A Dual Control Variate for doubly stochastic optimization and black-box variational inference

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Abstract

In this paper, we aim at reducing the variance of doubly stochastic optimization, a type of stochastic optimization algorithm that contains two independent sources of randomness: The subsampling of training data and the Monte Carlo estimation of expectations. Such an optimization regime often has the issue of large gradient variance which would lead to a slow rate of convergence. Therefore we propose Dual Control Variate, a new type of control variate capable of reducing gradient variance from both sources jointly. The dual control variate is built upon approximation-based control variates and incremental gradient methods. We show that on doubly stochastic optimization problems, compared with past variance reduction approaches that take only one source of randomness into account, dual control variate leads to a gradient estimator of significantly smaller variance and demonstrates superior performance on real-world applications, like generalized linear models with dropout and black-box variational inference.

1 Introduction

Various machine learning problems can be formulated as optimizing an objective of the form

\[ f(w) = \mathbb{E}_n \mathbb{E}_\epsilon f(w; n, \epsilon). \] (1)

Here, \( n \) is a discrete random variable uniformly distributed on \( \{1, \ldots, N\} \), which typically represents an index in a dataset. Meanwhile, \( \epsilon \) is a continuous random variable drawn from some fixed distribution, independent of \( w \) and \( n \). Objectives like this emerge in black-box variational inference (Paisley et al., 2012; Ranganath et al., 2014; Titsias and Lázaro-Gredilla, 2014) with reparameterization gradient and variational autoencoders (Kingma and Welling, 2014; Rezende et al., 2014) (where \( \epsilon \) corresponds to a sample from the latent space) and models that apply data augmentation or dropout during training (Srivastava et al., 2014) (where \( \epsilon \) corresponds to the random perturbation of the data).

Such objectives are typically addressed with stochastic optimization. The most obvious gradient estimator is given by drawing a random \( n \) and a random \( \epsilon \) and evaluating

\[ g_{\text{naive}}(w; n, \epsilon) = \nabla f(w; n, \epsilon). \] (2)

This estimator is adequate for many situations, but sometimes displays high variance, which slows optimization (Nemirovski et al., 2009; Bottou et al., 2018), as is shown by the blue lines in Fig. 1. In particular, when \( N \) is large, performing data subsampling could introduce a significant amount of gradient noise. When the variance is large, the step-size must be made very small, slowing optimization. For black-box variational inference, several recent works have thus been devoted to reducing the variance of this reparameterization estimator (Miller et al., 2017; Buchholz et al., 2018; Roeder et al., 2017; Wu et al., 2019; Geffner and Domke, 2018, 2020; Boustati et al., 2020).

Many methods have been developed to reduce the variance of related objectives. Problems without subsampling correspond to an objective \( f(w) = \mathbb{E}_\epsilon f(w; \epsilon) \). Many works have proposed to use control variate to control the gradient variance (Sec. 2.1). Other problems that only have subsampling can be written as \( f(w) = \mathbb{E}_n f(w; n) \). This is the incremental gradient setting, for which many methods have been developed, e.g. SVRG (Johnson and Zhang, 2013) and SAGA (Defazio et al., 2014a) (Sec. 2.2).

Unfortunately, as we explain in Sec. 3, these methods only address variance coming from a single source of randomness, meaning there are limitations on what they can accomplish when applied to doubly-stochastic problems.

In this work we propose a novel dual control variate (Sec. 3.4) that reduces the two types of gradient variance at the same time. We show theoretically that this can produce gradient estimators with lower variance than is
We empirically evaluate the effectiveness of the dual control variate on two applications: Generalized linear models with Gaussian dropout (Sec. 5.1) and black box variational inference (Sec. 5.2). We show that the dual control variate yields a gradient estimator with an order of magnitude smaller than the naive estimator or an approximation-based control variate. It is also superior to a baseline control variate based on incremental gradient ideas. (This baseline is too expensive to be practical.) This improvement in variance enables the use of larger learning rates, and thus yields a corresponding order of magnitude increase in optimization speed.

2 Preliminaries

2.1 Approximation-based control variate

Assume we have an objective of the form $f(w) = \mathbb{E}_\epsilon f(w; \epsilon)$, where $\epsilon$ is a random variable drawn from a fixed distribution independent of $w$. Computing the exact gradient is often intractable. A naive gradient estimator would be $\nabla f(w; \epsilon)$. The variance of this can often be reduced by instead using

$$g(w; \epsilon) = \nabla f(w; \epsilon) + c(w; \epsilon),$$

where $c(w; \epsilon)$ is a control variate, i.e. a zero-mean random variable. Ideally $c(w; \epsilon) \approx \nabla f(w) - \nabla f(w; \epsilon)$, in which case the variance could be reduced nearly to zero. This technique is widely adopted in variational inference (Paisley et al., 2012; Tucker et al., 2017; Grathwohl et al., 2018; Boustati et al., 2020) as well as in general Monte Carlo estimation (Owen, 2013) and statistical inference.

A general way to construct control variates involves using an approximation function $\tilde{f}$ for which the expectation $\mathbb{E}_\eta f(w; \eta)$ is available in closed-form (Miller et al., 2017; Geffner and Domke, 2020). Then, the control variate is defined as $c(w; \epsilon) = \mathbb{E}_\eta \nabla \tilde{f}(w; \eta) - \nabla \tilde{f}(w; \epsilon)$, which can be easily seen to have a mean zero. Using this control variate, the estimator from Eq. (3) becomes

$$g(w; \epsilon) = \nabla f(w; \epsilon) + \mathbb{E}_\eta \nabla \tilde{f}(w; \eta) - \nabla \tilde{f}(w; \epsilon).$$

The better the approximation $\tilde{f} \approx f$, the more the first and the last terms in Eq. (4) tend to cancel, meaning the lower the final variance tends to be.

