Pathwise gradient variance reduction in variational inference via zero-variance control variates

Anonymous authors
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Abstract

Stochastic gradient descent is a workhorse in modern deep learning. The gradient of interest is almost always the gradient of an expectation, which is unavailable in closed form. The pathwise and score-function gradient estimators represent the most common approaches to estimating the gradient of an expectation. When it is applicable, the pathwise gradient estimator is often preferred over the score-function gradient estimator because it has substantially lower variance. Indeed, the latter is almost always applied with some variance reduction techniques. However, a series of works suggest, in the context of variational inference, that pathwise gradient estimators may also benefit from variance reduction. Work in this vein generally rely on approximations of the integrand which necessitates the functional form of the variational family be simple. In this work, we apply zero-variance control variates for variance reduction of pathwise gradient estimators which have the advantage that very little is required of the variational distribution, except that we can sample from it.

1 Introduction

Stochastic optimisation, in particular stochastic gradient descent, is ubiquitous in modern machine learning. In many applications, deployment of stochastic gradient descent necessitates estimating the gradient of an expectation,

$$g(\lambda) = \nabla_\lambda \mathbb{E}_{q(z;\lambda)}[r(z;\lambda)], \tag{1}$$

where r is some real-valued function and $\lambda \in \mathbb{R}^{\dim_\lambda}$ is the parameter over which we optimise. Note that since the expectation is taken with respect to a distribution q that is parameterised by λ, we cannot simply push the gradient operator through the expectation. The two most common approaches to estimating $g(\lambda)$ are the **pathwise gradient estimator** and the **score-function gradient estimator**. We will introduce them in the context of variational inference (VI).

Given an observed dataset x that is governed by a data generating process which depends on latent variables $z \in \mathbb{R}^{\dim_z}$ and a prior $p(z)$ of the latent variables, the posterior distribution is given by

$$p(z|x) \propto p(x|z)p(z),$$

which is only known up to a normalising constant. VI seeks to approximate the posterior with a simple, tractable distribution in the variational family $\mathcal{Q} = \{q(z;\lambda) : \lambda \in \mathbb{R}^{\dim_\lambda}\}$. This is often done by finding the λ that minimises the Kullback-Leibler divergence between the variational distribution q and the posterior (in that order):

$$\lambda^* = \arg\min_\lambda \mathbb{E}_{q(z;\lambda)}[\log q(z;\lambda) - \log p(z|x)]. \tag{2}$$

In practice, this is done by maximising the so-called evidence lower bound (ELBO),

$$\lambda^* = \arg\max_\lambda \mathrm{ELBO}(\lambda), \tag{3}$$

where

$$\mathrm{ELBO}(\lambda) = \mathbb{E}_{q(z;\lambda)}[\log p(z,x) - \log q(z;\lambda)].$$

It is easy to see that minimising the KL divergence in (2) is equivalent to maximising the ELBO in (3). Notably, computation of the latter avoids the intractable normalising constant in the posterior $p(z|x)$.

The closed-form solution for λ^* is generally unavailable. Stochastic variational inference (Hoffman et al., 2013), which optimises with minibatch stochastic gradient descent, became a game changer and opened up new applications for VI. Stochastic VI requires gradient computation of the *minibatch ELBO*,

$$\text{mELBO}(\lambda) = \mathbb{E}_{q(z;\lambda)}\left[r(z;\lambda)\right],$$

where

$$r(z;\lambda) = \frac{N}{B}\sum_{i\in\text{batch}}\left[\log p(x_i|z)\right] + \log\frac{p(z)}{q(z;\lambda)}. \tag{4}$$

Here N and B are data and batch size respectively, and x_i denotes the i^{th} element of the dataset.

2 Gradient estimators for variational inference

There are two main types of gradient estimators in the variational inference literature for computing the gradient of mELBO: 1) the pathwise gradient, also known as the reparametrization trick; and 2) the score-function estimator, also known as REINFORCE. The latter is more broadly applicable than the former but comes at the cost of larger variance. Indeed, the score-function estimator is almost always used in conjunction with control variates to reduce its variance (see, for example Ranganath et al., 2014; Ji et al., 2021). It is far less common to see variance reduction employed for the pathwise gradient estimator but a series of recent works suggest potential benefits from doing so (Miller et al., 2017; Geffner & Domke, 2020). In this work, we propose a new variance reduction technique for the pathwise gradient estimator in the context of variational inference. But first in this section we review the pathwise graident estmator.

The pathwise gradient estimator is only readily applicable for *reparametrizable* distributions $q(z;\lambda)$, i.e. distributions where z can be equivalently generated from $z = T(\epsilon;\lambda)$ where $\epsilon \in \mathbb{R}^{\dim_z} \sim q_0(\epsilon)$ and q_0 is referred as the *base distribution* which is independent from λ. Take $z \sim \mathcal{N}(\mu, \sigma^2 I)$ as an example, the corresponding transformation is $T(\epsilon;\lambda) = \mu + \sigma\epsilon$ where ϵ is standard Gaussian and $\lambda = (\mu, \sigma)$.

When q is reparametrizable, the gradient operator can be pushed inside the expectation and we get that the gradient of mELBO is given by

$$\begin{aligned} g(\lambda) &\coloneqq \nabla_\lambda \,\text{mELBO}(\lambda) \\ &= \mathbb{E}_{q_0(\epsilon)}\varphi(\epsilon;\lambda), \end{aligned} \tag{5}$$

where we define

$$\varphi(\epsilon;\lambda) = \nabla_\lambda\left[r(T(\epsilon;\lambda);\lambda)\right]. \tag{6}$$

The pathwise gradient estimator is then simply a Monte Carlo estimator of (5) using a set of samples $\{\epsilon_{[l]}\}_{l=1}^L$ from q_0:

$$\hat{g}(\epsilon_{[1]},\ldots,\epsilon_{[L]};\lambda) \coloneqq \frac{1}{L}\sum_{l=1}^{L}\varphi(\epsilon_{[l]};\lambda). \tag{7}$$

We will refer to L as the number of gradient samples.

The variance of the gradient estimator is thought to play an important factor in the convergence properties of stochastic gradient descent. Henceforth, any expectations or variances without a subscript refer to q_0. Define the variance of the pathwise gradient estimator to be

$$\mathbb{V}[\hat{g}] = \mathbb{E}\|\hat{g}\|^2 - \|\mathbb{E}\hat{g}\|^2 = \frac{1}{L}(\mathbb{E}\|\varphi\|^2 - \|\mathbb{E}\varphi\|^2) = \frac{1}{L}\mathbb{V}[\varphi].$$

To reduce the variance of (7), we may add a *control variate* (CV) to the pathwise gradient estimator estimator

$$\frac{1}{L}\sum_{l=1}^{L}\left[\varphi(\epsilon_{[l]};\lambda) + c(\epsilon_{[l]})\right], \tag{8}$$

where the control variance $c(\cdot) \in \mathbb{R}^{\dim_\lambda}$ is a random variable with zero expectation, i.e. $\mathbb{E}[\varphi + c] = \mathbb{E}\varphi$. Let $\mathrm{Tr}(\mathbb{C}[\varphi, c])$ be the trace of the covariance matrix $\mathbb{C}[\varphi, c] = \mathbb{E}[(\varphi - \mathbb{E}\varphi)(c - \mathbb{E}c)^\top]$. A good control variate c has a strong, negative correlation with φ, since

$$\begin{aligned} \mathbb{V}[\tfrac{1}{L}\textstyle\sum_{l=1}^{L} \varphi(\epsilon_{[l]}; \lambda) + c(\epsilon_{[l]})] &= \tfrac{1}{L}\mathbb{V}[\varphi + c] \\ &= \tfrac{1}{L}(\mathbb{V}[\varphi] + \mathbb{V}[c] + 2\,\mathrm{Tr}(\mathbb{C}[\varphi, c])) \\ &= \mathbb{V}[\hat{g}] + \tfrac{1}{L}(\mathbb{V}[c] + 2\,\mathrm{Tr}(\mathbb{C}[\varphi, c])) \end{aligned} \tag{9}$$

Therefore, as long as $\mathrm{Tr}(\mathbb{C}[\varphi, c]) < 0$ and $|\,\mathrm{Tr}(\mathbb{C}[\varphi, c])| < \frac{1}{2}\mathbb{V}[c]$, the control variate adjusted estimator (8) will have a smaller variance than (7).

