Stochastic Variance-Reduced Hamilton Monte Carlo Methods

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Abstract

We propose a fast stochastic Hamilton Monte Carlo (HMC) method, for sampling from a smooth and strongly log-concave distribution. At the core of our proposed method is a variance reduction technique inspired by the recent advance in stochastic optimization. We show that, to achieve $\epsilon$ accuracy in 2-Wasserstein distance, our algorithm achieves $\tilde{O}(n + \kappa^2 d^{1/2}/\epsilon + \kappa^{4/3} d^{1/3} n^{2/3}/\epsilon^{2/3})$ gradient complexity (i.e., number of component gradient evaluations), which outperforms the state-of-the-art HMC and stochastic gradient HMC methods in a wide regime. We also extend our algorithm for sampling from smooth and general log-concave distributions, and prove the corresponding gradient complexity as well. Experiments on both synthetic and real data demonstrate the superior performance of our algorithm.

1 Introduction

Past decades have witnessed increasing attention of Markov Chain Monte Carlo (MCMC) methods in modern machine learning problems (Andrieu et al., 2003). An important family of Markov Chain Monte Carlo algorithms is called Langevin Monte Carlo method (Neal et al., 2011), which is based on Langevin dynamics (Parisi, 1981). Langevin dynamics was used for mathematical modeling of the dynamics of molecular systems, and can be described by the following Itô’s stochastic differential equation (SDE) (Øksendal, 2003),

$$dX_t = -\nabla f(X_t) dt + \sqrt{2\beta} dB_t,$$  \hspace{1cm} (1.1)

where $X_t$ is a $d$-dimensional stochastic process, $t \geq 0$ denotes the time index, $\beta > 0$ is the temperature parameter, and $B_t$ is the standard $d$-dimensional Brownian motion. Under certain assumptions on the drift coefficient $\nabla f$, Chiang et al. (1987) showed that the distribution of $X_t$ in (1.1) converges to its stationary distribution, a.k.a., the Gibbs measure $\pi_\beta \propto \exp(-\beta f(x))$. Note that $\pi_\beta$ is smooth and log-concave (resp. strongly log-concave) if $f$ is smooth and convex (resp.

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strongly convex). A typical way to sample from the density function $\pi_\beta$ is applying Euler-Maruyama discretization scheme (Kloeden and Platen, 1992) to (1.1), which yields

$$X_{k+1} = X_k - \nabla f(X_k)\eta + \sqrt{2\eta\beta} \cdot \epsilon_k,$$

where $\epsilon_k \sim N(0, I_{d\times d})$ is a standard Gaussian random vector, $I_{d\times d}$ is a $d \times d$ identity matrix, and $\eta > 0$ is the step size. (1.2) is often referred to as the Langevin Monte Carlo (LMC) method. In total variation (TV) distance, LMC has been proved to be able to produce approximate sampling of density $\pi_\beta \propto e^{-f/\beta}$ under arbitrary precision requirement in Dalalyan (2014); Durmus and Moulines (2016b), with properly chosen step size. The non-asymptotic convergence of LMC has also been studied in Dalalyan (2017); Dalalyan and Karagulyan (2017); Durmus et al. (2017), which shows that the LMC algorithm can achieve $\epsilon$-precision in 2-Wasserstein distance after $\tilde{O}(\kappa^2d/\epsilon^2)$ iterations if $f$ is $L$-smooth and $\mu$-strongly convex, where $\kappa = L/\mu$ is the condition number.

In order to accelerate the convergence of Langevin dynamics (1.1) and improve its mixing time to the unique stationary distribution, Hamiltonian dynamics (Duane et al., 1987; Neal et al., 2011) was proposed, which is also known as underdamped Langevin dynamics and is defined by the following system of SDEs

$$dV_t = -\gamma V_t dt - u \nabla f(X_t) dt + \sqrt{2\gamma u} dB_t,$$

$$dX_t = V_t dt,$$

where $\gamma > 0$ is the friction parameter, $u$ denotes the inverse mass, $X_t, V_t \in \mathbb{R}^d$ are the position and velocity of the continuous-time dynamics respectively, and $B_t$ is the Brownian motion. Let $W_t = (X_t^T, V_t^T)^T$, under mild assumptions on the drift coefficient $\nabla f(x)$, the distribution of $W_t$ converges to an unique invariant distribution $\pi_w \propto e^{-f(x)-\|v\|^2/(2u)}$ (Neal et al., 2011), whose marginal distribution on $X_t$, denoted by $\pi$, is proportional to $e^{-f(x)}$. Similar to the numerical approximation of the Langevin dynamics in (1.2), one can also apply the same Euler-Maruyama discretization scheme to Hamiltonian dynamics in (1.3), which gives rise to

$$v_{k+1} = v_k - \gamma \eta v_k - \eta u \nabla f(x_k) + \sqrt{2\gamma u \eta} \epsilon_k,$$

$$x_{k+1} = x_k + \eta v_k,$$

(1.4) is called Hamiltonian Monte Carlo (HMC) method, which provides an alternative way to sample from the target distribution $\pi \propto e^{-f(x)}$. While HMC has been observed to outperform LMC in a number of empirical studies (Chen et al., 2014, 2015), there does not exist a non-asymptotic convergence analysis of the HMC method until very recent work by Cheng et al. (2017). More specifically, Cheng et al. (2017) proposed a variant of HMC based on a novel discretization approach, and showed that it achieves $\epsilon$ sampling accuracy in 2-Wasserstein distance within $\tilde{O}(\kappa^2d^{1/2}/\epsilon)$ iterations for smooth and strongly convex function $f$. This improves upon the convergence rate of LMC by a factor of $(d^{1/2}/\epsilon)$.