2.2 Incremental gradient methods

We now consider a stochastic optimization problem with only subsampling noise, whose objective is given by $f(w) = \mathbb{E}_n f(w; n)$, where $n$ is a random variable uniformly distributed on $\{1, \ldots, N\}$. While one could compute $f$ exactly, this may be costly when $N$ is large. The naive gradient estimator $\nabla f(w; n)$ where $n$ is randomly chosen. Incremental gradient methods (Roux et al., 2012; Shalev-Shwartz and Zhang, 2013; Johnson and Zhang, 2013; Defazio et al., 2014b; Gower et al., 2020) were developed to reduce the variance of this gradient estimator. While details vary by algorithm, the basic idea is to "recycle" previous evaluations. For example, SAGA (Defazio et al., 2014a) stores the gradients $\nabla f(w^m; n)$ where $w^m$ is $w$ at the most recent time $f(w; n)$ was evaluated. Then, a gradient step is taken as

$$w \leftarrow w - \lambda \left( \nabla f(w; n) + \mathbb{E} \nabla f(w^m; m) - \nabla f(w^m; n) \right),$$

where $\lambda$ is a step size. When $w^m \approx m$, the first and last terms in Eq. (5) will approximately cancel. The fi-
nal expectation over \( m \) is tracked as a running average of \( \nabla f(w^m; m) \), meaning the cost per iteration is independent of \( N \).

3 Doubly stochastic optimization

This section introduces our method, the dual control variate, used to reduce the variance of gradient estimators for doubly stochastic objectives of the form

\[
    f(w) = \mathbb{E}_n \mathbb{E}_\epsilon f(w; n, \epsilon).
\]

We begin by explaining why approximation based control variates and incremental gradient methods are unable to reduce variance coming from both MC sampling and data subsampling in sections 3.1 and 3.2. We then introduce an approach that naively combines approximation based control variates and incremental gradient methods and discuss this limitation in section 3.3. Lastly we introduce dual control variates in section 3.4, a method able to jointly reduce variance coming from both MC sampling and data subsampling, thus addressing the limitations of current methods.

3.1 Approximation-based control variates in the doubly-stochastic setting

Approximation-based control variates can be applied to the doubly-stochastic objective using an approximation \( \hat{f}(w; n, \epsilon) \approx f(w; n, \epsilon) \) with tractable expectation with respect to \( \epsilon \). Then, using this approximation, we can define the unbiased gradient estimator

\[
    g_{cv}(w; n, \epsilon) = \nabla f(w; n, \epsilon) + \mathbb{E}_n \nabla \hat{f}(w; n, \epsilon) - \nabla \hat{f}(w; n, \epsilon),
\]

where the second term defines a control variate. We call this the \( cv \) estimator. Many existing algorithms can be seen as instances of this strategy (Grathwohl et al., 2018; Boustati et al., 2020). One strategy is to learn a neural network that takes as input the \( n \)-th datum and outputs a quadratic over \( \epsilon \).

Approximation-based control variates have limitations in how much they can reduce variance. The (trace of) variance of the above estimator is

\[
    \mathbb{V}[g_{cv}] = \mathbb{E}_n \mathbb{V}[\nabla f(w; n, \epsilon) - \nabla \hat{f}(w; n, \epsilon)] + \mathbb{V}[\nabla \hat{f}(w; n)],
\]

where \( f(w; n) = \mathbb{E}_\epsilon f(w; n, \epsilon) \). Appendix A.1 shows that this follows from the law of total variance \( \mathbb{V}[g_{cv}] = \mathbb{E}_n \mathbb{V}_\epsilon g_{cv} + \mathbb{V}_n \mathbb{E}_\epsilon g_{cv} \) plus a few simple manipulations. Intuitively, the first part of this expression could be arbitrarily small, depending on how well \( \hat{f} \) approximates \( f \). However, the second term is irreducible. This is the variance that subsampling would create if one could exactly evaluate \( f(w; n) = \mathbb{E}_\epsilon f(w; n, \epsilon) \). In other words, approximation-based control variates cannot reduce subsampling noise.

3.2 Incremental gradient methods in the doubly-stochastic setting

Incremental gradient methods can also be adapted to the doubly-stochastic setting. We do this by reinterpreting them not as algorithms but as control variate techniques. Take the setting of Sec. 2.2 where the objective \( f(w) = \mathbb{E}_n f(w; n) \) only has \( n \) as a source of randomness. Then, the SAGA (Defazio et al., 2014a) update from Eq. 5 can be viewed as performing stochastic gradient descent with the gradient estimator

\[
    g_{inc}(w; n) = \nabla f(w; n) + \mathbb{E}_m \nabla f(w^m; m) - \nabla f(w^n; n),
\]

In fact, this gradient estimator can be employed with any optimization algorithm.

If we extend this technique to the doubly-stochastic setting, we get what we call the inc estimator

\[
    g_{inc}(w; n, \epsilon) = \nabla f_n(w; n, \epsilon) + \mathbb{E}_m \nabla f(w^m; n, \epsilon) - \nabla f(w^n; n, \epsilon).
\]

This estimator has two limitations. First, while it can be implemented, it is not practical. This is because the value of \( \nabla f(w^n; n, \epsilon) \) is dependent on \( \epsilon \), which is resampled at each iteration. This means that it is not possible to efficiently maintain \( \mathbb{E}_m \nabla f(w^m; m, \epsilon) \), and so each gradient estimate, it requires a full pass over the dataset. Of course, doing this would be pointless—it would be better to simply explicitly sum out \( n \) and solve an optimization problem that only has randomness due to \( \epsilon \).