Finally, a control variate may also be formed as a linear combinations of control variates. Let $C : \mathbb{R}^{\dim_z} \to \mathbb{R}^{\dim_\lambda \times J}$ be a matrix with J control variates in the columns. This leads to the control-variate adjusted estimator

$$\hat{h}(\epsilon_{[1]}, \ldots, \epsilon_{[L]}; \lambda) \coloneqq \frac{1}{L}\sum_{l=1}^{L} \left[\varphi(\epsilon_{[l]}; \lambda) + C(\epsilon_{[l]})\beta\right], \tag{10}$$

which remains a valid control variate due to the linearity of expectation operators, i.e. $\mathbb{E}[C\beta] = 0$. Here $\beta \in \mathbb{R}^J$ is a vector of coefficients corresponding to each control variates. This construction allows us to combine multiple weak control variates into a strong one by adjusting β.

For obvious reasons, applying control variates is only worthwhile if the computation of control variates is cheaper than increasing the number of samples in (7). From (9), we can see that, for example, the estimator variance can be reduced by half either by doubling L or halving $\mathbb{V}[\varphi + c]$. This presents a unique challenge when applying control variates in the low L regime (such as the gradient estimator of VI where L is often very low), since the cost of applying control variates will more likely outweigh the cost of increasing L to achieve the same variance reduction. The control variates that were developed in the Markov Chain Monte Carlo (MCMC) community cannot be easily applied in our work because 1) they require large L but in stochastic VI L can be as small as one, and 2) MCMC variance reduction is usually done at the very end while in stochastic VI we need it per gradient update.

In our work, we are motivated by the gap in the VI literature on gradient variance reduction when q is reparametrizable but the mean and covariance of q are not available in closed form. A good example is when q is the result of pushing forward some base distribution through a normalizing flow. In Section 3, we provide a review of the latest advancements in variance reduction techniques for pathwise gradient estimators in the context of VI. This is followed by discussions on methods, including a novel method based on zero-variance control variates, for selecting β and C of (10) in Sections 4 and 5, respectively. Finally, we present the experimental results in Section 6.

3 Related work

Variance reduction for the pathwise gradient estimator in variational inference has been explored in Miller et al. (2017) and Geffner & Domke (2020). These works focused on designing a single control variate (i.e. C only has a column) with the form of $C = \mathbb{E}\tilde{\varphi} - \tilde{\varphi}$, where $\tilde{\varphi}(\epsilon; \lambda)$ is an approximation of $\varphi(\epsilon; \lambda)$. The expectation $\mathbb{E}\tilde{\varphi}$ is designed to be theoretically tractable, but this usually implies that there is some restriction imposed on T (and therefore q) to make this expectation easy to compute.

Miller et al. (2017) proposed $\tilde{\varphi}$ that is based on the first-order Taylor expansion of $\nabla_z \log p(z, x)$. However, this Taylor expansion requires the expensive computation of the Hessian $\nabla_z^2 \log p(z, x)$. Geffner & Domke (2020) improved upon their work and proposed using a quadratic function to approximate $\log p(z, x)$. Their method only requires the first-order gradient $\nabla_z \log p(z, x)$, and their $\mathbb{E}\tilde{\varphi}$ is available in closed-form as a function of the mean and covariance of q. A direct modification of their method is to estimate $\mathbb{E}\tilde{\varphi}$ empirically when the mean and covariance of q are unavailable; see Section 5.1 for more details. Both Miller et al. (2017) and Geffner & Domke (2020) only considered Gaussian q in their work, although the latter can be applied to a larger class of variational families where the mean and covariance of the variational distribution is known.

Our work is similar in spirit to another work from the same group in Geffner & Domke (2020). Like Geffner & Domke (2018), we propose combining weak control variates into a stronger one, but our work differs in the construction of the individual control variates and the optimisation criterion for β.

In our work, we are motivated by the gap in the literature of gradient variance reduction when q is reparametrizable but the mean and covariance are unknown. A good example of such a variational distribution q is normalizing flow, where z is the result of pushing forward a base distribution q_0 through a neural network parameterised by λ, $z = T(\epsilon; \lambda)$ where $\epsilon \sim q_0$.

4 Selecting β for the CV-adjusted pathwise gradient estimator

The utility of control variates depends on the choice of β and C. In this section, we will discuss various strategies to pick an appropriate β given a family of control covariates C.

4.1 A unique set of β for each dimension of λ

The formulation in (10) suggests that the same set of β is used across the dimensions of φ. This can be too restrictive for C that are weakly-correlated to φ. In such instance, having a unique set of β coefficients for each dimension of φ can be beneficial, as it allows the coefficients to be selected on a per-dimension basis. In fact, this can be easily done by turning C into a $\dim_\lambda \times (J\dim_\lambda)$-dimensional, block diagonal matrix

$$\begin{bmatrix} C_{1,:} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & C_{\dim_\lambda,:} \end{bmatrix},$$

where $C_{i,:}$ is the i^{th} row of the original C. In other words, we expand the number of control variates to $J\dim_\lambda$, and each control variate will only reduce the variance of a single dimension of φ.

4.2 Optimisation criteria for β

The β is usually chosen to minimise the variance of $\hat{h}$. In practice, this variance is usually replaced by an empirical approximation due to the lack of its closed-form expression. There are three approximations in the literature, the first of which is a direct approximation of the variance with samples $\{\epsilon_{[l]}\}_{l=1}^L$,

$$\mathbb{V}[\varphi + C\beta] \approx \tfrac{1}{L(L-1)} \textstyle\sum_{l>l'} \|\varphi(\epsilon_{[l]}) + C(\epsilon_{[l]})\beta - \varphi(\epsilon_{[l']}) - C(\epsilon_{[l']})\beta\|^2, \tag{11}$$

as seen in Belomestny et al. (2018). The second approximation is based on the definition of variance

$$\mathbb{V}[\varphi + C\beta] = \mathbb{E}\|\varphi - \mathbb{E}[\varphi + C\beta] + C\beta\|^2 \approx \min_{\alpha \in \mathbb{R}^{\dim_\lambda}} \tfrac{1}{L} \textstyle\sum_{l=1}^L \|\varphi(\epsilon_{[l]}) + \alpha + C(\epsilon_{[l]})\beta\|^2, \tag{12}$$

where $\alpha \in \mathbb{R}^{\dim_\lambda}$ is an intercept term in place of the unknown $\mathbb{E}[\varphi + C\beta]$. The second approximation in (12) is generally cheaper to compute than the first approximation in (11) as it only requires $O(L)$ operations rather than $O(L^2)$; see Si et al. (2022) for details.

