Multi-level Monte Carlo Variational Inference

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Abstract

In many statistics and machine learning frameworks, stochastic optimization with high variance gradients has become an important problem. For example, the performance of Monte Carlo variational inference (MCVI) seriously depends on the variance of its stochastic gradient estimator. In this paper, we focused on this problem and proposed a novel framework of variance reduction using multi-level Monte Carlo (MLMC) method. The framework is naturally compatible with reparameterization gradient estimators, which are one of the efficient variance reduction techniques that use the reparameterization trick. We also proposed a novel MCVI algorithm for stochastic gradient estimation on MLMC method in which sample size $N$ is adaptively estimated according to the ratio of the variance and computational cost for each iteration. We furthermore proved that, in our method, the norm of the gradient could converge to 0 asymptotically. Finally, we evaluated our method by comparing it with benchmark methods in several experiments and showed that our method was able to reduce gradient variance and sampling cost efficiently and be closer to the optimum value than the other methods were.

1 Introduction

Variational inference (VI) (Jordan et al., 1999) has been successful in the context of approximate Bayesian inference. The object of VI is to seek out the distribution from a variational family of distributions that best approximates an intractable posterior distribution (Miller et al., 2017), but the objective function of VI itself is often intractable and cannot be computed in closed form. In this case, we often use stochastic gradient methods that are estimated by using Monte Carlo methods, called Monte Carlo variational inference (MCVI). In MCVI, sampling from a posterior distribution is key to estimating the gradient stochastically. However, the performance of MCVI depends on controlling the variance of the stochastic gradient estimator.

There are two common MCVI gradient estimators. One is the score function gradient estimator (Paisley et al., 2012; Ranganath et al., 2014) and the other is the reparameterization gradient estimator (Titsias & Lázaro-Gredilla, 2014;
The score function gradient estimator can be applied to both discrete and continuous random variables, but it often has high variance. In contrast, the reparameterization gradient estimator often has lower variance on continuous random variables. Recently, Ruiz et al. (2016b) has bridged these two gradient estimators, and Tokui & Sato (2016) and Jang et al. (2017) has proposed the reparameterization trick for discrete or categorical variables. Therefore, the reparameterization gradient has become a more useful way to reduce gradient variance.

In this context, Miller et al. (2017) have proposed an approach to controlling the variance of reparameterization gradient estimators by linearizing a part of the gradient, but it was only applied to a Gaussian variational family of distribution. Buchholz et al. (2018) have proposed using a randomized quasi-Monte Carlo method for MCVI, which can reduce the variance of samples to lower than the MC method, but the selection of sequence is difficult.

In this paper, we give a novel framework for reducing gradient variance and the cost of sampling in the context of MCVI. The multi-level Monte Carlo (MLMC) method makes use of the linearity of expectation, and therefore it is derived on the reparameterization gradient estimator based on the reparameterization trick (Kingma & Welling, 2014).

Our contributions are as follows:

- We investigated the idea of using the MLMC method for MCVI on reparameterization gradient estimators.
- We proposed an algorithm that estimates the optimal number of samples to reduce the gradient variance while also reducing the sampling cost.
- We showed that when using the MLMC method, the stochastic gradient is unbiased and its variance is asymptotically reduced as levels of expectation per iteration increases. We also showed that when using stochastic gradient descent (SGD) with a constant learning rate, the magnitude of update-term variance calculated from stochastic gradient estimator on each iteration is reduced by a factor of $2^{\beta t}$ and therefore converges to 0.
- Through two different experiments, we illustrated that our method reduces the gradient variance and sampling cost more efficiently than standard MCVI does.

The rest of this paper is organized as follows. We overview the related work and back ground in Sections 2 and 3. In Section 4, we introduce our framework and theoretical properties. We give experimental results in Section 5 and conclude in Section 6.
2 Related work

2.1 Monte Carlo Variational Inference (MCVI)

Since the score function gradient estimator for variational inference (VI) was proposed (Paisley et al., 2012; Ranganath et al., 2014), MCVI has been receiving a lot of attention (see a recent review (Zhang et al., 2017)). The introduction of the gradient estimator showed that VI could be applied to non-conjugate models. However, the accuracy of MCVI crucially depends on the variance of the gradient estimator because of Monte Carlo estimation. As a result, various techniques for variance reduction have been introduced, such as Rao-Blackwellization, control variates (Ranganath et al., 2014), and importance sampling (Ruiz et al., 2016a; Burda et al., 2016; Sakaya & Klami, 2017).

In this context, Kingma & Welling (2014) and Rezende et al. (2014) introduced reparameterization gradients for MCVI, which enabled lower variance than the score function gradient did. The extensions of reparameterization gradients have also been proposed, such as the generalized reparameterization gradients (Ruiz et al., 2016b) and control variates on reparameterization gradients (Miller et al., 2017). Roeder et al. (2017) proposed a lower variance reparameterization gradient estimator from another point of view: removing a part of the total derivative with respect to the variational parameters that correspond to the score function (called the stop gradient).

The idea of using another Monte Carlo method to reduce the variance of the estimator has also been investigated recently. Ranganath et al. (2014) and Ruiz et al. (2016a) suggested using Quasi-Monte Carlo (QMC), and Tran et al. (2017) used this for a specific model. Recently, Buchholz et al. (2018) have proposed a variance reduction method by using Randomized QMC (RQMC) on an MCVI framework. However, this method has only confirmed the optimization path of training ELBO and not checked the predictive performance on a test data in experiments.

2.2 Multi-level Monte Carlo (MLMC)

When approximating posterior distributions, Monte Carlo methods are often used for estimating expectation of intractable objects with several random samples. The mean squared error (MSE) of the approximation with random samples is a rate of $O(N^{-1})$, and an accuracy of $\epsilon$ requires $N = O(\epsilon^{-2})$ samples. This rate can be too high for application. One approach to addressing this high cost is the use of QMC or RQMC methods, in which the samples are not chosen randomly and independently, instead being selected very carefully to reduce the error (Giles, 2015). In the best cases, the error rate is $O(N^{-2} \log N^{2d-2})$ or $O(N^{-2})$. There are many reviews about the QMC approach provided by Niederreiter (1992); L’Ecuyer & Lemieux (2005); Dick et al. (2013); Leobacher & Pillichshammer (2014).

Another approach to improving the computational efficiency is the MLMC method proposed by Heinrich (2001). The MLMC method has been used
Table 1: Relationship between existing work and this work. CV stands for Control Variates, RB for Rao-Blackwellization, and IS for Importance Sampling. \( N \) is the number of samples, and \( t \) is iteration step.

| Method                        | Order of sampling Variance | Gradient Estimator                      |
|-------------------------------|----------------------------|-----------------------------------------|
| Ranganath et al. (2014)       | \( CV \) & \( RB \)       | \( O(N^{-1}) \)                          |
| Ruiz et al. (2016a)           | \( CV \) & \( IS \)       | \( O(N^{-1}) \)                          |
| Roeder et al. (2015)          | Stop Gradient             | \( O(N^{-1}) \)                          |
| Miller et al. (2017)          | \( CV \)                   | \( O(N^{-1}) \)                          |
| Sakaya & Klami (2017)         | \( IS \)                   | \( O(N^{-1}) \)                          |
| Li et al. (2018)              | Adaptive IS               | \( O(N^{-1}) \)                          |
| Buchholz et al. (2018)        | RQMC sampling             | \( O(N^{-1}) \)                          |
| This Work                     | MLMC method               | \( O(2^{-\delta}N^{-1}) \)              |

| The number of samples | Theoretical analysis of gradient norm |
|-----------------------|--------------------------------------|
| Stay                  | -                                    |
| Stay                  | -                                    |
| Stay                  | -                                    |
| Stay                  | -                                    |
| Stay                  | -                                    |
| Increase              | ✓                                    |
| Decrease              | ✓                                    |

frequently in stochastic differential equations for options pricing (Giles, 2008; Cliffe et al., 2011; Rhee & Glynn, 2015). In statistics, there are many applications in approximate Bayesian computation (Giles et al., 2016; Jasra et al., 2017; Warne et al., 2018). More detail about MLMC method is in Appendix A.