Both LMC and HMC are gradient based Monte Carlo methods, and are effective in sampling from smooth and strongly log-concave distributions using only gradient evaluations. However, they can be slow if the evaluation of the gradient is computationally expensive, especially on large datasets. This motivates using stochastic gradient instead of full gradient in LMC and HMC, which gives rise to Stochastic Gradient Langevin Dynamics (SGLD) (Welling and Teh, 2011; Ahn et al.,
2012; Durmus and Moulines, 2016b; Dalalyan, 2017) and Stochastic Gradient Hamilton Monte Carlo (SG-HMC) method (Chen et al., 2014; Ma et al., 2015; Chen et al., 2015) respectively. For smooth and strongly log-concave distributions, Dalalyan and Karagulyan (2017); Dalalyan (2017) proved that the convergence rate of SGLD is $(\kappa^2 d \sigma^2 / \epsilon^2)$, where $\sigma^2$ denotes the upper bound of the variance of the stochastic gradient. Cheng et al. (2017) proposed a variant of SG-HMC and proved that it converges after $\tilde{O}(\kappa^2 d \sigma^2 / \epsilon^2)$ iterations. It is worth noting that although using stochastic gradient evaluations reduces the per-iteration cost, it comes at a cost that the convergence rates of SGLD and SG-HMC are slower than LMC and HMC. Thus, a natural question is:

**Does there exist an algorithm that can leverage stochastic gradients, but also achieve faster rate of convergence?**

In this paper, we answer this question affirmatively, when the function $f$ can be written as the finite sum of $n$ smooth component functions $f_i$

$$f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x). \quad (1.5)$$

It is worth noting that the finite sum structure is prevalent in machine learning, as the log-likelihood function of a dataset (e.g., $f$) is the sum of the log-likelihood over each data point (e.g., $f_i$) in the dataset. We propose a stochastic variance-reduced HMC (SVR-HMC), which incorporates the variance reduction technique into stochastic HMC. Our algorithm is inspired by the recent advance in stochastic optimization (Roux et al., 2012; Johnson and Zhang, 2013; Xiao and Zhang, 2014; Defazio et al., 2014; Allen-Zhu and Hazan, 2016; Reddi et al., 2016; Lei and Jordan, 2016; Lei et al., 2017), which use semi-stochastic gradients to accelerate the optimization of the finite-sum function, and to improve the runtime complexity of full gradient methods. We also notice that the variance reduction technique has already been employed in a recent work Dubey et al. (2016) on SGLD. Nevertheless, it does not show an improvement in terms of dependence on the sampling accuracy $\epsilon$.

In detail, our proposed algorithm uses a multi-epoch scheme to reduce the variance of the stochastic gradient. In the beginning of each epoch, it computes the full gradient or an estimation of the full gradient based on the entire data. Within each epoch, it performs semi-stochastic gradient descent, and outputs the last iterate as the warm up starting point in the next epoch. Thorough experiments on both synthetic and real data demonstrate the advantage of our proposed algorithm.

**Our Contributions** The major contributions of our work are highlighted as follows.

- We propose a new algorithm that incorporates variance-reduction technique into HMC. Our algorithm does not require the variance of the stochastic gradient is bounded. We proved that our algorithm has a better gradient complexity than the state-of-the-art LMC and HMC methods for sampling from smooth and strongly log-concave distributions, when the sampling error is measured by 2-Wasserstein distance. In particular, to achieve $\epsilon$ sampling error in 2-Wasserstein distance, our algorithm only needs $\tilde{O}(n + \kappa^2 d^{1/2} / \epsilon + \kappa^{4/3} d^{1/3} n^{2/3} / \epsilon^{2/3})$ number of component gradient evaluations. This improves upon the state-of-the-art result by (Cheng et al., 2017), which is $\tilde{O}(n\kappa^2 d^{1/2} / \epsilon)$ in a large regime.

- We extend the proposed algorithm to sampling from smooth and general log-concave distributions by adding a diminishing regularizer term $\lambda \|x\|_2^2 / 2$. We prove that the gradient complexity...
of the extended algorithm to achieve $\epsilon$ 2-Wasserstein distance is $(n + d^{11/2}/\epsilon^6 + d^{11/3}n^{2/3}/\epsilon^{10/3})$.

As far as we know, this is the first convergence result of LMC methods in 2-Wasserstein distance.

The remainder of this paper is organized as follows: In Section 2, we review some related work on gradient-based Langevin Monte Carlo algorithms. Then we present our algorithm in Section 3. In section 4, we provide theoretical analysis of the proposed algorithm for sampling from both strongly log-concave and general log-concave distributions. To validate our theory, both simulation and thorough real data for Bayesian logistic classification and linear regression are presented in Section 5. Finally, we conclude this paper in Section 6 with future work.