Minimising (12) with respect to β is essentially a least squares problem with a well-known closed-formed solution

$$\begin{aligned} \begin{bmatrix} \alpha^* \\ \beta^* \end{bmatrix} &= \arg\min_{\alpha,\beta} \sum_{l=1}^L \left\| \varphi(\epsilon_{[l]}) + \begin{bmatrix} \mathbb{I}_{\dim_\lambda} & C(\epsilon_{[l]}) \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right\|^2 \\ &= -(\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{\varphi}, \end{aligned} \tag{13}$$

where $\mathbb{I}_{\dim_\lambda}$ is an identity matrix of size $\dim_\lambda$, and $\boldsymbol{\varphi}$ and the design matrix $\boldsymbol{X}$ are given by

$$\boldsymbol{\varphi} = \begin{bmatrix} \varphi(\epsilon_{[1]}) \\ \vdots \\ \varphi(\epsilon_{[L]}) \end{bmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} \mathbb{I}_{\dim_\lambda} & C(\epsilon_{[1]}) \\ \vdots & \vdots \\ \mathbb{I}_{\dim_\lambda} & C(\epsilon_{[L]}) \end{bmatrix}.$$

However, the matrix inversion in (13) can be problematic to compute, especially when $\boldsymbol{X}^T\boldsymbol{X}$ is rank-deficient. In such instance, we can include a penalty in (12) and solve for the penalised least squares solution (see, for example, South et al., 2022), or use an iterative optimisation algorithm to minimise (12), as suggested in Si et al. (2022).

Finally the third approach relies on the assumption that $\mathbb{E}[C\beta] = 0$ and is based on the observation that

$$\mathbb{V}[\varphi + C\beta] = \mathbb{E}\|\varphi + C\beta\|^2 - \|\mathbb{E}\varphi\|^2.$$

This suggests that the variance can be equivalently minimised by minimising simply the expected squared norm component, $\mathbb{E}\|\varphi + C\beta\|^2$. Geffner & Domke (2018) shows that the minimiser $\beta^* = \arg\min_\beta \mathbb{E}\|\varphi + C\beta\|^2$ is given by

$$\beta^* = -\mathbb{E}[C^\top C]^{-1}\mathbb{E}[C^\top \varphi], \tag{14}$$

and suggests replacing $\mathbb{E}[C^\top C]$ and $\mathbb{E}[C^\top \varphi]$ with their empirical estimates. This approach, however, requires inverting a costly inversion of size J matrix.

4.3 Potential bias in the gradient estimator

The unbiasedness of the CV-adjusted Monte Carlo estimator (10) relies on the assumption that the β are independent of C, since $\mathbb{E}[C(\epsilon)\beta(\epsilon)] \neq 0$ in general. This necessitates that β and C should be estimated with independent sets of ϵ samples. However, in practice, the β is estimated with the same set of ϵ in C to save computational time at the cost of introducing bias in the gradient estimates.

5 Control variates

Having reviewed methods to select β given a family of control variates C, we now turn our attention to constructing C. We will first propose a simple modification of Geffner & Domke (2020) that will enable it to work for variational distributions q with unknown mean and covariance. Subsequently, we will introduce zero-variance control variates, which can be constructed without the knowledge of q or T.

5.1 Quadratic approximation control variates

In this section we review the quadratic-approximation control variates proposed in Geffner & Domke (2020). An important distinction at the outset is their assumption that the entropy term in mELBO,

$$-\mathbb{E}_{q(z)} \log q(z;\lambda),$$

is *known*. As such the focus of Geffner & Domke (2020) is to reduce the variance of

$$\mathbb{E}\nabla_\lambda f(T(\epsilon;\lambda)),$$

where

$$f(z) = \frac{N}{B}\sum_{i\in\text{batch}} [\log p(x_i|z)] + \log p(z). \tag{15}$$

Geffner & Domke (2020) proposed control variates of the form

$$C(\epsilon) = \mathbb{E}[\nabla_\lambda \tilde{f}(T(\epsilon;\lambda))] - \nabla_\lambda \tilde{f}(T(\epsilon;\lambda)), \tag{16}$$

where

$$\tilde{f}(z;v) = b_v^\top (z - z_0) + \frac{1}{2}(z - z_0)^\top B_v (z - z_0)$$

is a quadratic approximation of (15). Here, $v = \{B_v, b_v\}$ are the parameters of the quadratic equation that are chosen to minimise the L^2 difference between $\nabla f(z)$ and $\nabla\tilde{f}(z)$. We will drop v in $\tilde{f}$ for the sake of brevity. The location parameter z_0 is set to $\mathbb{E}T(\epsilon;\lambda)$. This quadratic approximation of f can also be viewed as a linear approximation on ∇f.

Algorithm 1 Quadratic CV (with empirical estimates of $\mathbb{E}\tilde{f}$)

1.3

Require: Learning rates $\gamma^{(\lambda)}$, $\gamma^{(v)}$.
  Initialise λ, v and control variate weight $\beta = 0$.
  for $k = 0, 1, 2, \cdots$ **do**
    Sample $\epsilon_{[1]}, \dots \epsilon_{[L]} \sim q_0$ to compute $\varphi(\epsilon_{[l]}; \lambda_k)$
    Generate an independent set of 100 ϵ samples to estimate $z_0 = \mathbb{E}T(\epsilon; \lambda)$
    Generate an independent set of 100 ϵ samples to estimate $\mathbb{E}\nabla_\lambda \tilde{f}(T(\epsilon; \lambda); v_k)$
    Compute $h = \frac{1}{L}\sum_{l=1}^{L}\left[\varphi(\epsilon_{[l]}; \lambda_k) + C(\epsilon_{[l]})\beta\right]$ See (16)
    Take an ascent step $\lambda_{k+1} \leftarrow \lambda_k + \gamma^{(\lambda)} h$
    Estimate $\mathbb{E}[C^\top C]$ and $\mathbb{E}[C^\top \varphi]$ with $\epsilon_{[1]}, \dots \epsilon_{[L]}$, and update β with (14).
    Take a descent step $v_{k+1} \leftarrow v_k - \gamma^{(v)} \frac{1}{2L}\sum_{l=1}^{L} \nabla_v \|\nabla_z f(T(\epsilon_{[l]}; \lambda_k)) - \nabla_z \tilde{f}(T(\epsilon_{[l]}; \lambda_k); v_k)\|^2$
  end for

The first term in (16) has a closed-form expression that depends on the mean and covariance of $q(z; \lambda)$, making the expectation cheap to evaluate when they are readily available. However, this is not the case when $T(\epsilon; \lambda)$ is arbitrarily complex, e.g. normalizing flow. A direct workaround of this limitation is to replace $\mathbb{E}\nabla_\lambda \tilde{f}(T(\epsilon; \lambda))$ with its empirical estimate based on a sample of ϵ's. Note that $\tilde{f}$ requires $z_0 = \mathbb{E}T(\epsilon; \lambda)$, which we estimate using another independent set of ϵ's. See Algorithm 1 for a summary of the procedure.

As (15) is a part of the Monte Carlo estimator (10), it could be tempting to estimate $\mathbb{E}\nabla_\lambda \tilde{f}(T(\epsilon; \lambda))$ with an average of the $\nabla_\lambda \tilde{f}(T(\epsilon; \lambda))$ evaluations that have been computed in (10). This is to be avoided as it will result in the two terms in (16) cancelling each other out.

As (16) is designed to be strongly correlated with φ when $\tilde{f}$ is reasonably close to f, the choice of β becomes less significant. Geffner & Domke (2020) opted to minimise the expected squared norm with a scalar β (note that C is a column vector in this case), the solution of which is given in (14). In their work, the expectations $\mathbb{E}[C^\top \varphi]$ and $\mathbb{E}[C^T C]$ are replaced with their empirical estimates computed from C and φ in (10), instead of fresh evaluations. However, as discussed in Section 4.2, the resulting gradient estimate is biased due to the dependency of between β and C.

While this bias is not mentioned explicitly in Geffner & Domke (2020), we conjecture that they overcame the issue by estimating the expectations with C and φ computed from previous iterations, as specified in Algorithm 1. Therefore, their β is independent from C in the current iteration. This will avoid introducing bias to the gradient estimate at the cost of having sub-optimal β. They also claimed that their estimates of $\mathbb{E}[C^\top \varphi]$ and $\mathbb{E}[C^T C]$ (and by extension, β) do not differ much across iterations. Moreover, their β is largely acting as an auxiliary 'switch' of the control variate when $\tilde{f}$ is a poor approximation of f, rather than the primary mechanism to reduce the estimator variance, since the β will be almost 0 when $\tilde{f}$ is not approximating well (i.e. $\mathbb{C}[\varphi, C] \approx 0$). Their C only kicks in when it is sufficiently correlated to φ.