The relationship between our work and existing work is organized in Table 1.

3 Monte Carlo Variational Inference (MCVI)

In this section, we review Monte Carlo Variational Inference (MCVI). First, we give a background of VI in Section 3.1. Next, we introduce two major gradient estimators in Section 3.2. Finally, we outline MCVI in Section 3.3.

3.1 Background of Variational Inference

The object in Bayesian inference is estimating a posterior distribution of latent variable \( z \) given observation data \( x \). Computing the exact posterior distribution of a model requires to sum or integrate over all \( z \) and it can be complex (e.g. non-conjugate model) or large-scale. Therefore, exact inference is typically intractable, and approximation is needed in these models. Consequently, the central idea of VI is to approximate the model posterior by a simpler distribution (Zhang et al., 2017).

In more detail, VI constructs an approximation of the posterior \( p(z|x) \) by minimizing the Kullback-Leibler (KL) divergence between a variational distribution \( q(\lambda) \), where \( \lambda \in \mathbb{R}^d \) is a free parameter, and the true posterior distribution. This is equal to maximizing the evidence lower bound (ELBO):

\[
\mathcal{L}(\lambda) = \mathbb{E}_{q(z|\lambda)}[\log p(x, z) - \log q(z|\lambda)].
\]
However, it is hard to compute a differentiation of the objective (1) with respect to $\lambda$ directly because the measure of the expectation depends on this parameter (Buchholz et al., 2018). There are two major approaches to handling this problem: the score function gradient estimator and the reparameterization gradient estimator.

### 3.2 Gradient Estimator

#### 3.2.1 Score Function Gradient

The first approach is based on the score function gradient, also known as REINFORCE gradient, (Ranganath et al., 2014). The score function gradient expresses the gradient of the ELBO as expectation with respect to $q(z|\lambda)$ and is given by

$$\nabla_\lambda L(\lambda) = \mathbb{E}_{q(z|\lambda)}[\nabla_\lambda \log q(z|\lambda)(\log p(x, z) - \log q(z|\lambda))].$$

(2)

The gradient estimator is obtained by approximating expectation by sampling $z$ from variational distribution $q(z|\lambda)$. However, this estimator tends to be noisy because of the variance of the samples, which can negatively affect its performance.

#### 3.2.2 Reparameterization Gradient

One of the notable approaches for reducing gradient variance is using the reparameterization gradient based on the reparameterization trick (Kingma & Welling, 2014). The reparameterization gradient expresses the distribution over $z$ as a deterministic transformation of other distribution over a noise variable $\epsilon$. Therefore, $z$ can be expressed $z = T(\epsilon; \lambda)$ where $\epsilon \sim p(\epsilon)$. By using the reparameterization trick, the ELBO is expressed as expectation with respect to $p(\epsilon)$ instead of $q(z|\lambda)$ and it’s derivation is given by

$$\nabla_\lambda L(\lambda) = \mathbb{E}_{p(\epsilon)}[\nabla_\lambda \log p(x, T(\epsilon; \lambda)) - \nabla_\lambda \log q(T(\epsilon; \lambda)|\lambda)].$$

(3)

Thus, the gradient estimator is obtained by approximating the expectation with independent random variables $\epsilon$ from $p(\epsilon)$.

### 3.3 Monte Carlo Variational Inference (MCVI)

In general setting of MCVI, the gradient of the ELBO is represented as an expectation $\nabla_\lambda L(\lambda) = \mathbb{E}[g_\lambda(\tilde{z})]$ over a random variable $\tilde{z}$. For the score function estimator, we choose $g$ in accordance with Equation (2) with $\tilde{z} = z$ as:

$$g_\lambda(z) = \nabla_\lambda \log q(z|\lambda)(\log p(x, z) - \log q(z|\lambda)).$$

(4)

For reparameterization estimator, we choose $g$ in accordance with Equation (3) with $\tilde{z} = \epsilon$ as:

$$g_\lambda(\epsilon) = \nabla_\lambda \log p(x, T(\epsilon; \lambda)) - \nabla_\lambda \log q(T(\epsilon; \lambda)|\lambda)).$$

(5)
This allows us to obtain a stochastic unbiased estimator of the gradient by an average over a finite sample $\{\tilde{z}_1, \tilde{z}_2, \cdots, \tilde{z}_N\}$ as:

$$\hat{\nabla}_\lambda L(\lambda) = \hat{g}_\lambda(\tilde{z}) = \frac{1}{N} \sum_{n=1}^{N} g_\lambda(\tilde{z}_n),$$

where $t$ represents the optimization step. Then, the ELBO can be optimized by using stochastic optimization (e.g. SGD, AdaGrad etc.). For example, optimization is achieved by iterating SGD updates with decreasing step size $\alpha_t$:

$$\lambda_{t+1} = \lambda_t - \alpha_t \hat{g}_\lambda(\tilde{z})$$

The convergence of the stochastic optimization scheme as in (7) tends to be slow when gradient estimators have a high variance. Therefore, various approaches for reducing the gradient variance exist (e.g. control variates (Glasserman, 2003), Rao-Blackwellization (Ranganath et al., 2014), importance sampling (Ruiz et al., 2016; Sakaya & Klami, 2017; Li et al., 2018), and others (Miller et al., 2017; Titsias & Lázaro-Gredilla, 2015)). However, these variance reduction techniques do not improve the $O(N^{-1})$ rate of the MSE of the estimator, except under some restricted conditions (Oates et al., 2017; Miller et al., 2017).

### 4 Multi-level Monte Carlo Variational Inference (MLMCVI)

In this section, we introduce MLMCVI.

#### 4.1 Multi-level Monte Carlo

Because of the linearity of expectation, given a sequence $P_0, P_1, \cdots, P_{L-1}$ which approximates $P_L$ with increasing accuracy, we have the simple identity:

$$\mathbb{E}[P_L] = \mathbb{E}[P_0] + \sum_{l=1}^{L} \mathbb{E}[P_l - P_{l-1}].$$

We can thus use the following unbiased estimator for $\mathbb{E}[P_L]$,

$$\mathbb{E}[P_L] \approx N_0^{-1} \sum_{n=1}^{N_0} P_0^{(0,n)} + \sum_{l=1}^{L} \left\{ N_l^{-1} \sum_{n=1}^{N_l} (P_l^{(l,n)} - P_{l-1}^{(l,n)}) \right\}$$

with the inclusion of $l$ in $(l,n)$ indicating that independent samples are used at each level of correction. This method is the previously mentioned MLMC method (Heinrich, 2001; Giles, 2008, 2015).

