Faster Convergence of Stochastic Gradient Langevin Dynamics for Non-Log-Concave Sampling

Difan Zou∗ and Pan Xu† and Quanquan Gu‡

Abstract

We establish a new convergence analysis of stochastic gradient Langevin dynamics (SGLD) for sampling from a class of distributions that can be non-log-concave. At the core of our approach is a novel conductance analysis of SGLD using an auxiliary time-reversible Markov Chain. Under certain conditions on the target distribution, we prove that $O(d^4 \epsilon^{-2})$ stochastic gradient evaluations suffice to guarantee $\epsilon$-sampling error in terms of the total variation distance, where $d$ is the problem dimension, which improves existing results on the convergence rate of SGLD (Raginsky et al., 2017; Xu et al., 2018). We further show that provided an additional Hessian Lipschitz condition on the log-density function, SGLD is guaranteed to achieve $\epsilon$-sampling error within $O(d^{15/4} \epsilon^{-3/2})$ stochastic gradient evaluations. Our proof technique provides a new way to study the convergence of Langevin based algorithms, and sheds some light on the design of fast stochastic gradient based sampling algorithms.

1 Introduction

We study the problem of sampling from a target distribution using Langevin dynamics (Langevin, 1908) based algorithms. Mathematically, Langevin dynamics (a.k.a., overdamped Langevin dynamics) is defined by the following stochastic differential equation (SDE)

$$dX(t) = -\nabla f(X(t))dt + \sqrt{2/\beta} dB(t),$$

where $\beta > 0$ is called the inverse temperature parameter and $B(t) \in \mathbb{R}^d$ is the Brownian motion at time $t$. It has been proved in Chiang et al. (1987); Roberts and Tweedie (1996) that under certain conditions on the drift term $-\nabla f(X(t))$, the Langevin dynamics will converge to a unique stationary distribution $\pi(dx) \propto e^{-\beta f(x)} dx$. To approximately sample from such a target distribution $\pi$, we can apply the Euler-Maruyama discretization onto (1.1), leading to the Langevin Monte Carlo algorithm (LMC), which iteratively updates the parameter $x_k$ as follows

$$x_{k+1} = x_k - \eta \nabla f(x_k) + \sqrt{2\eta/\beta} \epsilon_k,$$
where $k = 0, 1, \ldots$ denotes the time step, $\{\epsilon_k\}_{k=0,1,\ldots}$ are i.i.d. standard Gaussian random vectors in $\mathbb{R}^d$, and $\eta > 0$ is the step size of the discretization.

In large scale machine learning problems that involve a large amount of training data points, the log-density function $f(x)$ can be typically formulated as the average of the log-density functions over all the training data points, i.e., $f(x) = n^{-1} \sum_{i=1}^{n} f_i(x)$, where $n$ is the size of training dataset and $f_i(x)$ denotes the log-density function for the $i$-th training data point. In these problems, the computation of the full gradient over the entire dataset can be very time consuming. In order to save the cost of gradient computation, one can replace the full gradient $\nabla f(x)$ with a stochastic gradient computed only over a small subset of the dataset, which gives rise to stochastic gradient Langevin dynamics (SGLD) (Welling and Teh, 2011).

When the target distribution $\pi$ is log-concave, SGLD provably converges to $\pi$ at a sublinear rate in 2-Wasserstein distance (Dalalyan and Karagulyan, 2019; Dalalyan, 2017a; Wang et al., 2019). However, it becomes much more challenging to establish the convergence of SGLD when the target distribution is not log-concave. When the negative log-density function $f(x)$ is smooth and dissipative, the global convergence guarantee of SGLD has been firstly established in Raginsky et al. (2017) via optimal control theory and further improved in Xu et al. (2018) by a direct analysis of the ergodicity of LMC. Nonetheless, these two works require extremely large mini-batch size (e.g., $B = \Omega(\epsilon^{-4})$) to ensure sufficiently small sampling error, which is prohibitively large or even unrealistic compared with the practical setting. Zhang et al. (2017) studied the hitting time of SGLD for nonconvex optimization, but can only provide the convergence guarantee for finding a local minimum rather than converging to the target distribution. Recently, Chau et al. (2019); Zhang et al. (2019b) studied the global convergence of SGLD for nonconvex stochastic optimization problems and proved sharper convergence rates than those in Raginsky et al. (2017); Xu et al. (2018). However, their convergence results require additional data-based Lipschitz conditions on the stochastic gradients, which restricts their applications from a wide class of SGLD-based sampling problems.

In this paper, we consider the same setting in Raginsky et al. (2017); Xu et al. (2018) and aim to establish faster convergence rates for SGLD with an arbitrary mini-batch size. In particular, we establish a new convergence analysis for SGLD based on an auxiliary time-reversible Markov chain called Metropolized SGLD (Zhang et al., 2017), which is constructed by adding a Metropolis-Hasting step to SGLD. We show that as long as the transition kernel of the constructed Metropolized SGLD chain is sufficiently close to that of SGLD, we can prove the convergence of SGLD to the target distribution. Compared with existing proof approaches that typically take LMC or Langevin dynamics as an auxiliary sequence, Metropolized SGLD is closer to SGLD as its transition distribution also covers the randomness of stochastic gradients, thus can better characterize the convergence behavior of SGLD and lead to sharper convergence guarantees. To sum up, we highlight our main contributions as follows:

- We provide a new convergence analysis of SGLD for sampling a large class of distributions.

\[1\text{In some cases, the log-density function } f(x) \text{ is formulated as the sum of the log-density functions for training data points instead of the average. To cover these cases, we can simply transform the temperature parameter } \beta \rightarrow n\beta \text{ and thus the target distribution remains the same.}\]

\[2\text{Although this paper mainly focuses on the convergence analysis of SGLD for nonconvex optimization, part of its theoretical results also reveal the convergence rate for sampling from a target distribution.}\]

\[3\text{This Markov chain is practically intractable and is only used for the sake of theoretical analysis.}\]
that can be non-log-concave. In contrast to Raginsky et al. (2017); Xu et al. (2018) that require a very large mini-batch size, our convergence guarantee holds for arbitrary choice of mini-batch size.

- We prove that SGLD can achieve $\epsilon$-sampling error in total variation distance within $\tilde{O}(d^4\beta^2\rho^{-4}\epsilon^{-2})$ stochastic gradient evaluations, where $d$ is the problem dimension, $\beta$ is the inverse temperature parameter, and $\rho$ is the Cheeger constant (See Definition 4.2) of the target distribution. We also prove the convergence of SGLD under the measure of polynomial growth functions, which suggests that the number of required stochastic gradient evaluations is $\tilde{O}(\epsilon^{-2})$. This improves the state-of-the-art result proved in Xu et al. (2018) by a factor of $\tilde{O}(\epsilon^{-3})$.

- We further establish sharper convergence guarantees for SGLD provided with an additional Hessian Lipschitz condition on the log density function $f(x)$. We show that $\tilde{O}(d^{15/4}\beta^{7/4}\rho^{-7/4}\epsilon^{-3/2})$ stochastic gradient evaluations suffice to achieve $\epsilon$-sampling error in total variation distance. Our proof technique is much simpler and more intuitive than existing analysis for proving the convergence of Langevin algorithms under the Hessian Lipschitz condition (Dalalyan and Karagulyan, 2019; Mou et al., 2019; Vempala and Wibisono, 2019), which can be of independent interest.

