Subsampled Stochastic Variance-Reduced Gradient Langevin Dynamics

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Abstract

Stochastic variance-reduced gradient Langevin dynamics (SVRG-LD) was recently proposed to improve the performance of stochastic gradient Langevin dynamics (SGLD) by reducing the variance of the stochastic gradient. In this paper, we propose a variant of SVRG-LD, namely SVRG-LD+, which replaces the full gradient in each epoch with a subsampled one. We provide a nonasymptotic analysis of the convergence of SVRG-LD+ in 2-Wasserstein distance, and show that SVRG-LD+ enjoys a lower gradient complexity than SVRG-LD, when the sample size is large or the target accuracy requirement is moderate. Our analysis directly implies a sharper convergence rate for SVRG-LD, which improves the existing convergence rate by a factor of $\kappa^{1/6} n^{1/6}$, where $\kappa$ is the condition number of the log-density function and $n$ is the sample size. Experiments on both synthetic and real-world datasets validate our theoretical results.

1 INTRODUCTION

Markov chain Monte Carlo (MCMC) methods used for posterior sampling have achieved great successes in Bayesian machine learning and Bayesian statistics. Recently, a family of gradient-based MCMC algorithms derived from Langevin dynamics (Parisi, 1981) has become a research hotspot in both Bayesian sampling (Welling & Teh, 2011; Ahn et al., 2012; Wang et al., 2013; Dalalyan, 2014) and optimization (Raginsky et al., 2017; Zhang et al., 2017; Xu et al., 2017). The Langevin dynamics is defined by the following stochastic differential equation (SDE)

$$
\text{d}X_t = -\nabla f(X_t) \text{d}t + \sqrt{2} \text{d}B_t,
$$

(1.1)

where $X_t \in \mathbb{R}^d$ is a $d$-dimensional stochastic process, $B_t \in \mathbb{R}^d$ represents the standard $d$-dimensional Brownian motion and $-\nabla f(x)$ is called the drift coefficient. It can be shown that the Langevin dynamics converges to an invariant stationary distribution $\pi \propto \exp(-f)$ (Chang et al., 1987). Based on this observation, various Langevin dynamics based numerical algorithms (Roberts & Tweedie, 1996; Mattingly et al., 2002) have been designed to sample from the target distribution $\pi$. Directly applying Euler-Maruyama discretization (Kloeden & Platen, 1992) to SDE (1.1) gives rise to

$$
x_{k+1} = x_k - \nabla f(x_k) \eta + \sqrt{2\eta} \epsilon_k,
$$

(1.2)

where $\eta$ denotes the step size, and $\epsilon_k \sim N(0, I_{d \times d})$ is a $d$-dimensional standard Gaussian random vector. The sampling algorithm using (1.2) as its update formula is typically known as the Langevin Monte Carlo (LMC) algorithm, which has been extensively studied when the target distribution is both log-smooth and strongly log-concave, or even log-Hessian-Lipschitz (Dalalyan, 2014; Durmus & Moulines, 2016; Dalalyan, 2017; Dalalyan & Karagulyan, 2017).

On the other hand, modern machine learning problems often involve an extremely large amount of data. Suppose the dataset consists of $n$ observations, it is often assumed that the function $f$ in the drift term of (1.1) can be written as an average of $n$ finite component functions, i.e.,

$$
f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x),
$$

(1.3)

where each $f_i$ is smooth and $f$ is strongly convex. When $n$ is very large, the LMC algorithm can be inefficient
since the gradient evaluation is computationally very expensive. Following the same idea in stochastic optimization, Welling & Teh (2011) proposed the stochastic gradient Langevin dynamics (SGLD) algorithm by replacing the full gradient in (1.2) with a stochastic gradient computed only on a minibatch of data. The SGLD algorithm has been successfully applied to Bayesian learning (Welling & Teh, 2011; Ahn et al., 2012) and training deep neural networks (Chaudhari et al., 2016; Ye et al., 2017), because it can dramatically decrease the number of stochastic gradient evaluations and save a lot of computation in practice. Nevertheless, the convergence rate of SGLD is much slower than LMC, which may lead to a worse runtime complexity in certain regime. Regarding the true computational cost of SGLD, Nagapetyan et al. (2017) argued that SGLD is at most better by a constant factor relative to an Euler discretization with full gradients, and raised questions about the good performance of SGLD under the big-data setting. In order to fairly evaluate the performances of stochastic algorithms, one often uses gradient complexity to indicate the efficiency of a sampling algorithm in large scale machine learning problems. When f is smooth, strongly convex and Hessian Lipschitz, Dalalyan & Karagulyan (2017) proved that the gradient complexity of LMC to converge to the stationary distribution π in 2-Wasserstein distance is \(O(n\kappa d^{1/2}/\epsilon)\), where \(\epsilon\) represents the target accuracy and \(\kappa\) is the condition number of \(f\). In comparison, the gradient complexity of SGLD is \(\tilde{O}(\kappa^2 d\sigma^2 / \epsilon^2)\) (Dalalyan, 2017; Dalalyan & Karagulyan, 2017), which is slower than LMC when \(n \lesssim d^{1/2} \sigma^2 / \epsilon\), where \(d\sigma^2\) is an upper bound on the variance of the stochastic gradient.