If we define $C_0, V_0$ to be the cost and variance of one sample of $P_0$, and $C_l, V_l$ to be the cost and variance of one sample of $P_l - P_{l-1}$, then the total cost and variance of the multi-level estimator are $\sum_{l=0}^{L} N_l C_l$ and $\sum_{l=0}^{L} N_l^{-1} V_l$, respectively.
Table 2: Order of variance and cost of each method

| Method | Variance     | Cost          |
|--------|--------------|---------------|
| MC     | $N^{-1}$     | $N$           |
| QMC    | $N^{-2} \log N^{2d-2}$ | $N \log N$   |
| MLMC   | $2^{-ln}N^{-1}$ | $2^n N$     |

In Table 2, we give the order of variance and cost of MC, QMC and MLMC on an unbiased estimator. Where $d$ is a dimension of parameter space and $\beta, \gamma$ is constant.

4.2 MLMCVI

We find from Equation (3) that reparameterization gradient can be applied to MLMC framework because expectation is always dependent on fixed distribution $p(\epsilon)$ and therefore can be used by the linearity of expectation. When $g_\lambda(\epsilon) = \nabla_\lambda \log p(x, T(\epsilon; \lambda)) - \nabla_\lambda \log q(T(\epsilon; \lambda)|\lambda)$, multi-level reparameterization gradient (MRG) in iteration $T$ of optimization is expressed,

$$\nabla_\lambda T L_{MRG}(\lambda) = \mathbb{E}_{p(\epsilon)}[g_{\lambda T}(\epsilon)] = \mathbb{E}_{p(\epsilon)}[g_{\lambda 0}(\epsilon)] + \sum_{t=1}^{T} \left( \mathbb{E}_{p(\epsilon)}[g_{\lambda t}(\epsilon) - g_{\lambda t-1}(\epsilon)] \right), \quad (10)$$

where $t, T$ is a natural number.

For the MCVI framework, we must construct an unbiased estimator in Equation (10). Thus, the following lemma is necessary.

**Lemma 1.** If the MRG estimator in iteration $T$ of optimization is constructed by,

$$\hat{\nabla}_\lambda T L_{MRG}(\lambda) = N_0^{-1} \sum_{n=1}^{N_0} g_{\lambda 0}(\epsilon^{(n)}) + \sum_{t=1}^{T} \left( N_t^{-1} \sum_{n=1}^{N_t} [g_{\lambda t}(\epsilon^{(n)}) - g_{\lambda t-1}(\epsilon^{(n)})] \right), \quad (11)$$

where $N_t (t = 0, 1, \ldots, T)$ is sample size for each iteration, then the MRG estimator is an unbiased estimator for $\nabla_\lambda T \mathcal{L}(\lambda)$.

**Proof.** Now we set

$$\hat{\nabla}_\lambda T L_{MRG}(\lambda) = \sum_{t=0}^{T} \left( N_t^{-1} \sum_{n=1}^{N_t} [g_{\lambda t}^{(n)}(\epsilon) - g_{\lambda t-1}^{(n)}(\epsilon)] \right) \text{ s.t. } g_{\lambda t-1}(\epsilon) = 0.$$
then,

\[
\mathbb{E}[\hat{\nabla}_T \mathcal{L}_{\text{MRG}}(\lambda)] = \mathbb{E}\left[ \sum_{t=0}^{T} \left( N_t^{-1} \sum_{n=1}^{N_t} [g^{(n)}_{\lambda_t}(\epsilon) - g^{(n)}_{\lambda_{t-1}}(\epsilon)] \right) \right]
\]

\[
= \sum_{t=0}^{T} \mathbb{E}\left[ N_t^{-1} \sum_{n=1}^{N_t} [g^{(n)}_{\lambda_t}(\epsilon) - g^{(n)}_{\lambda_{t-1}}(\epsilon)] \right]
\]

\[
= \sum_{t=0}^{T} N_t^{-1} \sum_{n=1}^{N_t} \mathbb{E}[g^{(n)}_{\lambda_t}(\epsilon) - g^{(n)}_{\lambda_{t-1}}(\epsilon)]
\]

\[
= \sum_{t=0}^{T} \mathbb{E}[g_{\lambda_t}(\epsilon) - g_{\lambda_{t-1}}(\epsilon)]
\]

\[
= \mathbb{E}[g_{\lambda_T}(\epsilon)].
\]

Thus,

\[
\mathbb{E}[\hat{\nabla}_T \mathcal{L}_{\text{MRG}}(\lambda)] = \mathbb{E}[g_{\lambda_T}(\epsilon)].
\]

Then, Equation (11) is an unbiased estimator for \( \nabla_\lambda \mathcal{L}(\lambda) \).

For algorithm derivation, it is important to estimate optimal sample size \( N_t \). When we defined optimal sample size to minimize the variance of the MRG estimator, the following theorem was derived.

**Theorem 1.** If we define \( C_0, V_0 \) to be the cost and variance of one sample of \( g_{\lambda_0}(\epsilon) \), and \( C_t, V_t \) to be the cost and variance of one sample of \( g_{\lambda_t}(\epsilon) - g_{\lambda_{t-1}}(\epsilon) \) in iteration \( t \), then the overall cost and variance of \( \hat{\nabla}_T \mathcal{L}_{\text{MRG}}(\lambda) \) is \( \sum_{t=0}^{T} N_t C_t \) and \( \sum_{t=0}^{T} N_t^{-1} V_t \), respectively. In this setting, the variance is minimized by choosing sample size as

\[
N_{t+1} = \sqrt{\frac{V_{t+1}/C_{t+1}}{V_t/C_t}} N_t.
\]  \hspace{1cm} (12)

(Proof sketch): This theorem is proved by solving the constrained optimization problem that is minimizing the overall variance as follows:

\[
\min_{N_t} \sum_{t=0}^{T} N_t^{-1} V_t \quad \text{s.t.} \quad \sum_{t=0}^{T} N_t C_t = M,
\]  \hspace{1cm} (13)

where \( M \) is constant.

The details of proof for Theorem 1 is in Appendix B.1 of supplementary materials.

Further, referring to Giles (2013), the following corollary is obtained straightforwardly with this theorem.

8
Corollary 1. The optimal number of $N_t$ is estimated by

$$N_t \propto 2^{-\delta t/2}N_0,$$  \hspace{1cm} (14)

where $N_0 = N$ is the initial number of Monte Carlo samples and $\delta = \beta + \gamma$.

Proof. By Equation (12), the estimated sample-size $N_t$ is expressed as

$$N_t = \sqrt{\frac{V_t/C_t}{V_{t-1}/C_{t-1}}} N_{t-1}
= \sqrt{\frac{V_t/C_t}{V_{t-1}/C_{t-1}}} \times \sqrt{\frac{V_{t-1}/C_{t-1}}{V_{t-2}/C_{t-2}}} \times \cdots \times \sqrt{\frac{V_1/C_1}{V_0/C_0}} N_0
= \sqrt{\frac{V_t/C_t}{V_0/C_0}} N_0.$$

We now use the fact that the order of variance and cost in MLMC method is $O(2^{-\beta t}N^{-1})$ and $O(2^{\gamma t}N)$. Then,

$$N_t = \sqrt{\frac{V_t/C_t}{V_0/C_0}} N_0
\propto \sqrt{\frac{2^{-\beta t}N^{-1}}{2^{\gamma t}N}} \cdot \frac{N}{N^t} N_0
= 2^{-(\beta + \gamma)t/2}N_0.$$

Thus, if we set $\delta = \beta + \gamma$, Equation (14) is obtained. $\square$

The estimated sample size $N_t$ must be positive integer. Thus, it is determined $N_t$ by using Equation (14) and floor function as follows,

$$N_t = \left\lfloor 2^{-\delta t/2}N_0 \right\rfloor.$$  \hspace{1cm} (15)

By this corollary, the optimal number of samples is estimated and decreased as optimization proceeds. However, optimization of the MRG estimator can be heavy because the number of levels in Equation (11) increases with the number of iterations. To handle this problem, we derived the following two lemmas.