**Notation.** We use the notation $x \wedge y$ and $x \vee y$ to denote $\min\{x, y\}$ and $\max\{x, y\}$ respectively. We denote by $B(u, r)$ the Euclidean of radius $r > 0$ centered at $u \in \mathbb{R}^d$. For any distribution $\mu$ and set $A$, we use $\mu(A)$ to denote the probability measure of $A$ under the distribution $\mu$. For any two distributions $\mu$ and $\nu$, we use $\|\mu - \nu\|_{TV}$ and $D_{KL}(\mu, \nu)$ to denote the total variation distance and Kullback–Leibler divergence between $\mu$ and $\nu$ respectively. For $u, v \in \mathbb{R}^d$, we use $T_u(v)$ to denote the probability of transiting to $v$ after one step SGLD update from $u$. Similarly, $T_u(A)$ and $T_{\mathcal{A}}(A)$ are the probabilities of transiting to a set $A \subseteq \mathbb{R}^d$ after one step SGLD update starting from $u$ and the set $\mathcal{A}$ respectively. For any two sequences $\{a_n\}$ and $\{b_n\}$, we denote $a_n = O(b_n)$ and $a_n = \Omega(b_n)$ if $a_n \leq C_1 b_n$ or $a_n \geq C_2 b_n$ for some absolute constants $C_1$ and $C_2$. We use notations $\tilde{O}(\cdot)$ and $\tilde{\Omega}(\cdot)$ to hide polylogarithmic factors in $O(\cdot)$ and $\Omega(\cdot)$.

## 2 Related Work

Markov Chain Monte Carlo (MCMC) methods, such as random walk Metropolis (Mengersen et al., 1996), ball walk (Lovász and Simonovits, 1990), hit-and-run (Smith, 1984) and Langevin algorithms (Rossky et al., 1978; Parisi, 1981), have been extensively studied for sampling from a target distribution, and widely used in many machine learning applications. There are a large number of literature focusing on developing fast MCMC algorithms and establishing sharp theoretical guarantees. We will review the most related works among them due to the space limit.

Langevin dynamics (1.1) based algorithms have recently aroused as a promising method for accurate and efficient Bayesian sampling in both theory and practice (Welling and Teh, 2011; Dalalyan, 2017b). The non-asymptotic convergence rate of LMC has been extensively investigated in the literature when the target distribution is strongly log-concave (Durmus and Moulines, 2016; Dalalyan, 2017b; Durmus et al., 2017b), weakly log-concave (Dalalyan, 2017a; Mangoubi and Vishnoi, 2019), and non-log-concave but admits certain good isoperimetric properties (Raginsky et al., 2017; Ma et al., 2018; Lee et al., 2018; Xu et al., 2018; Vempala and Wibisono, 2019), to mention a few.
The stochastic variant of LMC, i.e., SGLD, is often studied together in the above literature and
the convex/nonconvex optimization field (Raginsky et al., 2017; Zhang et al., 2017; Xu et al., 2018;
Gao et al., 2018b; Chen et al., 2019a, 2020; Deng et al., 2020). Another important Langevin based
algorithm is the Metropolis Adjusted Langevin Algorithms (MALA) (Roberts and Tweedie, 1996),
which is developed by introducing a Metropolis-Hasting step into LMC. Theoretically, it has been
proved that MALA converges to the target distribution at a linear rate for sampling from both
strongly log-concave (Dwivedi et al., 2018) and non-log-concave (Bou-Rabee and Hairer, 2013; Ma
et al., 2018) distributions.

Beyond first-order MCMC methods, there has also emerged extensive work on high-order MCMC
methods. One popular algorithm among them is Hamiltonian Monte Carlo (HMC) (Neal et al.,
2011), which introduces a Hamiltonian momentum and leapfrog integrator to accelerate the mixing
rate. From the theoretical perspective, Durmus et al. (2017a) established general conditions under
which HMC can be guaranteed to be geometrically ergodic. Mangoubi and Vishnoi (2018, 2019)
proved the convergence rate of HMC for sampling log-concave distributions. Bou-Rabee et al.
(2018); Chen et al. (2019b) studied the convergence of Metropolized HMC (MHMC) for sampling
strongly log-concave distributions. Another important high-order MCMC methods are built upon
the underdamped Langevin dynamics, which incorporates the velocity into the Langevin dynamics
(1.1). For continuous-time underdamped Langevin dynamics, its mixing rate has been studied in
Eberle (2016); Eberle et al. (2017). The convergence of its discrete version has also been widely
studied for sampling from both log-concave (Chen et al., 2017; Dalalyan and Riou-Durand, 2018)
and non-log-concave distributions (Chen et al., 2015; Cheng et al., 2018a; Gao et al., 2018b,a).

3 The SGLD Algorithm

In this section, we introduce the SGLD algorithm, as displayed in Algorithm 1, which is built upon
the Euler-Maruyama discretization of the continuous-time Langevin dynamics (1.1) while using
mini-batch stochastic gradient in each iteration.

In the k-th iteration, SGLD samples a mini-batch of data points without replacement, denoted by
\( \mathcal{I} \), and computes the stochastic gradient at the current iterate \( \mathbf{x}_k \), i.e.,
\[
\nabla f(x_k) = \frac{1}{B} \sum_{i \in \mathcal{I}} \nabla f_i(x_k),
\]
where \( B = |\mathcal{I}| \) is the mini-batch size. Based on the stochastic gradient, the model parameter is
updated using the following rule,
\[
\mathbf{x}_{k+1} = \mathbf{x}_k - \eta g(x_k, \mathcal{I}) + \sqrt{2\eta/\beta} \cdot \mathbf{\epsilon}_k,
\]
where \( \mathbf{\epsilon}_k \) is randomly drawn from a standard normal distribution \( N(0, I) \) and \( \eta > 0 \) is the step size.

For the sake of analysis, we follow the same idea in Zhang et al. (2017) and add an extra step in
Algorithm 1 with the following accept/reject rule:
\[
\mathbf{x}_{k+1} = \begin{cases} 
\mathbf{x}_{k+1} & \mathbf{x}_{k+1} \in B(x_k, r) \cap B(0, R); \\
\mathbf{x}_k & \text{otherwise.}
\end{cases}
\]
(3.1)

This step ensures each new iterate \( \mathbf{x}_{k+1} \) does not go too far away from the previous iterate and all
iterates are restricted in a (relatively) large region \( B(0, R) \). Due to the above accept/reject rule,
Algorithm 1 is slightly different from the standard SGLD algorithm (Welling and Teh, 2011). This
Algorithm 1 Stochastic Gradient Langevin Dynamics (SGLD)

**input:** step size $\eta$; mini-batch size $B$; inverse temperature parameter $\beta$; radius $R$, $r$; maximum iteration number $k_{\text{max}}$

Randomly draw $x_0$ from initial distribution $\mu_0$.

for $k = 0, 1, \ldots, k_{\text{max}}$ do

    Randomly pick a subset $I$ from $\{1, \ldots, n\}$ of size $|I| = B$; randomly draw $\epsilon_k \sim N(0, I)$

    Compute the stochastic gradient $g(x_k, I) = 1/B \sum_{i \in I} \nabla f_i(x_k)$

    Update: $x_{k+1} = x_k - \eta g(x_k, I) + \sqrt{2\eta/\beta} \epsilon_k$

    if $x_{k+1} \notin B(x_k, r) \cap B(0, R)$ then
        $x_{k+1} = x_k$
    end if

end for

**output:** $\{x_i\}_{i=0,\ldots,k_{\text{max}}}$

A variant of SGLD was first proposed and investigated in Zhang et al. (2017). In fact, given proper choices of the radii $R$ and $r$, with high probability Algorithm 1 will accept all iterates, thus generate exactly the same outputs as the standard SGLD (see Appendix A for more details).