In order to achieve the best of both worlds, i.e., save the gradient computation of LMC as well as boost the convergence rate of SGLD, Dubey et al. (2016) proposed stochastic variance-reduced gradient Langevin dynamics (SVRG-LD) and stochastic average gradient Langevin dynamics (SAGA-LD), which adapts the idea of variance reduction in stochastic optimization such as SVRG (Johnson & Zhang, 2013; Allen-Zhu & Hazan, 2016; Reddi et al., 2016) and SAGA (Defazio et al., 2014) to gradient-based Monte Carlo methods. However, Dubey et al. (2016) only investigated the performance of both algorithms in terms of mean square error (MSE) of the averaged sample path. Baker et al. (2017) applied zero variance control variates to stochastic MCMC method, and showed that such technique is able to reduce the computational cost of stochastic gradient Langevin dynamics to \(O(1)\). Recently, Chatterji et al. (2018) analyzed the convergence rates of SVRG-LD and SAGA-LD to the stationary distribution in 2-Wasserstein distance, and showed that SAGA-LD has a lower gradient complexity compared with SVRG-LD. However, they also observed that when considering low target accuracy regime or the samples size is very large, both of these variance reduction based LMC algorithms perform worse than SGLD, which can converge even within a single data pass. However, their theoretical results suggest that SAGA-LD attains a faster convergence rate than SVRG-LD, which is not consistent with the convergence analyses of SAGA and SVRG for optimization, where both methods have been proved to have the same gradient complexity (Johnson & Zhang, 2013; Defazio et al., 2014). Therefore, Chatterji et al. (2018) raised a question that whether SVRG is less suited than SAGA to work with sampling methods.

In this paper, in order to overcome the shortcomings of SVRG-LD and SAGA-LD, we propose a variant of SVRG-LD, namely SVRG-LD+, by replacing the full gradient computation in the outer loop of SVRG-LD with a subsampled one. The idea of using subsampled gradient instead of full gradient in variance reduction algorithms is originated from the recent work on variance reduction for stochastic optimization (Harikandeh et al., 2015; Lei & Jordan, 2016; Lei et al., 2017), and has also been adopted to Langevin based algorithm by Chen et al. (2017). It is worthy noting that the algorithm proposed in Chen et al. (2017), namely practical vrSG-MCMC, is similar to our algorithm. Nevertheless, the practical SVRG-LD algorithm needs to output all the iterates because its theoretical guarantee is on the sample path. In contrast, our algorithm only needs to output the last iterate, because our theory holds for the last iterate.

### 1.1 OUR CONTRIBUTIONS

We highlight the major contributions of our work as follows.

- We propose the SVRG-LD+ algorithm and analyze its convergence rate to the target distribution in Wasserstein distance. Specifically, we prove that the SVRG-LD+ algorithm requires \(O((n + \kappa^3/2 n^{1/2} d^{1/2}/\epsilon) \land \kappa^2 d \sigma^2 / \epsilon^2)\) stochastic gradient evaluations to converge to the target distribution in 2-Wasserstein distance within \(\epsilon\)-accuracy. Our result suggests that when the sample size \(n\) is large or the target accuracy \(\epsilon\) is moderate, the gradient complexity of SVRG-LD+ is better than that of SVRG-LD and SAGA-LD (Chatterji et al., 2018). In addition, the gradient complexity of SVRG-LD+ is never worse than that of SGLD.

- Since SVRG-LD is a special case of SVRG-LD+ when the subsampled gradient is chosen to be the full gradient, our analysis of SVRG-LD+ directly implies a sharp convergence rate of SVRG-LD,
which improves the recent result in Chatterji et al. (2018) by a factor of \( n^{1/6} n^{1/6} \), and matches the convergence rate of SAGA-LD (Chatterji et al., 2018). This suggests that both SVRG and SAGA are equally suited to work with sampling methods, and therefore answers the question raised in (Chatterji et al., 2018). Our experiments on both synthetic and real data also show that SVRG-LD and SAGA-LD have comparable performance, which verifies our theory.

We summarize the gradient complexities of existing LMC methods in Table 1, from which we can see that SVRG-LD\(^+\) achieves the lowest gradient complexity among all methods. Detailed discussions will be provided in the main theory section.

1.2 ADDITIONAL RELATED WORK

Another line of research that is related to LMC is Hamiltonian Monte Carlo (HMC) method (Neal, 2011), which is based on Hamiltonian dynamics by introducing fictitious momentum variables. Recently, the HMC method has been widely studied and developed experimentally and theoretically. Specifically, Chen et al. (2014) proposed a stochastic gradient HMC (SG-HMC) algorithm and demonstrated its better performance than SGLD in learning Bayesian neural networks. Chen et al. (2015) conducted a comprehensive analysis for a family of SG-MCMC algorithms including SG-HMC in terms of MSE, and showed that SG-HMC attains a better performance than SGLD if adopting an appropriate discretization method. Ma et al. (2015) proposed a general framework to design samplers from the target distribution, and generated a new state-adaptive sampler on the Riemannian manifold. The nonasymptotic convergence analysis of HMC and SG-HMC was provided in Cheng et al. (2017), where the authors analyzed an underdamped Langevin MCMC algorithm and proved the convergence guarantees in 2-Wasserstein distance. Zou et al. (2018) proposed a stochastic variance-reduced HMC algorithm and proved its convergence rate in 2-Wasserstein distance. Li et al. (2018) analyzed the mean square error of the HMC based algorithm for different discretization schemes. Our work is focused on LMC and is complementary to this line of research.

1.3 NOTATION

We use \([n]\) to denote the index set \( \{1, \ldots, n\} \). For a random vector \( x_k \in \mathbb{R}^d \), we denote its probability distribution function by \( P(x_k) \). The 2-Wasserstein distance between two probability measures \( u \) and \( v \) is defined as follows,

\[
W_2(u, v) = \left( \inf_{\zeta \in \Gamma(u, v)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \| x_u - x_v \|^2 \, d\zeta(x_u, x_v) \right)^{1/2},
\]

where the infimum is over all joint distributions \( \zeta \). We use \( a_n = O(b_n) \) to denote that \( a_n \leq C b_n \) for some constant \( C > 0 \) independent of \( n \), and use \( a_n = \tilde{O}(b_n) \) to hide the logarithmic terms of \( b_n \). We also make use of the notation \( a_n \lesssim b_n \) (\( a_n \gtrsim b_n \)) if \( a_n \) is less than (larger than) \( b_n \) up to a constant. We use \( a \wedge b \) and \( a \vee b \) to denote \( \min\{a, b\} \) and \( \max\{a, b\} \) respectively.