Lemma 2. The MRG estimator in iteration $T$ can be represented as

$$\hat{\nabla}_{\lambda_T} \mathcal{L}_{\text{MRG}}(\lambda) = \hat{\nabla}_{\lambda_{T-1}} \mathcal{L}_{\text{MRG}}(\lambda) + N_T^{-1} \sum_{n=1}^{N_T} [g_{\lambda_T}(\epsilon^{(n)}) - g_{\lambda_{T-1}}(\epsilon^{(n)})].$$  \hspace{1cm} (16)

When $\hat{\nabla}_{\lambda_T} \mathcal{L}_{\text{MRG}}(\lambda)$ is expressed as Equation (16), the random variable in iteration $T$ is only included in $N_T^{-1} \sum_{n=1}^{N_T} [g_{\lambda_T}(\epsilon^{(n)}) - g_{\lambda_{T-1}}(\epsilon^{(n)})]$. Consequently, in stochastic optimization frameworks, parameter $\lambda_{T+1}$ must be updated only using this term. Then, we focused on SGD with a constance learning rate $\alpha$ and derived the update rule for the MRG estimator.
Lemma 3. In the SGD update rule, the following holds.

\[ \lambda_{t+1} = \lambda_t - \alpha \nabla \lambda_t \mathcal{L}_{\text{MRG}}(\lambda) \]

\[ = \lambda_t + (\lambda_t - \lambda_{t-1}) - \alpha N_t^{-1} \sum_{n=1}^{N_t} [g_{\lambda_t}(\epsilon^{(n)}) - g_{\lambda_{t-1}}(\epsilon^{(n)})]. \tag{17} \]

The proof of Lemma 2 and Lemma 3 is in Appendix B.2 and B.3 of supplementary materials.

From the above theorem and corollary, algorithm of MLMCVI is derivated as Algorithm 1, where \( \hat{g}_{\lambda_t}(\epsilon) = \nabla_{\lambda} \mathcal{L}_{\text{MRG}}(\lambda) \).

### Algorithm 1 Multi-level Monte Carlo Variational Inference

Require: Data \( x \), random variable \( \epsilon \sim p(\epsilon) \), transform \( z = T(\epsilon; \lambda) \), model \( p(x, z) \), variational family \( q(z|\lambda) \)

Ensure: Variational parameter \( \lambda^* \)

1. Initialize: \( N_0, \lambda_0, \alpha_0 \) and \( \delta \)
2. for \( t = 0 \) to \( T \) do
3:   if \( t = 0 \) then
4:     \( \epsilon^{(n)} \sim p(\epsilon) \) \( (n = 1, 2, \ldots, N_0) \) \( \triangleq \) sampling \( \epsilon \)
5:     \( \hat{g}_{\lambda_0}(\epsilon) = N_0^{-1} \sum_{n=1}^{N_0} g_{\lambda_0}(\epsilon^{(n)}) \) \( \triangleq \) calc. RG estimator
6:     \( \lambda_1 = \lambda_0 - \alpha_0 \hat{g}_{\lambda_0}(\epsilon) \) \( \triangleq \) grad-update
7:   else
8:     estimate \( N_t \) by (15)
9:     \( \epsilon^{(n)} \sim p(\epsilon) \) \( (n = 1, 2, \ldots, N_t) \) \( \triangleq \) sampling \( \epsilon \)
10:    \( \hat{g}_{\lambda_t}(\epsilon) = N_t^{-1} \sum_{n=1}^{N_t} [g_{\lambda_t}(\epsilon^{(n)}) - g_{\lambda_{t-1}}(\epsilon^{(n)})] \) \( \triangleq \) calc. multi-level term
11:   if \( \lambda_{t+1} \) is converged to \( \lambda^* \) then
12:      break
13:   end if
14: end if
15: end for
16: return \( \lambda^* \)

#### 4.3 Theoretical Properties

In the following theoretical analysis, we focused on SGD with a constant learning rate \( \alpha \). The optimal parameter \( \lambda^* \) is obtained with SGD using the update rule,

\[ \lambda_{t+1} = \lambda_t - \alpha \hat{g}_{\lambda_t}(\epsilon). \tag{18} \]

Bottou et al. (2016) provided many comprehensive theorems based on SGD in the stochastic approximation literature. In this context, Buchholz et al. (2018) proved the following upper bound on the norm of gradients in the situations where using RQMC method.

**Theorem 2** (Buchholz et al. (2018)). Let \( F \) be a function with Lipschitz continuous derivatives, i.e. there exists \( L > 0 \) s.t. \( \forall \lambda, \tilde{\lambda}, \| \nabla F(\lambda) - \nabla F(\tilde{\lambda}) \|^2 \leq L \| \lambda - \tilde{\lambda} \|^2 \), let \( U_N = \{u_1, \cdots, u_N\} \) be an RQMC sequence and let \( \forall \lambda, G : u \mapsto g_{\Gamma(u)}(\lambda) \) has cross partial derivatives of up to order \( d \). Let the constant learning rate \( \alpha < 2/L \)
and let $\mu = 1 - \alpha L / 2$. Then, $\forall \lambda, \text{tr} V_{U_N} [\hat{g}_\lambda (\epsilon)] \leq M_V \times r(N)$, where $M_V < \infty$ and $r(N) = O(N^{-2})$ and

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\|\nabla F(\lambda_t)\|_2^2] \leq \frac{1}{2\mu} \alpha L M_V r(N) + \frac{F(\lambda_1) - F(\lambda^*)}{\alpha \mu T}, \tag{19}$$

where $\lambda_t$ is iteratively defined in (18). Consequently,

$$\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\|\nabla F(\lambda_t)\|_2^2] \leq \frac{1}{2\mu} \alpha L M_V r(N). \tag{20}$$

Theorem 2 can be extended in the situations where using MLMC method on the assumption of Lipschitz continuous derivatives. We proved the following upper bound of the norm of gradients.

**Theorem 3.** Let $F$ be a function with Lipschitz continuous derivatives, i.e.:

$$\exists L > 0 \text{ s.t. } \forall \lambda, \tilde{\lambda} \quad \|\nabla F(\lambda) - \nabla F(\tilde{\lambda})\|_2 \leq L \|\lambda - \tilde{\lambda}\|_2.$$ 

Let the constant learning rate $\alpha < 2 / L$ and let $\mu = 1 - \alpha L / 2$. Then,

$$\forall \lambda_t, \text{tr} N [\hat{g}_{\lambda_t} (\epsilon)] \leq \kappa \cdot 2^{-\beta t} N^{-1},$$

where $\kappa, \beta$ is constant and $\kappa < \infty, \beta < \infty, t = 1, 2, \ldots, T$, and the upper bound of the norm of the gradient on SGD is

$$\frac{!}{!} \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\|\nabla F(\lambda_t)\|_2^2] \leq \frac{1}{T \alpha \mu} \left[ F(\lambda_1) - F(\lambda^*) \right] + \frac{\alpha L}{2 \mu (2^\beta - 1) T N} (1 - 2^{-\beta T}), \tag{21}$$

where $\lambda_t$ is iteratively defined in (18). Consequently,

$$\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\|\nabla F(\lambda_t)\|_2^2] = 0. \tag{22}$$

The proof of Theorem 3 is in Appendix B.4 of supplementary materials.

In Equation (21), the sum of the norm of gradients is bounded by the factor of optimization step $T$ and the order of MLMC variance $2^{-\beta T}$. Therefore, it converges to 0 asymptotically as the number of iterations increases (Equation (22)).