Essentially, Algorithm 1 will approximately generate samples from the following truncated target distribution (i.e., the restriction of $\pi$ to a set $\Omega = B(0, R)$).

$$
\pi^*(dx) = \begin{cases} 
\frac{e^{-\beta f(x)}}{\int_{\Omega} e^{-\beta f(y)} dy} dx & x \in \Omega; \\
0 & \text{otherwise.}
\end{cases} \tag{3.2}
$$

In the later analysis, we will show that with a proper choice of $R$, $\pi^*$ can be sufficiently close to $\pi$, if the target distribution has an exponential tail. Thus the output of Algorithm 1 can well approximate the target distribution $\pi$ (see Lemma 6.5 for more details).

## 4 Main Theory

In this section, we present our main theoretical results on the convergence rate of Algorithm 1. To begin with, we first provide the following two definitions. The first one quantifies the goodness of the initial distribution compared with the target distribution, and the second one characterizes the isoperimetric profile of a given distribution. Both definitions are widely used in the convergence analysis of MCMC methods (Lovász and Simonovits, 1993; Vempala, 2007; Dwivedi et al., 2018; Mangoubi and Vishnoi, 2019).

**Definition 4.1** ($\lambda$-warm start). Let $\nu$ be a distribution on $\Omega$. We say the initial distribution $\mu_0$ is a $\lambda$-warm start with respect to $\nu$ if

$$
\sup_{\mathcal{A} \subseteq \Omega} \frac{\mu_0(\mathcal{A})}{\nu(\mathcal{A})} \leq \lambda.
$$
Definition 4.2 (Cheeger constant). Let $\mu$ be a probability measure on $\Omega$. We say $\mu$ satisfies the isoperimetric inequality with Cheeger constant $\rho$ if for any $A \in \Omega$, it holds that

$$\lim_{h \to 0^+} \inf \frac{\mu(A_h) - \mu(A)}{h} \geq \rho \min \{\mu(A), 1 - \mu(A)\},$$

where $A_h = \{x \in \Omega : \exists y \in A, \|x - y\|_2 \leq h\}$.

Next, we introduce some common assumptions on the log density function $f(x)$ and stochastic gradients $g(x, I)$ that are used in Algorithm 1.

Assumption 4.3 (Dissipativeness). There are absolute constants $m > 0$ and $b \geq 0$ such that

$$\langle \nabla f(x), x \rangle \geq m\|x\|^2 - b,$$

for all $x \in \mathbb{R}^d$.

This assumption has been conventionally made in the convergence analysis for sampling form non-log-concave distributions (Raginsky et al., 2017; Xu et al., 2018; Zou et al., 2019a). Basically, this assumption implies that the log density function $f(x)$ grows like a quadratic function when $x$ is outside a ball centered at the origin. Note that a strongly convex function $f(x)$ simply satisfies Assumption 4.3, but not vice versa.

Assumption 4.4 (Smoothness). There exists a positive constant $L$ such that for any $x, y \in \mathbb{R}^d$ and all functions $f_i(x)$, it holds that

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

This assumption has also been made in many related papers (Raginsky et al., 2017; Zhang et al., 2017; Xu et al., 2018).

We now define the following function that will be repeatedly used in the subsequent theoretical results:

$$\bar{R}(\zeta) = \left[\max\left\{\frac{4d \log(4L/m)}{m\beta}, \frac{4d + 8\sqrt{d \log(1/\zeta)} + 8 \log(1/\zeta)}{m\beta}\right\}\right]^{1/2}. \quad (4.1)$$

Then based on all aforementioned assumptions, we present the convergence result of Algorithm 1 in the following theorem.

Theorem 4.5. Under Assumptions 4.3 and 4.4, for any $\zeta \in (0, 1/2)$, set $R = \bar{R}(\zeta)$, $\eta = O(R^{-1} \wedge \rho^2 d^{-2})$ and $r = \sqrt{10\eta d/\beta}$. Let $\pi^*$ be the truncated target distribution in $\Omega = B(0, R)$. Then for any $\lambda$-warm start with respect to $\pi^*$, the output of Algorithm 1 satisfies

$$\|\mu_k - \pi\|_{TV} \leq \lambda(1 - C_0\eta)^k + 3\zeta + \frac{C_1\eta^{1/2}}{B} + C_2\eta^{1/2},$$

where $\mu_k$ denotes the distribution of $x_k$, $\rho$ is the Cheeger constant of $\pi^*$, $C_0 = \bar{O}(\rho^2 \beta^{-1})$, $C_1 = \bar{O}(Rd\rho^{-1}\beta^{3/2})$ and $C_2 = \bar{O}(d\rho^{-1}\beta^{1/2})$ are problem-dependent constants.

Remark 4.6. Theorem 4.5 shows that the total variation distance between the distributions $\mu_k$ and $\pi$ can be upper bounded by the sum of four terms. In specific, the first term corresponds to
the sampling error of Metropolized SGLD, which converges to zero at a linear rate. The second term represents the difference between the target distribution $\pi(x)e^{-\beta f(x)}$ and its truncated version $\pi^*$. The last two terms correspond to the approximation error between SGLD and Metropolized SGLD, which is in the order of $O(\eta^{1/2})$. Moreover, regarding the approximation error, the third term corresponds to the variance of stochastic gradients, and will diminish if we use full gradient in each iteration.

**Remark 4.7.** If we set $\zeta = O(\eta^{1/2})$, then it can be observed that when $k \to \infty$, SGLD achieves sampling error at most $O(\eta^{1/2})$, suggesting that the stationary distribution of SGLD (if exists) is $\eta^{1/2}$-close to the stationary distribution of the Langevin dynamics (1.1). This bypasses the drawback of a large body of existing works (Raginsky et al., 2017; Xu et al., 2018; Gao et al., 2018b; Zou et al., 2019a; Nguyen et al., 2019; Zhang et al., 2019a) where the sampling error bound usually diverges when the number of iterations goes to infinity.

Note that the upper bound of the sampling error proved in Theorem 4.5 relies on the step size, mini-batch size, and the goodness of the initialization (i.e., $\lambda$). In order to guarantee $\epsilon$-sampling error of Algorithm, we need to specify the choices of these hyper-parameters. In particular, we present the iteration complexity of Algorithm 1 in the following Corollary.