2 ALGORITHM

In this section, we present our SVRG-LD\(^+\) algorithm, which is displayed in Algorithm 1.

The algorithm contains multiple epochs. At the beginning of the \( j \)-th epoch, we uniformly choose \( B \) samples from all training data and obtain a gradient estimator:

\[
\tilde{g}_j = \nabla f_{I_j}(\tilde{x}_j) = \frac{1}{|I_j|} \sum_{i \in I_j} \nabla f_i(\tilde{x}_j),
\]

where \( |I_j| = B \). At the \( l \)-th iteration in the \( j \)-th epoch, we define the semi-stochastic gradient as \( g_k = \nabla f_{I_k}(x_k) - \nabla f_{I_k}(\tilde{x}_j) + \tilde{g}_j \), where \( k = jm + l \) is the total iteration of the algorithm, \( m \) is the length of each epoch, and \( \nabla f_{I_k}(x) = 1/|I_k| \sum_{i \in I_k} \nabla f_i(x) \). Then we perform the following update:

\[
x_{k+1} = x_k - \eta g_k + \sqrt{2\eta} \epsilon_k,
\]

where \( \eta \) is the step size and \( \epsilon \sim N(0, I_{d \times d}) \) is a Gaussian random vector.

\[
x_{k+1} = x_k - \eta g_k + \sqrt{2\eta} \epsilon_k,
\]

where \( \eta \) is the step size and \( \epsilon \sim N(0, I_{d \times d}) \) is a Gaussian random vector.

It is worth noting that the major difference between SVRG-LD\(^+\) and SVRG-LD (Dubey et al., 2016) is that we replace the full gradient computation in the beginning of each epoch with a subsampled one. On one hand,
this leads to the consequence that the stochastic gradient \( g_j \) is not an unbiased estimator of the true gradient \( \nabla f(x) \), which introduces extra error that poses additional challenge in the analysis. On the other hand, compared with SVRG-LD, it saves gradient computations especially when the sample size \( n \) is large. Therefore, the crucial idea of SVRG-LD+ is to make an appropriate trade-off between extra error and saving gradient computation, and the batch size \( B \) is a vital parameter which should be carefully designed.

**Algorithm 1 SVRG-LD+**

1: **input:** initial point \( x_0 \), step size \( \eta \), batch size \( B \), mini-batch size \( b \), epoch length \( m \)
2: **initialization:** \( x_0 = x_0 \)
3: for \( j = 0, \ldots, \lceil K/m \rceil \)
4: Uniformly sample \( I_j \subseteq [n] \) with \( |I_j| = B \)
5: \( \tilde{g}_j = \nabla f_{\bar{I}_j} (\bar{x}_j) \)
6: for \( k = 0, \ldots , m - 1 \)
7: \( k = jm + l \)
8: Uniformly sample \( \bar{I}_k \subseteq [n] \) where \( |\bar{I}_k| = b \)
9: \( g_k = \nabla f_{\bar{I}_k} (x_k) - \nabla f_{\bar{I}_k} (\bar{x}_j) + \tilde{g}_j \)
10: \( x_{k+1} = x_k - \eta g_k + \sqrt{2\eta} e_k \)
11: end for
12: \( \bar{x}_{j+1} = x_{(j+1)m-1} \)
13: end for
14: **output:** \( x_K \)

### 3 MAIN THEORY

In this section, we are going to present our main theoretical results on the convergence rate of Algorithm 1 in 2-Wasserstein distance. We will first establish the convergence guarantees of Algorithm 1. Then, we will show that SVRG-LD+ reduces to SVRG-LD when choosing \( B = n \), and our analysis leads to a sharp convergence result of SVRG-LD that improves the recent result in Chaudhari et al. (2016).

For the target distribution \( \pi \propto e^{-f} \), we first lay down the following assumptions on function \( f(x) \), which are required in our analysis.

**Assumption 3.1** (Smoothness). There exists a positive constant \( M \) such that for each component function \( f_i(x) \), the following holds for all \( x, y \in \mathbb{R}^d \),

\[
\|\nabla f_i(x) - \nabla f_i(y)\|_2 \leq M\|x - y\|_2.
\]

Note that Assumption 3.1 immediately implies that the function \( f \) is also \( M \)-smooth, and consequently the target distribution \( \pi \) is \( M \)-log-smooth.

**Assumption 3.2** (Strong convexity). There exists a positive constant \( \mu \) such that for function \( f \), the following holds for all \( x, y \in \mathbb{R}^d \),

\[
f(x) \geq f(y) + \langle \nabla f(y), x - y \rangle + \frac{\mu}{2}\|x - y\|_2^2.
\]

The above assumption states that function \( f \) is strongly convex, which indicates that the distribution \( \pi \propto e^{-f} \) is strongly log-concave.

**Assumption 3.3** (Hessian Lipschitz). There exists a positive constant \( L \) such that for function \( f \), the following holds for all \( x, y \in \mathbb{R}^d \),

\[
\|\nabla^2 f(x) - \nabla^2 f(y)\|_2 \leq L\|x - y\|_2.
\]

This assumption is essential and useful for proving a faster convergence rate of Langevin Monte Carlo methods (Dalalyan & Karagulyan, 2017; Chatterji et al., 2018).