Further, to study the impact of variance reduction by using MLMC method on SGD with a fixed step size and strongly convex functions, we proved an upper bound on the optimality gap. The detail of this theorem is in Appendix B.5 of supplementary materials.
5 Experiments

We conducted experiments to analyze the effectiveness and to confirm the results of theoretical properties and the performance of our method. We used two different models: a hierarchical linear regression and a Bayesian neural network (BNN). We compared our method with benchmark methods in terms of the performance of prediction by using the converged value of the ELBO of the test dataset. We used the update-term variance to compare the performance of variance reduction because, in our method, the parameter is updated in a special manner.

Experimental Settings  In our experiments, we optimized the ELBO using the Adam optimizer (Kingma & Ba, 2015) with the initial step size set to 0.1. We reduced the learning rate by a factor of 0.9 every iterations. We calculated the gradients by using an automatic differentiation toolbox such as Pytorch. The test-ELBO values were calculated by 2000 MC samples, and the variance of the update-term was estimated by resampling MC samples and calculating the gradient and the learning rate 1000 times, and computing the empirical variance in each optimization step.

Benchmark methods  We used two benchmark methods : the vanilla MCVI based on MC sampling and the QMCVI based on RQMC sampling (Buchholz et al., 2018). We implemented QMCVI based on the code presented in the author’s Github\textsuperscript{1}.

Results  We found that our method resulted in a significantly closer to the optimal values and lower update-term variance compared to the benchmark methods. Futher, as stated in Corollary 1, our method can reduce the sampling cost, whereas the cost of the MC-based method is fixed and that of the RQMC-based method proposed by Buchholz et al. (2018) is increased.

5.1 Hierarchical Linear Regression

We began the experiments with a hierarchical linear regression on a toy data. The sampling process for output \( y_i \) is \( y_i \sim \mathcal{N}(x_i^T b_i, \epsilon) \), \( b_i \sim \mathcal{N}(\mu_\beta, \sigma_\beta) \). We set a Gaussian hyper prior on \( \mu_\beta \), and lognormal hyper priors on the variance of intercepts \( \sigma_\beta \) and the noise \( \epsilon \).

\textsuperscript{1}https://github.com/alexanderbuchholz/qmcvi-pytorch
The generative process of this model is as follows.

\[
egin{align*}
    \mu_{\beta} & \sim \mathcal{N}(0, 10^2), & \text{intercept hyper prior} \\
    \sigma_{\beta} & \sim \text{LogNormal}(0.5), & \text{intercept hyper prior} \\
    \epsilon & \sim \text{LogNormal}(0.5), & \text{noise} \\
    b_i & \sim \mathcal{N}(\mu_{\beta}, \sigma_{\beta}), & \text{intercepts} \\
    y_i & \sim \mathcal{N}(x_i^T b_i, \epsilon). & \text{output}
\end{align*}
\]

We set \( I = 100 \) and \( k = 10 \), where \( k \) denotes the dimension of the data \( x_i \) and \( I \) is the number of observations. In this settings, the dimension of the whole parameter space is \( d = I \times k + k + 2 = 1012 \), and we approximate it by using a variational diagonal Gaussian distribution.

We optimized the ELBO based on the reparameterization gradient estimator by using the Adam optimizer (Kingma & Ba, 2015). We compared the MC- and RQMC-based approaches using 10 and 100 samples with our MLMC-based approach using 10 and 100 MC samples. In the optimization step, we set the hyper parameter \( \delta \) for sample size estimation to 0.005.

The results are shown in Figure 1. We found that our method using \( N = 10, 50 \) samples (dashed and solid blue line) gets closer to the optimum value than the benchmark methods do using \( N = 50 \) samples. In addition, our method significantly reduces variance of the update-terms calculated from reparameterization gradient estimator. Further, our method achieved better predictive performance and variance reduction while reducing the cost of sampling (See Figure 2).

Figure 1: Hierarchical Linear Regression: experiments 5.1: Left is the ELBO value of test data using Adam optimizer with the MC-, RQMC-, and MLMC-based reparameterization gradient estimator (higher is better). Right is the log-scale empirical variance of update-term on each iteration (lower is better). It shows that the stability of convergence in our method using 10 and 100 MC samples (dashed and solid blue line) is better than MC- and RQMC-based method. Further, our method converges closer to the optimal value than the benchmark methods do, while having lower update-term variance.
5.2 Bayesian Neural Network (BNN)

As a second example, we conducted experiments with the proposed and benchmark methods in the context of a BNN. The network consisted of a 50-unit hidden layer with ReLU activations. We set a normal prior over each weight, and placed an inverse Gamma hyper prior over each weight prior. We also set an inverse Gamma prior over the observation variance.

The generate process is as follows.

\[
\alpha \sim \text{Gamma}(1, 0.1), \quad \text{weight hyper prior}
\]
\[
\tau \sim \text{Gamma}(1, 0.1), \quad \text{noise hyper prior}
\]
\[
w_i \sim \mathcal{N}(0, 1/\alpha), \quad \text{weights}
\]
\[
y \sim \mathcal{N}(\phi(x, w), 1/\tau). \quad \text{output distributions}
\]

In this settings, \( \phi(x, w) \) is a multi-layer perceptron which maps input data \( x \) to output \( y \) by using the set of weights \( w \). We express the set of parameters as \( \theta := (w, \alpha, \tau) \). The model exhibits a posterior of dimension \( d = 653 \), and was applied to a 100-row dataset subsampled from the wine dataset in the UCI repository\(^2\).

We approximated the posterior by using a variational diagonal Gaussian distribution and we set the hyper parameter \( \delta \) for sample size estimation to 0.005.

The results are shown in Figure 3. We found that our method using \( N = 10, 50 \) samples (dashed and solid blue line) also gets closer to the optimum value than the benchmark methods do using \( N = 50 \) samples. In addition, our method significantly reduces variance of the update-terms calculated from reparameterization gradient estimator. Furthermore, the performance of prediction and variance reduction of our method is better while reducing the cost of sampling (See Figure 4).

\(^2\)https://archive.ics.uci.edu/ml/datasets/Wine+Quality
Figure 3: Bayesian neural network: experiments 5.2: Left is the ELBO value of test data using Adam optimizer with the MC-, RQMC-, and MLMC-based reparameterization gradient estimator (higher is better). Right is the log-scale empirical variance of update-term on each iteration (lower is better). It shows that the stability of convergence in our method using 10 and 50 MC samples (dashed and solid blue line) is better than MC- and RQMC-based method. Further, our method converges closer to the optimal value than the benchmark methods do, while having lower update-term variance.

Figure 4: Bayesian neural network: the number of samples in experiments 5.2 when we set $\delta = 0.005$. Our method reduces the cost of sampling per iteration.
6 Conclusion

We proposed MLMCVI, a novel framework of variance and cost reduction for MCVI with reparameterization gradient estimator that uses MLMC method. Under MLMCVI framework, the optimal number of samples and the update scheme are naturally derived, and they provide the minimum total variance per optimization steps. Further, our method has a theoretical guarantees, which is that the norm of the gradient provably converges to 0 under the assumptions: Lipschitz continuous derivatives and SGD with constant learning rate.

We also confirmed that our method achieves better performances of prediction and variance reduction by two experiments. Our future research direction is to determine how to set $\delta$ because it can be affects the efficiency of variance reduction.

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A The Detail Information on MLMC

We introduce the detail information on MLMC to help understand background, our method, algorithm and theoretical analysis.