**Notation**

We denote the discrete update by lower case bold symbol $x_k$ and the continuous-time dynamics by upper case italicized bold symbol $X_t$. For a vector $x \in \mathbb{R}^d$, we denote by $\|x\|_2$ the Euclidean norm. For a random vector $X_t \in \mathbb{R}^d$ or $x_k \in \mathbb{R}^d$, we denote its probability distribution function by $P(X_t)$ or $P(x_k)$ respectively. For a probability measure $u$, we denote by $E_u(X)$ the expectation of $X$ under probability measure $u$. We denote the 2-Wasserstein distance between two probability measures $u$ and $v$ as

$$W_2(u, v) = \left( \inf_{\zeta \in \Gamma(u, v)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|X_u - X_v\|_2^2 d\zeta(X_u, X_v) \right)^{1/2},$$

where the infimum is over all joint distributions $\zeta$ with $u$ and $v$ being its marginal distributions. We use $a_n = O(b_n)$ to denote that $a_n \leq Cb_n$ for some constant $C > 0$ independent of $n$, and use $a_n = \bar{O}(b_n)$ to hide the logarithmic terms of $b_n$. We also make use of the notation $a_n \preceq b_n$ ($a_n \succeq b_n$) if $a_n$ is less than (larger than) $b_n$ up to a constant. We use $a \wedge b$ to denote $\min\{a, b\}$.

## 2 Related Work

In this section, we briefly review the relevant work in the literature.

Langevin Monte Carlo (LMC) methods (a.k.a., Unadjusted Langevin Algorithms), and its Metropolis adjusted version, have been studied in a number of papers (Roberts and Tweedie, 1996; Roberts and Rosenthal, 1998; Stramer and Tweedie, 1999a,b; Jarner and Hansen, 2000; Roberts and Stramer, 2002), which have been proved to attain asymptotic exponential convergence. In the past few years, there has emerged quite a few studies on proving the non-asymptotic convergence of LMC methods. Dalalyan (2014) first proposed the theoretical guarantee for approximate sampling using Langevin Monte Carlo method for strongly log-concave and smooth distributions, where he proved rate $O(d/\epsilon^2)$ for LMC algorithm with warm start in total variation (TV) distance. This result has later been extended to Wasserstein metric by Dalalyan and Karagulyan (2017); Durmus and Moulines (2016b), where the same convergence rate in 2-Wasserstein distance holds without the warm start assumption. Recently, Cheng and Bartlett (2017) also proved an $(d/\epsilon)$ convergence rate of the LMC algorithm in KL-divergence. Regarding to the stochastic gradient based extensions of LMC methods, Dalalyan (2017); Dalalyan and Karagulyan (2017) analyzed the convergence rate for the LMC algorithm based on both unbiased and biased stochastic gradients. In particular, they proved that the computational complexity for unbiased stochastic gradient LMC is $O(k^2 d/\epsilon^2)$, and showed that the LMC may not converge to the target distribution if the stochastic gradient has non-negligible bias.
In order to improve convergence speed of LMC methods, the Hamiltonian Monte Carlo (HMC) method was proposed Duane et al. (1987), which introduces a momentum term in its dynamics. Please refer to Neal et al. (2011) for a detailed introduction to HMC. To deal with large datasets, stochastic gradient HMC has been proposed for Bayesian learning (Chen et al., 2014; Ma et al., 2015). Chen et al. (2015) investigated the generic stochastic gradient MCMC algorithms with high-order integrators, and provided a comprehensive convergence analysis. For strongly log-concave and smooth distribution, a non-asymptotic convergence guarantee was proved by Cheng et al. (2017) for underdamped Langevin MCMC, which is a variant of stochastic gradient HMC method.

Our proposed algorithm is motivated by the stochastic variance reduced gradient (SVRG) algorithm, was first proposed in Johnson and Zhang (2013), and later extended to different problem setups Xiao and Zhang (2014); Defazio et al. (2014); Reddi et al. (2016); Allen-Zhu and Hazan (2016); Lei and Jordan (2016); Lei et al. (2017). Inspired by this line of research, Dubey et al. (2016) applied the variance reduction technique to stochastic gradient Langevin dynamics, and proved a slightly tighter convergence bound than SGLD. Nevertheless, the dependence of the convergence rate on the sampling accuracy $\epsilon$ is not improved. Thus, it remains open whether variance reduction technique can indeed improve the convergence rate of MCMC methods. Our work answers this question in the affirmative and provides rigorously faster rates of convergence for sampling from log-concave and smooth density functions.

