Efficient Debiased Variational Bayes by Multilevel Monte Carlo Methods

Kei Ishikawa, Takashi Goda

January 15, 2020

Abstract

Variational Bayes is a method to find a good approximation of the posterior probability distribution of latent variables from a parametric family of distributions. The evidence lower bound (ELBO), which is nothing but the model evidence minus the Kullback-Leibler divergence, has been commonly used as a quality measure in the optimization process. However, the model evidence itself has been considered computationally intractable since it is expressed as a nested expectation with an outer expectation with respect to the training dataset and an inner conditional expectation with respect to latent variables. Similarly, if the Kullback-Leibler divergence is replaced with another divergence metric, the corresponding lower bound on the model evidence is often given by such a nested expectation. The standard (nested) Monte Carlo method can be used to estimate such quantities, whereas the resulting estimate is biased and the variance is often quite large. Recently the authors provided an unbiased estimator of the model evidence with small variance by applying the idea from multilevel Monte Carlo (MLMC) methods. In this article, we give more examples involving nested expectations in the context of variational Bayes where MLMC methods can help construct low-variance unbiased estimators, and provide numerical results which demonstrate the effectiveness of our proposed estimators.

1 Introduction

Variational inference, or variational Bayes, is a very powerful optimization tool in Bayesian computations to find a good approximation of the posterior probability distribution of latent variables from a parametric family of distributions [13]. Let $z$ be a vector of latent variables following a prior distribution $p(z)$. Given a set of i.i.d. observations $x$, Bayes’ theorem leads to the posterior distribution of $z$, that is

$$p(z|x) = \frac{p(z, x)}{p(x)} = \frac{p(z)p(x|z)}{\mathbb{E}_{z \sim p(z)}[p(x|z)]}.$$
To approximate $p(z|x)$ by $q(z;x)$ from some parametric family of distributions with parameters $\phi$ (here and in what follows, we omit the dependence on such parameters from the notation for simplicity), we need to measure the divergence between $p(z|x)$ and $q(z;x)$. Typically, the Kullback-Leibler (KL) divergence has been considered:

$$KL(q(z;x)\|p(z|x)) = \mathbb{E}_{z \sim q(z;x)} \left[ \log \frac{q(z;x)}{p(z|x)} \right].$$

Minimizing the KL divergence is equivalent to maximizing the evidence lower bound (ELBO):

$$\text{ELBO}(q) = \log p(x) - KL(q(z;x)\|p(z|x)) = \mathbb{E}_{z \sim q(z;x)} \left[ \log \frac{p(z)p(x|z)}{q(z;x)} \right]$$

$$= \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q(z_n;x_n)} \left[ \log \frac{p(z_n)p(x_n|z_n)}{q(z_n;x_n)} \right],$$

where the last equality holds when $z_1, \ldots, z_N$ are i.i.d. random variables and each $x_n$ depends only on $z_n$ and under the mean-field approximation for $q$. The key ingredient of employing the ELBO is that, although both the model evidence, or the log marginal likelihood, $\log p(x)$ and the KL divergence have been considered computationally hard to estimate, only the computable quantities $p(z_n), p(x_n|z_n)$ and $q(z_n;x_n)$ appear on the right-most side above so that one can estimate the ELBO by the standard Monte Carlo sampling for $n \in \{1, \ldots, N\}$ and $z_n \sim q(z_n;x_n)$. This is key to realizing so-called stochastic variational inference as in [13]. Even for the case where one wants to estimate the parameters $\theta$ of $p(z)$ and $p(x|z)$ via maximum likelihood estimation simultaneously, maximization of the ELBO with respect to both $\theta$ and $\phi$ is reasonable. However, looking at learning $\theta$ only, the ELBO is a downward-biased quantity of the true model evidence.

Recently there have been several attempts to reduce the bias in the Monte Carlo estimation of the model evidence. For instance, the importance weighted autoencoders proposed in [4] use an intermediate quantity between the model evidence and the ELBO. A more recent study from [19] applies the Jackknife method to reduce the bias of the estimator of the model evidence further. However, how to remove the bias from the evidence estimator completely has not been known until the work by the authors [10]. In fact, an independent work [18] undertook the same problem, but in contrast to the estimator proposed by the authors, the expected cost and the variance per one sample of the resulting estimator of [18] are both infinite. The main tool to introduce an unbiased low-variance Monte Carlo estimator comes from multilevel Monte Carlo (MLMC) methods due to Giles [7] and their randomized version due to Rhee & Glynn [24]. We refer to a recent review article [8] for comprehensive information on MLMC methods.

In this article, we push forward the idea of applying multilevel Monte Carlo methods to various Bayesian computations in the context of stochastic variational inference. The common underlying problem is that a quantity we want to
estimate, such as the model evidence or an evidence lower bound based on some divergence metrics other than the KL divergence, is expressed as a nested expectation, where an outer expectation is taken with respect to observations and an inner conditional expectation is with respect to latent variables. If only affine transformations are applied to an inner expectation before taking an outer expectation, two expectations can be concatenated into a single expectation with respect to both observations and latent variables, so that a standard (single-loop) Monte Carlo estimator does work. This is indeed the case for the ELBO. However, if there exists a non-affine transformation between two expectations, they cannot be concatenated inherently. A nested Monte Carlo estimator is probably the most straightforward approach to estimate such a nested expectation. The algorithm goes like: first generate a set of random samples on outer variables, and then generate a set of random samples on inner variables for each outer sample conditionally. However, as the paper [22] clearly shows a degraded rate of convergence for nested Monte Carlo estimators, nested Monte Carlo estimators are generally inefficient, and, needless to say, biased.