Nevertheless, \( g_{inc} \) serves as an important point of reference. Surprisingly, when we introduce our dual control variate below, this computational issue disappears. Thus, we will compare to \( g_{inc} \) when possible to give more insight into which source of variance is more important.

The second limitation of \( g_{inc} \) is that it is limited in how much variance it can reduce. The (trace of) variance is

\[
    \mathbb{V}[g_{inc}] = \mathbb{E}_n \mathbb{V}[\nabla f(w; n, \epsilon) - \nabla f(w^n; n, \epsilon)] + \mathbb{V}[\nabla f(w^n)],
\]

where \( \nabla f(w; \epsilon) = \nabla \mathbb{E}_n f(w; n, \epsilon) \). Appendix A.2 shows that this follows from the law of total variance \( \mathbb{V}[g_{inc}] = \mathbb{E}_n \mathbb{V}_\epsilon g_{inc} + \mathbb{V}_n \mathbb{E}_\epsilon g_{inc} \). Essentially, the goal of the estimator is to reduce the first term, which could be arbitrarily
We now introduce a new approach for controlling the variance of gradient estimators for doubly stochastic optimization problems, the central contribution of this paper. The idea is to introduce an approximation \( \hat{f} \approx f \) and take an expectation over \( \epsilon \) as with approximation-based control variates, but to also recycle past evaluations at different values of \( n \) as in incremental gradient methods. We propose the estimator

\[
g_{\text{dual}}(w; n, \epsilon) = \nabla f(w; n, \epsilon) + \mathbb{E}_m \mathbb{E}_\eta \nabla \hat{f}(w^m; m, \eta) - \nabla \hat{f}(w^m; n, \epsilon) .
\]

Note that \( g_{\text{dual}} \) does not suffer from the same computational issue as \( g_{\text{inc}} \). The approximation \( \hat{f} \) is designed so that \( \mathbb{E}_m \nabla \hat{f}(w^m; n, \eta) \) can be computed in closed-form. By caching these values, the expectation over \( m \) can be computed using a running average, rather than iterating though all possible values of \( n \).

The variance of \( g_{\text{dual}} \) is trivial to calculate. It is

\[
\mathbb{V}[g_{\text{dual}}] = \mathbb{V}_\epsilon \mathbb{V}_n \nabla f(w; n, \epsilon) + \mathbb{E}_m \mathbb{E}_\eta \mathbb{V}[\nabla \hat{f}(w^m; m, \eta) - \nabla \hat{f}(w^m; n, \epsilon)]
\]

\[
= \mathbb{V}_\epsilon [\nabla f(w; n, \epsilon) - \nabla \hat{f}(w^m; n, \epsilon)],
\]

where the second line follows from the fact that the middle term on the right of Eq. 15 is constant with respect to \( \epsilon \) and \( n \), and thus makes no contribution to the variance.

The equation above indicates that (unlike \( g_{\text{cv}} \), \( g_{\text{inc}} \), or \( g_{\text{combo}} \)) the variance of \( g_{\text{dual}} \) can in principle be arbitrarily small. The variance is only limited by how close \( \hat{f} \) is to \( f \) and how close the previously evaluated values \( w^m \) are to \( w \).

### 4 Related work

Recent work Boustati et al. (2020) proposes to approximate the optimal batch-dependent control variate for doubly stochastic optimization using a recognition network. Similar to our work, they take into account the usage of subsampling when designing their variance reduction techniques for doubly stochastic problems. However, their approach is essentially different from ours: Their control variate reduces the conditional variance of MC noise (conditioned on the mini-batch samples) but it is unable to reduce the subsampling noise itself and suffers in the same way as \( g_{\text{cv}} \).

There is also a line of work aiming at applying incremental gradient methods on doubly stochastic problems Zheng and Kwok (2018); Bietti and Mairal (2017). However, their approaches only aim to reduce the subsampling noise in doubly stochastic problems which are different from our goal. These approaches resolve the impracticality issue of \( g_{\text{inc}} \) but still leave MC variance unchanged.

The closest prior work is Geffner and Domke (2018) which proposes to use an ensemble of different types of control

### Table 1: Different estimators

| Estimator | Minimum Variance | \( \nabla f \) evals per iteration |
|-----------|------------------|---------------------------------|
| naive     | \( \mathbb{V}_{n, \epsilon} \nabla f(w; n, \epsilon) \) | 1                               |
| cv        | \( \mathbb{V}_n \nabla f(w; n) \) | 2                               |
| inc       | \( \mathbb{V}_{\epsilon} \nabla f(w; \epsilon) \) | \( n+2 \)                        |
| dual      | 0                | 3                               |

small if all the values \( w^n \) are close to the current optimization value \( w \). However, the estimator is unable to reduce the second term, which is the irreducible variance that comes from sampling \( \epsilon \).

### 3.3 Combination of control variates

Given that \( c_{\text{cv}} \) reduces Monte Carlo noise and \( c_{\text{inc}} \) reduces subsampling noise, one might hope that using them together could reduce total noise. This section argues that such a strategy has its limits. Consider an estimator based on a control variate that is a convex combination of the previous control variates, i.e.

\[
g_{\text{combo}}(w; n, \epsilon) = \nabla f(w; n, \epsilon) + \beta c_{\text{cv}}(w; n, \epsilon) + (1 - \beta) c_{\text{inc}}(w; n, \epsilon) \]

(12)

where \( \beta \in (0, 1) \).