For the ease of comparison, we summarize the gradient complexity\(^1\) in 2-Wasserstein distance for different gradient-based Monte Carlo methods in Table 1. Evidently, for sampling from smooth and strongly log-concave distributions, our proposed algorithm (SVR-HMC) outperforms the existing algorithms.

| Methods                  | Gradient Complexity          |
|--------------------------|------------------------------|
| LMC (Dalalyan, 2017)     | $\left( \frac{n\kappa^2 d}{\epsilon^2}, \frac{n\kappa^2 d^{1/2}}{\epsilon} \right)$ |
| HMC (Cheng et al., 2017) | $\left( \frac{\kappa^2 d^2}{\epsilon^2}, \frac{\kappa^2 d^{1/2}}{\epsilon} \right)$ |
| SGLD (Dalalyan, 2017)    | $\left( \frac{\kappa^2 d^2}{\epsilon^2}, \frac{\kappa^2 d^{1/2}}{\epsilon} \right)$ |
| SG-HMC (Cheng et al., 2017)| $\left( \frac{\kappa^2 d^2}{\epsilon^2}, \frac{\kappa^2 d^{1/2}}{\epsilon} \right)$ |
| SVR-HMC (this paper)     | $\tilde{O}\left(n + \frac{\kappa^2 d^{1/2}}{\epsilon} + \frac{\kappa^{3/4} d^{1/3} n^{2/3}}{\epsilon^{2/3}}\right)$ |

3 The Proposed Algorithm

In this section, we propose a novel HMC algorithm that leverages variance reduced stochastic gradient to sample from the target distribution $\pi = e^{-f(x)}/Z$, where $Z = \int e^{-f(x)}dx$ is the partition function.

\(^1\)The gradient complexity is defined as number of stochastic gradient evaluations to achieve $\epsilon$ sampling accuracy.
Recall that function $f(x)$ has the finite-sum structure in (1.5). When $n$ is large, the full gradient $1/n \sum_{i=1}^{n} \nabla f_i(x)$ in (1.4) can be expensive to compute. Thus, the stochastic gradient is often used to improve the computational complexity per iteration. However, due to the non-diminishing variance of the stochastic gradient, the convergence rate of gradient-based MC methods using stochastic gradient is often no better than that of gradient-based MC using full gradient.

In order to overcome the drawback of stochastic gradient, and achieve faster rate of convergence, we propose a Stochastic Variance-Reduced Hamiltonian Monte Carlo algorithm (SVR-HMC), which leverages the advantages of both HMC and variance reduction. The outline of the algorithm is displayed in Algorithm 1. We can see that the algorithm performs in a multi-epoch way. At the beginning of each epoch, it computes the full gradient of the $f$ at some snapshot of the iterate $\tilde{x}_j$. Then it performs the following update for both the velocity and the position variables in each epoch

$$
\begin{align*}
\mathbf{v}_{k+1} &= \mathbf{v}_k - \gamma \eta \mathbf{v}_k - \eta u g_k + \epsilon^v_k, \\
\mathbf{x}_{k+1} &= \mathbf{x}_k + \eta \mathbf{v}_k + \epsilon^x_k,
\end{align*}
$$

where $\gamma, \eta, u > 0$ are tuning parameters, $g_k$ is a semi-stochastic gradient that is an unbiased estimator of $\nabla f(x_k)$ and defined as follows,

$$
g_k = \nabla f_{i_k}(x_k) - \nabla f_{i_k}(\tilde{x}_j) + \nabla f(\tilde{x}_j),
$$

where $i_k$ is uniformly sampled from $\{1, \ldots, n\}$, and $\tilde{x}_j$ is a snapshot of $x_k$ that is only updated every $m$ iterations such that $k = jm + l$ for some $l = 0, \ldots, m - 1$. And $\epsilon^v_k$ and $\epsilon^x_k$ are Gaussian random vectors with zero mean and covariance matrices equal to

$$
\begin{align*}
E[\epsilon_k^v(\epsilon_k^v)^	op] &= u(1 - e^{-2\gamma \eta}) \cdot I_{d \times d}, \\
E[\epsilon_k^x(\epsilon_k^x)^	op] &= u(2\gamma \eta + 4e^{-\gamma \eta} - e^{-2\gamma \eta} - 3) \cdot I_{d \times d}, \\
E[\epsilon_k^x(\epsilon_k^v)^	op] &= u \gamma (1 - 2e^{-\gamma \eta} + e^{-2\gamma \eta}) \cdot I_{d \times d},
\end{align*}
$$

where $I_{d \times d}$ is a $d \times d$ identity matrix.

The idea of semi-stochastic gradient has been successfully used in stochastic optimization in machine learning to reduce the variance of stochastic gradient and obtains faster convergence rates (Johnson and Zhang, 2013; Xiao and Zhang, 2014; Reddi et al., 2016; Allen-Zhu and Hazan, 2016; Lei and Jordan, 2016; Lei et al., 2017). Apart from the semi-stochastic gradient, the second update formula in (3.1) also differs from the direct Euler-Maruyama discretization (1.4) of Hamiltonian dynamics due to the additional Gaussian noise term $\epsilon_k^x$. This additional Gaussian noise term is pivotal in our theoretical analysis to obtain faster convergence rates of our algorithm than LMC methods. Similar idea has been used in Cheng et al. (2017) to prove the faster rate of convergence of HMC (underdamped MCMC) against LMC.

4 Main Theory

In this section, we analyze the convergence of our proposed algorithm in 2-Wasserstein distance between the distribution of the iterate in Algorithm 1, and the target distribution $\pi \propto e^{-f}$. 