MLMC methods are an excellent rescue for estimating nested expectations efficiently. We refer to [8, Section 9] for a brief discussion on MLMC methods applied to estimate nested expectations. Most relevant works to this article are [9] and [11], in which MLMC methods are applied to special classes of nested expectations, although the latter work was studied in a quite different context from machine learning. These works provide the theoretical bases of using MLMC methods for estimating nested expectations appearing in the context of stochastic variational inference. In this article, we first present various problems in Bayesian computations related to variational inference where nested expectations appear, and after explaining MLMC methods applied to nested expectations, we provide numerical results that examine whether MLMC methods are efficient to estimate such expectations in a practical setting.

2 Nested expectations in variational Bayes

In this section, we provide various examples of nested expectations appearing in the context of variational inference. Those quantities have been traditionally estimated by using nested Monte Carlo estimators, whereas MLMC methods are usefully applicable to estimate them more efficiently as shown later in this article.

2.1 Model evidence

In this section, except for the locally marginalized ELBO introduced in Section 2.2, we assume a latent variable model that corresponds to the following i.i.d. data generating process for $n = 1, \ldots, N$:

\[
Z_n \sim p(z) \\
X_n | Z_n = z_n \sim p(x | z_n)
\]
This latent variable model can be expressed as a graphical model presented in Figure 1. In the Bayesian statistics, the model evidence, or the log marginalized likelihood is a fundamental quantity. However, the computation of this quantity has been infeasible in the standard framework of variational Bayes, because the exact posterior is not available. One solution for making the evidence estimation feasible is to use a nested Monte Carlo estimator with an importance distribution \( q \) to estimate \( p(x_n) \) for each data point \( x_n \) as:

\[
\sum_{n=1}^{N} \log p(x_n) = N \cdot \mathbb{E}_X \left[ \log \mathbb{E}_{Z \sim q(Z; X)} \left[ \frac{p(X, Z)}{q(Z; X)} \right] \right],
\]

where the random variable \( X \) in the outer expectation is uniformly distributed over \( x_1, ..., x_N \). This scheme works well in the framework of variational inference because the variational distribution itself serves as a good approximation of the posterior of the latent variables, so that it can be used as an importance distribution \( q \). However, as is evident, this quantity is expressed as a nested expectation with an outer expectation with respect to \( X \) and an inner conditional expectation with respect to \( Z \). Thus, an efficient estimation of the evidence has been considered computationally hard. Instead, by fixing the number of inner samples on \( Z \), this scheme was recently applied to variational autoencoders to obtain a tighter lower bound on the evidence [4]. In [10] upon which our present work is built, the use of the so-called randomized MLMC method is proposed to obtain a completely unbiased estimator of the evidence.

### 2.2 Locally marginalized ELBO

In this example, we consider the following i.i.d. data generating process with local latent variables \( z_1, ..., z_N \) and a vector of global latent variables \( \beta \). The data of the observable variables are denoted by \( x_1, ..., x_N \). This model can be considered as an extension of the first example with additional global latent variables.

\[
\begin{align*}
\beta & \sim p(\beta) \\
Z_n|\beta & \sim p(z|\beta) \\
X_n|Z_n = z_n & \sim p(x|z_n)
\end{align*}
\]

Only in this example, global latent variables are considered, and this model can be represented as a graphical model in Figure 2.
We define the locally marginalized ELBO (LM-ELBO) in the following. By definition, this lower bound on the evidence is tighter than the ELBO.

$$\text{LM-ELBO} := \log p(x_{1:N}) - \text{KL}[q(\beta)||p(\beta|x_{1:N})]$$

$$\geq \log p(x_{1:N}) - \text{KL}[q(z_{1:N}, \beta)||p(z_{1:N}, \beta|x_{1:N})] =: \text{ELBO}.$$  

As the locally marginalized ELBO is tighter than the normal ELBO, this can help approximate the evidence better and help the M-step in the variational Bayes [13, 23]. Furthermore, this tighter lower bound can potentially help to compute the criterion for model selection such as perplexity used in topic modeling. Theoretically, we can claim that the locally marginalized ELBO is asymptotically equivalent to the evidence if an estimator for the posterior of $\beta$ converges to the true posterior. Such estimation of the posterior is possible by starting around the neighborhood of the global optimal parameter, if we carry out variational inference using noisy gradient of the locally marginalized ELBO as described in Section 3.3. This lower bound can be written as a nested expectation as follows.

$$\text{LM-ELBO} = \log p(x_{1:N}) - \text{KL}[q(\beta)||p(\beta|x_{1:N})]$$

$$= \mathbb{E}_{\beta \sim q(\beta)} \left[ \log \prod_{n=1}^{N} \frac{p(x_n|\beta)p(\beta)}{q(\beta)} \right]$$

$$= \sum_{n=1}^{N} \mathbb{E}_{\beta \sim q(\beta)} \left[ \log \mathbb{E}_{Z \sim q(z|x_n)} \left[ \frac{p(x_n, Z|\beta)}{q(Z|x_n)} \right] \right] + \mathbb{E}_{\beta \sim q(\beta)} \left[ \log \frac{p(\beta)}{q(\beta)} \right]$$

$$= N \cdot \mathbb{E}_{X} \mathbb{E}_{\beta \sim q(\beta)} \left[ \log \mathbb{E}_{Z \sim q(z|X)} \left[ \frac{p(X, Z|\beta)}{q(Z|X)} \right] \right] + \mathbb{E}_{\beta \sim q(\beta)} \left[ \log \frac{p(\beta)}{q(\beta)} \right].$$

Here an outer expectation is taken with respect to both $X$ and $\beta$ simultaneously, whereas an inner conditional expectation is with respect to $Z$.