A.1 Multi-level Monte Carlo (MLMC)

As we showed in Section 4.1., given a sequence \( P_0, P_1, \cdots, P_{L-1} \) which approximates \( P_L \) with increasing accuracy, we have the simple identity by linearity of expectation:

\[
E[P_L] = E[P_0] + \sum_{l=1}^{L} E[P_l - P_{l-1}].
\] (23)

So, we can use the following unbiased estimator for \( E[P_L] \),

\[
E[P_L] \approx N_0^{-1} \sum_{n=1}^{N_0} r_0^{(0,n)} + \sum_{l=1}^{L} \left\{ N_l^{-1} \sum_{n=1}^{N_l} (P_l^{(l,n)} - P_{l-1}^{(l,n)}) \right\}
\] (24)

with the inclusion of \( l \) in \((l, n)\) indicating that independent samples are used at each level of correction.

If \( Y \) is an approximation to \( E[P] \), then the mean squared error (MSE) is

\[
\text{MSE} \equiv E[(Y - E[P])^2] = V[Y] + (E[Y] - E[P])^2.
\] (25)

So, if \( Y \) is multi-level estimator

\[
Y = \sum_{l=0}^{L} Y_l, \quad Y_l = N_l^{-1} \sum_{n=1}^{N_l} (P_l^{(l,n)} - P_{l-1}^{(l,n)}),
\]

with \( P_{-1} \equiv 0 \), then

\[
E[Y] = E[P_L], \quad V[Y] = \sum_{l=0}^{L} N_l^{-1} V_l, \quad V_l \equiv V[P_l - P_{l-1}].
\]

To ensure that the MSE is less than \( \epsilon^2 \), it is important that \( V[Y] \) and \( (E[P_L] - P)^2 \) are both less than \( \frac{1}{2} \epsilon^2 \). According to this idea, we can see that the cost increases exponentially with level \( l \), while both the weak error \( E[Y] - E[P] \) and the multi-level correction of variance \( V_l \) decrease exponentially (Giles, 2008).

A.2 Control variates and Relationship to two-level MLMC

One of the classic method to reduce variance of Monte Carlo samples is using control variates method (Glasserman, 2003). When we want to estimate \( E[f] \) and there is a function \( h \) which is high correlated to \( f \) with a known expectation
\(E[h]\), we can use the unbiased estimator for \(E[f]\) based on \(N\) i.i.d samples \(\omega^{(n)}\) as follows,

\[
N^{-1} \sum_{n=1}^{N} \{ f(\omega^{(n)}) - a(h(\omega^{(n)}) - E[h]) \}. \tag{26}
\]

Then, variance is expressed as: \(V[f(\omega^{(n)})] = V[f(\omega^{(n)})] + a^2 V[h(\omega^{(n)})] - 2a \text{Cov}(f(\omega^{(n)}), h(\omega^{(n)}))\) and the optimal value for \(a\) is \(\rho \sqrt{V[f]/V[h]}\), where \(\rho\) is the correlation between \(f\) and \(h\). So, the variance of this estimator is reduced by factor \(1 - \rho^2\) (see Giles (2008)).

Two-level MLMC is very similar to this method. According to Giles (2013), if we want to estimate \(E[P_1]\) but it is much cheaper to simulate \(P_0\) which approximates \(P_1\), then since

\[
E[P_1] = E[P_0] + E[P_1 - P_0], \tag{27}
\]

we can use the unbiased two-level estimator

\[
N_0^{-1} \sum_{n=1}^{N_0} P_n^{(n)} + N_1^{-1} \sum_{n=1}^{N_1} (P_1^{(n)} - P_0^{(n)}). \tag{28}
\]

There are two different points from control variates methods. One is that the value of \(E[P_0]\) is unknown, so has to be estimated. The other is using \(a = 1\).

### A.3 Theoretical Property on MLMC

The following theorem is important to understand how to set hyperparameter \(\delta = \beta + \gamma\) on our algorithm.

**Theorem 4** (Giles (2008)). Let \(P\) denote a random variable, and let \(P_l\) denote the corresponding level \(l\) numerical approximation. If there exist independent estimators \(Y_l\) based on \(N_l\) Monte Carlo samples, each with expected cost \(C_l\) and variance \(V_l\), and positive constants \(\alpha, \beta, \gamma, c_1, c_2, c_3\) such that \(\alpha \geq \frac{1}{2} \min(\beta, \gamma)\) and

1. \(|E[P_l - P]| \leq c_1 2^{-\alpha l}\)
2. \(E[Y_l] = \begin{cases} E[P_0], & (l = 0) \\ E[P_l - P_{l-1}], & (l > 0) \end{cases}\)
3. \(V_l \leq c_2 2^{-\beta l}\)
4. \(C_l \leq c_3 2^{-\gamma l}\),

then there exists a positive constant \(c_4\) such that for any \(\epsilon < e^{-1}\) there are values \(L\) and \(N_l\) for which the multi-level estimator \(Y = \sum_{l=0}^{L} Y_l\) has a mean-squared-error with bound

\[
\text{MSE} = E[(Y - E[P])^2] < \epsilon^2 \tag{29}
\]
with a computational complexity $C$ with bound

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

B Proofs of Lemmas and Theorems

B.1 Proof of Theorem 1

Proof. Now we consider the constrained minimization problem as follow,

$$\min_{N_t} \sum_{t=0}^{T} N_t^{-1} V_t \quad \text{s.t.} \quad \sum_{t=0}^{T} N_t C_t = M,$$

where $M$ is constant.

For a fixed cost, the variance is minimized by choosing $N_t$ to minimize

$$f = \sum_{t=0}^{T} N_t^{-1} V_t + \mu^2 \left( \sum_{t=0}^{T} N_t C_t - M \right)$$

for some value of the Lagrange multiplier $\mu^2 (\mu > 0)$. Thus,

$$\frac{\partial f}{\partial N_t} = -N_t^{-2} V_t + \mu^2 C_t = 0$$

$$\Rightarrow N_t^2 = \frac{1}{\mu^2} \frac{V_t}{C_t}$$

$$\therefore N_t = \frac{1}{\mu} \sqrt{\frac{V_t}{C_t}} \quad (\because \mu > 0, C_t > 0, V_t > 0).$$

(31)

Now, we substitute (31) for (30),

$$f = \sum_{t=0}^{T} \mu \sqrt{V_t C_t} + \sum_{t=0}^{T} \mu \sqrt{V_t C_t} - \mu^2 M$$

$$= 2\mu \sum_{t=0}^{T} \sqrt{V_t C_t} - \mu^2 M.$$  

(32)

We differentiate (32) by $\mu$,

$$\frac{\partial f}{\partial \mu} = 2 \sum_{t=0}^{T} \sqrt{V_t C_t} - 2\mu M = 0$$

$$\Rightarrow \mu = \frac{1}{M} \sum_{t=0}^{T} \sqrt{V_t C_t}.$$  

(33)
Thus, we substitute (33) for (31),

$$N_t = \frac{M}{\sum_{t=0}^{T} \sqrt{V_tC_t}} \sqrt{\frac{V_t}{C_t}}. \quad (34)$$

We consider the ratio of $N_{t+1}$ to $N_t$,

$$\frac{N_{t+1}}{N_t} = \frac{M}{\sum_{t=0}^{T} \sqrt{V_tC_t}} \sqrt{\frac{V_{t+1}}{C_{t+1}}} \cdot \frac{\sum_{t=0}^{T} \sqrt{V_tC_t}}{M \sqrt{\frac{V_t}{C_t}}} \cdot \frac{\sqrt{C_t}}{\sqrt{V_t}}.$$ 