Again, there are limits to how much \( c_{\text{combo}} \) could reduce variance. Imagine an ideal situation, created to make both \( c_{\text{cv}} \) and \( c_{\text{inc}} \) maximally effective: Suppose that the approximation used by \( c_{\text{cv}} \) is exact (i.e. \( f = \hat{f} \)) and that the stored parameter values used by \( c_{\text{inc}} \) are all fully up to date (i.e. \( w^n = w \) for all \( n \)). Then, as we show in Appendix A.3, the variance is

\[
\mathbb{V}[g_{\text{combo}}] = \beta^2 \mathbb{V}_n [\nabla f(w; n)] + (1 - \beta)^2 \mathbb{V}_\epsilon [\nabla f(w; \epsilon)] .
\]

(13)

Even in this idealized scenario, such a control variate cannot reduce variance to zero. The problem is intuitively that \( c_{\text{cv}} \) tries to reduce variance with respect to \( \epsilon \) for each \( n \), but does not care about the variance of the resulting estimator with respect to \( n \). Similarly, \( c_{\text{inc}} \) tries to reduce variance with respect to \( n \) for each \( \epsilon \), but does not care about the variance of the resulting estimator with respect to \( \epsilon \). Thus, one can only hope for so much by combining them. The solution is to develop a single control variate that \textit{jointly} reduces both types of noise.

### 3.4 Dual control variate

We now introduce a new approach for controlling the variance of gradient estimators for doubly stochastic optimiza-
we can find an approximation to Eq. (18) by applying the
algorithm with Gaussian dropout and Gaussian mean-field black
box variates to reduce the gradient variance of BBVI. In par-
icular, they demonstrate that it is possible to combine a
gradient estimator with MC variance controlled and a gradi-
et estimator with subsampling noise controlled to form a
new unbiased gradient estimator. This approach shows an
improved convergence rate but it does not reduce the two
types of variance jointly.

5 Experiments

In this section, we empirically evaluate the proposed dual
control variate on two applications: Generalized linear mod-
els with Gaussian dropout and Gaussian mean-field black
box variational inference. On each application, we compare
the performance of dual estimator with naive and cv. We
additionally adopt the inc estimator as a baseline estima-
tor that only controls the subsampling noise for tasks of
small scale, in which iterating through the whole dataset is
tractable. Overall, we find that the dual estimator demon-
strates a significantly smaller variance compared with other
estimators, which aligns with our theory in Sec. 3.4.

5.1 Application: Generalized linear model with
Gaussian dropout

We first consider generalized linear models with Gaussian
dropout, with an objective function defined as

\[
 f(w) = \mathbb{E}_n \mathbb{E}_\epsilon f(w; n, \epsilon), \tag{17}
\]

\[
 f(w; n, \epsilon) := \mathcal{L}(y_n, \phi(x_n; w, \epsilon)) \tag{18}
\]

\[
 \phi(x_n; w, \epsilon) = w(\epsilon \circ x_n), \tag{19}
\]

where \( x_n \in \mathbb{R}^D, y_n \in \mathbb{R}^K, w \in \mathbb{R}^{K \times D} \) and \( \epsilon \in \mathbb{R}^D \) is a
sample from \( \mathcal{N}(1, \sigma I) \), \( \circ \) stands for element-wise
product and \( \mathcal{L} \) is a loss function such as mean-squared error.

We can find an approximation to Eq. (18) by applying
second-order Taylor expansion around \( \epsilon = 1 \), given by

\[
 \tilde{f}(w; n, \epsilon) = f(w; n, 1) + (\epsilon - 1)^T \nabla_{\epsilon} f(w; n, 1) + \\
 \frac{1}{2} (\epsilon - 1)^T \nabla^2_{\epsilon} f(w; n, 1)(\epsilon - 1), \tag{20}
\]

whose expectation with respect to \( \epsilon \) can be given in closed-
form as

\[
 \mathbb{E}_\epsilon \tilde{f}(w; n, \epsilon) = f(w; n, 1) + \frac{\sigma^2}{2} \text{tr} \left( \nabla^2 f(w; n, 1) \right). \tag{21}
\]

Note that Eq. (20) can be computed efficiently using Hessian
vector product while Eq. (21) can also be evaluated without
explicitly instantiating the Hessian matrix with respect to \( \epsilon \)
(see Appendix B).

Results We compare the performance of \( g_{\text{naive}}, g_{\text{cv}}, \) and
\( g_{\text{dual}} \) on CIFAR-10 (Krizhevsky et al., 2009) classification,
where we apply dropout on features extracted from a
LeNet (LeCun et al., 1998) pretrained on CIFAR-10 and
then fine-tune the output layer using the cross-entropy loss
with \( \sigma = 0.5 \). We use a batch size of 100, and optimize
using standard gradient descent without momentum for a
wide range of learning rates.

We present the results in Figure 2 and Figure 3. Since the
true gradient variance is too expensive to estimate, we com-
pute the expected squared gradient norm as an approxima-
tion. The dual estimator shows a gradient norm significantly
smaller than \( g_{\text{cv}} \) and \( g_{\text{naive}} \), which coincides with our anal-
ysis in Sec. 3.1. Additionally, we show the trace of objective
evaluated on the full training set under different learning

\begin{algorithm}
\caption{Stochastic gradient descent with the dual control variate.}
\begin{algorithmic}
\Require Learning rate \( \lambda \).
\State Initialize the parameter \( w_0 \), the parameter table \( W = \{w^1, \ldots, w^N\} \) and the running mean \( M = \mathbb{E}_m \mathbb{E}_\eta \nabla \tilde{f}(w_0; m, \eta) \).
\For{\( k = 1, 2, \ldots \)}
\State Sample \( n \) and \( \epsilon \).
\State Extract the value of \( \tilde{w} \) from the table \( W \).
\State Compute the base gradient \( g \leftarrow \nabla \tilde{f}(w_k; n, \epsilon) \).
\State Compute the control variate \( \epsilon \leftarrow M - \nabla \tilde{f}(w^0; n, \epsilon) \).
\State Update the running mean \( M \leftarrow M + \frac{1}{\epsilon} \left( \mathbb{E}_n \nabla \tilde{f}(w_k; n, \eta) - \mathbb{E}_n \nabla \tilde{f}(w^0; n, \eta) \right) \)
\State Update the table \( w \leftarrow w_k \) and update the parameter \( w_{k+1} \leftarrow w_k - \lambda(g + \epsilon) \).
\EndFor
\end{algorithmic}
\end{algorithm}
rates and different numbers of iterations. We can see that $g_{\text{dual}}$ always reaches objectives smaller than the baseline estimators, displaying significantly better convergence for large learning rates.