### 2.3 Reversed KL upper bound

In the standard variational inference, we minimize the average of the KL divergence between $q(z|x_n)$ and $p(z|x_n)$, given the observations $x_1, ..., x_N$. However, the use of the reversed KL divergence can offer several advantages over the standard variational inference, such as avoidance of the mode seeking behavior that
In particular, we recover the \( \chi \) Pearson’s divergence. Because of the ratio of two inner conditional expectations with respect to \( \gamma \), when \( \gamma = 1 \), the negative of this quantity, \( \gamma > 0 \), on the model evidence based on the reversed KL divergence is given by

\[
N \cdot \mathbb{E}_X \left[ \log p(X) + \text{KL}[p(z|X)||q(z; X)] \right]
\]

\[
= N \cdot \mathbb{E}_X \mathbb{E}_{Z \sim p(z|X)} \left[ \log \frac{p(X, Z)}{q(Z; X)} \right]
\]

\[
= N \cdot \mathbb{E}_X \mathbb{E}_{Z \sim q(z; X)} \left[ \frac{p(X, Z)}{p(X)q(Z; X)} \log \frac{p(X, Z)}{q(Z; X)} \right]
\]

\[
= N \cdot \mathbb{E}_X \left[ \mathbb{E}_{Z \sim q(z; X)} \left[ \frac{p(X, Z)}{q(Z; X)} \log \frac{p(X, Z)}{q(Z; X)} \right] \right].
\]

Because of the ratio of two inner conditional expectations with respect to \( Z \), this quantity is inherently given by the nested form.

### 2.4 Rényi and \( \chi \) bounds

Other than the KL divergence, various divergence metrics can be used to carry out variational inference. One of such examples is \( \alpha \)-divergence, which is a general class of divergence metrics including the KL divergence as a special case. Though there are various definitions of the \( \alpha \)-divergence family, we adopt Rényi’s \( \alpha \)-divergence as described in [17]. We also use its extension to negative value of \( \alpha \), as this definition allows for the derivation of the variational \( \chi \)-upper bound proposed in [5]. The divergence metric used here can be written as

\[
D_\gamma[p(z)||q(z)] := \frac{1}{\gamma} \log \mathbb{E}_{Z \sim q(z)} \left[ \left( \frac{p(Z)}{q(Z)} \right)^\gamma \right].
\]

This quantity is called the \( \alpha \)-divergence when we choose \( \gamma = 1 - \alpha \) for \( \alpha > 0 \). When \( \gamma = 1 \), the model evidence as described in Section 2.1 is recovered. When \( \gamma > 1 \), the negative of this quantity, \( -D_\gamma[p(z)||q(z)] \), becomes the logarithm of Neyman’s \( \chi \) divergence.

Replacing the KL divergence with \( D_\gamma[p(z)||q(z)] \) in the definition of the normal ELBO, we obtain various upper/lower bounds on the model evidence as follows.

\[
\log p(x_{1:N}) + D_\gamma[p(z_{1:N}|x_{1:N})||q(z_{1:N}; x_{1:N})]
\]

\[
= N \cdot \mathbb{E}_X \left[ \log p(X) + \frac{1}{\gamma} \log \mathbb{E}_{Z \sim q(z; X)} \left[ \left( \frac{p(Z|X)}{q(Z; X)} \right)^\gamma \right] \right]
\]

\[
= N \cdot \mathbb{E}_X \left[ \frac{1}{\gamma} \log \mathbb{E}_{Z \sim q(z; X)} \left[ \left( \frac{p(Z|X)}{q(Z; X)} \right)^\gamma \right] \right].
\]

In particular, we recover the \( \chi^2 \) upper bound if \( \gamma = 2 \), which corresponds to the Pearson’s \( \chi^2 \) divergence

\[
\chi^2_P[q(z)||p(z)] = \int \frac{(q(z) - p(z))^2}{q(z)} \, dz,
\]
as proposed in [5]. Moreover, when $\gamma = 1/2$ and $-1$, we recover the variational Rényi lower bounds corresponding to the Hellinger distance
\[
\text{Hel}[q(z)||p(z)] = \frac{1}{2} \int (\sqrt{p(z)} - \sqrt{q(z)})^2 \, dz,
\]
and the Neyman’s $\chi^2$ divergence
\[
\chi^2_N[q(z)||p(z)] = \int \frac{(q(z) - p(z))^2}{p(z)} \, dz,
\]
respectively, as in [17].

We can also consider the reversed metric $D_\gamma[q(z)||p(z)]$ and the corresponding upper/lower bound on the model evidence.

\[
\log p(x_{1:N}) - D_\gamma[q(z_{1:N}; x_{1:N})||p(z_{1:N}|x_{1:N})] = N \cdot \mathbb{E}_X \left[ \log p(X) - \frac{1}{\gamma} \log \mathbb{E}_{Z \sim p(z|x)} \left[ \left( \frac{q(Z; X)}{p(Z; X)} \right)^\gamma \right] \right]
\]
\[
= N \cdot \mathbb{E}_X \left[ -\frac{1}{\gamma} \log \mathbb{E}_{Z \sim p(z|x)} \left[ \left( \frac{q(Z; X)}{p(Z; X)} \right)^\gamma \frac{p(Z; X)}{q(Z; X)} \right] \right]
\]
\[
= N \cdot \mathbb{E}_X \left[ -\frac{1}{\gamma} \frac{\mathbb{E}_{Z \sim q(z;x)} \left[ \left( \frac{q(Z; X)}{p(Z; X)} \right)^\gamma \frac{p(Z; X)}{q(Z; X)} \right]}{\mathbb{E}_{Z \sim q(z;x)} \left[ \frac{p(Z; X)}{q(Z; X)} \right]} \right]
\]

When $\gamma = 2$, we recover the $\chi^2$ lower bound corresponding to the reversed Pearson’s $\chi^2$ divergence $\chi^2_p[q(z)||p(z)]$ (or Neyman’s $\chi^2$ divergence). When $\gamma = 1/2$ and $-1$, we recover the variational Rényi upper bounds corresponding to Hellinger distance $\text{Hel}[p(z)||q(z)]$ and reversed Neyman’s $\chi^2$ divergence $\chi^2_N[q(z)||p(z)]$ (or Pearson’s $\chi^2$ divergence), respectively.

