t g_{\boldsymbol{\psi}}$      with step-size $\rho_t$, $\eta_t$
9 end
```

Since $\frac{d\sigma(\phi)}{d\phi} = \sigma(\phi)(1 - \sigma(\phi))$, the expectation for the REINFORCE gradient is

$$\begin{aligned}
&\mathbb{E}_{z \sim \text{Bernoulli}(\sigma(\phi))}[g_R(z, \phi)] = \mathbb{E}_{z \sim \text{Bernoulli}(\sigma(\phi))}[f(z) \nabla_\phi \log(\sigma(\phi)^z (1 - \sigma(\phi))^{1-z})] \\
=&\mathbb{E}_{z \sim \text{Bernoulli}(\sigma(\phi))}[f(z)(z(1 - \sigma(\phi)) - \sigma(\phi)(1 - z))] \\
=&\sigma(\phi)(1 - \sigma(\phi))[f(1) - f(0)].
\end{aligned}$$

Thus $\mathbb{E}[g_A] = \mathbb{E}[g_R]$ and $g_A(u, \phi)$ is an unbiased estimator for the true gradient.

(iii): The second moment of $g_A(u, \phi)$ can be expressed as

$$\begin{aligned}
&\mathbb{E}_{u \sim \text{Uniform}(0,1)}[g_A^2(u, \phi)] = \mathbb{E}_{u \sim \text{Uniform}(0,1)}[f_\Delta^2(u, \phi)(u - 1/2)^2] \\
=&\int_{\sigma(|\phi|)}^{1} [f(1) - f(0)]^2 (u - 1/2)^2 du + \int_{0}^{\sigma(-|\phi|)} [f(0) - f(1)]^2 (u - 1/2)^2 du \\
=&\frac{1}{12}[1 - (\sigma(|\phi|) - \sigma(-|\phi|))^3][f(1) - f(0)]^2
\end{aligned}$$

Denoting $t = \sigma(|\phi|) - \sigma(-|\phi|) = P(f_\Delta = 0)$, we can re-express (39) as $\mathbb{E}_{u \sim \text{Uniform}(0,1)}[g_A(u, \phi)] = \frac{1}{4}(1 - t^2)[f(1) - f(0)]$. Thus, the variance of $g_A(u, \phi)$ can be expressed as

$$\begin{aligned}
\text{Var}[g_A(u, \phi)] =& \frac{1}{4}\left[\frac{1}{3}(1 - t^3) - \frac{1}{4}(1 - t^2)^2\right][f(1) - f(0)]^2 \\
=& \frac{1}{16}(1 - t)(t^3 + \frac{7}{3}t^2 + \frac{1}{3}t + \frac{1}{3})[f(1) - f(0)]^2 \\
\leq& 0.039788[f(1) - f(0)]^2 \\
\leq& \frac{1}{25}[f(1) - f(0)]^2,
\end{aligned}$$

where $\text{Var}(g_A)$ reaches its maximum at $0.039788[f(1) - f(0)]^2$ when $t = \frac{\sqrt{5}-1}{2}$, which means $\frac{P(f_\Delta = 0)}{P(f_\Delta \neq 0)} = \frac{\sqrt{5}+1}{2}$.

(iv): For the REINFORCE gradient, we have

$$\begin{aligned}\mathbb{E}_{z\sim\text{Bernoulli}(\sigma(\phi))}[g_R^2(z,\phi)] =&\mathbb{E}_{z\sim\text{Bernoulli}(\sigma(\phi))}\left[f^2(z)(z(1-\sigma(\phi))-\sigma(\phi)(1-z))^2\right]\\ =&f^2(1)(1-\sigma(\phi))^2\sigma(\phi)+f^2(0)(-\sigma(\phi))^2(1-\sigma(\phi))\\ =&\sigma(\phi)(1-\sigma(\phi))[(1-\sigma(\phi))f^2(1)+\sigma(\phi)f^2(0)].\end{aligned}$$

Therefore the variance can be expressed as

$$\begin{aligned}&\text{Var}[g_R(u,\phi)]\\ =&\sigma(\phi)(1-\sigma(\phi))\left[(1-\sigma(\phi))f^2(1)+\sigma(\phi)f^2(0)-\sigma(\phi)(1-\sigma(\phi))[f(1)-f(0)]^2\right]\\ =&\sigma(\phi)(1-\sigma(\phi))[(1-\sigma(\phi))f(1)+\sigma(\phi)f(0)]^2\end{aligned}$$

The largest variance satisfies

$$\sup_\phi \text{Var}[g_R(z,\phi)] \geq \text{Var}[g_R(z,0)] = \frac{1}{16}(f(1)+f(0))^2,$$

and hence when $f\geq 0$ a.s. or $f\leq 0$ a.s., we have

$$\sup_\phi \text{Var}[g_R(z,\phi)] \geq \text{Var}[g_R(z,0)] > \frac{1}{25}(f(1)-f(0))^2 \geq \sup_\phi \text{Var}[g_A(u,\phi)],$$

which means the ARM spike gradient has a variance that is bounded by $\frac{1}{25}(f(1)-f(0))^2$, and its worst-case variance is smaller than that of the REINFORCE gradient.