Lastly, let us return to the discussion of the entropy term at the beginning of this section. Our setup is more general than Geffner & Domke (2020) as we does not assume the entropy term $-\mathbb{E}_{q(z)} \log q(z; \lambda)$ to necessarily have a closed-form expression, i.e. our $r(z, \lambda)$ includes $-\log q(z; \lambda)$. Although it was claimed in Geffner & Domke (2020) that their quadratic approximation control variate can also be similarly designed for $r(z, \lambda)$ in (4) rather than $f(z, \lambda)$ in (15), we found the implementation difficult because the updating step of v requires the gradient $\nabla_z \log q(z; \lambda)$, and in turn $\frac{\partial \lambda}{\partial z}$, which is challenging to compute.

5.2 Zero-variance control variates

The control variates in Geffner & Domke (2020) require one to know the mean and covariance of $q(z; \lambda)$. To avoid this requirement, we propose the use of gradient-based control variates (Assaraf & Caffarel, 1999; Mira et al., 2013; Oates et al., 2017). These control variates are generated by applying a so-called Stein operator $\mathcal{L}$ to a class of user-specified functions $P(z)$. Typically the Stein operator uses $\nabla_z \log q(z)$, the gradients of

the log probability density function for the distribution over which the expectation is taken, but it does not require any other information about φ or T.

We will focus on the form of gradient-based control variates known as zero-variance control variates (ZVCV, Assaraf & Caffarel, 1999; Mira et al., 2013). ZVCV uses the second order Langevin Stein operator and a polynomial $P(z) = \sum_{j=1}^{J} \beta_j P_j(z)$, where $P_j(z)$ is the jth monomial in the polynomial and J is the number of monomials. The control variates are

$$\{\mathcal{L}P_j(z)\}_{j=1}^{J} = \{\Delta_z P_j(z) + \nabla_z P_j(z) \cdot \nabla_z \log q(z)\}_{j=1}^{J},$$

where Δ_z is the Laplacian operator and $q(z)$ is the probability density function for the distribution over which the expectation is taken. A sufficient condition for these control variates to have zero expectation is that the tails of q decay faster than polynomially (Appendix B of Oates et al., 2016), which is satisfied by Gaussian q for example.

In this paper, we only consider first-order polynomials so there are $J = \dim_z$ control variates of the form

$$\left\{ \frac{\partial}{\partial z_j} \log q(z) \right\}_{j=1}^{\dim_z}.$$

Here, z_j refers to the j^{th} dimension of z. For pathwise gradient estimators using a standard Gaussian as the base distribution, these control variates simplify further to

$$\left\{ \frac{\partial}{\partial \epsilon_j} \log q_0(\epsilon) \right\}_{j=1}^{\dim_z} = \{-\epsilon_j\}_{j=1}^{\dim_z}.$$

We are also using the same set of control variates across different dimensions of φ, but assigning each dimension with a unique set of β. That is, the matrix of control variates C is a block-diagonal matrix of size $\dim_\lambda \times \dim_\lambda \dim_z$

$$C(\epsilon) = \begin{bmatrix} -\epsilon^\top & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & -\epsilon^\top \end{bmatrix}. \tag{17}$$

This is in contrast to Geffner & Domke (2020) where the values in C is different across dimensions, but their β is shared. The simplicity of ZVCV comes with the drawback that it is often not as correlated as the integrand. This makes the choice of β crucial.

5.2.1 Exact least squares

As discussed in Section 4.2, the optimal β can be selected by optimising (12), the solution of which is given in (13). We can further exploit the block-diagonal structure of (17) and decompose (12) into a series of linear regression that corresponds to each dimension of λ. In other words, we can solve β for each dimension of λ individually

$$\begin{bmatrix} \alpha_i^* \\ \beta_i^* \end{bmatrix} = -(\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{\varphi}_i, \quad i = 1, \dots, \dim_\lambda, \tag{18}$$

where i denotes the dimension of λ which α_i^*, β_i^* and $\boldsymbol{\varphi}_i$ correspond to, e.g. $\boldsymbol{\varphi}_i = [\varphi_i(\epsilon_{[1]}), \dots, \varphi_i(\epsilon_{[L]})]^\top$ is a subset of $\boldsymbol{\varphi}$ in (13) that corresponds to the i^{th} dimension of λ, and

$$\boldsymbol{X} = \begin{bmatrix} 1 & -\epsilon_{[1]}^\top \\ \vdots & \vdots \\ 1 & -\epsilon_{[L]}^\top \end{bmatrix}.$$

Note that the inversion of $\boldsymbol{X}^\top \boldsymbol{X}$ only needs to be performed once and can be used across different φ_i, thereby scaling well to models with high-dimensional λ. The control variate for φ_i can then be computed as $\varphi_i(\epsilon) = -\epsilon^\top \beta_i^*$. We also propose using $\epsilon_{[1]}, \dots, \epsilon_{[L]}$ that have already been generated in (10) to compute β^*, as the resulting control variate tends to have a lower mean squared error.

Algorithm 2 ZVCV-GD

1.3

Require: Learning rates $\gamma^{(\lambda)}$, $\gamma^{(\alpha,\beta)}$.
  Initialise λ
  for $k = 0, 1, 2, \cdots$ **do**
    Sample $\epsilon_{[1]}, \dots \epsilon_{[L]} \sim q_0$
    Compute $\varphi(\epsilon_{[l]}; \lambda_k), \forall l = 1, \dots, L$ See (5)
    Initialise $\alpha_0 = -\frac{1}{L}\sum_{l=1}^{L} \varphi(\epsilon_{[l]}; \lambda_k)$ and β_0 at the zero vector
    for $m = 0, 1, 2, \cdots$ **do**
      Take a descent step $(\alpha_{m+1}, \beta_{m+1}) \leftarrow (\alpha_m, \beta_m) - \gamma^{(\alpha,\beta)} \frac{1}{L}\sum_{l=1}^{L} \nabla_{\alpha,\beta} \|\varphi(\epsilon_{[l]}; \lambda_k) + \alpha_m + C(\epsilon_{[l]})\beta_m\|^2$
    end for
    Set β^* as the final value of β from the previous inner loop
    Compute $h = \frac{1}{L}\sum_{l=1}^{L} \varphi(\epsilon_{[l]}; \lambda_k) + C(\epsilon_{[l]})\beta^*$ See (17)
    Take an ascent step $\lambda_{k+1} \leftarrow \lambda_k + \gamma^{(\lambda)} h$.
  end for

5.2.2 Least squares with gradient descent

There are several challenges we face in applying ZVCV. For example, $\boldsymbol{X}^T\boldsymbol{X}$ in (18) must be invertible. This is often not the case for models with large $\dim_z$, as we usually keep L low and thus the column space of $\boldsymbol{X}$ is rank-deficient. This can be solved by adding a penalty term in (12) (i.e. shrinking β towards 0), and empirical evidence suggests that is more effective than using a subset of these control variates to achieve better performance (Geffner & Domke, 2018; South et al., 2022). However, penalised least squares remains prohibitively expensive to solve as it still involves inverting a matrix of size $\dim_z$.

Instead, we propose mimicking penalised least squares by minimising (12) with respect to α and β with gradient descent. This is done by

1. Initialise α at $-\frac{1}{L}\sum_{l=1}^{L} \varphi(\epsilon_{[l]})$ and β at the zero vector. Set $\gamma^{(\alpha,\beta)}$ to a low value;
2. Take a descent step $(\alpha_{m+1}, \beta_{m+1}) \leftarrow (\alpha_m, \beta_m) - \gamma^{(\alpha,\beta)} \frac{1}{L}\sum_{l=1}^{L} \nabla_{\alpha,\beta} \|\varphi(\epsilon_{[l]}) + \alpha_m + C(\epsilon_{[l]})\beta_m\|^2$;
3. Repeat Step 2 for a few times.