We would like to emphasize here that the divergence metrics and the corresponding lower/upper bounds on the model evidence are defined as nested expectations. This point is not shared by the normal ELBO, which makes a crucial difference in estimating them from a computational viewpoint.

2.5 Mutual Information
Let us recall that the mutual information is defined by $I(X; Z) := \int \log \frac{p(x, z)}{p(x)p(z)} \, dp(x, z)$. Mutual information has long been studied in the context of machine learning [26, 20]. As is evident below, the mutual information is inherently expressed as
a nested expectation, and thus its more computable variational bounds are often used instead, in situations where we need to optimize the mutual information.

Though various specifications of \( p(x, z) \) are possible, we only consider the same model as that in Section 2.1, so that we have \( p(x, z) = p(x | z)p(z) \). Then we can rewrite the mutual information in this model as:

\[
I(X; Z) = \mathbb{E}_{(X, Z) \sim p(x, z)} \left[ \log \frac{p(X, Z)}{p(Z)} - \log p(X) \right]
\]

\[
= \mathbb{E}_X \left[ \mathbb{E}_{Z \sim p(z|X)} [\log p(X|Z) - \log \mathbb{E}_{Z \sim p(z)} [p(X|Z)]] \right]
\]

\[
= \mathbb{E}_X \left[ \mathbb{E}_{Z \sim q(z;X)} \left[ \frac{p(X|Z)}{q(Z; X)} \log p(X|Z) \right] - \log \mathbb{E}_{Z \sim q(z;X)} \left[ \frac{p(X|Z)p(Z)}{q(Z; X)} \right] \right]
\]

Here the first term appearing in each line above corresponds to the negative conditional entropy \(-H(X|Z)\) and the second term corresponds to the entropy \(H(X)\), which both result in the nested expectations with an outer expectation with respect to \( X \) and an inner conditional expectation with respect to \( Z \). This way, in most of the specifications of \( p(x, z) \), the mutual information is represented as nested expectations.

Another possible specification of \( p(x, z) \) is \( p(x, z) \propto e^{T(x, z)} \) with a mapping from the data space \( X \) to the latent space \( Z \) being \( z = \epsilon(x) \). Even though this is an unnormalized statistical model, we can compute the empirical mutual information of data \( \{x_1, ..., x_N\} \) and its mapped representation \( \{\epsilon(x_1), ..., \epsilon(x_N)\} \) as follows.

\[
I(X; Z) = \mathbb{E}_{(X, Z)} [\log p(X, Z) - \log p(X) - \log p(Z)]
\]

\[
= \mathbb{E}_X [\log p(X, \epsilon(X)) - \log p_x(X) - \log p_z(\epsilon(X))]
\]

\[
= \mathbb{E}_X \left[ T(X, \epsilon(X)) - \log \mathbb{E}_{X'}[e^{T(X', \epsilon(X'))}] - \log \mathbb{E}_{X'}[e^{T(X', \epsilon(X))}] \right]
\]

\[
+ \log \mathbb{E}_X \left[ e^{T(X, \epsilon(X))} \right],
\]

where \( X \) and \( X' \) appearing in the expectations are uniformly distributed random variables over the data \( x_1, ..., x_N \) and mutually independent. Although an inner expectation with respect to \( X' \) is no longer conditional on the outer variable \( X \), the nested structure still holds, so that an efficient estimation of \( I(X; Z) \) is not straightforward.

### 3 Monte Carlo methods for nested expectations

As we observed in Section 2, many quantities appearing in variational Bayes which we want to estimate are given by nested expectations of the form either

\[
I = \mathbb{E}_X \left[ f \left( \mathbb{E}_{Z \sim q(z;X)} [g(p(Z), p(X|Z), q(Z; X))] \right) \right],
\]
or

\[ I = \mathbb{E}_X \mathbb{E}_\beta \sim q(\beta) \left[ f \left( \mathbb{E}_{Z \sim q(z; X)} [g(p(\beta), p(X, Z|\beta), q(Z; X))] \right) \right], \]

where \( X \) denotes the discrete uniform random variable of the data \( x_1, \ldots, x_N \) and the random variable \( Z \) follows the probability distribution \( q(z; X) \) conditional on \( X \). For the latter, \( \beta \) denotes the vector of global latent variables. Here the inner function \( g \) has possibly multiple outputs and so the outer function \( f \) can be multivariate. It should be noted that the above form does not cover the second representation of the mutual information, so that readers should properly amend it when implementing. In this section we provide an (possibly unbiased) MLMC estimator of such nested expectations after briefly reviewing the standard nested Monte Carlo estimator. For simplicity we shall focus on nested expectations written in the former form.

### 3.1 Nested Monte Carlo estimator

For positive integers \( K, M \), the nested Monte Carlo estimator approximates \( I \) simply by

\[ \hat{I}_{K,M} = \frac{1}{M} \sum_{m=1}^{M} f \left( \frac{1}{K} \sum_{k=1}^{K} g(p(Z_{m,k}), p(X_m|Z_{m,k}), q(Z_{m,k}; X_m)) \right), \]

where \( X_1, \ldots, X_M \) are i.i.d. random samples of \( X \), and for each \( X_m \), we denote by \( Z_{m,1}, \ldots, Z_{m,K} \) conditionally i.i.d. random samples of \( Z \sim q(z; X_m) \). If \( f \) is not a linear function, \( \hat{I}_{K,M} \) is obviously a biased estimator of \( I \), i.e., \( \mathbb{E}[\hat{I}_{K,M}] \neq I \).