<table>
<thead>
<tr>
<th>METHOD</th>
<th>GRADIENT COMPLEXITY</th>
<th>HESSIAN LIPSCHITZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMC (Dalalyan &amp; Karagulyan, 2017)</td>
<td>( \tilde{O}\left(\frac{m^2d^{1/2}}{\epsilon}\right) )</td>
<td>Yes</td>
</tr>
<tr>
<td>SGLD (Dalalyan, 2017)</td>
<td>( \tilde{O}\left(\frac{\epsilon^2d^2}{\epsilon^{1/2}}\right) )</td>
<td>No^2</td>
</tr>
<tr>
<td>SAGA-LD (Chatterji et al., 2018)^3</td>
<td>( \tilde{O}\left(n + \frac{\kappa^2/2}{\epsilon}d^{1/2}\right) )</td>
<td>Yes</td>
</tr>
<tr>
<td>SVRG-LD (Chatterji et al., 2018)</td>
<td>( \tilde{O}\left(n + \frac{\kappa n/2}{\epsilon}d^{1/2}\right) )</td>
<td>Yes</td>
</tr>
<tr>
<td>SVRG-LD (this paper)</td>
<td>( \tilde{O}\left(n + \frac{\kappa^2/2}{\epsilon}d^{1/2}\right) )</td>
<td>Yes</td>
</tr>
<tr>
<td>SVRG-LD+ (this paper)</td>
<td>( \tilde{O}\left(\left(n + \frac{\kappa^2/2}{\epsilon}d^{1/2}\right) \land \frac{n^2}{\epsilon}\right) )</td>
<td>Yes</td>
</tr>
</tbody>
</table>

^3Different from the definition in (1.3), the finite-sum function \( f \) is defined as \( f = \sum_{i=1}^n f_i(x) \) in Chatterji et al. (2018), which leads to a difference in the results by a factor of \( n \). To make a fair comparison, we translate their results with the same definition in (1.3).
**Assumption 3.4** (Bounded Variance). There exists a constant $\sigma$, such that the following holds for all $x \in \mathbb{R}^d$, 
\[
\mathbb{E}_i[\|\nabla f_i(x) - \nabla f(x)\|^2_2] \leq d\sigma^2.
\]

Assumption 3.4 is necessary and widely made in stochastic Langevin dynamics based methods such as SGLD (Dalalyan, 2017; Dalalyan & Karagulyan, 2017) and SGHMC (Cheng et al., 2017). However, it should be noted that this assumption is only required for the analysis of the SVRG-LD algorithm but not required for SVRG-LD$^+$.

In what follows, we will present the convergence results of Algorithm 1. Following the literature (Dalalyan, 2017; Dalalyan & Karagulyan, 2017; Cheng & Bartlett, 2017; Zou et al., 2018; Chatterji et al., 2018), we will focus on the 2-Wasserstein distance between the target distribution $\pi \propto e^{-f}$ and the distribution of the $k$-th iterate in Algorithm 1. Specifically, we have the following theorem for SVRG-LD$^+$.

**Theorem 3.5.** Under Assumptions 3.1-3.4, let $P(x_k)$ denote the distribution of the $k$-th iterate $x_k$ in Algorithm 1. Set the step size $\eta$ to satisfy
\[
\eta \leq \min\left\{\left(\frac{b\mu}{2AM^4\mu^2}\right)^{1/3}, \frac{1}{6m(\sigma^2/B + M)}\right\}.
\]
The 2-Wasserstein distance between $P(x_k)$ and $\pi$ is bounded by
\[
\mathcal{W}_2(P(x_k), \pi) \\
\leq (1 - \eta\mu/4)^k \mathcal{W}_2(P(x_0), \pi) + \frac{3\sigma d^{1/2}}{\mu B^{1/2}} \mathcal{W}_2(\pi, x_k) + \frac{2\mu(\mu d + M^{3/2}d^2)}{\mu B^{1/2}} \mathcal{W}_2(x_k, \pi) + \frac{4\eta M\mu d^{1/2}M^{1/2}d^{1/2}}{(b\mu)^{1/2}}.
\]

It is worth noting that the mini-batch size $b$ and the batch size $B$ are two independent parameters in the algorithm that can be chosen separately. In practice, one typically chooses $b \ll B$ (see for example, Harikandeh et al. (2015); Lei & Jordan (2016); Chen et al. (2017) in order to obtain a good convergence result. If we intentionally choose $b > B$ in the algorithm, the evaluation of the semi-stochastic gradient will be even more expensive than that of the subsampled/full gradient in the outer loop, which makes variance reduction techniques no longer effective. The optimal choices of $b$ and $B$ in two different regimes of sample size $n$ will be specified in the following corollaries.

Theorem 3.5 implies that in order to achieve $\epsilon$-accuracy in 2-Wasserstein distance, the step size $\eta$ should be set to be sufficiently small, and the batch size $B$ should be sufficiently large. To address these requirements, we present the following corollaries to show the optimal selections of $\eta$ and $B$, and compute the gradient complexity of SVRG-LD$^+$ under different regimes.

We first consider the regime where $n \gtrsim \frac{d\sigma^2}{(\mu^2\epsilon^2)}$.

**Corollary 3.6.** Under the same assumptions as in Theorem 3.5, suppose the sample size satisfies $n \gtrsim \frac{d\sigma^2}{(\mu^2\epsilon^2)}$, if we set $B = O(\frac{d^2}{\epsilon^2} \mu^2 \sigma^2)$, $b = O(1)$, $m = O(B)$ and $\eta = O(\frac{(d\sigma^2)}{(\mu^2\epsilon^2)})$. Algorithm 1 achieves $\epsilon$-accuracy in 2-Wasserstein distance after
\[
T = \tilde{O}\left(\frac{d\sigma^2}{\mu^2\epsilon^2}\right)
\]

stochastic gradient evaluations.