□

Proof of Theorem 6. First, to compute the gradient with respect to $\boldsymbol{w}_1$, since

$$\mathcal{E}(\boldsymbol{w}_{1:T}) = \mathbb{E}_{q(\boldsymbol{b}_1)}\mathbb{E}_{q(\boldsymbol{b}_{2:T}\,|\,\boldsymbol{b}_1)}[f(\boldsymbol{b}_{1:T})] \tag{39}$$

we have

$$\nabla_{\boldsymbol{w}_1}\mathcal{E}(\boldsymbol{w}_{1:T}) = \mathbb{E}_{\boldsymbol{u}_1\sim\text{Uniform}(0,1)}[f_\Delta(\boldsymbol{u}_1,\mathcal{T}_{\boldsymbol{w}_1}(\boldsymbol{x}))(\boldsymbol{u}_1-1/2)]\nabla_{\boldsymbol{w}_1}\mathcal{T}_{\boldsymbol{w}_1}(\boldsymbol{x}), \tag{40}$$

where

$$\begin{aligned}f_\Delta(\boldsymbol{u}_1,\mathcal{T}_{\boldsymbol{w}_1}(\boldsymbol{x})) =& \mathbb{E}_{\boldsymbol{b}_{2:T}\sim q(\boldsymbol{b}_{2:T}\,|\,\boldsymbol{b}_1),\ \boldsymbol{b}_1=\mathbf{1}[\boldsymbol{u}_1>\sigma(-\mathcal{T}_{\boldsymbol{w}_1}(\boldsymbol{x}))])}[f(\boldsymbol{b}_{1:T})]\\ &-\mathbb{E}_{\boldsymbol{b}_{2:T}\sim q(\boldsymbol{b}_{2:T}\,|\,\boldsymbol{b}_1),\ \boldsymbol{b}_1=\mathbf{1}[\boldsymbol{u}_1<\sigma(\mathcal{T}_{\boldsymbol{w}_1}(\boldsymbol{x}))])}[f(\boldsymbol{b}_{1:T})]\end{aligned} \tag{41}$$

Second, to compute the gradient with respect to $\boldsymbol{w}_t$, where $2\leq t\leq T-1$, since

$$\mathcal{E}(\boldsymbol{w}_{1:T}) = \mathbb{E}_{q(\boldsymbol{b}_{1:t-1})}\mathbb{E}_{q(\boldsymbol{b}_t\,|\,\boldsymbol{b}_{t-1})}\mathbb{E}_{q(\boldsymbol{b}_{t+1:T}\,|\,\boldsymbol{b}_t)}[f(\boldsymbol{b}_{1:T})] \tag{42}$$

we have

$$\nabla_{\boldsymbol{w}_t}\mathcal{E}(\boldsymbol{w}_{1:T}) = \mathbb{E}_{q(\boldsymbol{b}_{1:t-1})}\left[\mathbb{E}_{\boldsymbol{u}_t\sim\text{Uniform}(0,1)}[f_\Delta(\boldsymbol{u}_t,\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}),\boldsymbol{b}_{1:t-1})(\boldsymbol{u}_t-1/2)]\nabla_{\boldsymbol{w}_t}\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1})\right], \tag{43}$$

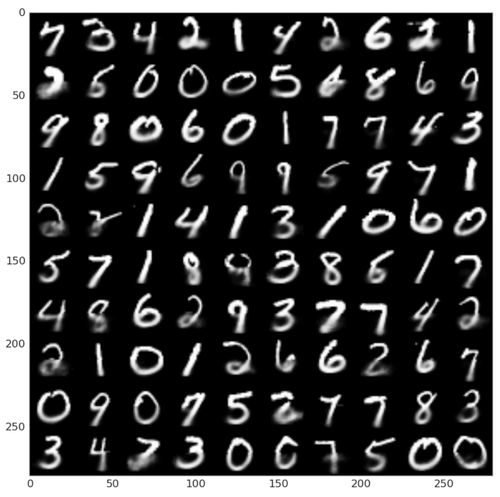


Figure 4: Randomly selected example results of predicting the lower half of a MNIST digit given its upper half, using a binary stochastic network, which has two binary stochastic hidden layers and is trained by ARM maximum likelihood inference.