For simplicity of notation, let us introduce a random functional of \( X \):

\[ f_K(X) = f \left( \frac{1}{K} \sum_{k=1}^{K} g(p(Z_k), p(X|Z_k), q(Z_k; X)) \right), \]

where \( Z_1, \ldots, Z_K \sim q(z; X) \). Under mild assumptions on \( f \), the law of large numbers leads to the equality \( I = \mathbb{E}_X [f_\infty(X)] \) and the mean squared error of \( \hat{I}_{K,M} \) is decomposed into the sum of the variance and the squared bias:

\[
\mathbb{E} \left[ (\hat{I}_{K,M} - I)^2 \right] = \mathbb{V} \left[ \hat{I}_{K,M} \right] + \left( \mathbb{E} [\hat{I}_{K,M}] - I \right)^2 \\
= \frac{\mathbb{V}_X[f_K(X)]}{M} + (\mathbb{E} [(f_K - f_\infty)(X)])^2.
\]

In order to estimate \( I \) with mean squared accuracy \( \varepsilon^2 \), it suffices to have

\[
\frac{\mathbb{V}_X[f_K(X)]}{M} \leq \frac{\varepsilon^2}{2}, \quad (\mathbb{E} [(f_K - f_\infty)(X)])^2 \leq \frac{\varepsilon^2}{2}.
\]

Assuming that \( \mathbb{V}_X[f_K(X)] \approx \mathbb{V}_X[f_\infty(X)] \) and that the bias \( |\mathbb{E} [(f_K - f_\infty)(X)]| \) decays with the order \( 1/K \), we need \( M = O(\varepsilon^{-2}) \) and \( K = O(\varepsilon^{-1}) \), resulting in the total computational cost \( MN = O(\varepsilon^{-3}) \).
3.2 Multilevel Monte Carlo estimator

To reduce the necessary cost to \(O(\varepsilon^{-2})\) for estimating nested expectations, let us consider applying MLMC methods. The main difference from nested Monte Carlo methods is to use the telescoping sum

\[
E[f_{2L}(X)] = E[f_1(X)] + \sum_{\ell=1}^{L} (E[f_{2\ell}(X)] - E[f_{2\ell-1}(X)]).
\]

In order to estimate the difference of expectations \(E[f_{2\ell}(X)] - E[f_{2\ell-1}(X)]\), one can use the common random samples of \(X\) and also the common random samples of \(Z \sim q(z; X)\). Recall that \(f_{2\ell}(X)\) is computed based on \(2^\ell\) random samples of \(Z \sim q(z; X)\). Dividing those samples into two disjoint subsets both with \(2^{\ell-1}\) samples, one can compute \(f_{2\ell-1}(X)\) twice, which we denote by \(f_{2\ell-1}^{(a)}(X)\) and \(f_{2\ell-1}^{(b)}(X)\). Because they are independent each other, it is obvious to see that

\[
E[f_{2\ell-1}^{(a)}(X)] = E[f_{2\ell-1}^{(b)}(X)] = E[f_{2\ell-1}(X)].
\]

By introducing a random functional on the difference:

\[
\Delta_{\ell}f(X) = \begin{cases} f_1(X) & \text{if } \ell = 0, \\ f_{2\ell} - \frac{f_{2\ell-1}^{(a)} + f_{2\ell-1}^{(b)}}{2} & \text{otherwise}, \end{cases}
\]

we have

\[
E[f_{2\ell}(X)] = E[f_1(X)] + \sum_{\ell=1}^{L} \left( E[f_{2\ell}(X)] - \frac{E[f_{2\ell-1}^{(a)}(X)] + E[f_{2\ell-1}^{(b)}(X)]}{2} \right)
\]

\[
= E[f_1(X)] + \sum_{\ell=1}^{L} E\left[ (f_{2\ell} - \frac{f_{2\ell-1}^{(a)} + f_{2\ell-1}^{(b)}}{2}) (X) \right]
\]

\[
= \sum_{\ell=0}^{L} E[\Delta_{\ell}f(X)].
\]

MLMC methods estimate each term on the rightmost side independently:

\[
\hat{I}_{L,M_0,\ldots,M_L}^{\text{MLMC}} = \sum_{\ell=0}^{L} \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \Delta_{\ell}f(X_{\ell,m}).
\]

where \(X_{0,1}, \ldots, X_{0,M_0}, \ldots, X_{L,1}, \ldots, X_{L,M_L}\) are i.i.d. random samples of \(X\). Because of the independence between different levels \(\ell\), the mean squared error of \(\hat{I}_{L,M_0,\ldots,M_L}^{\text{MLMC}}\) is decomposed into

\[
E\left[ (\hat{I}_{L,M_0,\ldots,M_L}^{\text{MLMC}} - I)^2 \right] = \sum_{\ell=0}^{L} \frac{\mathcal{V}[\Delta_{\ell}f(X)]}{M_\ell} + (E[(f_{2L} - f_{2\infty})(X)])^2.
\]
Since $f_1, f_2, \ldots$ approximate $f_\infty$ with increasing accuracy, the variance of the difference $\Delta_\ell f$ is expected to get smaller as the level $\ell$ increases. Thus fewer number of outer samples $M_\ell$ is needed to estimate $E[\Delta_\ell f(X)]$ accurately for larger $\ell$ where the computational cost per one sample is as large as $O(2^\ell)$. This way, we can allocate most of outer samples to smaller levels and make the total computational cost to estimate $I$ significantly small as compared to the nested Monte Carlo estimator.

The following fundamental theorem on MLMC methods is proven in [7, 8].