6
Algorithm 1 Stochastic Variance-Reduced Hamiltonian Monte Carlo (SVR-HMC)

1: initialization: $\tilde{x}_0 = x_0$, $\tilde{v}_0 = v_0$
2: for $j = 0, \ldots, \lceil K/m \rceil$
3:  $g = \nabla f(\tilde{x}_j)$
4:  for $l = 0, \ldots, m - 1$
5:     $k = jm + l$
6:     Generate Gaussian random variable $\epsilon_{x_k}$ and $\epsilon_{v_k}$ satisfying (3.3)
7:     Uniformly sample $i_k \in [n]$
8:     $g_k = \nabla f_{i_k}(x_k) - \nabla f_{i_k}(\tilde{x}_j) + \tilde{g}$
9:     $x_{k+1} = x_k + \eta v_k + e_{x_k}^\gamma$
10:    $v_{k+1} = v_k - \gamma \eta v_k - \eta u g_k + e_{v_k}^\gamma$.
11:   if $l = m - 1$
12:      $\tilde{x}_j = x_{k+1}$
13: end
14: end for
15: end for
16: output: $x_K$

Following the recent work Durmus and Moulines (2016a); Dalalyan and Karagulyan (2017); Dalalyan (2017); Cheng et al. (2017), we use the 2-Wasserstein distance to measure the convergence rate of Algorithm 1, since it directly provides the level of approximation of the first and second order moments (Dalalyan, 2017; Dalalyan and Karagulyan, 2017). It is arguably more suitable to characterize the quality of approximate sampling algorithms than the other distance metrics such as total variation distance. In addition, while Algorithm 1 performs update on both the position variable $x_k$ and the velocity variable $v_k$, only the convergence rate of the position variable $x_k$ is of central interest.

4.1 SVR-HMC for Sampling from Strongly Log-concave Distributions

We first present the convergence rate and gradient complexity of SVR-HMC when $f$ is smooth and strongly convex, i.e., the target distribution $\pi \propto e^{-f}$ is smooth and strongly log-concave. We start with the following formal assumptions on the objective function.

Assumption 4.1 (Smoothness). There exists a constant $L > 0$, such that for any $x, y \in \mathbb{R}^d$, the following holds for any $i$,

$$
\|\nabla f_i(x) - \nabla f_i(y)\|_2 \leq L\|x - y\|_2.
$$

Under Assumption 4.1, it can be easily verified that function $f(x)$ is also $L$-smooth.

Assumption 4.2 (Strong Convexity). There exists a constant $\mu > 0$, such that for any $x, y \in \mathbb{R}^d$, the following holds for any $i$,

$$
\|\nabla f(x) - \nabla f(y)\|_2 \geq \mu\|x - y\|_2.
$$
Note that the strong convexity assumption is only made on the finite sum function \( f \), instead of the individual component function \( f_i \)'s. This is in contrast to the smoothness assumption, which is made on each individual function \( f_i \).

Now, we are ready to deliver the main result.

**Theorem 4.3.** Under Assumptions 4.1 and 4.2. Let \( P(x_K) \) denote the distribution of the last iterate \( x_K \), and \( \pi \propto e^{-f(x)} \) denote the stationary distribution of (1.3). If setting \( u = 1/L \) and \( \gamma = 2 \), the output of in Algorithm 1 satisfies,

\[
W_2(P(x_K), \pi) \leq e^{-K\eta/(2\kappa)}w_0 + 4\eta\kappa(2\sqrt{D_1} + \sqrt{D_2}) + 2\sqrt{\kappa D_3\eta^{3/2}},
\]

where \( w_0 = W_2(P(x_0), \pi) \), \( \kappa = L/\mu \) is the condition number, \( \eta \) is the step size, and \( m \) denotes the epoch (i.e., inner loop) length of Algorithm 1. \( D_1, D_2 \) and \( D_3 \) are defined as follows,

\[
\begin{align*}
D_1 &= \left( \frac{8\eta^2}{5} + \frac{4}{3} \right)U_v + \frac{4}{3L}U_f + \frac{16dn}{3L}, \\
D_2 &= 13U_v + \frac{8U_f}{L} + \frac{28dn}{L}, \\
D_3 &= U_v + 4ud,
\end{align*}
\]

in which parameters \( U_v \) and \( U_f \) are in the order of \( O(d/\mu) \) and \( O(d\kappa) \), respectively.

**Remark 4.4.** In existing stochastic Langevin Monte Carlo methods (Dalalyan and Karagulyan, 2017; Zhang et al., 2017) and stochastic Hamiltonian Monte Carlo methods (Chen et al., 2014, 2015; Cheng et al., 2017), their convergence analyses require that the variance of stochastic gradient is bounded, i.e., the inequality \( \mathbb{E}_i \| \nabla f_i(x) - \nabla f(x) \|_2^2 \leq \sigma^2 \) holds uniformly for all \( x \in \mathbb{R}^d \). In stark contrast, our analysis does not need this assumption, which implies that our algorithm is applicable to a larger class of target density functions.

In the following corollary, by providing a specific choice of step size \( \eta \), and epoch length \( m \), we present the gradient complexity of Algorithm 1 in 2-Wasserstein distance.