According to this result, the optimal sample size $N_{t+1}$ is,

$$N_{t+1} = \sqrt{\frac{V_{t+1}/C_{t+1}}{V_t/C_t}} N_t.$$

\[\Box\]

**B.2 Proof of Lemma 2**

*Proof.* Because of the linearity of expectation, multi-level reparameterization gradient in iteration $T$ of optimization is expressed

$$\nabla_{\lambda_T} \mathcal{L}_{\text{MRG}}(\lambda) = \mathbb{E}_{p(\epsilon)}[g_{\lambda_T}(\epsilon)]$$

$$= \mathbb{E}_{p(\epsilon)}[g_{\lambda_0}(\epsilon)] + \sum_{t=1}^{T} \mathbb{E}_{p(\epsilon)}[g_{\lambda_t}(\epsilon) - g_{\lambda_{t-1}}(\epsilon)]$$

$$= \left( \mathbb{E}_{p(\epsilon)}[g_{\lambda_0}(\epsilon)] + \sum_{t=1}^{T-1} \mathbb{E}_{p(\epsilon)}[g_{\lambda_t}(\epsilon) - g_{\lambda_{t-1}}(\epsilon)] \right)$$

$$+ \mathbb{E}_{p(\epsilon)}[g_{\lambda_T}(\epsilon) - g_{\lambda_{T-1}}(\epsilon)].$$

Then, by constructing the unbiased estimator in the above equation, we obtain

$$\hat{\nabla}_{\lambda_T} \mathcal{L}_{\text{MRG}}(\lambda) = \hat{\nabla}_{\lambda_{T-1}} \mathcal{L}_{\text{MRG}}(\lambda) + N_{T-1} \sum_{n=1}^{N_T} [g_{\lambda_T}(\epsilon^{(n)}) - g_{\lambda_{T-1}}(\epsilon^{(n)})].$$

\[\Box\]
B.3 Proof of Lemma 3

Proof. From Theorem 2 and the update rule in iteration $t - 1$,

$$
\lambda_t - \alpha \tilde{\nabla}_{\lambda_t} \mathcal{L}_{\text{MRG}}(\lambda)
= \lambda_t - \alpha \left( \tilde{\nabla}_{\lambda_{t-1}} \mathcal{L}_{\text{MRG}}(\lambda) + N_t^{-1} \sum_{n=1}^{N_t} [g_{\lambda_t}(\epsilon(n)) - g_{\lambda_{t-1}}(\epsilon(n))] \right)
= \lambda_t - \alpha \tilde{\nabla}_{\lambda_{t-1}} \mathcal{L}_{\text{MRG}}(\lambda) - \alpha N_t^{-1} \sum_{n=1}^{N_t} [g_{\lambda_t}(\epsilon(n)) - g_{\lambda_{t-1}}(\epsilon(n))]
= \lambda_t + (\lambda_t - \lambda_{t-1}) - \alpha N_t^{-1} \sum_{n=1}^{N_t} [g_{\lambda_t}(\epsilon(n)) - g_{\lambda_{t-1}}(\epsilon(n))].
$$

We obtain relationship (17).

B.4 Proof of Theorem 3

Proof. By the Lipschitz assumption, we have that $F(\lambda) \leq F(\bar{\lambda}) + \nabla F(\bar{\lambda})^\top (\lambda - \bar{\lambda}) + \frac{1}{2} L \| \lambda - \bar{\lambda} \|_2^2, \forall \lambda, \bar{\lambda}$. By using the SGD update-rule, we obtain $\lambda_{t+1} - \lambda_t = -\alpha \tilde{g}_{\lambda_t}(\epsilon)$. Thus,

$$
F(\lambda_{t+1}) - F(\lambda_t)
\leq \nabla F(\lambda_t)^\top (\lambda_{t+1} - \lambda_t) + \frac{1}{2} L \| \lambda_{t+1} - \lambda_t \|_2^2
= -\alpha \nabla F(\lambda_t)^\top \tilde{g}_{\lambda_t}(\epsilon) + \frac{\alpha^2 L}{2} \| \tilde{g}_{\lambda_t}(\epsilon) \|_2^2.
$$

Taking expectation by $\epsilon \sim p(\epsilon)$, we obtain

$$
\mathbb{E}_{p(\epsilon)}[F(\lambda_{t+1}) - F(\lambda_t)]
\leq -\alpha \mathbb{E}_{p(\epsilon)}[\nabla F(\lambda_t)^\top \tilde{g}_{\lambda_t}(\epsilon)] + \frac{\alpha^2 L}{2} \mathbb{E}_{p(\epsilon)}[\| \tilde{g}_{\lambda_t}(\epsilon) \|_2^2].
$$

Using the fact that $\mathbb{E}_{p(\epsilon)}[\| \tilde{g}_{\lambda_t}(\epsilon) \|_2^2] = V[\tilde{g}_{\lambda_t}(\epsilon)] + \mathbb{E}_{p(\epsilon)}[\| \tilde{g}_{\lambda_t}(\epsilon) \|_2^2]$ and after exploiting the fact that $\mathbb{E}_{p(\epsilon)}[\tilde{g}_{\lambda_t}(\epsilon)] = \nabla F(\lambda_t)$, we obtain

$$
\mathbb{E}_{p(\epsilon)}[F(\lambda_{t+1}) - F(\lambda_t)]
\leq -\alpha \| \nabla F(\lambda_t) \|_2^2 + \frac{\alpha^2 L}{2} \left( V[\tilde{g}_{\lambda_t}(\epsilon)] + \mathbb{E}_{p(\epsilon)}[\| \tilde{g}_{\lambda_t}(\epsilon) \|_2^2] \right)
= \frac{\alpha^2 L}{2} V[\tilde{g}_{\lambda_t}(\epsilon)] + \left( \frac{\alpha^2 L}{2} - \alpha \right) \| \nabla F(\lambda_t) \|_2^2.
$$

(35)

Summing for $t = 1, 2, \ldots, T$ and we take the total expectation,

$$
\mathbb{E}[F(\lambda_T) - F(\lambda_1)]
\leq \frac{\alpha^2 L}{2} \sum_{t=1}^{T} \mathbb{E}[V[\tilde{g}_{\lambda_t}(\epsilon)]] + \left( \frac{\alpha^2 L}{2} - \alpha \right) \sum_{t=1}^{T} \mathbb{E}[\| \nabla F(\lambda_t) \|_2^2].
$$

24
We use the fact that $F(\lambda^*) - F(\lambda_1) \leq \mathbb{E}[F(\lambda_T) - F(\lambda_1)]$, where $\lambda_1$ is deterministic and $\lambda^*$ is the true minimizer. Dividing the inequality by $T$, we have

$$\frac{1}{T}[F(\lambda^*) - F(\lambda_1)] \leq \frac{\alpha^2 L}{2} \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[V[\hat{g}_{\lambda_t}(\epsilon)]] + \left(\frac{\alpha^2 L}{2} - \alpha\right) \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\|\nabla F(\lambda_t)\|^2].$$

By using $\alpha < 2/L$ and $\mu = 1 - \alpha L/2$, we obtain

$$\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\|\nabla F(\lambda_t)\|^2] \leq \frac{1}{T\alpha\mu} [F(\lambda_1) - F(\lambda^*)] + \frac{\alpha L}{2\mu T} \sum_{t=1}^{T} \mathbb{E}[V[\hat{g}_{\lambda_t}(\epsilon)]].$$

(36)

We now use $V[\hat{g}_{\lambda_t}(\epsilon)] \leq \kappa \cdot 2^{-\beta t} N^{-1}$ for all $t$. Then,

$$\sum_{t=1}^{T} \mathbb{E}[V[\hat{g}_{\lambda_t}(\epsilon)]] \leq \sum_{t=1}^{T} \mathbb{E}[\kappa \cdot 2^{-\beta t} N^{-1}]$$

$$= \frac{\kappa}{N} \sum_{t=1}^{T} \mathbb{E}[2^{-\beta t}]$$

$$= \frac{\kappa}{N} \sum_{t=1}^{T} 2^{-\beta t}$$

$$= \frac{\kappa}{N} \frac{2^{-\beta T} - 1}{2^{-\beta} - 1}$$

$$= \frac{\kappa}{N} \frac{1 - 2^{-\beta T}}{2^{\beta} - 1}.$$ 

(37)

By substituting (37) for (36), Equation (21) is obtained. Straightforwardly, we obtain Equation (22) by taking $T \to \infty$ on Equation (21).