**Theorem 1.** Assume that there exist constants $c_1, c_2, \alpha, \beta > 0$ such that

1. $\alpha \geq \min(\beta, 1)/2$,
2. $\mathbb{E}[|f_{2^\ell} - f_\infty(X)|] \leq c_1 2^{-\alpha \ell}$ (decay of bias) and
3. $V_\ell = \mathbb{V}[\Delta_\ell f(X)] \leq c_2 2^{-\beta \ell}$ (decay of variance on difference).

Then, for any accuracy $\varepsilon < \exp(-1)$, there exists a constant $c_3 > 0$ such that there are corresponding maximum level $L$ and numbers of outer samples $M_0, M_1, \ldots, M_L$ for which the mean squared error of the MLMC estimator $\hat{I}_{L,M_0,\ldots,M_L}^{\text{MLMC}}$ is less than $\varepsilon^2$ with the total computational cost $C$ bounded by

$$\mathbb{E}[C] \leq \begin{cases} c_4 \varepsilon^{-2}, & \beta > 1, \\ c_4 \varepsilon^{-2} \log \varepsilon^{-1}^2, & \beta = 1, \\ c_4 \varepsilon^{-2-(1-\beta)/\alpha}, & \beta < 1. \end{cases}$$

**Remark 1.** Some comments are in order.

1. If we are in the regime $\beta > 1$, MLMC methods can estimate nested expectations with the cost of $O(\varepsilon^{-2})$, which compares favorably with nested Monte Carlo methods. As proven in [9][11], there are several examples on nested expectations for which $\alpha = 1$ and $\beta = 2$ hold. In our experiments, it is expected that the same rates of convergence on the bias and the variance are observed, respectively.

2. Given the maximum level $L$, the method of Lagrange multipliers leads to an optimal allocation of outer samples $M_0, M_1, \ldots, M_L$ by minimizing the variance for a fixed computational cost:

$$\sum_{\ell=0}^{L} \frac{V_\ell}{M_\ell} + \lambda \sum_{\ell=0}^{L} C_\ell M_\ell,$$

where $C_\ell$ is the computational cost per sample of $\Delta_\ell f(X)$, which is essentially proportional to $2^\ell$. Then we have

$$M_\ell \propto \sqrt{\frac{V_\ell}{C_\ell}} = O(2^{-(\beta+1)/2}).$$
3. In particular, if $\beta > 1$, the MLMC estimator can be made unbiased by applying the idea from [24] as follows. For any sequence $\omega = (\omega_0, \omega_1, \ldots)$ such that $\omega_\ell > 0$ and $\|\omega\|_1 = 1$, we have

$$I = \mathbb{E}[f_\infty(X)] = \sum_{\ell=0}^{\infty} \mathbb{E}[\Delta_\ell f(X)] = \sum_{\ell=0}^{\infty} \omega_\ell \cdot \mathbb{E}[\Delta_\ell f(X)] / \omega_\ell.$$  

For any batch size $M > 0$, let $\mathcal{L}_1, \ldots, \mathcal{L}_M \geq 0$ be a sequence of i.i.d. random samples from a discrete probability distribution $\omega = (\omega_0, \omega_1, \ldots)$. Then it is easy to see that

$$\frac{1}{M} \sum_{m=1}^{M} \frac{\Delta_{\mathcal{L}_m} f(X_m)}{\omega_{\mathcal{L}_m}}$$

is an unbiased estimator of $I$. The expected computational cost and the variance per one sample of this estimator are given by

$$\sum_{\ell=0}^{\infty} \omega_\ell C_\ell \quad \text{and} \quad \sum_{\ell=0}^{\infty} \frac{V_\ell}{\omega_\ell},$$

respectively. In order for these quantities to be both finite, it suffices to have $\omega_\ell \propto 2^{-(\beta+1)\ell/2}$ if $\beta > 1$ is satisfied.

Regarding the first item above, we can make some precise statements in the present context. First, the following result directly comes from [9, Theorem 5.2 and Remark 3]:

**Theorem 2.** If there exist $s > 4$ and $t > 2$ with $(s-4)(t-2) \geq 8$ such that

$$\mathbb{E}_X \mathbb{E}_{Z \sim q(z; x)} \left[ \log \frac{p(Z)p(X|Z)}{p(X)q(Z; X)} \right]^s, \mathbb{E}_X \mathbb{E}_{Z \sim q(z; x)} \left[ \log \frac{p(Z)p(X|Z)}{p(X)q(Z; X)} \right]^t < \infty,$$

then the MLMC estimator for the model evidence satisfies $\alpha = 1$ and $\beta = 2$. The same result on $\alpha$ and $\beta$ holds for the MLMC estimator for the locally marginalized ELBO if

$$\mathbb{E}_X \mathbb{E}_{Z \sim q(z; x)} \left[ \frac{p(X,Z|\beta)p(\beta)}{p(X)q(\beta)q(Z; X)} \right]^s < \infty,$$

and

$$\mathbb{E}_X \mathbb{E}_{Z \sim q(z; x)} \left[ \log \frac{p(X,Z|\beta)p(\beta)}{p(X)q(\beta)q(Z; X)} \right]^t < \infty.$$

By applying the result from [11, Lemma 2], we also have the following:

**Theorem 3.** Assume that we have

$$\mathbb{E}_X \mathbb{E}_{Z \sim q(z; x)} \left[ \frac{p(Z)p(X|Z)}{p(X)q(Z; X)} \right]^4, \sup_{X,Z} \left| \log \frac{p(Z)p(X|Z)}{q(Z; X)} \right| < \infty.$$

Then the MLMC estimator for the reversed KL divergence satisfies $\alpha = 1$ and $\beta = 2$. 