### 5.2 Application: Gaussian mean-field black box variational inference

In this section, we demonstrate that dual control variate can be applied on black box variational inference (BBVI) (Ranganath et al., 2014; Kucukelbir et al., 2017) with mean-field Gaussian as the variational posterior.

We begin with a brief introduction of mean-field Gaussian BBVI. Assume we have a latent variable model

$$p(x, z) = \prod_{n=1}^{N} p(x_n | z)p(z),$$

where $\{x_1, \ldots, x_N\}$ denotes the observed data and $z \in \mathbb{R}^d$ represents the latent variable.

We are interested in the posterior distribution of the latent variable $p(z | x)$, which is typically intractable. A potential approach to sidestep this issue involves using variational inference, which uses a variational distribution $q_w(z)$ parameterized by $w$ to approximate the true posterior. The parameter of $q_w(z)$ can be obtained by maximizing the evidence lower bound (ELBO), which is equivalent to minimizing the following objective

$$f(w) = -\mathbb{E}_{n \sim q_w(z)} \left[ N \log p(x_n | z) + \log p(z) \right] - \mathbb{H}(w),$$

where $\mathbb{H}(w)$ denotes the entropy of $q_w$. One widely adopted choice of $q_w(z)$ is the mean-field Gaussian, with diagonal covariance, i.e.

$$q_w(z) \sim \mathcal{N}(\mu, \text{diag}(\sigma)), \quad (24)$$

where we would have $w = (\mu, \sigma)$. In order to estimate the objective’s gradient with respect to $w$ via Monte Carlo sampling, one typically has to apply the reparameterization trick (Kingma and Welling, 2014; Rezende et al., 2014; Titsias and Lázaro-Gredilla, 2014) on $z$, which aims to represent the sampling routine $z \sim q_w(z)$ as a deterministic and differentiable function $z = T_w(\epsilon)$ of a $w$-independent base random variable $\epsilon$. With the reparameterized form, we can rewrite the function inside the nested expectation as

$$k_n(T_w(\epsilon)) = N \log p(x_n | T_w(\epsilon)) + \log p(T_w(\epsilon)). \quad (25)$$

Then, we can rewrite the objective as:

$$f(w) = -\mathbb{E}_{n \sim \epsilon} f(w; n, \epsilon), \quad (26)$$

where we define

$$f(w; n, \epsilon) = k_n(T_w(\epsilon)) + \mathbb{H}(w). \quad (27)$$

Next, we will derive the approximation function for BBVI, which can lead us to $g_{\text{cv}}(w; n, \epsilon)$ and $g_{\text{dual}}(w; n, \epsilon)$. Inspired by previous work (Miller et al., 2017), we propose to get an approximation for $f(w; n, \epsilon)$ using a second order Taylor expansion for $k_n(\cdot)$ around $z_0 = T_w(0)^1$, which yields

$$\tilde{f}(w; n, \epsilon) = k_n(z_0) + (T_w(\epsilon) - z_0)^\top \nabla k_n(z_0) + \frac{1}{2} (T_w(\epsilon) - z_0)^\top \nabla^2 k_n(z_0)(T_w(\epsilon) - z_0) + \mathbb{H}(w), \quad (28)$$

\footnote{1We use $z_0 = \text{stop gradient}(T_w(0))$ so that the gradient does not backpropagate from $z_0$ to $w$.}
Figure 4: For mean-field black-box variational inference, the dual estimator leads to improved convergence at higher learning rates. This improvement is a consequence of lower variance (Fig. 1). Australian and Sonar are small datasets, included because it is possible to compute the inc estimator using brute force, which gives some insight into where the improvement in the dual estimator comes from. MNIST and FMNIST are larger-scale problems where the inc estimator is intractable. Given the small improvement of the cv estimator over the naive estimator on these problems, we suspect that most of the improvement in the dual estimator comes from reduced subsampling variance.
in which we assume the entropy can be computed in closed-form. It is worth noting that, in the case of mean-field Gaussian, the expected gradient of the approximation Eq. (28) can only be computed efficiently (via Hessian-vector product) only with respect to the mean parameter $\mu$ but not for the scale parameter $\sigma$, which means $g_{\text{cv}}(w; n, \epsilon)$ and $g_{\text{dual}}(w; n, \epsilon)$ can only be used as the gradient estimator for $\mu$. Fortunately, controlling only the gradient variance on $\mu$ is sufficient here because the total gradient is dominated by the variance from $\mu$, as is pointed out by Geffner and Domke (2020).

**Results** On BBVI, we first experiment with two small-scale tasks: Bayesian logistic regression on the Australian dataset and the sonar dataset. These are small enough to allow us to explicitly compute $g_{\text{inc}}$ as a baseline. The prior on the weights is a standard Gaussian. We estimate gradients using a minibatch size of 5 all using a single shared value of $\epsilon$. We optimize using stochastic gradient descent (without momentum) with learning rates ranging from $10^{-5}$ to $5 \times 10^{-3}$ (See Appendix. C for details). The weights $w$ are initialized from a standard Gaussian, with the results shown averaging over 10 independent trials. We report the gradient variance of the different estimators using a single shared optimization trace collected (using the dual estimator) with a learning rate of $1e-3$. Additionally, we show the ELBO (evaluated on the full dataset) trace under different learning rates and number of iterations.