**Corollary 4.8.** Under the same assumptions made in Theorem 4.5, consider Gaussian initialization $\mu_0 = N(0, I/(2\beta L))$, then for any mini-batch size $B \leq n$, if set the step size and maximum iteration number as

$$\eta = \tilde{O}\left(\frac{\rho^2 \epsilon^2}{d^2 \beta} \wedge \frac{B^2 \rho^2 \epsilon^2}{d^4 \beta}\right), \quad k_{\max} = \tilde{O}\left(\frac{d^3 \beta^2}{\rho^4 \epsilon^2} \vee \frac{d^5 \beta^2}{B^2 \rho^4 \epsilon^2}\right).$$

Algorithm 1 can achieve an $\epsilon$ sampling error in total variation distance.

**Remark 4.9.** Note that the iteration complexity in Corollary 4.8 holds for any mini-batch size $1 \leq B \leq n$, as opposed to Raginsky et al. (2017); Xu et al. (2018) that require the mini-batch size to be $O(\rho^{-1})$ in order to guarantee diminishing sampling error. Moreover, if we set the mini-batch size to be $B = O(d)$, the number of stochastic gradient evaluations needed to achieve $\epsilon$-sampling error is $\tilde{O}(d^1 \beta^2 \rho^{-4} \epsilon^{-2})$.

For a general non-log-concave distribution, it is difficult to prove a tight bound on the Cheeger constant $\rho$. One possible lower bound of $\rho$ can be obtained via Buser’s inequality (Buser, 1982; Ledoux, 1994), which shows that the Cheeger constant $\rho$ can be lower bounded by $\Omega(d^{-1/2} c_p)$ under Assumption 4.4, where $c_p$ is the Poincaré constant of the distribution $\pi^*$. Moreover, Bakry et al. (2008) gave a simple lower bound of $c_p$, showing that $c_p \geq e^{-\beta \text{Osc}_RF} / (2R^2)$, where $\text{Osc}_RF = \sup_{x\in B(0, R)} f(x) - \inf_{x\in B(0, R)} f(x) \leq LR^2/2$. Assuming $R = \tilde{O}(d^{1/2})$, this further implies that $\rho = \tilde{O}(d^{-1}) \cdot e^{-\tilde{O}(R^2)} = e^{-\tilde{O}(d)}$. In addition, better lower bounds of $\rho$ can be proved when the target distribution enjoys better properties. When the target distribution is a mixture of strongly log-concave distributions, the lower bound of $\rho$ can be improved to $1/poly(d)$ (Lee et al., 2018). Strengthening Assumption 4.3 to a local nonconvexity condition yields $\rho = e^{-\tilde{O}(L)}$ (Ma et al., 2018). For log-concave distributions, Lee and Vempala (2017) proved that the Cheeger constant $\rho$ can be lower bounded by $\rho = \Omega(1/(\text{Tr}(\Sigma^2))^{1/4})$, where $\Sigma$ is the covariance matrix of the distribution.
\( \pi^* \). When the target distribution is \( m \)-strongly log-concave, based on Cousins and Vempala (2014); Dwivedi et al. (2018), it can be shown that \( \rho = \Omega(\sqrt{m}) \).

Based on Corollary 4.8, we further show that the convergence of SGLD can also be established under the measure of any polynomial growth function.

**Corollary 4.10.** Under the same assumptions and hyper-parameter configurations as in Corollary 4.8, let \( h(x) \) be a polynomial growth function with degree \( H \), i.e., \( h(x) \leq C(1 + \|x\|_2^H) \) for some constant \( C \), and \( k_{\text{max}} \) be defined in Corollary 4.8, then for any \( k \geq k_{\text{max}} \), the output of Algorithm 1 satisfies

\[
\mathbb{E}[h(x_k)] - \mathbb{E}[h(x^\pi)] \leq C' \epsilon,
\]

where \( x^\pi \sim \pi \) denotes the random vector that follows the target distribution \( \pi \) and \( C' = O(d^{H/2}) \) is a problem-dependent constant.

**Remark 4.11.** Similar results have been presented in Sato and Nakagawa (2014); Chen et al. (2015); Vollmer et al. (2016); Erdogdu et al. (2018). However, Sato and Nakagawa (2014) only analyzed the finite-time approximation error between SGLD and the SDE (1.1) rather than the convergence to the target distribution. The convergence results in Chen et al. (2015); Vollmer et al. (2016); Erdogdu et al. (2018) also differ from ours as their guarantees are made on the sample path average rather than the last iterate. In addition, these works assume that the Poisson equation solution of the SDE (1.1) has polynomially bounded \( i \)-th order derivative \( (i \in \{2, 3, 4\}) \), which is not required in our result.

**Remark 4.12.** Let us consider a special case that \( h(\cdot) = f(\cdot) \), which was studied in Raginsky et al. (2017); Xu et al. (2018). Assumption 4.4 implies that \( h(x) \) is a quadratic growth function. Then Corollary 4.10 shows that in order to guarantee \( \mathbb{E}[f(x_k)] - \mathbb{E}[f(x^\pi)] \leq \epsilon \), Algorithm 1 requires \( \tilde{O}(\epsilon^{-2}) \) stochastic gradient evaluations. In contrast, in order to achieve the same error, Raginsky et al. (2017); Xu et al. (2018) require \( \tilde{O}(\epsilon^{-8}) \) and \( \tilde{O}(\epsilon^{-5}) \) stochastic gradient evaluations respectively, both of which are worse than ours.

### 5 Improved Convergence Rates under Hessian Lipschitz Condition

In this section, we will show that the convergence rate of SGLD can be improved by invoking Hessian Lipschitz condition, which is defined as follows.

**Assumption 5.1 (Hessian Lipschitz).** There exists a positive constant \( M \) such that for any \( x, y \in \mathbb{R}^d \), it holds that

\[
\|\nabla^2 f(x) - \nabla^2 f(y)\|_{\text{op}} \leq M \|x - y\|_2.
\]

This assumption has been made in many recent papers to prove faster convergence rate of LMC (Dalalyan and Karagulyan, 2019; Vempala and Wibisono, 2019; Mou et al., 2019) for sampling from both log-concave and non-log-concave distributions.
With this additional assumption, we state the convergence result of Algorithm 1 in the following theorem.

**Theorem 5.2.** Under Assumptions 4.3, 4.4, and 5.1, for any $\zeta \in (0, 1/2]$ and $\lambda$-warm start with respect to $\pi^*$, if set $R = R(\zeta)$, $r = \sqrt{10\eta d/\beta}$, and the step size $\eta = O(d^{-1}R^{-1} \wedge \rho^{2}d^{-2})$, then the output of Algorithm 1 satisfies

$$
\|\mu_k - \pi\|_{TV} \leq \lambda(1 - C_0\eta)^k + 3\zeta + C_1B^{-1}\eta^{1/2} + C_2\eta,
$$

where $C_0 = O(\beta^{-1}\rho^2)$, $C_1 = O(R^2d\rho^{-1}\beta^{3/2})$ and $C_2 = O(d^{3/2}\rho^{-1} + Rd^{1/2}\beta\rho^{-1})$ are problem-dependent constants.