**Corollary 4.5.** Under the same assumptions as in Theorem 4.3, let \( m = n \) and \( \eta = O(\epsilon/(\kappa^{-1}d^{-1/2})\wedge \epsilon^{2/3}/(\kappa^{1/3}d^{1/3}n^{2/3})) \). Then the output of Algorithm 1 satisfies \( W_2(P(x_K), \pi) \leq \epsilon \) after

\[
\tilde{O}\left(n + \frac{\kappa^2d^{1/2}}{\epsilon} + \frac{n^{2/3}\kappa^{4/3}d^{1/3}}{\epsilon^{2/3}}\right)
\]

stochastic gradient evaluations.

**Remark 4.6.** Recall that the gradient complexity of HMC is \( n\kappa^2d^{1/2}/\epsilon \) and the gradient complexity of SG-HMC is \( \tilde{O}(\kappa^2d\sigma^2/\epsilon^2) \), both of which are recently proved in Cheng et al. (2017). It can be seen from Corollary 4.5 that the gradient complexity of our SVR-HMC algorithm has a better dependence on dimension \( d \).

Note that the gradient complexity of SVR-HMC in (4.2) depends on the relationship between sample size \( n \) and precision parameter \( \epsilon \). To make a thorough comparison with existing algorithms, we discuss our result for SVR-HMC in the following three regimes:
• When \( n \lesssim \kappa d^{1/4}/\epsilon^{1/2} \), the gradient complexity of our algorithm is dominated by \( (\kappa^2 d^{1/2}/\epsilon) \), which is lower than that of the HMC algorithm by a factor of \( (n) \) and lower than that of the SG-HMC algorithm by a factor of \( (d^{1/2}/\epsilon) \).

• When \( \kappa d^{1/4}/\epsilon^{1/2} \lesssim n \lesssim \kappa d^2 \sigma^2 d/\epsilon^2 \), the gradient complexity of our algorithm is dominated by \( (n^{2/3} \kappa^{4/3} d^{1/3}/\epsilon^{2/3}) \). It improves that of HMC by a factor of \( (n^{1/3} \kappa^{2/3} d^{1/6}/\epsilon^{1/3}) \), and is lower than that of SG-HMC by a factor of \( (\kappa^{2/3} d^{2/3} \sigma^2 n^{-2/3}/\epsilon^{4/3}) \). Plugging in the upper bound of \( n \) into (4.2) yields \( (\kappa^2 d^2 \sigma^2 /\epsilon^2) \) gradient complexity, which still matches that of SG-HMC.

• When \( n \gtrsim \kappa^4 d/\epsilon^2 \), i.e., the sample size is super large, the gradient complexity of our algorithm is dominated by \( (n) \). It is still lower than that of HMC by a factor of \( (\kappa^2 d^{1/2}/\epsilon) \). Nonetheless, our algorithm has a higher gradient complexity than SG-HMC due to the extremely large sample size. This suggests that SG-HMC (Cheng et al., 2017) is the most suitable algorithm in this regime.

4.2 SVR-HMC for Sampling from General Log-concave Distributions

In this section, we show that the proposed algorithm SVR-HMC can also be used for sampling from distributions, which are only general log-concave but not strongly log-concave.

In detail, we want to sample from the distribution \( \pi \propto e^{-f(x)} \), where \( f \) is general convex and \( L \)-smooth. We follow the similar idea in Dalalyan (2014) to construct a strongly log-concave distribution by adding a quadratic regularizer to the convex and \( L \)-smooth function \( f \), which yields

\[
\tilde{f}(x) = f(x) + \lambda \|x\|^2/2,
\]

where \( \lambda > 0 \) is a regularization parameter. Apparently, \( \tilde{f} \) is \( \lambda \)-strongly convex and \( (L + \lambda) \)-smooth. Then we can apply Algorithm 1 to function \( \tilde{f} \), which amounts to sampling from the modified target distribution \( \tilde{\pi} \propto e^{-\tilde{f}} \). We will obtain a sequence \( \{x_k\}_{k=0}^{K} \), whose distribution converges to a unique stationary distribution of Hamiltonian dynamics (1.3), denoted by \( \bar{\pi} \). According to Neal et al. (2011), \( \tilde{\pi} \) is propositional to \( e^{-f(x)} \), i.e.,

\[
\tilde{\pi} \propto \exp(-\tilde{f}(x)) = \exp\left(-f(x) - \frac{\lambda}{2} \|x\|^2\right).
\]

Denote the distribution of \( x_k \) by \( P(x_k) \). By triangle inequality we have

\[
W_2(P(x_k, \pi)) \leq W_2(P(x_k, \bar{\pi})) + W_2(\bar{\pi}, \pi).
\]

(4.3)

To bound the 2-Wasserstein distance between \( P(x_k) \) and the desired distribution \( \pi \), we only need to upper bound the 2-Wasserstein distance between two Gibbs distribution \( \tilde{\pi} \) and \( \pi \). Before we present our theoretical characterization on this distance, we first lay down the following assumption.