See Algorithm 2 for a complete description. The combination of learning rate and number of iterations is analogous to the penalty in penalised least squares: a lower number of iterations and learning rate $\gamma^{(\alpha,\beta)}$ will result in a near-zero β that results from a stronger penalty (more shrinkage of β towards 0). This procedure is also similar in spirit to Si et al. (2022).

6 Experiments

In these experiments, we assess the efficacy of various control variate strategies. We perform variational inference on the following model-dataset pairs: logistic regression on the *a1a* dataset, a hierarchical Poisson model on the *frisk* dataset, and Bayesian neural network (BNN) on the *redwine* dataset. For the BNN model, we consider a full-batch gradient estimator trained on a subset of 100 data points of the *redwine* dataset following the experimental setup in Geffner & Domke (2020) and Miller et al. (2017). We also consider a mini-batch estimator of size 32 but trained on the full *redwine* dataset, see Appendix A for more details. With the exception of mini-batch BNN, these models appeared in either Geffner & Domke (2020) or Miller et al. (2017).

Three classes of variational families are considered:

- **Mean-field Gaussian** The covariance of the Gaussian distribution $\mathcal{N}(\mu, \Sigma)$ is parameterised by log-scale parameters, i.e. $\Sigma = \operatorname{diag}(\exp(2\log\sigma_1, \dots, 2\log\sigma_{\dim_z}))$. The mean and log-scale parameters are initialised with a zero-mean Gaussian with a 0.5 scale;

- **Rank-5 Gaussian** The covariance of the Gaussian distribution $\mathcal{N}(\mu, \Sigma)$ is parameterised by a factor $F \in \mathbb{R}^{\dim_z \times 5}$ and diagonal components, i.e. $\Sigma = FF^\top + \operatorname{diag}(\exp(2\log\sigma_1, \ldots, 2\log\sigma_{\dim_z}))$. The mean, log-scale and F parameters are initialised with a zero-mean Gaussian with a 0.5 scale;
- **Real NVP** We use a real NVP normalizing flow (Dinh et al., 2017) with two coupling layers and compose the layers in alternate pattern. The flow has a standard multivariate Gaussian as its base distribution. The scale and translation networks have the same architecture of $8 \times 16 \times 16$ hidden units with ReLU activations, followed by a fully connected layer. There is an additional tanh activation at the tail of the scale network to prevent the exponential term from blowing up. The weights and biases of the networks are initialised with Glorot Gaussian (Glorot & Bengio, 2010) and standard Gaussian initialisers respectively.

We only present the results for mean-field Gaussian and real NVP in the main section. The results for rank-5 Gaussian are included in Appendix C, as they are largely similar to those obtained for mean-field Gaussian.

We use an Adam optimiser and set its learning rate $\gamma^{(\lambda)} = 0.01$ to maximise mELBO. The gradient estimator is equipped with the following control variate strategies:

- **No CV** No control variates, i.e. the vanilla gradient estimator.
- **ZVCV-GD** A ZVCV with β minimising least squares with an inner gradient descent, as described in Algorithm 2 and Section 5.2.2. We set the learning rate $\gamma^{(\alpha,\beta)} = 0.001$ and iterated the inner gradient descent 4 times for each outer Adam step.
- **Quadratic CV** This is the original algorithm presented in Geffner & Domke (2020) when q is Gaussian (i.e. the mean and covariance of q are readily available). When q is real NVP, we use Algorithm 1 and 100 samples to estimate $\mathbb{E}T(\epsilon;\lambda)$ and $\mathbb{E}\nabla_\lambda \tilde{f}(T(\epsilon;\lambda))$.

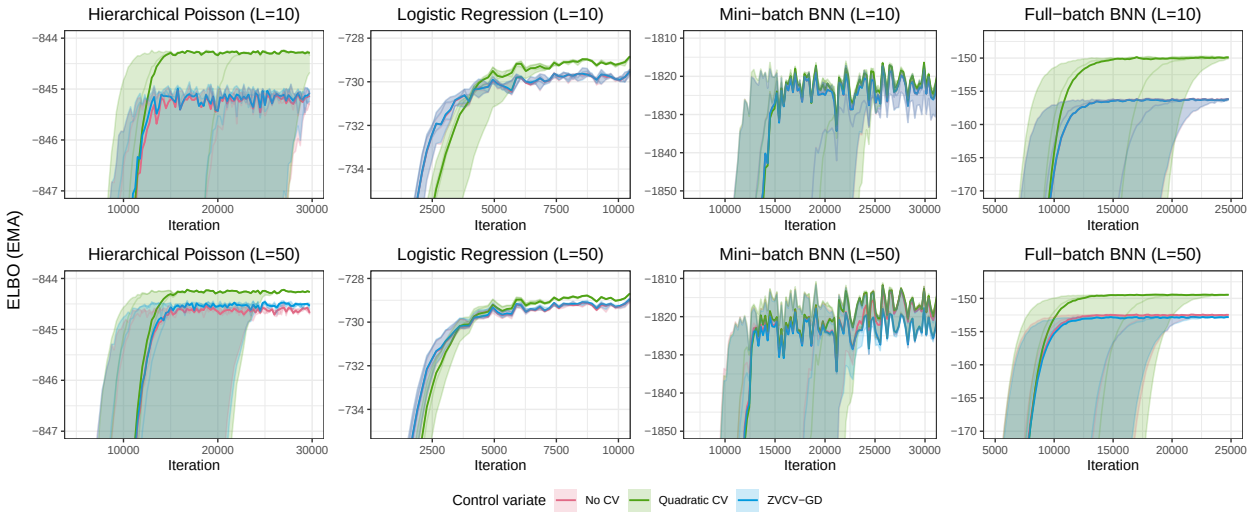
Note that above we only compare our method in detail with Geffner & Domke (2020) as it is a direct improvement of Miller et al. (2017).

For evaluation, the experiment is repeated 5 times with different initial values of the variational parameter λ to assess the robustness of the optimisers under different initialisation. We report the ELBO and variance of the gradient estimators. The ELBO for evaluation purpose is always computed with the full dataset (even when using mini-batched ELBO for optimisation) and 500 samples from q. The variance of the gradient estimators is computed by repeatedly sampling 100 gradients (say, $\hat{g}_{[1]}, \ldots, \hat{g}_{[100]}$) from the estimator and computed with $\mathbb{V}[\hat{g}] \approx \frac{1}{100}\sum_j \|\hat{g}_{[j]} - (\frac{1}{100}\sum_i \hat{g}_{[i]})\|^2$. Our code is implemented in JAX 0.4.6 (jaxlib 0.4.6, CUDA 11.8, CuDNN 8.8) and ran on Nvidia A100 80GB.