Regarding the upper bound proved in Theorem 5.2, the four terms have the same meaning as those in Theorem 4.5. Compared with the convergence result in Theorem 4.5, the improvement brought by Hessian Lipschitz condition lies in the approximation error between the transition distributions of SGLD and Metropolized SGLD, which is improved from $O(\eta^{1/2})$ to $O(B^{-1}\eta^{1/2} + \eta)$.

Dalalyan and Karagulyan (2019); Mou et al. (2019); Vempala and Wibisono (2019) also improved the convergence rate of LMC using the additional Hessian Lipschitz condition. However, Dalalyan and Karagulyan (2019) only focused on strongly log-concave distributions and the theoretical results in Mou et al. (2019); Vempala and Wibisono (2019) cannot be easily extended to SGLD. Moreover, we would like to emphasize that compared with these prior works, our proof (see Lemma B.2 for more details) to show such an improvement is much simpler and more intuitive, which may be of independent interest.

**Corollary 5.3.** Under the same assumptions made in Theorem 5.2, consider Gaussian initialization $\mu_0 = N(0, I/(2\beta L))$, then for any mini-batch size $B \leq n$, if set the step size and maximum iteration number as

$$
\eta = \tilde{O}\left(\frac{\rho^2B^2\epsilon^2}{d^2\beta} \wedge \frac{\rho\epsilon}{d^{3/2} + d\beta^{1/2}}\right), \quad k_{\text{max}} = \tilde{O}\left(\frac{d^5\beta^2}{\rho^4B^2\epsilon^2} + \frac{d^{5/2}\beta + d^2\beta^{3/2}}{\rho^3\epsilon}\right),
$$

Algorithm 1 can achieve an $\epsilon$ sampling error in terms of total variation distance.

Note that the required number of stochastic gradient evaluations is $Bk_{\text{max}} = \tilde{O}(d^{5/2}\beta^2/(B\rho^4\epsilon^2) + Bd^{5/2}\beta^{3/2}/(\rho^3\epsilon))$. Therefore, if set the mini-batch size as $B = \tilde{O}([d^{5/2}\beta^{1/2}\rho\epsilon]^{1/2})$, it can be derived that the gradient complexity of Algorithm 1 is $\tilde{O}(d^{15/4}\beta^{7/4}\rho^{-7/2}\epsilon^{-3/2})$. This strictly improves the stochastic gradient complexity (i.e., number of stochastic gradient evaluations to achieve $\epsilon$-sampling error) of Algorithm 1 without Assumption 5.1 by a factor of $\tilde{O}(d^{1/4}\beta^{1/4}\rho^{-1/2}\epsilon^{-1/2})$.

### 6 Proof Sketch of the Main Results

In this section, we first provide the construction of an auxiliary Metropolized SGLD chain, then present the proof roadmap of our main theory, and finally we discuss the technical novelty of our proof compared with existing works.
6.1 Construction of Metropolized SGLD

As mentioned before, our proof is based on Metropolized SGLD, i.e., SGLD with a Metropolis-Hasting step. In this subsection, we will provide a detailed characterization on the transition distributions of SGLD and Metropolized SGLD.

**Transition distribution of Algorithm 1.** Let $g(x, I)$ denote the stochastic gradient computed at the point $x$, where $I$ denotes the stochastic mini-batch of data points queried in the gradient computation. Then it is clear that Algorithm 1 can be described as a Markov process. More specifically, let $u$ and $w$ be the starting point and the point obtained after one-step iteration of Algorithm 1, the Markov chain in this iteration can be formed as $u \rightarrow v \rightarrow w$, where $v$ is generated based on the following conditional probability density function,

$$P(v|u) = \mathbb{E}_I[P(v|u, I)] = \mathbb{E}_I\left[\frac{1}{(4\pi \eta/\beta)^{d/2}} \exp \left(-\frac{\|v - u + \eta g(u, I)\|^2}{4\eta/\beta}\right)\right]u,$$  \hspace{1cm} (6.1)

which is exactly the transition probability of standard SGLD (i.e., without any accept/reject step). Let $R > 0$ be a user defined radius and recall that $\Omega = B(0, R)$, the process $v \rightarrow w$ can be formulated as

$$w = \begin{cases} 
    v & v \in B(u, r) \cap \Omega; \\
    u & \text{otherwise}.
\end{cases}$$  \hspace{1cm} (6.2)

Let $p(u) = P_{v \sim P(v|u)}[v \in B(u, r) \cap \Omega]$ be the acceptance probability in (6.2), and $Q(w|u)$ be the conditional PDF that describes $u \rightarrow w$, we have

$$Q(w|u) = (1 - p(u))\delta_u(w) + P(w|u) \cdot 1 \left[w \in B(u, r) \cap \Omega\right],$$

where $P(w|u)$ is computed by replacing $v$ with $w$ in (6.1). Similar to Zhang et al. (2017); Dwivedi et al. (2018), we consider the 1/2-lazy version of the above Markov process, i.e., we consider the Markov process with the following transition distribution

$$T_u(w) = \frac{1}{2} \delta_u(w) + \frac{1}{2} Q(w|u),$$  \hspace{1cm} (6.3)

where $\delta_u(\cdot)$ is the Dirac-delta distribution at $u$. However, it is difficult to directly prove the ergodicity of the Markov process with transition distribution $T_u(w)$, and it is also difficult to tell whether its stationary distribution exists or not.

**Metropolized SGLD.** Note that SGLD is known to be asymptotically biased (Teh et al., 2016; Vollmer et al., 2016), which does not converge to the target distribution $\pi$ even when it runs for infinite steps.

In order to quantify the sampling error for the output of Algorithm 1 and prove its convergence, we follow the high-level idea of Zhang et al. (2017), which constructs a auxiliary Markov process by adding an extra Metropolis-Hasting correction step into Algorithm 1. We call it Metropolized SGLD. Given the starting point $u$, let $w$ be the candidate state generated from the distribution
\( T_u(\cdot) \). Metropolized SGLD will accept the candidate \( w \) with the following probability,

\[
\alpha_u(w) = \min \left\{ 1, \frac{T_w(u)}{I_u(w)} \cdot \exp \left[ -\beta(f(w) - f(u)) \right] \right\}.
\]

Let \( T_u^*(\cdot) \) denote the transition distribution of such auxiliary Markov process, i.e.,

\[
T_u^*(w) = (1 - \alpha_u(w))\delta(u) + \alpha_u(w)T_u(w),
\]

which is time-reversible and easy to verify. Due to this Metropolis-Hastings correction step, the Markov chain can converge to a unique stationary distribution \( \pi^* \) up to some approximation error; and (3) We prove that with a proper choice of the truncation radius \( R \), the total variation distance between the truncated target distribution \( \pi^* \) and the target distribution \( \pi \) can be sufficiently small.

**Bounding the difference between \( T_u(\cdot) \) and \( T_u^*(\cdot) \).** Similar to Lemma 3 in Zhang et al. (2017), we will show that the transition distribution \( T_u(\cdot) \) of Algorithm 1 (SGLD) can be \( \delta \)-close to that of Metropolized SGLD \( T_u^*(\cdot) \) by some small quantity \( \delta \), which is formally stated in the following lemma.