12
3.3 Computations of Noisy Gradient

If the derivatives of a nested expectation with respect to parameters $\phi$ of $q(z; x)$ as well as $\theta$ of $p(x, z)$ or of $p(x, z, \beta)$ are again given by the nested form as considered above, the derivatives of the nested Monte Carlo/MLMC estimators for the nested expectation can be used as noisy gradient estimators. Therefore if the true derivatives satisfy the conditions as discussed above, MLMC methods can be applied to estimate the derivatives and the resulting estimates can be used in the stochastic optimization process. Moreover, we can make the MLMC estimators unbiased as mentioned in the third item of Remark [1]. In many applications, some automatic differentiation software can be used to compute the derivatives via reparametrization trick [15, 25, 16, 6]. Another method to compute the noisy gradient is to use the score function to compute the noisy gradient [23]. This way the use of noisy gradient enables combinations of MLMC methods with various variational inference techniques.

4 Experiments

In this section, we provide the results of numerical experiments to see the performance of MLMC estimators in the applications discussed in Section 2.

4.1 Comparison of multilevel and nested estimators

First, we plotted the computational costs of both nested Monte Carlo and MLMC estimators required to estimate the model evidence with a certain accuracy $\varepsilon$ in Figure 3. In this figure, the accuracy $\varepsilon$ at each maximum level $L$ is estimated by the standard Monte Carlo method as $\varepsilon = 4\sqrt{E[|\Delta_{L+1}|^2]}$. The required cost for each estimator was estimated by the number of samples required in the inner Monte Carlo sampling. Then the required cost for the MLMC estimator with the maximum level $L$ is estimated by

$$\frac{\mathbb{V}[\hat{I}^{\text{MLMC}}_{L, M_0, \ldots, M_L}]}{(\varepsilon/2)^2} \cdot \sum_{\ell=0}^{L} M_\ell 2^\ell,$$

whereas the required cost for the nested Monte Carlo estimator is estimated by

$$\frac{\mathbb{V}[\hat{I}^{L,M}]}{(\varepsilon/2)^2} \cdot M^2L,$$

for the same $L$, where both $\mathbb{V}[\hat{I}^{\text{MLMC}}_{L, M_0, \ldots, M_L}]$ and $\mathbb{V}[\hat{I}^{L,M}]$ are estimated by i.i.d. sampling of $\hat{I}^{\text{MLMC}}_{L, M_0, \ldots, M_L}$ and $\hat{I}^{L,M}$. Here the runtime required for computing each estimator is not used because an efficient implementation of MLMC estimators depends on the computing environment, which we leave open for future work. When the total computational cost is fixed, the authors observed so far that the MLMC estimators tend to be more accurate but slow as compared to the nested Monte Carlo estimators in general due to its complex model structure.
Figure 3: The relation of the required computational cost of evidence and its accuracy. Relative accuracy is chosen to equal one at level 0. Required cost is the cost where the estimated bias is expected to equal the estimated variance at each level. We estimated the bias and the variance using 100 samples at each level (0 to 9).

4.2 Convergence of MLMC coupling

Next, we evaluated the convergence behavior of differences $\Delta f$ for the MLMC estimators of the following metrics: evidence, locally marginalized ELBO, variational Rényi and $\chi$ bound (both $\gamma = 1/2$), reversed KL divergence and mutual information. We also evaluated the convergence behavior of the gradients of the corresponding MLMC estimators mentioned above, except for the locally marginalized ELBO. The gradients were estimated by the reparametrization technique. Except for the locally marginalized ELBO, for the data $x_1, ..., x_N$ and the model $p(x, z)$, we used the MNIST dataset and the (convolutional) variational autoencoder. The weights of the model were trained for 200 iterations, although 1200 iterations are required for the convergence of the variational objective function. For the locally marginalized ELBO, we chose latent Dirichlet allocation as an example. The model was trained by online variational inference on the dataset of random Wikipedia articles. The locally marginalized ELBO was evaluated after 100 steps of training with the batch size of 64.

Figure 4 shows the convergence behaviors of $\mathbb{E}[\Delta f]$ and $\mathbb{V}[\Delta f]$ for the MLMC estimators described above. The requirements for the MLMC method, i.e., the exponential decays of both $\mathbb{E}[\Delta f]$ and $\mathbb{V}[\Delta f]$, are satisfied for most
of the estimators presented, except for the mutual information and the locally marginalized ELBO. In general, \( \mathbb{E}[\Delta_\ell f] \) and \( \mathbb{V}[\Delta_\ell f] \) decay with the orders of \( 2^{-\ell} \) and \( 2^{-2\ell} \), respectively, implying that we have \( \alpha = 1 \) and \( \beta = 2 \) in the assumptions of Theorem 1. On the other hand, \( \mathbb{E}[\Delta_\ell f] \) for the mutual information converges much faster than expected. This might be caused by the relatively complex structure inside the nested expectation, which involves both log and fraction. For the locally marginalized ELBO, the difference variable \( \Delta_\ell f \) does not converge at the assumed rate both in the expectation and the variance. However, huge declines in the expectations and the variances are observed between \( \ell = 0 \) and \( \ell = 1 \), and so most of the samples can be allocated only for the smallest level \( \ell = 0 \) if a required accuracy is not so small. Thus, despite such an abnormal convergence behavior of \( \Delta_\ell f \), the MLMC method is still applicable.

Figure 5 shows the convergence behavior of \( \mathbb{E}[\nabla (\Delta_\ell f)] \) and \( \mathbb{V}[\nabla (\Delta_\ell f)] \) in \( L_1 \) norm and in trace norm, respectively. Again we can see the expected exponential decays, implying that we have \( \alpha = 1 \) and \( \beta = 2 \) in the assumptions of Theorem 1 even for the gradient estimation.

It should be pointed out, however, that we observed such good exponential decays of \( \mathbb{E}[\Delta_\ell f] \) and \( \mathbb{V}[\Delta_\ell f] \) to be violated as the training of the variational autoencoder progresses. This obstacle is problematic when applying MLMC methods to deep neural networks, which we leave open for future research.