B.5 Theorem for an upper bound on the optimality gap

We proved the following upper bound on the optimality gap to study the impact of variance reduction by using MLMC method on SGD with a fixed step size and strongly convex functions.

**Theorem 5.** Let $F$ have Lipschitz continuous derivatives and be a strongly convex function, i.e. there exist a constant $c > 0$ s.t.:

$$\forall \lambda, \tilde{\lambda} \quad F(\tilde{\lambda}) \geq F(\lambda) + \nabla F(\lambda)^\top (\lambda - \tilde{\lambda}) + \frac{1}{2} c \|\lambda - \tilde{\lambda}\|^2.$$
Let the constant learning rate $\alpha < \frac{1}{2e}$ and $\alpha < \frac{2}{T}$. Then,

$$\forall \lambda_t, \quad V[\hat{g}_{\lambda_t}(\epsilon)] \leq \kappa \cdot 2^{-\beta t} N^{-1},$$

where $\kappa, \beta$ is constant and $\kappa < \infty, \beta < \infty, t = 1, 2, \ldots, T$, and the expected optimality gap satisfies, $\forall t \geq 0$,

$$E[F(\lambda_{t+1}) - F(\lambda^*)] \leq \left[\left(\frac{\alpha^2 L}{2} - \alpha\right)2c + 1\right]E[F(\lambda_t) - F(\lambda^*)] + \frac{\alpha^2 \kappa L}{2^{1+\beta t} N}.$$  \tag{38}$$

Consequently,

$$\lim_{T \rightarrow \infty} E[F(\lambda_T) - F(\lambda^*)] = 0.$$ \tag{39}$$

Proof. Based on Equation (35) from the previous proof of Theorem 3, we got

$$E_p(\epsilon)[F(\lambda_{t+1}) - F(\lambda_t)] \leq \frac{\alpha^2 L}{2} V[\hat{g}_{\lambda_t}(\epsilon)] + \left(\frac{\alpha^2 L}{2} - \alpha\right)\|\nabla F(\lambda_t)\|^2_2$$

$$\leq \frac{\alpha^2 L}{2} V[\hat{g}_{\lambda_t}(\epsilon)] + \left(\frac{\alpha^2 L}{2} - \alpha\right)2c(F(\lambda_t) - F(\lambda^*)).$$

by using the fact that $\frac{\alpha L}{2} - 1 < 0$ and the optimality gap can be upper bounded by the gradient in the current point $\lambda$, e.g. $2c(F(\lambda) - F(\lambda^*)) \leq \|\nabla F(\lambda)\|^2_2, \forall \lambda$ on the strong convexity situation. By subtracting $F(\lambda^*)$ from both sides, taking total expectations and rearranging, we obtain

$$E[F(\lambda_{t+1}) - F(\lambda^*)] \leq \frac{\alpha^2 L}{2} E[V[\hat{g}_{\lambda_t}(\epsilon)]] + \left[\left(\frac{\alpha^2 L}{2} - \alpha\right)2c + 1\right]E[F(\lambda_t) - F(\lambda^*)] \tag{40}$$

$$\leq \left[\left(\frac{\alpha^2 L}{2} - \alpha\right)2c + 1\right]E[F(\lambda_t) - F(\lambda^*)] + \frac{\alpha^2 \kappa L}{2N} 2^{-\beta t}.$$ 

This is the result (38). Now we define $\delta = \left[\left(\frac{\alpha^2 L}{2} - \alpha\right)2c + 1\right]$. We add

$$\frac{\alpha^2 L E[V[\hat{g}_{\lambda_t}(\epsilon)]]}{2(\delta - 1)}$$

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to both sides of the equation (40). This yields

\[ E[F(\lambda_{t+1}) - F(\lambda^*)] + \frac{\alpha^2 L E[V[\hat{g}_{\lambda_t}(\epsilon)]]}{2(\delta - 1)} \]

\[ \leq \frac{\alpha^2 L}{2} E[V[\hat{g}_{\lambda_t}(\epsilon)]] + \delta E[F(\lambda_t) - F(\lambda^*)] \]

\[ + \frac{\alpha^2 L E[V[\hat{g}_{\lambda_t}(\epsilon)]]}{2(\delta - 1)} \]

\[ \leq \delta \left( E[F(\lambda_t) - F(\lambda^*)] + \frac{\alpha^2 L E[V[\hat{g}_{\lambda_t}(\epsilon)]]}{2(\delta - 1)} \right). \]

Now we show that \( \delta < 1 \). We formally define

\[ \delta = \left( \frac{\alpha L}{2} - 1 \right) 2\alpha c + 1, \]
and as \( \frac{\alpha L}{2} < 1 \) we obtain \( \delta < 1 - 2\alpha c \). Using \( \alpha < 1/2c \) we obtain \( \delta < 1 \). Thus, we have a contracting equation, when iterating over \( t \),

\[ E[F(\lambda_{t+1}) - F(\lambda^*)] \]

\[ \leq \delta^t \left( F(\lambda_1) - F(\lambda^*) + \frac{\alpha^2 L E[V[\hat{g}_{\lambda_t}(\epsilon)]]}{2(\delta - 1)} \right) \]

\[ + \frac{\alpha^2 L E[V[\hat{g}_{\lambda_t}(\epsilon)]]}{2(\delta - 1)} \]

\[ \leq \delta^t \left( F(\lambda_1) - F(\lambda^*) + \frac{\alpha^2 \kappa L}{2^{1+\beta t}(\delta - 1)N} \right) \]

\[ + \frac{\alpha^2 \kappa L}{2^{1+\beta t}(1 - \delta)N}. \]

After simplification, we have

\[ E[F(\lambda_{t+1}) - F(\lambda^*)] \]

\[ \leq \delta^t \left( F(\lambda_1) - F(\lambda^*) + \frac{\alpha \kappa L}{(2\alpha c - 4c)2^{2\beta t}N} \right) \]

\[ + \frac{\alpha \kappa L}{(4c - 2\alpha c L)2^{2\beta t}N}. \]

Thus, if we take \( t + 1 = T \to \infty \), we obtain

\[ \lim_{T \to \infty} E[F(\lambda_T) - F(\lambda^*)] = 0. \]

In the above theorem, Equation (38) shows that the expected optimality gap between \( \lambda_T \) in iteration \( T \) and the true optimal \( \lambda^* \) is upper bounded by a factor of the order of variance \( 2^{-\beta t} \). Therefore, the estimated parameter converges to the optimal value asymptotically (Equation (39)).