**Lemma 6.1.** Under Assumption 4.4, let \( G = \max_{i \in [n]} \| \nabla f_i(0) \|_2 \) and set \( r = \sqrt{10Ld/\beta} \). Then there exists a constant

\[
\delta = 10Ld\eta + 10L(LR + G)d^{1/2}1/2\eta 2/2, 12\beta(LR + G)^2d\eta B + 2\beta^2(LR + G)^2d\eta B
\]

such that for any set \( A \subseteq \Omega \) and any point \( u \in \Omega \), it holds that

\[
(1 - \delta)T_u^*(A) \leq T_u(A) \leq (1 + \delta)T_u^*(A).
\]

**Proving the convergence of \( T_u(\cdot) \).** We first state the definition of the conductance of a time-reversible Markov chain as follows.

**Definition 6.2 (conductance).** The conductance of a time-reversible Markov chain with transition distribution \( T_u^*(\cdot) \) and stationary distribution \( \pi^* \) is defined by,

\[
\phi := \inf_{A: A \subseteq \Omega, \pi^*(A) \in (0,1)} \frac{\int_A T_u^*(\Omega \setminus A)\pi^*(du)}{\min\{\pi^*(A), \pi^*(\Omega \setminus A)\}},
\]
where \( \Omega \) is the support of the state of the Markov chain.

In Lemma 6.1, we have already shown that the transition distribution of Algorithm 1, i.e., \( \mathcal{T}_u(\cdot) \) is \( \delta \)-close to that of Metropolized SGLD, i.e., \( \mathcal{T}_u^*(\cdot) \), for some small quantity \( \delta \). Besides, from Lovász and Simonovits (1993); Vempala (2007), we know that a time-reversible Markov chain can converge to its stationary distribution at a linear rate depending on its conductance. Therefore, we aim to characterize the convergence rate of \( \mathcal{T}_u(\cdot) \) based on the ergodicity of \( \mathcal{T}_u^*(\cdot) \). In this part, we utilize the conductance parameter of \( \mathcal{T}_u^*(\cdot) \), denoted by \( \phi \), and establish the convergence of \( \mathcal{T}_u(\cdot) \) in total variation distance in the following lemma.

**Lemma 6.3.** Under Assumption 4.4, if \( \mathcal{T}_u(\cdot) \) is \( \delta \)-close to \( \mathcal{T}_u^*(\cdot) \) with \( \delta \leq \min\{1 - \sqrt{2}/2, \phi/16\} \), then for any \( \lambda \)-warm start initial distribution with respect to \( \pi^* \), it holds that

\[
\|\mu_k - \pi^*\|_{TV} \leq \lambda \left(1 - \phi^2/8\right)^k + 16\delta/\phi,
\]

where \( \mu_k \) denotes the distribution of iterate \( x_k \) generated by Algorithm 1.

By Lemma 6.3, it is clear that the convergence rate of Algorithm 1 relies on the conductance of \( \mathcal{T}_u^*(\cdot) \). Therefore, in order to establish a explicit convergence rate, it requires to characterize the value of \( \phi \). The following lemma provides a lower bound of \( \phi \).

**Lemma 6.4.** Under Assumptions 4.3 and 4.4, if the step size satisfies \( \eta \leq \left[35(Ld + (LR + G)^2\beta d/B)\right]^{-1} \land \left[25\beta(LR + G)^2\right]^{-1} \), there exists an absolute constant \( c_0 \) such that

\[
\phi \geq c_0 \rho \sqrt{\eta/\beta},
\]

where \( \rho \) is the Cheeger constant of the distribution \( \pi^* \).

**Bounding the difference between \( \pi \) and \( \pi^* \).** Lemmas 6.3 and 6.4 state that Algorithm 1 can be guaranteed to converge to the truncated target distribution \( \pi^* \). Thus the last thing remaining to be done is ensuring that \( \pi^* \) is sufficiently close to \( \pi \). The following lemma characterizes the total variation distance between the target distribution \( \pi \) and its truncated version in \( \mathcal{B}(0, \tilde{R}(\zeta)) \) for some \( \zeta \in (0, 1/2) \), where the function \( \tilde{R}(\cdot) \) is defined in (4.1).

**Lemma 6.5.** For any \( \zeta \in (0, 1/2) \), let \( \Omega = \mathcal{B}(0, \tilde{R}(\zeta)) \) and \( \pi^* \) be the truncated target distribution in \( \Omega \), the total variation distance between \( \pi^* \) and \( \pi \) can be upper bounded by \( \|\pi^* - \pi\|_{TV} \leq 3\zeta \).

Lemma 6.5 suggests that as long as the radius is \( R = \tilde{\Omega}(d^{1/2}) \), the truncated distribution \( \pi^* \) can be sufficiently close to the target distribution \( \pi \).

**Completing the proof of Theorem 4.5.** Based on Lemmas 6.1-6.5, the rest proof of Theorem 4.5 is straightforward. We defer the detailed proofs of all theorems and corollaries to Appendix B.

### 6.3 Discussion on the Technical Novelty

Our analysis framework is essentially different from that in existing works (Raginsky et al., 2017; Xu et al., 2018) and their variants. We illustrate the analysis roadmaps of different approaches in Figure 1. It can be seen that both Raginsky et al. (2017); Xu et al. (2018) make use of the LMC iterate \( x_k^{LMC} \) to characterize the convergence of SGLD (while they bound the error between \( x_k^{LMC} \))
and $x^\pi$ in different ways). However, their results on the error between $x_k$ and $x_k^{LMC}$ diverges as $k$ increases, due to the uncertainty of stochastic gradients. This suggests that LMC may not be an adequate auxiliary chain for studying SGLD. In our paper, we directly treat SGLD itself (including the randomness of stochastic gradients and Brownian term) as a Markov chain and study its convergence to the target distribution based on a different auxiliary chain, i.e., Metropolized SGLD ($x_k^{MH}$) (green arrows in Figure 1), which is closer to SGLD as its transition distribution also covers the randomness of stochastic gradients (see Section 6.1 for more details). Besides, Metropolized SGLD is a time-reversible Markov chain and thus provably converges to the (truncated) target distribution exponentially fast. Consequently, combining these results we are able to prove a faster convergence rate.

We would also like to point out that the construction of Metropolized SGLD follows the same spirit of Zhang et al. (2017) but with a different goal and thus the analyses are not the same. Different from Zhang et al. (2017) that only characterizes the hitting time of SGLD to a certain set by lower bounding the restricted conductance of SGLD (but cannot ensure its convergence to $\pi$), we focus on sampling from a certain target distribution and thus need to bound the approximation error between $x_k$ and $x_k^{MH}$. As a consequence, we show that the sampling error of SGLD to the target distribution can be upper bounded by $O(\sqrt{\eta})$, while the conductance analysis in Zhang et al. (2017) can only give $O(1)$ sampling error.

## 7 Conclusion and Future Work

We proved a faster convergence rate of SGLD for sampling from a broad class of distributions that can be non-log-concave. In particular, we developed a new proof technique for characterizing the convergence of SGLD. Different from the existing works that mainly study the convergence of SGLD based on LMC or continuous Langevin dynamics, we made use of a more accurate auxiliary Markov chain, namely Metropolized SGLD, and proved the convergence rate of SGLD by bounding the approximation error between the transition distributions of SGLD and Metropolized SGLD.