**Remark 3.7.** According to Corollary 3.6, if $n \gtrsim \frac{d\sigma^2}{(\mu^2\epsilon^2)}$, then the gradient complexity of SVRG-LD$^+$ in (3.1) matches that of SGLD (Dalalyan, 2017; Dalalyan & Karagulyan, 2017). Note that the gradient complexities of LMC, SAGA-LD and SVRG-LD are at least $\tilde{O}(n)$ due to the use of full gradients, which indicates that SVRG-LD$^+$ achieves lower gradient complexity than LMC, SAGA-LD and SVRG-LD in this regime.

When the sample size satisfies $n \lesssim \frac{d\sigma^2}{(\mu^2\epsilon^2)}$, we choose the batch size $B$ to be $n$, i.e., compute the full gradient in the beginning of each epoch in Algorithm 1. In this regime, Algorithm 1 reduces to SVRG-LD (Dubey et al., 2016), and its gradient complexity is characterized by the following corollary.

**Corollary 3.8.** Under the same assumptions as in Theorem 3.5, suppose the sample size satisfies $n \lesssim \frac{d\sigma^2}{(\mu^2\epsilon^2)}$, if we set $b = 1$ and
\[
\eta = \min\left\{\frac{\mu\epsilon}{Ld + M^{3/2}d^{1/2}}, \frac{\mu^{1/2}\epsilon}{\mu^{1/2}d^{1/2}n^{1/2}}\right\},
\]

SVRG-LD$^+$ achieves $\epsilon$-accuracy in 2-Wasserstein distance after
\[
T = \tilde{O}\left(n + \frac{Ld + M^{3/2}d^{1/2}}{\mu^2\epsilon} + \frac{Md^{1/2}n^{1/2}}{\mu^{3/2}\epsilon}\right)
\]

stochastic gradient evaluations.

**Remark 3.9.** According to Corollary 3.6, if $n \lesssim \frac{d\sigma^2}{(\mu^2\epsilon^2)}$, following Chatterji et al. (2018), if we further assume $n \gtrsim \frac{L^2d}{(M^2\mu) + \kappa}$, and treat $1/M$ and $\mu$ as constants of order $O(1)$, then the complexity in (3.2) can be simplified as
\[
T = \tilde{O}\left(n + \frac{\kappa^{3/2}d^{1/2}n^{1/2}}{\epsilon}\right).
\]
It is worth noting that in this regime, Algorithm 1 does not need Assumption 3.4. Moreover, combining the results in Corollaries 3.6 and 3.8, the gradient complexity of SVRG-LD+ can be derived as follows

\[ \tilde{O}\left(\left(n + \frac{\kappa^3/2n^{1/2}d^{1/2}}{\epsilon}\right) \wedge \frac{\kappa^2d^2}{\epsilon^2} \right), \]  

(3.3)

where \( O(1/\mu^2) = O(\kappa^2/M^2) = O(\kappa^2) \) as \( 1/M = O(1) \).

**Remark 3.10.** Corollary 3.8 essentially provides the gradient complexity for SVRG-LD, which is lower than that proved in Chatterji et al. (2018). Recall that their result is \( O(f(n)/\mu + f(n)/M^2) \). Last but not the least, our proof gradient complexity of SVRG-LD matches that of SAGA-LD (Chatterji et al., 2018), which suggests that SVRG-LD and SAGA-LD enjoy the same performance.

### 4 PROOF OF THE MAIN THEORY

In this section, we provide the proof for our main theory. We first define an operator \( \mathcal{L} \) derived from the Langevin dynamics. Specifically, let \( x_0 \) be any starting position, and we denote by \( \mathcal{L}_t x_0 \) the random position of the Markov process generated by Langevin dynamics (1.1) after time \( t \). Let \( x^\pi \) denote the random variable that satisfies the stationary distribution \( \pi \propto e^{-f}. \) In addition, we define \( \Delta_k = \mathcal{L}_t x^\pi \) and \( \Delta_k = \mathcal{L}_n x_\pi \), where \( \Delta_{k+1} = \mathcal{L}_n x^{\pi} - x_{k+1} \), \( \Delta_k = \mathcal{L}_n x^{\pi} - x_{k} \), \( \Delta_{k+1} = \mathcal{L}_n x^{\pi} - x_{k+1} \), \( \Delta_k = \mathcal{L}_n x^{\pi} - x_{k+1} \) are due to Markov property of \( \mathcal{L} \). Then the following holds trivilly

\[ \Delta_{k+1} = \mathcal{L}_n x^{\pi} - x_{k+1} = \mathcal{L}_n x^{\pi} - x_k + \mathcal{L}_n x^{\pi} - \mathcal{L}_n x^{\pi} - (x_{k+1} - x_k). \]

Consider two synchronously coupled Markov processes \( \mathcal{L}_n x^{\pi} \) and \( x_k \) which have shared Brownian motion term in updates \( \mathcal{L}_n x^{\pi} \to \mathcal{L}_n x^{\pi} \) and \( x_k \to x_{k+1} \), we further have

\[ \Delta_{k+1} = \Delta_k + \eta \left( g_k - \nabla f(x_k) \right) - \int_0^\eta \nabla f(L_{k+1} x^{\pi}) dt = \Delta_k + \eta \left( g_k - \nabla f(x_k) \right) - \nabla f(L_{k+1} x^{\pi}) - \nabla f(x_k) \]

\[ - \int_0^\eta \left( \nabla f(L_{k+1} x^{\pi}) - \nabla f(L_{k+1} x^{\pi}) \right) dt = \Delta_k + \eta \Phi_k - \eta U_k - S_k - V_k, \]  