The results are presented in the left two columns in Fig. 1, Figs. 4(a) and 4(b). Note that both the inc and cv estimators have lower variance on the naive estimator, but this varies by the dataset. The excellent performance of the inc estimator on Australian shows the importance of reducing subsampling noise. The dual estimator has the lowest variance. This enables the use of larger learning rates, leading to faster optimization. (Even faster than the inc estimator which makes a full pass through the data in each iteration.)

Next, we experiment with two larger-scale tasks: MNIST (LeCun et al., 1998) and Fashion-MNIST (Xiao et al., 2017) (FMNIST). We estimate the gradients using a mini-batch of 100 samples with a single shared $\epsilon$. Because of the scale of the datasets, we are forced to use the expected gradient norm as a proxy for the gradient variance. We again initialize the variational parameters randomly using standard Gaussian and average results over 5 independent trials.

| Datasets     | N      | Q    |
|--------------|--------|------|
| CIFAR-10     | 50,000 | 820  |
| Australian   | 690    | 14   |
| Sonar        | 208    | 60   |
| MNIST        | 60,000 | 7,840|
| FMNIST       | 60,000 | 7,840|

Table 2: Dataset size (N) and latent dimensionality (Q) of datasets used in experiments

We experiment with learning rates ranging from $4e-8$ to $1.5e-5$ and $2e-8$ to $7.5e-6$ for MNIST and FMNIST respectively (see Appendix. C for details).

Results are shown in the right two columns in Fig. 1, Fig. 4(c) and Fig. 4(d). Here $g_{\text{dual}}$ shows much lower variance than $g_{\text{naive}}$ or $g_{\text{cv}}$. (While $g_{\text{inc}}$ is too expensive to run, we conjecture that it would perform well.)

### 6 Efficiency analysis

In this section, we will study the computational cost of different estimators. First, a theoretical analysis in terms of “oracle” evaluations of $f(w; n, \epsilon)$: The naive estimator needs to compute a single gradient per iteration. The cv estimator computes one gradient and also one Hessian-vector product for the control variate. The dual estimator needs one gradient and two Hessian-vector products: One for evaluating the control variate, and one for updating the running mean $M$. Although there is no oracle cost, the dual estimator also has some overhead to maintain the parameter table $W$.

In Table. 3, we give actual measured runtimes based on a JAX implementation running on an Nvidia 2080ti GPU. For the inc estimator, the number is the averaged time by running 10 runs with 1 update step. For the rest estimators, these are the average time for a single update step of optimization, estimated by running 10 runs with 200 update steps each. Overall, each iteration with the dual estimator is around 1.5 to 2.5 times slower than naive and around 1.2 times slower than cv. Notice that, despite the cv and the dual estimator being 2/3 times more expensive than the naive estimator in oracle complexity, they are actually faster in practice. We believe this is an artifact of the usage of mini-batching and GPU computation. Lastly, recall that in Fig. 3 and Fig. 4, dual achieves a given objective in an order of magnitude fewer iterations, meaning it is the fastest in terms of wall-clock time.

| Datasets     | N      | Q    |
|--------------|--------|------|
| (F)MNIST     |        |      |
| CIFAR-10     |        |      |
| naive        | 11.5ms | 9.35ms|
| cv           | 12.8ms | 19.75ms|
| inc          | 711ms  | 499ms |
| dual         | 15.7ms | 23.8ms|

Table 3: Average time of a single update step.
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A Derivation of variance for different estimators

In this section, we will show the full derivation for the trace of the variance of $g_{cv}, g_{inc}$ and $g_{combo}$.

A.1 Variance of $g_{cv}$

In this section, we will derive the trace for the $cv$ estimator defined as

$$g_{cv}(w; n, \epsilon) = \nabla f(w; n, \epsilon) + \mathbb{E}_{\eta} \nabla \tilde{f}(w; n, \eta) - \nabla \tilde{f}(w; n, \epsilon), \quad (29)$$

where $\tilde{f}$ is an approximation function of $f$ with closed-form expectation with respect to $\epsilon$.

To start with, we will apply the law of total variance

$$\nabla [g_{cv}] = \mathbb{E}_{n} \nabla g_{cv} + \nabla \mathbb{E}_{\epsilon} g_{cv}. \quad (30)$$

The first term can be computed as

$$\mathbb{E}_{n} \nabla g_{cv} = \mathbb{E}_{n} [\nabla f(w; n, \epsilon) + \mathbb{E}_{\eta} \nabla \tilde{f}(w; n, \eta) - \nabla \tilde{f}(w; n, \epsilon)] \quad (31)$$

which follows since $\mathbb{E}_{\eta} \nabla \tilde{f}(w; n, \eta)$ is a constant with respect to $\epsilon$ and therefore does not affect the variance.