There are at least two future directions that are worth to study. First, it would be interesting to see whether we can directly implement a practical Metropolized SGLD algorithm instead of implicitly using it as an auxiliary chain for proving the convergence of SGLD. We expect this will greatly accelerate the sampling process due to the fast mixing rate of MH methods (Dwivedi et al.,

---

**Figure 1:** Illustration of the analysis framework of SGLD in different works: Raginsky et al. (2017), Xu et al. (2018), this work. The goal is to prove the convergence of SGLD iterates $x_k$ to the point following the target distribution $x^\pi$. Besides, $x_k^{LMC}$ and $x_k^{MH}$ denote the $k$-th iterates of LMC and Metropolized SGLD; $x_t^{LD}$ denotes the solution of (1.1) at time $t$; $x^{\pi LMC}$ denotes the point following the stationary distribution of LMC.
The challenge, however, lies in developing new stochastic gradient sampling algorithms that can accurately estimate MH acceptance probabilities. Second, it is also possible to extend our theoretical analysis to high-order stochastic gradient MCMC methods such as SGHMC (Chen et al., 2014), stochastic gradient UL-MCMC (Cheng et al., 2018b) and variance reduced SGHMC (Zou et al., 2019b).

**A Connection to Standard SGLD**

In this section we will discuss the connection between Algorithm 1 and the standard SGLD algorithm, i.e., removing the accept/reject step in Algorithm 1. In specific, we will show that when the radius $R$ and $r$ are properly chosen, with very high probability (say $1 - \delta$) all proposals in Algorithm 1 will be accepted. In this case, the output of Algorithm 1 will be exactly the same as that of the standard SGLD. Then it can be concluded that the total variation distance between the outputs of Algorithm 1 and the standard SGLD is at most $\delta$. We formally state this result in the following proposition.

**Proposition A.1.** Let $K$ be the number of iterations of Algorithm 1 and $\delta \in (0, 1)$ be an arbitrary constant. Set

$$R = C_1 \left( \frac{d \log(K/\delta)}{m \beta} \right), \quad r = C_2 \sqrt{\eta d / \beta} \left( 1 + \sqrt{\frac{\log(K/\delta)}{d}} \right)^{1/2},$$

for some absolute positive constants $C_1$ and $C_2$. Then with probability at least $1 - \delta$, Algorithm 1 generates the same output as that of the standard SGLD.

In order to prove Proposition A.1, it suffices to show that with probability at least $1 - \delta$, Algorithm 1 will accept all $K$ iterates. In other words, let $\{x_k\}_{k=0,...,K}$ be the iterates generated by the standard SGLD (without accept/reject step), our goal is to prove that with probability at least $1 - \delta$, all $x_k$’s stay inside the region $B(0, R)$, and $\|x_k - x_{k-1}\|_2 \leq r$ for all $k \leq K$. These properties are summarized in the following two facts.

**Fact 1:** With probability at least $1 - \delta/2$, all iterates stay inside the region $B(0, R)$

**Fact 2:** Given Fact 1, with probability at least $1 - \delta/2$, $\|x_k - x_{k-1}\|_2 \leq r$ for all $k \leq K$.

The following lemma will be useful to the proof.

**Lemma A.2** (Lemma 3.1 in Raginsky et al. (2017)). Under Assumption 4.4, there exists a constant $G = \max_{i \in [n]} \|\nabla f_i(0)\|_2$ such that for any $x \in \mathbb{R}^d$ and $i \in [n]$, it holds that

$$\|\nabla f_i(x)\|_2 \leq L\|x\|_2 + G.$$

Now we will proceed to proving these two facts.

**Proof of Proposition A.1.** Regarding Fact 1, we first take a look at $\|x_k\|_2^2$. By Assumption 4.3, we have

$$\mathbb{E}[\|x_{k+1}\|_2^2 \mid x_k] = \mathbb{E}[\|x_k - \eta g(x_k, i) + \sqrt{2\eta/\beta} \epsilon_k\|_2^2 \mid x_k]$$

14
= \|x_k\|^2 - 2\eta\mathbb{E}[x_k, g(x_k, I)]x_k + \eta^2\mathbb{E}[\|g(x_k, I)\|^2] + \frac{2\eta}{\beta} \\
\leq (1 - 2\eta^2)\|x_k\|^2 + 2\eta + \eta^2(L\|x_k\|^2 + G)^2 + \frac{2\eta}{\beta} \\
\leq (1 - 2\eta^2 + 2L^2\eta^2)\|x_k\|^2 + 2\eta + 2\eta^2G^2 + \frac{2\eta}{\beta},

where the first inequality follows from Assumption 4.3, the second inequality follows from Lemma A.2, and the last inequality is due to Young’s inequality. If we choose \(\eta \leq 1 / (4L^2)\), the above inequality implies that

\[
\mathbb{E}[\|x_{k+1}\|^2 | x_k] \leq (1 - 3\eta^2/2)\|x_k\|^2 + 2\eta + 2\eta^2G^2 + \frac{2\eta}{\beta}.
\]

Let \(D = (4b + 4G^2 + 4d\beta^{-1})/m\). We can verify that \(\mathbb{E}[\|x_{k+1}\|^2] \leq (1 - \eta^2)\|x_k\|^2\). Note that in order to prove \(\|x_k\|^2 \leq R\), we only need to consider \(x_k\) satisfying \(\|x_k\|^2 \geq D\) since our choice of \(R\) satisfies \(R > 2\sqrt{D}\), otherwise \(\|x_k\|^2 \leq \sqrt{D} \leq R\) naturally holds. Then by the concavity of the function \(\log(\cdot)\), for any \(\|x_k\|^2 \geq R/2\), we have

\[
\mathbb{E}[\log(\|x_{k+1}\|^2) | x_k] \leq \log(\mathbb{E}[\|x_{k+1}\|^2] | x_k]) \leq \log(1 - \eta^2) + \log(\|x_k\|^2) \leq \log(\|x_k\|^2) - \eta^2.
\]

Besides, it naturally holds that

\[
\|x_{k+1}\|^2 - \|x_k\|^2 \leq \eta\|g(x_k, I)\|^2 + \sqrt{\eta^2/\beta}\|e_k\|^2.
\]

Note that \(\|e_k\|^2\) follows \(\chi(d)\) distribution, which is subgaussian. Thus if \(\|x_k\|^2 \leq R\), we have \(\|x_{k+1}\|^2 - \|x_k\|^2\) is also subgaussian with mean less than \(\eta(LR + G) + \sqrt{\eta d/\beta}\). Combined with the fact that \(\|x_k\|^2 \geq R/2\) we have

\[
\log(\|x_{k+1}\|^2) - \log(\|x_k\|^2) = 2\log(\|x_{k+1}\|/\|x_k\|) \leq \|x_{k+1}\|^2/\|x_k\|^2 - 1 \leq \frac{2\|x_{k+1}\|^2 - 2\|x_k\|^2}{R}.
\]