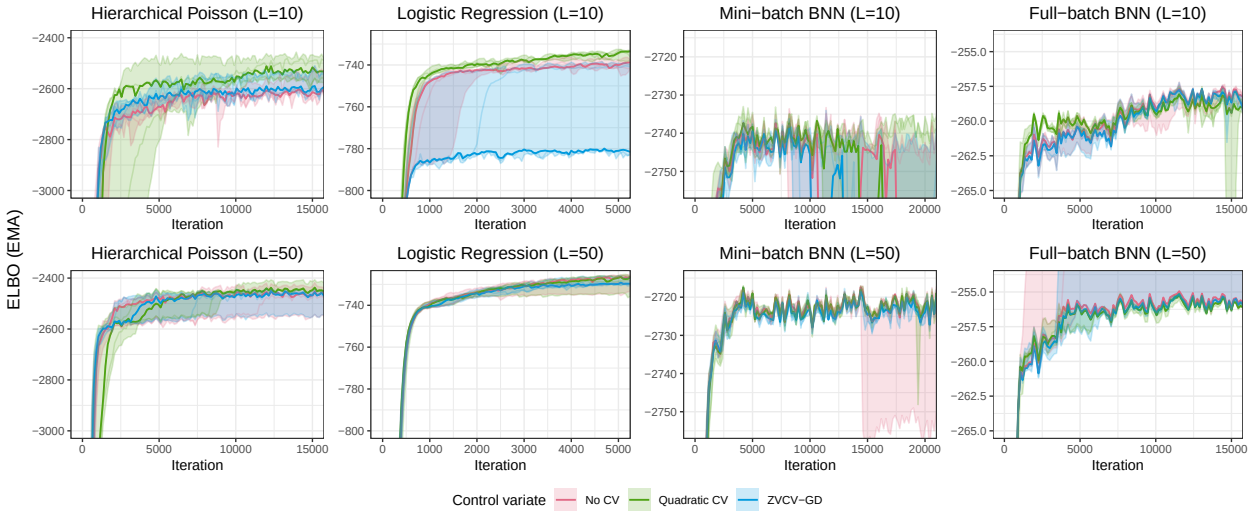
6.1 ELBO against iteration counts

The results in Figure 1 demonstrate that gradient estimators with quadratic CV generally outperform the vanilla estimator, while ZVCV-GD provides only marginal improvement and can even converge to a suboptimal maximum in some cases (e.g. logistic regression, real NVP 2, and $L = 10$). The performance gap between the estimators also decreases as the number of gradient samples L increases, as seen in the bottom rows of Figure 1a and 1b. It should be noted that quadratic CVs may perform poorly in the early stages of gradient descent (e.g. logistic regression on mean-field Gaussian and hierarchical Poisson on real NVP) as it takes time to learn the quadratic function $\tilde{f}$.

The variance of the gradient estimators can help explain the performance gap observed in Figure 1. We compute the variance ratio $\mathbb{V}[\hat{h}]/\mathbb{V}[\hat{g}]$ ($\hat{g}$ and $\hat{h}$ as defined in (7) and (10) respectively) in every 50 iterations and show them in Figure 2; a ratio less than 1 indicates a reduction in variance relative to the vanilla estimator. See Appendix B for more details on the calculation of the variance ratio. As shown in Figure 2, quadratic CV generally achieves a lower variance than ZVCV-GD, particularly for Gaussian q when $\mathbb{E}\tilde{f}$ can be computed exactly. The estimator with ZVCV-GD and larger L tends to perform better in models with fewer control variates (i.e. low $\dim_z$), as the β is less susceptible to overfitting when solving the least squares



(a) Mean-field Gaussian with 10 (top) and 50 (bottom) gradient samples.



(b) Real NVP with 10 (top) and 50 (bottom) gradient samples.

Figure 1: ELBO plotted against gradient descent steps for different number of gradient samples L and two families of variational distributions. Boldfaced lines are the median ELBO across 5 repetitions. Shaded area illustrates the range of ELBO across 5 repetitions. The ELBO values are smoothed with exponential moving average. Higher ELBO is better.

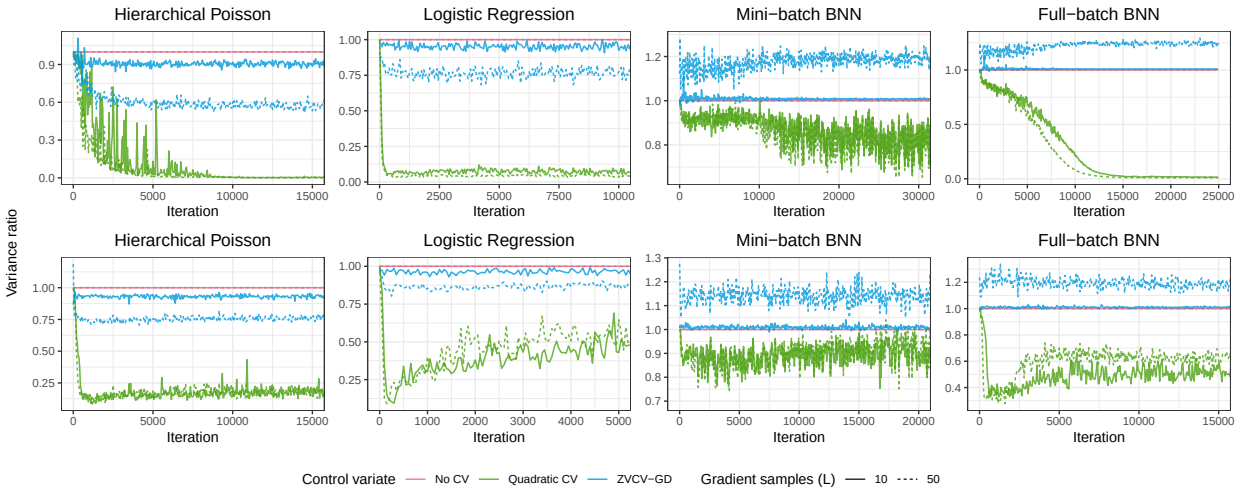


Figure 2: For $\hat{g}$, i.e. No CV, and $\hat{h}$ which is either ZVCV-GD or Quadratic CV, we plot the variance ratio $\mathbb{V}[\hat{h}]/\mathbb{V}[\hat{g}]$ at each iteration with mean-field Gaussian (top) and RealNVP (bottom) as variational distributions. Note the vanilla estimator (red) always has the ratio of 1. ZVCV-GD (blue) fails to reduce variance in BNN. There is a significant overlap in quadratic CV between $L = 10, 50$ (solid and dotted green respectively). Lower ratio is better.

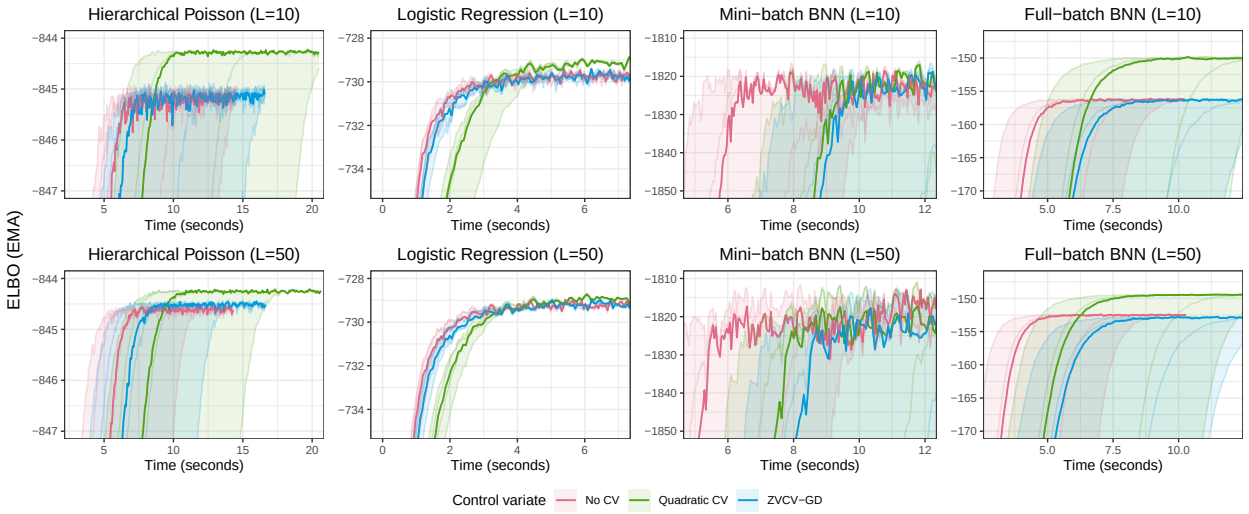
with the gradient descent algorithm discussed in Section 5.2.2. On the contrary, in models with large $\dim_z$, such as BNNs, ZVCV-GD fails to reduce variance.