Table 4: Comparison of the test negative ELBOs of various algorithms, using the same "Nonlinear" network structure.

	ARM	ST	1/2	Annealed ST	ST Gumbel-S.	SF	MuProp
VAE (Bernoulli)	**101.3**	116.0	110.9	111.5	111.5	112.2	109.7
VAE (Categorical)	**107.1**	110.9	128.8	107.8	107.8	110.6	107.8

where

$$f_\Delta(\boldsymbol{u}_t, \mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}), \boldsymbol{b}_{1:t-1}) = \mathbb{E}_{\boldsymbol{b}_{t+1:T}\sim q(\boldsymbol{b}_{t+1:T}\,|\,\boldsymbol{b}_t),\ \boldsymbol{b}_t = \mathbf{1}[\boldsymbol{u}_t > \sigma(-\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}))])}[f(\boldsymbol{b}_{1:T})] \\ - \mathbb{E}_{\boldsymbol{b}_{t+1:T}\sim q(\boldsymbol{b}_{t+1:T}\,|\,\boldsymbol{b}_t),\ \boldsymbol{b}_t = \mathbf{1}[\boldsymbol{u}_t < \sigma(\mathcal{T}_{\boldsymbol{w}_t}(\boldsymbol{b}_{t-1}))])}[f(\boldsymbol{b}_{1:T})] \quad (44)$$

Finally, to compute the gradient with respect to $\boldsymbol{w}_T$, we have

$$\nabla_{\boldsymbol{w}_T}\mathcal{E}(\boldsymbol{w}_{1:T}) = \mathbb{E}_{q(\boldsymbol{b}_{1:T-1})}\left[\mathbb{E}_{\boldsymbol{u}_T\sim\text{Uniform}(0,1)}[f_\Delta(\boldsymbol{u}_T, \mathcal{T}_{\boldsymbol{w}_T}(\boldsymbol{b}_{T-1}), \boldsymbol{b}_{1:T-1})(\boldsymbol{u}_T - 1/2)]\nabla_{\boldsymbol{w}_T}\mathcal{T}_{\boldsymbol{w}_T}(\boldsymbol{b}_{T-1})\right], \quad (45)$$