The second term can be computed as

$$\nabla \mathbb{E}_{\epsilon} g_{cv} = \nabla \mathbb{E}_{\epsilon} [\nabla f(w; n, \epsilon) + \mathbb{E}_{\eta} \nabla \tilde{f}(w; n, \eta) - \nabla \tilde{f}(w; n, \epsilon)]$$

$$= \nabla \mathbb{E}_{\epsilon} [\nabla f(w; n, \epsilon)] + \mathbb{E}_{\eta} \nabla \tilde{f}(w; n, \eta) - \nabla \tilde{f}(w; n, \epsilon) \quad (32)$$

Then we can combine the two terms together to get

$$\nabla [g_{cv}] = \mathbb{E}_{n} \nabla [\nabla f(w; n, \epsilon) - \nabla \tilde{f}(w; n, \epsilon)] + \nabla [\nabla f(w; n)] \quad (33)$$

A.2 Variance of $g_{inc}$

Here, we will derive the trace of the variance of the inc estimator defined as

$$g_{inc}(w; n, \epsilon) = \nabla f_n(w; n, \epsilon) + \mathbb{E}_{m} \nabla f(w^m; m, \epsilon) - \nabla f(w^n; n, \epsilon). \quad (34)$$

We can derive its variance by first applying the law of total variance

$$\nabla [g_{inc}] = \mathbb{E}_{n} \nabla g_{inc} + \nabla \mathbb{E}_{\epsilon} g_{inc}. \quad (35)$$

The first term can be computed as

$$\mathbb{E}_{n} \nabla g_{inc} = \mathbb{E}_{n} \nabla [\nabla f_n(w; n, \epsilon) + \mathbb{E}_{m} \nabla f(w^m; m, \epsilon) - \nabla f(w^n; n, \epsilon)] \quad (36)$$

$$= \mathbb{E}_{n} \nabla [\nabla f(w; n, \epsilon) - \nabla f(w^n; n, \epsilon)]. \quad (37)$$
where the second line follows because $\mathbb{E}_m \nabla f(w^m; m, \epsilon)$ is a constant with respect to $n$.

The second term can be computed as

$$\nabla \mathbb{E}_{\epsilon} g_{\text{inc}} = \nabla \mathbb{E}_{\epsilon} \nabla f_n(w; n, \epsilon) + \mathbb{E}_{\epsilon} \nabla f(w^m; m, \epsilon) - \nabla f(w^*; n, \epsilon)$$ (43)

$$= \nabla \mathbb{E}_{\epsilon} \nabla f_n(w; n, \epsilon) + \mathbb{E}_{\epsilon} \nabla f(w^m; m, \epsilon) - \mathbb{E}_{\epsilon} \nabla f(w^*; n, \epsilon)$$ (44)

$$= \nabla \mathbb{E}_{\epsilon} \nabla f_n(w; n, \epsilon)$$ (45)

$$= \nabla \mathbb{E}_{\epsilon} \nabla f(w; \epsilon),$$ (46)

which then leads us to

$$\nabla \mathbb{E}_{\epsilon} g_{\text{inc}} = \mathbb{E}_{\epsilon} \nabla f(w; n, \epsilon) - \nabla f(w^*; n, \epsilon) + \nabla \mathbb{E}_{\epsilon} \nabla f(w; \epsilon).$$ (47)

### A.3 Variance of $g_{\text{combo}}$

In this section, we will derive the variance for the estimator $g_{\text{combo}}$ defined as

$$g_{\text{combo}}(w; n, \epsilon) = \nabla f(w; n, \epsilon) + \beta_{\text{cv}}(w; n, \epsilon) + (1 - \beta) c_{\text{inc}}(w; n, \epsilon),$$ (49)

under the ideal assumption where we have $f = \tilde{f}$ and $w = w^*, \forall n$. The variance can be derived through

$$\nabla \mathbb{E}_{\epsilon} g_{\text{combo}} = \nabla \mathbb{E}_{\epsilon} \nabla f(w; n, \epsilon) + \beta_{\text{cv}}(w; n, \epsilon) + (1 - \beta) c_{\text{inc}}(w; n, \epsilon)$$ (50)

$$= \nabla \mathbb{E}_{\epsilon} \nabla f(w; n, \epsilon) + \beta \left( \mathbb{E}_{\eta} \nabla \tilde{f}(w; n, \eta) - \nabla \tilde{f}(w; n, \epsilon) \right) +$$

$$(1 - \beta) \left( \nabla \mathbb{E}_m f(w^m; m, \epsilon) - \nabla f(w^*; n, \epsilon) \right)$$ (51)

Then we replace $\tilde{f}$ with $f$ and $w^*$ with $w$ based on our assumption,

$$\nabla \mathbb{E}_{\epsilon} g_{\text{combo}} = \nabla \mathbb{E}_{\epsilon} \nabla f(w; n, \epsilon) + \beta \left( \mathbb{E}_{\eta} \nabla f(w; n, \eta) - \nabla f(w; n, \epsilon) \right) +$$

$$(1 - \beta) \left( \nabla \mathbb{E}_m f(w; m, \epsilon) - \nabla f(w; n, \epsilon) \right)$$ (52)

$$= \nabla \mathbb{E}_{\epsilon} \nabla f(w; n, \epsilon) + \beta (\nabla f(w; n) - \nabla f(w; n, \epsilon)) + (1 - \beta) (f(w; \epsilon) - f(w; n, \epsilon))$$ (53)

$$= \nabla \mathbb{E}_{\epsilon} \beta \nabla f(w; n) + (1 - \beta) \nabla f(w; \epsilon)$$ (54)

$$= \beta^2 \nabla \mathbb{E}_{\epsilon} \nabla f(w; n) + (1 - \beta)^2 \nabla \mathbb{E}_{\epsilon} \nabla f(w; \epsilon).$$ (55)

The last line follows because $\nabla f(w; n)$ is independent of $\nabla f(w; \epsilon)$. 
\section*{B Efficient computation of Hessian trace for Gaussian Dropout}

Recall that, when computing the expectation of the approximation function for Gaussian Dropout, we would like to compute the trace of the Hessian matrix with respect to $\epsilon$

$$\text{tr}(\nabla_{\epsilon}^2 f(w; n, \epsilon))$$

(56)