(4.1)

where we define

\[ \Phi_k = g_k - \nabla f(x_k), \]

\[ U_k = \nabla f(L_{k+1} x^{\pi}) - \nabla f(x_k), \]

\[ S_k = \sqrt{2} \int_0^\eta \int_0^\eta \nabla^2 f(L_{k+1} x^{\pi}) dB_s dt, \]

\[ V_k = \int_0^\eta \left( \nabla f(L_{k+1} x^{\pi}) - \nabla f(L_{k+1} x^{\pi}) \right) dt - S_k. \]

Note that in Algorithm 1, the semi-stochastic gradient \( g_k \) has the following property

\[ \mathbb{E}[ g_k | x_j ] = \mathbb{E}[ \nabla f_{2k}(x_k) - \nabla f_{2k}(x_j) + \nabla f_{2j}(x_j) | x_j ] \]

\[ = \mathbb{E}[ \nabla f(x_k) - \nabla f(x_j) + \nabla f_{2j}(x_j) ]. \]

Then we can decompose \( \Phi_k \) as follows

\[ \Phi_k = g_k - \nabla f(x_k) \]

\[ = \nabla f_{2k}(x_k) - \nabla f_{2k}(x_j) - \left( \nabla f(x_k) - \nabla f(x_j) \right) \]

\[ \Psi_k \]

\[ + \left( \nabla f_{2j}(x_j) - \nabla f(x_j) \right). \]  

(4.2)

Submitting the above equation into (4.1) yields

\[ \Delta_{k+1} = \Delta_k - \eta U_k + \eta \Psi_k + \eta e_j - S_k - V_k. \]  

(4.3)

Now, we have already obtained the recursive update of \( \Delta_k \). In what follows, we will upper bound the \( \ell_2 \)-norm of each term on the R.H.S of (4.3). To begin with, we provide the following technical lemmas.

**Lemma 4.1.** (Dalalyan & Karagulyan, 2017) Under Assumptions 3.1 and 3.2, we have

\[ \mathbb{E}[ \| \Delta_k - \eta U_k \|_2^2 ] \leq (1 - \mu)^2 \mathbb{E}[ \| \Delta_k \|_2^2 ], \]

where \( \eta \) denotes the step size, \( \mu \) is the strongly convex parameter on function \( f(x) \).

**Lemma 4.2.** Under Assumptions 3.1 and 3.2, we have the following upper bound on \( \| \Psi_k \|_2^2 \).

\[ \mathbb{E}[ \| \Phi_k \|_2^2 ] \]

\[ \leq \frac{4d\sigma^2}{b} \wedge \frac{M^2}{b} (6m^2\eta^2 M^2 \mathbb{E}[ \| \Delta_{jm} \|_2^2 ] + G_j ) e^{2m^2 M^2 \eta^2}, \]  

(4.4)

where

\[ G_j = 6m^2\eta^2 (\mathbb{E}[ \| e_j \|_2 ] + Md) + 2md\eta. \]

**Lemma 4.3.** Under Assumption 3.4, \( \| e_j \|_2 \) is bounded as follows,

\[ \mathbb{E}[ \| e_j \|_2 ] \]

\[ \leq \frac{da^2}{B}. \]

In addition, if \( B = n, \mathbb{E}[ \| e_j \|_2 ] = 0. \)
Lemma 4.4. (Dalalyan, 2017) Under Assumptions 3.1 and 3.3, regarding to terms $\mathcal{S}_k$ and $\mathcal{V}_k$ in (4.3), we have the following uniformly upper bound on their $\ell_2$-norms:

$$
E[\|\mathcal{V}_k\|_2^2] \leq \frac{\eta^4}{2}(L^2d^2 + M^3d),
$$

$$
E[\|\mathcal{S}_k\|_2^2] \leq \frac{\eta^3M^2d}{3},
$$

where $M$ and $L$ denotes the smoothness and Hessian Lipschitz parameters respectively.

Now, we are ready to present the proof for Theorem 3.5.

Proof of Theorem 3.5. Note that

$$
E[\Psi_k | x_k, \mathcal{L}_n \mathcal{X}^r, \mathcal{L}_{k+1} \mathbf{x}^r] = 0,
$$

which immediately implies

$$
E[\|\Delta_{k+1}\|_2^2] = E[\|\Delta_k - \eta \mathcal{U}_k + \eta \mathcal{V}_k - \mathcal{V}_k\|_2^2] + \eta^2E[\|\Psi_k\|_2^2]
$$

$$
\leq (1 + \alpha)E[\|\Delta_k - \eta \mathcal{U}_k - \mathcal{S}_k\|_2^2]
$$

$$
+ (1 + 1/\alpha)E[\|\eta \mathcal{V}_k\|_2^2] + \eta^2E[\|\Psi_k\|_2^2]
$$

$$
= (1 + \alpha)E[\|\Delta_k - \eta \mathcal{U}_k\|_2^2]
$$

$$
+ (1 + 1/\alpha)E[\|\eta \mathcal{V}_k\|_2^2] + \eta^2E[\|\Psi_k\|_2^2]
$$

$$
\leq (1 + \alpha)E[\|\Delta_k\|_2^2]
$$

$$
+ 2(1 + 1/\alpha)E[\|\mathcal{V}_k\|_2^2] + \eta^2E[\|\Psi_k\|_2^2],
$$

where $\alpha > 0$ is an arbitrary chosen parameter, the first inequality is by Young’s inequality, and the second equality follows from the fact $E[\mathcal{S}_k | \Delta_k, \mathcal{U}_k] = 0$. Applying Lemmas 4.1 and 4.2, we have

$$
E[\|\Delta_{k+1}\|_2^2]
$$

$$
\leq (1 + \alpha)(1 - \eta \mu)^2E[\|\Delta_k\|_2^2] + (1 + \alpha)E[\|\mathcal{S}_k\|_2^2]
$$

$$
+ 2(1 + 1/\alpha)E[\|\mathcal{V}_k\|_2^2] + \eta^2E[\|\Psi_k\|_2^2]
$$

$$
\leq \left(1 + \alpha\right)\left(1 - \eta \mu\right)^2 + \frac{6\eta^4M^4m^2}{b}e^{2\eta^2m^2\mu^2}
$$

$$
\times \max \left\{E[\|\Delta_k\|_2^2], E[\|\Delta_{jm}\|_2^2]\right\} + \Omega_1 + \Omega_2,
$$