$$f_\Delta(\boldsymbol{u}_T, \mathcal{T}_{\boldsymbol{w}_T}(\boldsymbol{b}_{T-1}), \boldsymbol{b}_{1:T-1}) = f(\boldsymbol{b}_{1:T-1}, \boldsymbol{b}_T = \mathbf{1}[\boldsymbol{u}_T > \sigma(-\mathcal{T}_{\boldsymbol{w}_T}(\boldsymbol{b}_{T-1}))])) \\ - f(\boldsymbol{b}_{1:T-1}, \boldsymbol{b}_T = \mathbf{1}[\boldsymbol{u}_T < \sigma(\mathcal{T}_{\boldsymbol{w}_T}(\boldsymbol{b}_{T-1}))]) \quad (46)$$

□

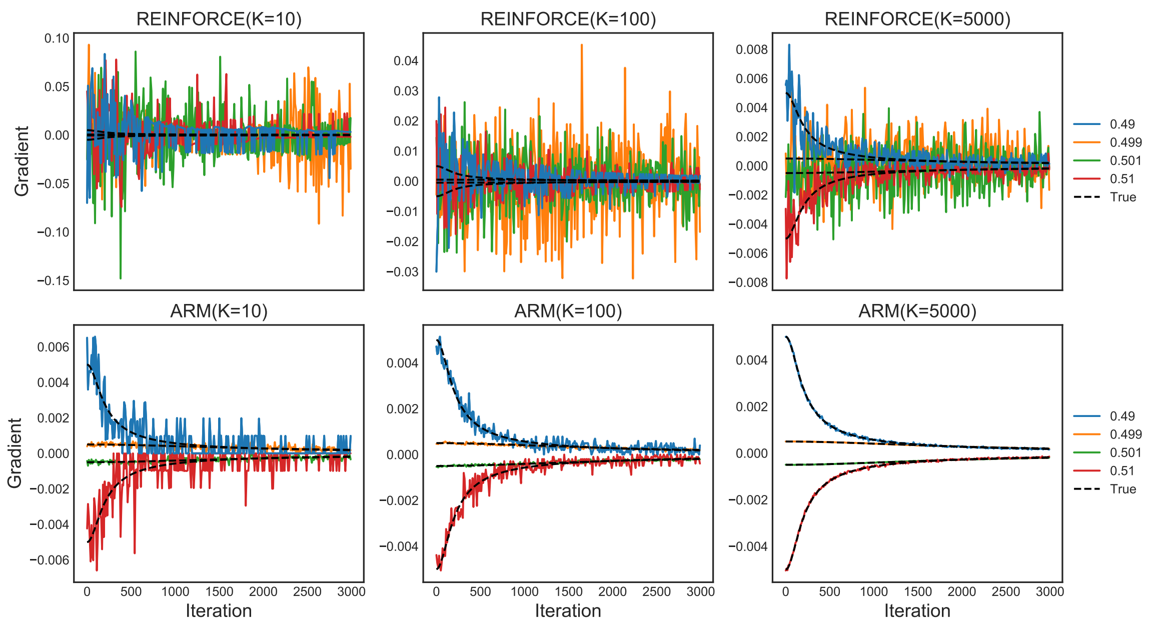
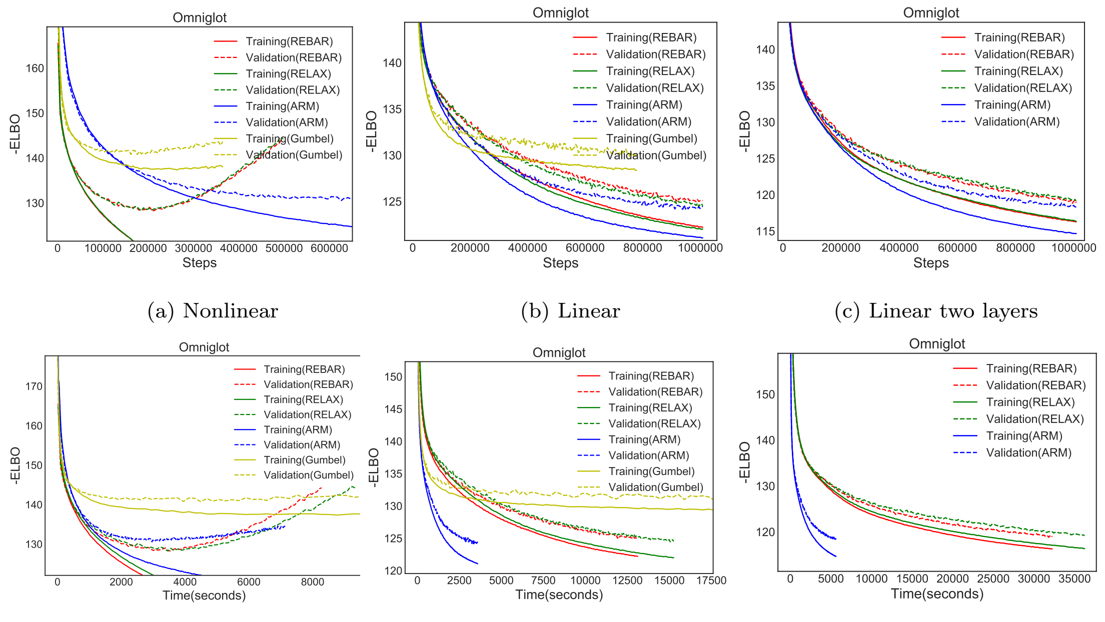


Figure 5: Estimation of the true gradient at each iteration using $K > 1$ Monte Carlo samples, using REINFORCE, shown in the top row, or ARM, shown in the bottom row. The ARM estimator exhibits significant lower variance given the same number of Monte Carlo samples.



(a) Nonlinear (b) Linear (c) Linear two layers

(d) Nonlinear (e) Linear (f) Linear two layers

Figure 6: Test negative ELBOs on OMNIGLOT with respect to training iterations, shown in the top row, and wall clock times on Tesla-K40 GPU, shown in the bottom row, for three differently structured Bernoulli VAEs.

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