To start with, we will derive the formula for the Hessian

$$\nabla_{\epsilon} f(w; n, \epsilon) = \frac{d\phi(x_n; w, \epsilon)^\top}{d\phi} \frac{dL}{d\phi}$$

(57)

$$\nabla_{\epsilon} f(w; n, \epsilon) = (\epsilon \circ x_n)^\top w^\top \frac{dL}{d\phi}$$

(58)

$$\nabla_{\epsilon} f(w; n, \epsilon) = \text{diag}(x_n) w^\top \frac{dL}{d\phi}$$

(59)

$$\nabla_{\epsilon}^2 f(w; n, \epsilon) = \text{diag}(x_n) w^\top \frac{dL}{d\phi}$$

(60)

$$\text{diag}(x_n) w^\top \frac{dL}{d\phi}$$

(61)

where $\frac{dL}{d\phi}$ is a shorthand for $\frac{dL(y_n, \phi(x_n; w, \epsilon))}{d\phi}$

The trace of the Hessian can be computed as

$$\text{tr} \left( \nabla_{\epsilon}^2 f(w; n, 1) \right) = \sum_{d=1}^{D} \left( \text{diag}(x_n) w^\top \right)_d \nabla_{\phi}^2 L(y_n, \phi(x_n; w, \epsilon)) \left( \text{diag}(x_n) w^\top \right)_d$$

(62)

where $\text{diag}(x_n) \in \mathbb{R}^{D \times D}$ is a diagonal matrix whose entries are the $D$ elements of the vector $x_n$ and $\left( \text{diag}(x_n) w^\top \right)_d$ represents the $d_{th}$ row of this $D \times K$ matrix. Note that we do not need to explicitly store the diagonal matrix $\text{diag}(x_n) w^\top$ because we can directly compute $\text{diag}(x_n) w^\top$ using the broadcasting mechanism. As such, the computation would cost $O(DK^2)$ in total, although this is of cubic complexity, $K$ is typically much smaller than $D$ in practice which makes the overall cost acceptable.

Now suppose we are using the logistic loss, such that

$$L(y, \phi) = \log \sum_{i=1}^{K} \exp(\phi_i) - \phi_y.$$  

(63)

We will show that the computation of the trace can be further accelerated. To start with, note that

$$\frac{dL}{d\phi} = \frac{\exp(\phi)}{\sum_{i=1}^{K} \exp(\phi_i)} - \delta_y,$$

(64)

where $\delta_y$ is a one-hot vector. The second derivative of this is

$$\frac{\ddot{L}}{d\phi d\phi^\top} = \frac{\text{diag}(\exp(\phi))}{\sum_{i=1}^{K} \exp(\phi_i)^2} - \frac{\exp(\phi) \exp(\phi)^\top}{(\sum_{i=1}^{K} \exp(\phi_i))^2}$$

(65)

For the purpose of simplicity, we will define $a = \frac{\exp(\phi)}{\sum_{i=1}^{K} \exp(\phi_i)}$ such that the second derivative can be rewritten as

$$\frac{d\dot{L}}{d\phi d\phi^\top} = \text{diag}(a) - aa^\top$$

(66)

In this case, we can compute the trace of the Hessian as

$$\text{tr}(\nabla_{\epsilon}^2 f(w; n, \epsilon)) = \text{tr} \left( \text{diag}(x_n) w^\top \left( \text{diag}(a) - aa^\top \right) \text{diag}(a) \right)$$

(67)

$$\text{tr}(\nabla_{\epsilon}^2 f(w; n, \epsilon)) = \text{tr} \left( \text{diag}(x_n) w^\top \text{diag}(a) \text{diag}(x_n) \right) - \text{tr} \left( \text{diag}(x_n) w^\top aa^\top \text{diag}(x_n) \right)$$

(68)
We can simplify the first term by having
\[
tr \left( \text{diag}(\text{diag}(x_n)) w^{\top} \text{diag}(\text{diag}(x_n)) \right) = tr \left( \left( \text{diag}(\sqrt{a}) \ right) w \text{diag}(x_n) \right)^{\top} \left( \text{diag}(\sqrt{a}) \text{diag}(x_n) \right) \right) 
\]
\[
= \| \text{diag}(\sqrt{a}) \text{diag}(x_n) \|_F^2
\] (69)
which can be computed efficiently without using any matrix product operation.

Next, we notice that the second term can be computed using
\[
tr \left( \text{diag}(\text{diag}(x_n)) w^{\top} aa^{\top} w \text{diag}(x_n) \right) = tr \left( a^{\top} w \text{diag}(x_n) \text{diag}(x_n) w^{\top} a \right) \]
\[
= a^{\top} w \text{diag}(x_n) \text{diag}(x_n) w^{\top} a \]
\[
= \| \text{diag}(x_n) w^{\top} a \|_2^2
\] (71)
This computation above costs \(O(DK)\) in total.

C Selection of learning rates

For CIFAR-10, we experiment with learning rates of
\{1e−1, 7.5e−2, 5e−2, 2.5e−2, 1e−2, 5e−3, 1e−3, 5e−4, 1e−4, 1e−5, 1e−6, 1e−7, 1e−8\}

For Australian and Sonar, we experiment with learning rates of
\{7.5e−3, 5e−3, 2.5e−3, 1e−3, 5e−4, 1e−4, 5e−5, 2.5e−5, 1e−5\}

For MNIST, we experiment with learning rates of
\{1.5e−05, 1e−05, 4e−06, 3e−06, 2e−06, 4e−07, 2e−07, 4e−08\}

For FMNIST, we experiment with learning rates of
\{7.5e−06, 5e−06, 2e−06, 1.5e−06, 1e−06, 2e−07, 1e−07, 2e−08\}