Assumption 4.7. Regarding distribution \( \pi \propto e^{-f} \), its fourth-order moment is upper bounded, i.e., there exists a constant \( \bar{U} \) such that \( \mathbb{E}_\pi[\|x\|_2^4] \leq \bar{U} d^2 \).

The following theorem spells out the convergence rate of SVR-HMC for sampling from a general log-concave distribution.
Theorem 4.8. Under Assumptions 4.1 and 4.7, in order to sample for a general log-concave density \( \pi \propto e^{-f(x)} \), the output of Algorithm 1 when applied to \( \tilde{f}(x) = f(x) + \lambda \|x\|_2^2/2 \) satisfies \( \mathcal{W}_2(P(x_k), \pi) \leq \epsilon \) after
\[
\tilde{O}\left(n + \frac{d^{11/2}}{\epsilon^6} + \frac{d^{11/3}n^{2/3}}{\epsilon^{10/3}}\right)
\]
gradient evaluations.

Regarding to sampling from a smooth and general log-concave distribution, to the best of our knowledge, there is no existing theoretical analysis on the convergence of LMC algorithms in 2-Wasserstein distance. Yet the convergence analyses of LMC methods in total variation distance (Dalalyan, 2014; Durmus et al., 2017) and KL-divergence (Cheng and Bartlett, 2017) have recently been established. In detail, Dalalyan (2014) proved a convergence rate of \( (d^3/\epsilon^4) \) in total variation distance for LMC with general log-concave distributions, which implies \( (nd^3/\epsilon^4) \) gradient complexity. Durmus et al. (2017) improved the gradient complexity of LMC in total variation distance to \( (nd^5/\epsilon^2) \). Cheng and Bartlett (2017) proved the convergence of LMC in KL-divergence, which attains \( (nd/\epsilon^3) \) gradient complexity. It is worth noting that our convergence rate in 2-Wasserstein distance is not directly comparable to the aforementioned existing results.

![Figure 1: Numerical results for synthetic data, where we compare 3 different algorithms, and show their convergence performance in 2-Wasserstein distance. (a)-(h) represent for different dimensions \( d \) and sample sizes \( n \).](image-url)
5 Experiments

In this section, we compare the proposed algorithm (SVR-HMC) with the state-of-the-art MCMC algorithms for Bayesian learning. To compare the convergence rates for different MCMC algorithms, we conduct the experiments on both synthetic data and real data. We compare our algorithm with SGLD (Welling and Teh, 2011), VR-SGLD (Reddi et al., 2016), HMC (Cheng and Bartlett, 2017) and SG-HMC (Cheng and Bartlett, 2017).

5.1 Simulation Based on Synthetic Data

On the synthetic data, we construct each component function to be \( f_i(x) = (x - a_i)\Sigma(x - a_i)/2 \), where each element in \( a_i \) is sampled i.i.d. from the Gaussian distribution \( \mathcal{N}(2, 4) \), and \( \Sigma \) is a positive definite symmetric matrix with maximum eigenvalue \( L = 3/2 \) and minimum eigenvalue \( \mu = 2/3 \). Then the target density \( \pi \propto \exp \left( 1/n \sum_{i=1}^{n} f_i(x) \right) \propto \exp \left( (x - \bar{a})\Sigma(x - \bar{a})/2 \right) \) is a multivariate Gaussian distribution with mean \( \bar{a} = 1/n \sum_{i=1}^{n} a_i \) and covariance matrix \( \Sigma \).

In our simulation, we investigate different dimension \( d \) and number of component functions \( n \), and show the 2-Wasserstein distance between the target distribution \( \pi \) and that of the output from different algorithms with respect to the number of data passes. In order to estimate the 2-Wasserstein distance between the distribution of each iterate and the target one, we repeat all algorithms for 20,000 times and obtain 20,000 random samples for each algorithm in each iteration. In Figure 1, we present the convergence results for three HMC based algorithms (HMC, SG-HMC and SVR-HMC). It is evident that SVR-HMC performs the best among these three algorithms when \( n \) is not large enough, and its performance becomes close to that of SG-HMC when the number of component function is increased. This phenomenon is well-aligned with our theoretical analysis, since the gradient complexity of our algorithm can be worse than SG-HMC when the sample size \( n \) is extremely large.

5.2 Bayesian Logistic Regression for Classification

Figure 2: Comparison of different algorithms for Bayesian logistic regression, where \( y \) axis shows the negative log-likelihood on the test data, and \( y \) axis is the number of data passes. (a)-(d) correspond to 4 datasets.
Table 2: Summary of datasets for Bayesian classification

| Dataset      | pima   | a3a   | gisette | mushroom |
|--------------|--------|-------|---------|----------|
| n (training) | 384    | 3185  | 6000    | 4062     |
| n (test)     | 384    | 29376 | 1000    | 4062     |
| d            | 8      | 122   | 5000    | 112      |