(4.5)

where

$$
\Omega_1 = (1 + \alpha)E[\|\mathcal{S}_k\|_2^2]
$$

$$
+ 2(1 + 1/\alpha)E[\|\mathcal{V}_k\|_2^2]
$$

$$
\Omega_2 = \frac{4d^2\sigma^2\eta^2}{b} \land \frac{M^2\eta^2G_j}{b}e^{2\eta^2m^2\mu^2}. \quad (4.6)
$$

Note that the step size $\eta$ satisfies $\eta \leq \min \left\{ (b\mu/(24M^2m^2))^{1/3}, 1/(6b\sigma^2/B) + 6mM \right\},$ we have $\exp(2m^2M^2\eta^2) \leq 2$ and $6\eta^4M^4m^2\exp(2m^2M^2\eta^2)/b \leq \eta \mu/2$. We choose $\alpha = \eta \mu$, which implies $(1 + \alpha)(1 - \eta \mu)^2 \leq 1 - \eta \mu$. Thus, (4.5) can be further rewritten as follows,

$$
E[\|\Delta_{k+1}\|_2^2] \leq (1 - \eta \mu/2)\max \left\{E[\|\Delta_k\|_2^2], E[\|\Delta_{jm}\|_2^2]\right\} + \Omega_1 + \Omega_2.
$$

(4.7)

In order to obtain the upper bound of $E[\|\Delta_k\|_2^2]$, we need to recursively call (4.7). Note that since $jm \leq k$, the number of calls to (4.7) must be smaller than $k$, thus we have

$$
E[\|\Delta_k\|_2^2] \leq (1 - \eta \mu/2)^k\left(E[\|\Delta_0\|_2^2]\right) + \frac{\Omega_1 + \Omega_2}{\eta \mu/2}.
$$

(4.8)

In what follows, we are going to upper bound $\Omega_1$ and $\Omega_2$. Note that $m \geq 1$ and $M \geq \mu$, we have $\eta \mu \leq 1$. Then by the application of Lemmas 4.3 and 4.4, we have

$$
\Omega_1 \leq \left(1 + \alpha\right)\eta \mu^2d^2 + 2(1 + 1/\alpha)
$$

$$
\times \left(\frac{\eta^2d^2}{B}\log n + \frac{\eta^4(L^2d^2 + M^3d)}{2}\right)
$$

$$
\leq \frac{2\eta^3M^2d}{3} + \frac{4d^2\sigma^2}{B\mu} + \frac{2\eta^4(L^2d^2 + M^3d)}{\mu},
$$

$$
\Omega_2 \leq \frac{4d^2\sigma^2\eta^2}{b} \land \frac{6M^2md\eta^3}{b}.
$$

Then we substitute the above upper bounds of $\Omega_1$ and $\Omega_2$ into (4.8), and obtain

$$
E[\|\Delta_k\|_2^2]
$$

$$
\leq (1 - \eta \mu/2)^k\left(E[\|\Delta_0\|_2^2]\right) + \frac{\Omega_1 + \Omega_2}{\eta \mu/2}
$$

$$
\leq (1 - \eta \mu/2)^k\left(E[\|\Delta_0\|_2^2]\right) + \frac{8d^2\sigma^2}{B\mu^2}\log n
$$

$$
+ \frac{4\eta^2(L^2d^2 + M^3d)}{\mu^2} + \frac{14d^2mM^2d^2}{b\mu} \land \frac{8d^2\eta^2}{b\mu}.
$$

Based on the definition of 2-Wasserstein distance, we have $W_2^2(P(x_k), \pi) \leq E[\|\Delta_k\|_2^2]$. Applying the inequality that $x^2 + y^2 + z^2 \leq (|x| + |y| + |z|)^2$ for all $x, y, z \in \mathbb{R}$, we complete the proof of Theorem 3.5. \hfill \square

5 EXPERIMENTS

In this section, we are going to verify our theoretical results and evaluate the performances of different Langevin based algorithms on both synthetic and real datasets.

5.1 SIMULATION ON SYNTHETIC DATA

We first validate our theoretical results based on synthetic data. In this simulation, we consider function $f(x) =$
1/n \sum_{i=1}^{n} f_i(x) = 1/n \sum_{i=1}^{n} (x - \theta_i)^T \Sigma (x - \theta_i) / 2,

where \Sigma is a symmetric matrix having largest eigenvalue \( M = 2 \) and smallest eigenvalue \( \mu = 1/2 \), and \( \theta_i \) is drawn from standard multivariate Gaussian distribution.

We first compare the convergence rates of four different algorithms (i.e., SGLD, SVRG-LD, SAGA-LD and SVRG-LD+) to the target distribution in 2-Wasserstein distance, which are reported in Figure 1. It can be seen that there is no obvious difference between the convergence rates of SAGA-LD and SVRG-LD, which verifies our theoretical result of SVRG-LD. Moreover, Figures 1(a) and 1(b) demonstrate that the best choice of \( B \) is \( B = n \) when the sample size \( n \) is small, while Figures 1(c) and 1(d) show that using subsampled gradient in SVRG-LD+ (i.e., \( B < n \)) is able to improve the performance of SVRG-LD when \( n \) is relatively large. This is well aligned with our theoretical analysis that the optimal batch size \( B \) is in the order of \( O(d\sigma^2 / (\epsilon \mu)^2 \wedge n) \).