5 Conclusion

In this article, we have shown that multilevel Monte Carlo methods can be used to efficiently estimate various nested expectations appearing in stochastic variational inference. Our numerical experiments have empirically shown that the assumptions for MLMC estimators to achieve the optimal order of computational cost are satisfied in most of the examples listed in the article. It follows from the previous works [9, 11] that we already have the corresponding theoretical results for some of the quantities, i.e., the model evidence, the locally marginalized ELBO and the variational lower bound based the reversed KL divergence, to explain such optimality of MLMC estimators, whereas we do not have for others yet. An accompanying theoretical analysis is a work in progress. Also, it is worth investigating whether MLMC methods are usefully applicable to more examples in the context of machine learning.

References

[1] Felix Vsevolodovich Agakov. Variational Information Maximization in Stochastic Environments. PhD thesis, University of Edinburgh, 2005.

[2] Alexander A Alemi, Ian Fischer, Joshua V Dillon, and Kevin Murphy. Deep variational information bottleneck. arXiv preprint arXiv:1612.00410, 2016.
Figure 4: Convergence rate of coupled estimators
Figure 5: Convergence rate of coupled estimators of the gradients

(a) Evidence
(b) Reversed KL
(c) Hellinger Upper bound
(d) Hellinger Lower bound
(e) Mutual Information
[3] Alexander A Alemi, Ben Poole, Ian Fischer, Joshua V Dillon, Rif A Saurous, and Kevin Murphy. Fixing a broken elbo. *arXiv preprint arXiv:1711.00464*, 2017.

[4] Yuri Burda, Roger Grosse, and Ruslan Salakhutdinov. Importance weighted autoencoders. *arXiv preprint arXiv:1509.00519*, 2015.

[5] Adji Bousso Dieng, Dustin Tran, Rajesh Ranganath, John Paisley, and David Blei. Variational inference via χ upper bound minimization. In *Advances in Neural Information Processing Systems*, pages 2732–2741, 2017.

[6] Mikhail Figurnov, Shakir Mohamed, and Andriy Mnih. Implicit reparameterization gradients. In *Advances in Neural Information Processing Systems*, pages 441–452, 2018.

[7] Michael B Giles. Multilevel Monte Carlo path simulation. *Operations Research*, 56(3):607–617, 2008.

[8] Michael B Giles. Multilevel Monte Carlo methods. *Acta Numerica*, 24:259–328, 2015.

[9] Takashi Goda, Tomohiko Hironaka, and Takeru Iwamoto. Multilevel Monte Carlo estimation of expected information gains. *Stochastic Analysis and Applications*, 2020.

[10] Takashi Goda and Kei Ishikawa. Multilevel Monte Carlo estimation of log marginal likelihood, 2019.

[11] Tomohiko Hironaka, Michael B Giles, Takashi Goda, and Howard Thom. Multilevel Monte Carlo estimation of the expected value of sample information. *arXiv preprint arXiv:1909.00549*, 2019.

[12] Matthew Hoffman, Francis R Bach, and David M Blei. Online learning for latent dirichlet allocation. In *advances in neural information processing systems*, pages 856–864, 2010.

[13] Matthew D Hoffman, David M Blei, Chong Wang, and John Paisley. Stochastic variational inference. *Journal of Machine Learning Research*, 14(1):1303–1347, 2013.

[14] Michael I Jordan, Zoubin Ghahramani, Tommi S Jaakkola, and Lawrence K Saul. An introduction to variational methods for graphical models. *Machine learning*, 37(2):183–233, 1999.

[15] Diederik P Kingma and Max Welling. Auto-encoding variational Bayes. *arXiv preprint arXiv:1312.6114*, 2013.

[16] Alp Kucukelbir, Dustin Tran, Rajesh Ranganath, Andrew Gelman, and David M Blei. Automatic differentiation variational inference. *The Journal of Machine Learning Research*, 18(1):430–474, 2017.
[17] Yingzhen Li and Richard E Turner. Rényi divergence variational inference. In *Advances in Neural Information Processing Systems*, pages 1073–1081, 2016.

[18] Yucen Luo, Alex Beatson, Mohammad Norouzi, Jun Zhu, David Duvenaud, Ryan P Adams, and Ricky TQ Chen. SUMO: Unbiased estimation of log marginal probability for latent variable models. 2019.

[19] Sebastian Nowozin. Debiasing evidence approximations: On importance-weighted autoencoders and Jackknife variational inference. 2018.

[20] Liam Paninski. Estimation of entropy and mutual information. *Neural computation*, 15(6):1191–1253, 2003.

[21] Ben Poole, Sherjil Ozair, Aaron van den Oord, Alexander A Alemi, and George Tucker. On variational bounds of mutual information. *arXiv preprint arXiv:1905.06922*, 2019.

[22] Tom Rainforth, Robert Cornish, Hongseok Yang, Andrew Warrington, and Frank Wood. On nesting Monte Carlo estimators. *arXiv preprint arXiv:1709.06181*, 2017.

[23] Rajesh Ranganath, Sean Gerrish, and David Blei. Black box variational inference. In *Artificial Intelligence and Statistics*, pages 814–822, 2014.

[24] Chang-han Rhee and Peter W Glynn. Unbiased estimation with square root convergence for SDE models. *Operations Research*, 63(5):1026–1043, 2015.

[25] Francisco J R Ruiz, Titsias K Michalis, and David Blei. The generalized reparameterization gradient. In *Advances in neural information processing systems*, pages 460–468, 2016.

[26] Naftali Tishby, Fernando C Pereira, and William Bialek. The information bottleneck method. *arXiv preprint physics/0004057*, 2000.