Table 3: Test error of different algorithms for Bayesian classification after 10 entire data passes on 4 datasets

| Dataset | pima   | a3a   | gisette | mushroom |
|---------|--------|-------|---------|----------|
| SGLD    | 0.2314 ± 0.0044 | 0.1594 ± 0.0018 | 0.0098 ± 0.0009 | (6.647 ± 2.251) × 10^{-4} |
| SGHMC   | 0.2306 ± 0.0079 | 0.1591 ± 0.0044 | 0.0096 ± 0.0006 | (5.916 ± 2.734) × 10^{-4} |
| VR-SGLD | 0.2299 ± 0.0056 | 0.1572 ± 0.0012 | 0.0105 ± 0.0006 | (7.755 ± 3.231) × 10^{-4} |
| SVR-HMC | 0.2289 ± 0.0043 | 0.1570 ± 0.0019 | 0.0093 ± 0.0011 | (6.278 ± 3.149) × 10^{-4} |

Now, we apply our algorithm to the Bayesian logistic regression problems. In logistic regression, given \( n \) i.i.d. examples \( \{a_i, y_i\}_{i=1,...,n} \), where \( a_i \in \mathbb{R}^d \) and \( y_i \in \{0,1\} \) denote the features and binary labels respectively, the probability mass function of \( y_i \) given the feature \( a_i \) is modelled as

\[
p(y_i|a_i, x) = 1/(1 + e^{-y_i a_i^\top x}),
\]

where \( x \in \mathbb{R}^d \) is the regression parameter. Considering the prior \( p(x) = \mathcal{N}(0, \lambda^{-1}I) \), the posterior distribution takes the form

\[
p(x|A, Y) \propto p(Y|A, x)p(x) = \prod_{i=1}^n p(y_i|a_i, \beta)p(x).
\]

where \( A = [a_1, a_2, \ldots, a_n]^\top \) and \( Y = [y_1, y_2, \ldots, y_n]^\top \). The posterior distribution can be written as

\[
p(x|A, Y) \propto e^{-\sum_{i=1}^n f_i(x)},
\]

where each \( f_i(x) \) is in the following form

\[
f_i(x) = n \log \left( 1 + \exp(-y_i a_i^\top x) \right) + \lambda/2\|x\|_2^2.
\]
We use four binary classification datasets from Libsvm (Chang and Lin, 2011) and UCI machine learning repository (Lichman, 2013), which are summarized in Table 3. Note that *pima* and *mushroom* do not have test data in their original version, and we split them into 50% for training and 50% for test. In order to compare the performance of different algorithms, we report log-likelihood results on the test data. Following Welling and Teh (2011); Chen et al. (2014, 2015), we report the sample path average and discard the first 50 iterations as burn-in. We run each algorithm 20 times and report the averaged results for comparison. Note that variance reduction based algorithms (i.e., VR-SGLD and SVR-HMC) require the first data pass to compute one full gradient. Therefore, in Figure 2, plots of VR-SGLD and VRHMC start from the second data pass while plots of SGLD and SGHMC start from the first data pass. It can be clearly seen that our proposed algorithm is able to converge faster than SGLD and SG-HMC on all datasets, which validates our theoretical analysis of the convergence rate. In addition, although there is no existing non-asymptotic theoretical guarantee for VR-SGLD when the target distribution is strongly log-concave, from Figure 2, we can observe that SVR-HMC also outperforms VR-SGLD on these four datasets, which again demonstrates the superior performance of our algorithm. This clearly shows the advantage of our algorithm for Bayesian learning.

### 5.3 Bayesian Linear Regression

We also apply our algorithm to Bayesian linear regression, and make comparison with the baseline algorithms. Similar to Bayesian classification, given i.i.d. examples \( \{ \mathbf{a}_i, y_i \}_{i=1}^n \) with \( y_i \in \mathbb{R} \), the likelihood of Bayesian linear regression is \( p(y_i | \mathbf{a}_i, \mathbf{x}) = \mathcal{N}(\mathbf{x}^\top \mathbf{a}_i, \sigma_a^2) \) and the prior is \( \mathcal{N}(\mathbf{0}, \lambda^{-1} \mathbf{I}) \). We use 4 datasets, which are summarized in Table 4. In our experiment, we set \( \sigma_a^2 = 1 \) and \( \lambda = 1 \), and conduct the normalization of the original data. In addition, we split each dataset into training and test data evenly. Similarly, we compute the sample path average while treating the first 50 iterates as burn in. In order to compare the performance of different algorithms, we report the mean square errors on the test data on these 4 datasets in Figure 3. It is evident that our algorithm is faster than all the other baseline algorithms on all the datasets, which further illustrates the advantage of our algorithm for Bayesian learning.

| Dataset   | geographical | noise | parkinson | toms  |
|-----------|--------------|-------|-----------|-------|
| \( n \)   | 1059         | 1503  | 5875      | 45730 |
| \( d \)   | 69           | 5     | 21        | 96    |

### 6 Conclusions and Future work

We propose a stochastic variance reduced Hamilton Monte Carlo (HMC) method, for sampling from a smooth and strongly log-concave distribution. We show that, to achieve \( \epsilon \) accuracy in 2-Wasserstein distance, our algorithm enjoys a faster rate of convergence and better gradient complexity than
state-of-the-art HMC and stochastic gradient HMC methods in a wide regime. We also extend our algorithm for sampling from smooth and general log-concave distributions. Experiments on both synthetic and real data verified the superior performance of our algorithm. In the future, we will extend our algorithm to nonconvex functions.

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