6.2 ELBO against wall-clock time

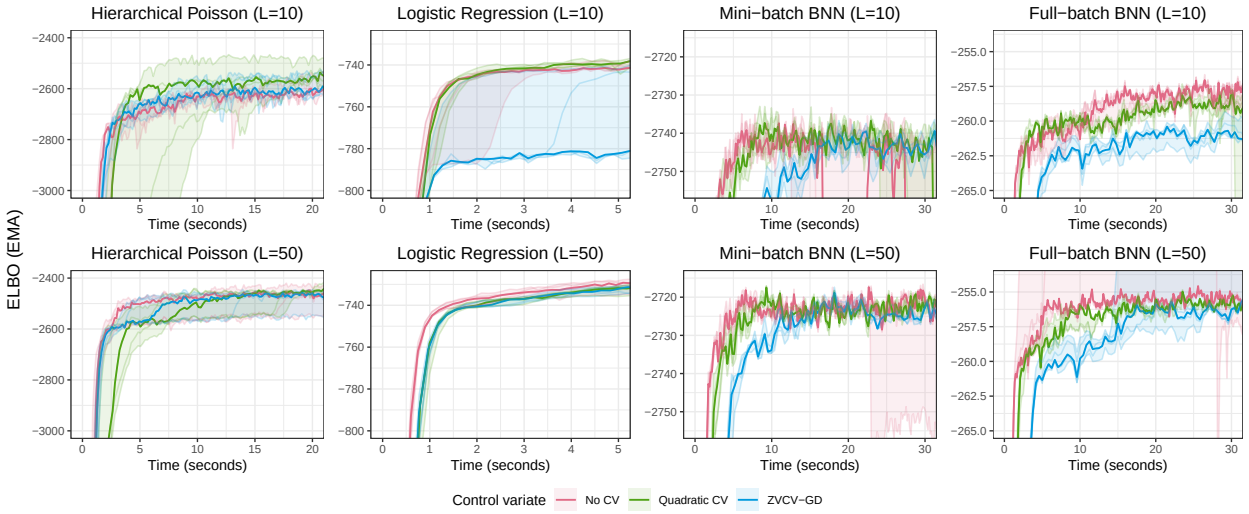
To evaluate whether the computational cost of computing control variates is justified by the potential improvement in ELBO, we measure the ELBO against wall-clock time in Figure 3. Our experiments show that vanilla estimators almost always converge earlier to a respectable maximum in our implementation of variational inference in JAX. Furthermore, the performance gap between the estimators is even narrower when $L = 50$. An unexpected finding is that increasing the number of gradient samples from 10 to 50 imposes almost no additional computational cost (as seen by comparing the top and bottom rows of Figure 3a and 3b). Therefore, increasing the number of gradient samples may be a better idea than implementing control variates, as the advantage of CVs decreases with increasing number of gradient samples. Additionally, the gain from using CV estimators is relatively small and not universal. For instance, the improvement of 0.5 nats in hierarchical Poisson and 3 nats in full-batch BNN achieved by Quadratic CV comes at a cost of approximately 50% more running time.

7 Conclusion

In our study of the pathwise gradient estimator in variational inference, we reviewed the existing state-of-the-art control variates for reducing gradient variance, namely the quadratic CV in Geffner & Domke (2020). We identified a gap in the literature of variance reduction of pathwise gradient estimators in stochastic VI resulting from the setting where the variational distribution has intractable mean and covariance, rendering the SOTA represented by Geffner & Domke (2020) not applicable directly. To address this gap, we proposed using ZVCV, which does not assume specific conditions on the variational distribution. However, our empirical results showed that neither the ZVCV-adjusted gradient estimator nor the quadratic CV-adjusted estimator provided substantial variance reduction that justifies their implementation. Instead, we found that increasing the number of gradient samples is a highly cost-effective method for reducing variance.



(a) Mean-field Gaussian as variational distributions.



(b) Real NVP as variational distributions.

Figure 3: ELBO plotted against wall-clock time for different number of gradient samples L and two families of variational distributions. Boldfaced lines are the median ELBO across 5 repetitions. Shaded area illustrates the range of ELBO across 5 repetitions. The ELBO values are smoothed with exponential moving average. Higher ELBO is better.

Taking a step back, it is worth discussing the fundamental value in performing variance reduction for pathwise gradient estimators in stochastic VI. For one, it is quite interesting that a dramatic reduction in gradient variance can fail to deliver any discernible effect on the ELBO. This is what was observed in the experiments section — even when the variance ratio was substantially lower than 1, the cv-adjusted gradient estimator, compared to the vanilla gradient, did not move the needle in a meaningful manner on the ELBO optimisation objective. As such, it can be expected that downstream metrics including predictive log likelihood or predictive MSE will also reveal the general futility of equipping the gradient estimator with a control variate. These findings seem to point to a negative phenomenon for pathwise gradients in stochastic VI — reducing the gradient variance is insufficient to improving downstream performance.

In future work, we hope to explore ZVCV-adjusted gradient estimators in generative models where it can truly shine. Namely, ZVCV is particularly powerful when the distribution of interest is difficult to sample from. One class of distribution models that fit this description are energy-based models (Song & Kingma, 2021).

Relatedly, there is a class of stochastic VI methods known as implicit VI. The variational distribution employed is still required to be reparametrizable but we drop the requirement that the so-called pathwise score, $\nabla_z \log q(z;\lambda)$, be known, e.g. as in normalizing flows. It was shown in Titsias & Ruiz (2019) that the pathwise score may itself be written as an expectation, $\nabla_z \log q(z;\lambda) = E_{q(\epsilon|z;\lambda)} \nabla_z \log q(z|\epsilon;\lambda)$ where $q(\epsilon|z;\lambda)$ is referred to as the reverse conditional. In Titsias & Ruiz (2019), the expectation with respect to the reverse conditional is based on MCMC samples. We could conceivably improve the efficiency by employing ZVCV here.

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A Models and datasets

Logistic regression with the *a1a* dataset We extracted the $a1a$ dataset from the repository hosting Geffner & Domke (2020). We used the full dataset $\{\boldsymbol{x}_i, y_i\}_{i=1}^{1605}$ and 90% of the dataset for training. The response y_i is binary and is modelled as

$$\begin{aligned} w_0, \boldsymbol{w} &\sim \mathcal{N}(0, 10^2) \\ p(y_i|\boldsymbol{x}_i, z) &= \text{Bernoulli}\left(\frac{1}{1+\exp(-w_0 - \boldsymbol{w}^T\boldsymbol{x}_i)}\right), \end{aligned}$$

where $z = \{w_0, \boldsymbol{w}\}$ and $\dim_z = 120$.

Hierarchical Poisson regression with the *frisk* dataset This example is coming from Gelman et al. (2007). We only used a subset of data (weapon-related crime, precincts with 10%-40% of black proportion), as in Miller et al. (2017) and Geffner & Domke (2020). The response y_{ep} denotes the number of frisk events due to weapons crimes within an ethnicity group e in precinct p over a 15-months period in New York City:

$$\begin{aligned} \mu &\sim \mathcal{N}(0, 10^2) \\ \log\sigma_\alpha, \log\sigma_\beta &\sim \mathcal{N}(0, 10^2) \\ \alpha_e &\sim \mathcal{N}(0, \sigma_\alpha^2) \\ \beta_p &\sim \mathcal{N}(0, \sigma_\beta^2) \\ \log\lambda_{ep} &= \mu + \alpha_e + \beta_p + \log N_{ep} \\ p(y_{ep}|z) &= \text{Poisson}(\lambda_{ep}), \end{aligned}$$

where $z = \{\alpha_1, \alpha_2, \beta_1, \ldots, \beta_{32}, \mu, \log\sigma_\alpha, \log\sigma_\beta\}$ and $\dim_z = 37$. N_{ep} is the (scaled) total number of arrests of ethnicity group e in precinct p over the same period of time.