In Figure 2, we further compare different choices of batch size \( B \) in SVRG-LD+ when \( n \) is large. Note that since the optimal batch size \( B = n \) when the sample size is small, we only perform this experiment on the synthetic datasets with big sample size \( n = 20000 \) and \( n = 50000 \). It can be inferred from Figure 2 that if we set \( \epsilon = 10^{-2} \), the optimal \( B \) in SVRG-LD+ for datasets with sample sizes \( n = 20000 \) and \( n = 50000 \) are both \( B = 20000/2 = 50000/5 = 10000 \). This phenomenon agrees with our theory that for a large \( n \), \( O(d\sigma^2 / (\epsilon \mu)^2) \) is independent of \( n \).

5.2 BAYESIAN LOGISTIC REGRESSION

We also collaborate our theoretical results with Bayesian logistic regression. Suppose we are given a dataset with \( n \) examples \( \{X_i, y_i\}_{i=1,2,...,n} \), where \( X_i \in \mathbb{R}^d \) denotes the \( d \)-dimensional feature of the \( i \)-th sample, and \( y_i \in \{-1, 1\} \) denotes the corresponding binary label. In Bayesian logistic regression, we assume that the input examples are independent, then the probability distribution of \( y_i \) given features \( X_i \) and regression coefficients \( \beta \in \mathbb{R}^d \) has the following form

\[ p(y_i | X_i, \beta) = \frac{1}{1 + e^{-\beta^T X_i}}. \]

Moreover, the prior of \( \beta \) is typically modelled as a Gaussian distribution with zero mean (Dubey et al., 2016; Chatterji et al., 2018), i.e., \( \beta \sim N(0, \lambda I_{d \times d}) \). Then we apply the Langevin based method to sample from the posterior distribution of \( \beta \), i.e., \( p(\beta | X, y) \propto p(\beta) \prod_{i=1}^{n} p(y_i | X_i, \beta) \), which implies that the component function \( f_i(\beta) \) can be written as

\[ f_i(\beta) = n \log (1 + e^{-y_i \beta^T X_i}) + \| \beta \|^2 \lambda. \]

We apply the Langevin based algorithm to four datasets: pima, mushroom, a9a and ijcnn1, which are available at UCI repository\(^4\) and Libsvm website\(^5\). It is worth noting that pima and mushroom do not have test datasets like a9a and ijcnn1, thus we manually partition them into train and test datasets. The basic information of all the datasets is summarized in Table 2. Again, we evaluate the performance of four different algorithms: SGLD,

\(^4\)https://archive.ics.uci.edu/ml/
\(^5\)https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/
SVRG-LD, SAGA-LD and SVRG-LD$^+$, and perform sample path average to estimate the optimal $\beta$, where the minibatch size for each algorithm is set to be 1.

Figure 3 shows the negative log-likelihood of the test examples on these 4 datasets, where each algorithm has been run 10 times to calculate the averaged result. It can be seen that there exists a lag of one data pass for SAGA-LD and SVRG-LD, since they need to scan the entire dataset to compute a full gradient in the beginning. As we can see from the results in Figure 3, SVRG-LD$^+$ converges faster than the other methods, which validates the superior performance of SVRG-LD$^+$. In detail, SVRG-LD$^+$ has a similar convergence rate as SAGA-LD and SVRG-LD when $n$ is small, e.g. datasets pima, and performs close to SGLD for relatively large datasets, e.g., a9a and ijcnn1. This is also consistent with our theoretical results, since the convergence rate of SVRG-LD$^+$ matches that of SGLD when $n \gtrsim d\sigma^2/(\epsilon \mu)^2$.

Figure 4: Bayesian Logistic regression results of SVRG-LD$^+$ using different batch size $B$, where y axis shows the negative log-likelihood on the test data, and x axis is the number of data passes. (a)-(d) correspond to 4 datasets.

Table 2: Summary of datasets for Bayesian logistic regression.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>pima</th>
<th>mushroom</th>
<th>a9a</th>
<th>ijcnn1</th>
</tr>
</thead>
<tbody>
<tr>
<td># training</td>
<td>600</td>
<td>6000</td>
<td>32561</td>
<td>49990</td>
</tr>
<tr>
<td># test</td>
<td>168</td>
<td>2124</td>
<td>16281</td>
<td>91701</td>
</tr>
<tr>
<td>$d$</td>
<td>8</td>
<td>112</td>
<td>123</td>
<td>22</td>
</tr>
</tbody>
</table>

Next, we evaluate the performance of SVRG-LD$^+$ algorithms when choosing different batch sizes $B$, which are reported in Figure 4. It can be observed that when the batch size is chosen appropriately, SVRG-LD$^+$ converges faster than SVRG-LD, but leading to a slightly higher error. Based on these observations, we can conclude that for Bayesian logistic regression, SVRG-LD$^+$ is more suitable than SVRG-LD when the dataset size is relatively large, and the required accuracy is moderate.

6 CONCLUSIONS

We propose the SVRG-LD$^+$ algorithm and analyze its convergence rate in 2-Wasserstein distance when the target distribution is log-smooth, strongly log-concave and log-Hessian-Lipschitz. Our result implies a sharper convergence analysis of SVRG-LD that improves the state-of-the-art. Experiments on synthetic and real data back up the theoretical results of this paper.

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