Bayesian neural network with the *redwine* dataset We push a vector input $\boldsymbol{x}_i$ through a 50-unit hidden layer and ReLU activation's to predict wine quality. The response y_i is an integer from 1 to 10 (inclusive) measuring the score of red wine. We place an uniform improper prior on the log-variance of the weights and error (see Section 5.7 of Gelman et al., 2013, for a discussion on the prior choice):

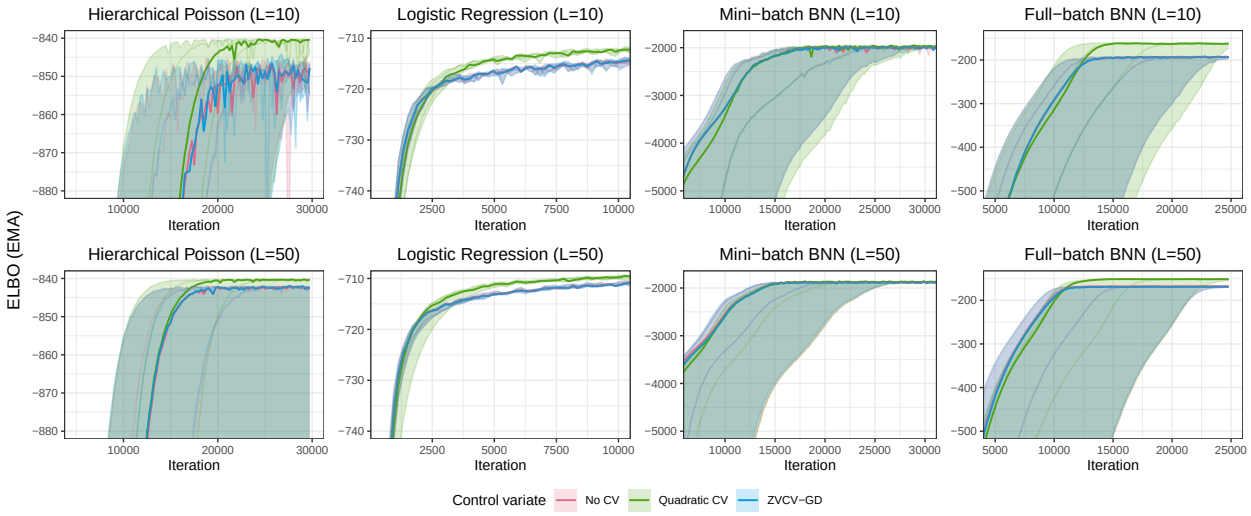
$$\begin{aligned} &p(\log\alpha^2) \propto 1, \quad \text{equivalent to } p(\alpha) \propto \alpha^{-1} \\ &p(\log\tau^2) \propto 1, \quad \text{equivalent to } p(\tau) \propto \tau^{-1} \\ &w_i \sim \mathcal{N}(0, \alpha^2), \quad i = 1, \ldots, 651 \\ &y_i|\boldsymbol{x}_i, \boldsymbol{w}, \tau \sim \mathcal{N}(\phi(\boldsymbol{x}, \boldsymbol{w}), \tau^2) \end{aligned}$$

where ϕ is a multi-layer perception. Here, $z = \{\log\alpha^2, \log\tau^2, \boldsymbol{w}\}$ and $\dim_z = 653$. For full-batch gradient descent, we use a subset of 100 data point as in Miller et al. (2017) and Geffner & Domke (2020). For mini-batch gradient descent, we use 90% of the full dataset for training (size of training set = 1431).

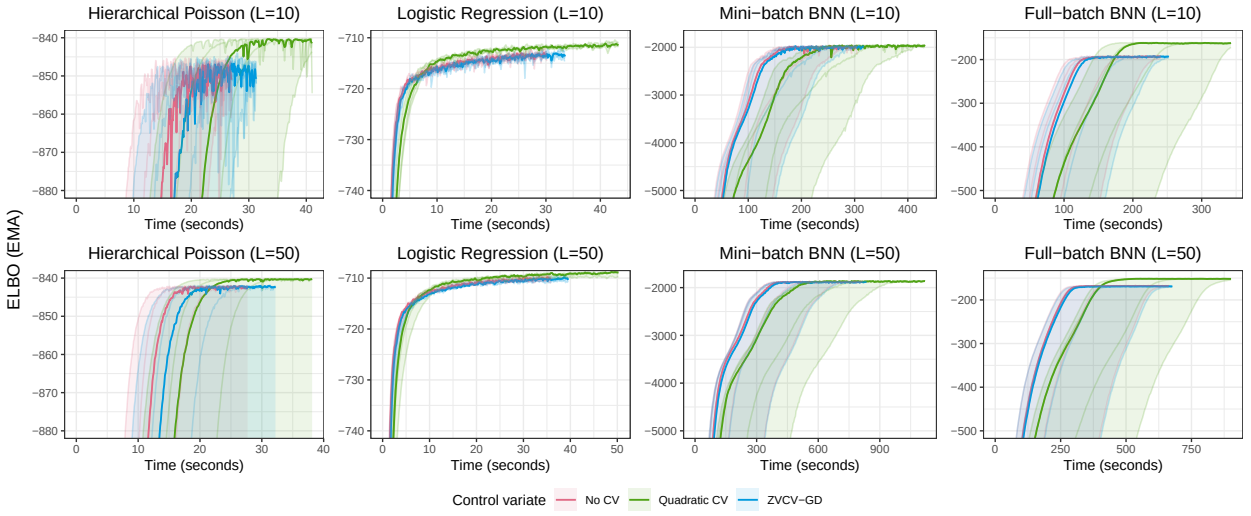
B Computation of variance ratio

The variance ratio $\mathbb{V}[\hat{h}]/\mathbb{V}[\hat{g}]$ was computed with the following step:

1. Collect 100 samples of $\hat{g}$ resulting in $\{\hat{g}_{[j]}\}_{j=1}^{100}$;
2. For each $\hat{g}_{[j]}$, compute its corresponding cv-adjusted gradient estimate $\hat{h}$ (10) to collect $\{\hat{h}_{[j]}\}_{j=1}^{100}$;
3. Estimate $\mathbb{V}[\hat{g}] \approx \frac{1}{100}\sum_j \|\hat{g}_{[j]} - (\frac{1}{100}\sum_i \hat{g}_{[i]})\|^2$. Repeat the same step for $\mathbb{V}[\hat{h}]$;
4. Calculate the ratio $\mathbb{V}[\hat{h}]/\mathbb{V}[\hat{g}]$.



(a) ELBO versus iteration counts.



(b) ELBO versus wall-clock time.

Figure 4: ELBO plotted against gradient descent steps and wall-clock time for different number of gradient samples L and rank-5 Gaussian. Boldfaced lines are the median ELBO across 5 repetitions. Shaded area illustrates the range of ELBO across 5 repetitions. The ELBO values are smoothed with exponential moving average. Higher ELBO is better.

(a) Variance ratio

Figure 5: For $\hat{g}$, i.e. No CV, and $\hat{h}$ which is either ZVCV-GD or Quadratic CV, we plot the variance ratio $\mathbb{V}[\hat{h}]/\mathbb{V}[\hat{g}]$ at each iteration with rank-5 Gaussian as variational distribution. Note the vanilla estimator (red) always has the ratio of 1. ZVCV-GD (blue) fails to reduce variance in both mini-batch and full-batch BNN. Lower ratio is better.

C Results from rank-5 Gaussian

The insight derived from Figure 4 and 5 below are similar to those obtained from Figure 1, 3 and 2. In most cases, the cost for evaluating control variates outweighs the improvement in ELBO achieved through variance reduction in the gradient estimator. We observe marginal gain in ELBO despite the estimators with control variates taking longer time to converge.