Then if we assume \(\eta \leq d(LR + G)^{-1}/\beta\), we have \(\log(\|x_{k+1}\|^2) - \log(\|x_k\|^2)\) is also a subgaussian random variable with mean less than \(4\sqrt{\eta d/\beta}R^{-1}\), i.e., there exist constants \(b > 1, c > 0\) such that for any \(t\),

\[
\mathbb{P}(\log(\|x_{k+1}\|^2) - \log(\|x_k\|^2) > 4\sqrt{\eta d/\beta}R^{-1} + 2tR^{-1}) \leq b \exp(-ct^2).
\]

We will consider any subsequence among \(\{x_k\}_{k=1,...,K}\), with all iterates, except the first one, staying outside the region \(B(0, R/2)\) \((R > 2\sqrt{D})\). Denote such subsequence by \(\{y_k\}_{k=1,...,K'}\), which clearly satisfies (A.1) and (A.2), where \(y_0\) satisfies \(\|y_0\|^2 \leq D\) and \(K' \leq K\). Then it suffices to prove that with high probability all points in \(\{y_k\}_{k=1,...,K'}\) will stay inside the region \(B(0, R)\). Then let \(E_k\) be the event that \(\|y_k\|^2 \leq R\) for all \(k' \leq k\), and \(\mathcal{F}_k = \{y_0, \ldots, y_k\}\) be the filtration, it is easy to see that \(E_k \subseteq E_{k-1}\) and thus the sequence \(\{1(E_{k-1}) \cdot \log(\|y_k\|^2) + km\eta)|\mathcal{F}_{k-1}\}_{k=1,...,K'}\) is a super-martingale. Besides, we can show that the martingale difference has a subgaussian tail, i.e., for any \(t \geq 0\),

\[
\mathbb{P}(\|y_{k+1}\|^2 + (k + 1)m\eta - \log(\|y_k\|^2) - km\eta \geq 5\sqrt{\eta d/\beta}R^{-1} + 2tR^{-1}) \leq b \exp(-ct^2),
\]
where $b > 1$, $c > 0$ are absolute constants. Then by Theorem 2 in Shamir (2011), we have for a given $k$, conditioned on the event $E_{k-1}$, it holds that with probability at least $1 - \delta'$,

$$\log(\|y_k\|^2) + km\eta \leq \log(\|y_0\|^2) + c_1\sqrt{k\eta d \log(1/\delta')/(\beta R^2)}$$

for some absolute positive constant $R$. Taking union bound over all $k = 1, \ldots, K'$ ($K' \leq K$) and defining $\delta = 2\delta' K'$, we have with probability at least $1 - \delta/2$, for all $k = 1, \ldots, K'$ it holds that

$$\log(\|y_k\|^2) \leq 2\log(R/2) + c_1\sqrt{k\eta d \log(2K/\delta)/(\beta R^2)} - mk\eta$$

$$\leq 2\log(R/2) + \frac{c_2d\log(2K/\delta)}{m\beta R^2},$$

where $c_2$ is an absolute positive constant. It is clear that our choice of $R$ implies that

$$\frac{c_2d\log(2K/\delta)}{m\beta R^2} \leq 2\log(2).$$

Therefore, for all $k = 1, \ldots, K$, we have with probability at least $1 - \delta/2$ that

$$\log(\|y_k\|^2) \leq 2\log(R/2) + 2\log(2) = \log(R^2).$$

This immediately implies that with probability at least $1 - \delta/2$, all iterates stay inside the region $B(0, R)$, which completes the proof of Fact 1.

Now we proceed to prove Fact 2, of which the key is to prove $\|x_k - x_{k-1}\|_2 \leq r$ for all $k \geq K$. Note that in each iteration, the proposal distribution of $x_{k+1}$ is an expected Gaussian distribution. Besides, note that for all possible mini-batch, the drift term satisfies

$$\eta\|g(x_k, z)\|_2 \leq \eta(\beta R + G).$$

This implies that the probability that $x_{k+1} \notin B(x_k, r)$ can be upper bounded by

$$\mathbb{P}[x_{k+1} \notin B(x_k, r)] \leq \mathbb{P}_{z \sim \chi_2^2}[2\eta\beta^{-1} z \preceq (r - \eta(\beta R + G))^2] = \mathbb{P}_{z \sim \chi_2^2}[\sqrt{z} \leq r - \eta(\beta R + G)/2\eta\beta^{-1}]^{1/2}].$$

By standard tail bound of Chi-square distribution and our choice of $r$,

$$\mathbb{P}[x_{k+1} \notin B(x_k, r)] \leq \mathbb{P}_{z \sim \chi_2^2}[\sqrt{z} \leq d^{1/2} + \sqrt{2\log(2K/\delta)}] \leq 1 - \frac{\delta}{(2K)}.$$

Taking union bound over all iterates, we are able to complete the proof of Fact 2.

Combining Fact 1 and Fact 2 completes the proof of Proposition A.1.

**B Proofs of the Main Theorems and Corollaries**

In this section, we present the detailed proofs of our main theorems and corollaries.
B.1 Proof of Theorem 4.5

Now we provide the detailed proof of Theorem 4.5 based on the key lemmas presented in our proof roadmap.

Proof of Theorem 4.5. We first characterize the condition on the step size required in Lemmas 6.1, 6.3 and 6.4. From Lemma 6.1, we know that if \( \eta \leq 10(LR + G) \delta \leq \beta^2 \eta^{3/2} \) and \( \beta \geq 1 \), the transition distribution \( T_u(\cdot) \) can be \( \delta \)-close to \( T^*(\cdot) \) with

\[
\delta = 10Ld\eta + 10(LR + G)d^{1/2}\beta^{1/2}\eta^{3/2} + 12\beta(LR + G)^2d\eta/B + 2\beta^2(LR + G)^4\eta^2/B \\
\leq 14Ld\eta + 14(LR + G)^2\beta d\eta/B. \tag{B.1}
\]

Besides, note that Lemma 6.3 requires \( \delta \leq \min\{1 - \sqrt{2}/2, \phi/16\} \), which can be satisfied if

\[
14Ld\eta + 14(LR + G)^2\beta d\eta/B \leq \min\{1 - \sqrt{2}/2, \phi/16\}.
\]

Then based on the requirement of \( \eta \) and the lower bound of \( \phi \) in Lemma 6.4, it suffices to set the step size to be

\[
\eta \leq \min\left\{ \frac{1}{25\beta(LR + G)^2}, \frac{1}{35(Ld + (LR + G)^2\beta d/B)^2}, \left(\frac{c_0\rho}{16\sqrt{3}(14Ld + 14(LR + G)^2\beta d/B)}\right)^2 \right\}.
\]

Now we are able to put the results of these lemmas together to establish the convergence of Algorithm 1. Combining Lemmas 6.3 and 6.5 and setting \( R = \hat{R}(\zeta) \) for some \( \zeta \in (0, 1/2] \), we have

\[
\|\mu_k - \pi\|_{TV} \leq \|\pi - \pi^*\|_{TV} + \|\mu_k - \pi^*\|_{TV} \\
\leq 3\zeta + \lambda(1 - \phi^2/8)^k + \frac{16\delta}{\phi} \\
\leq 3\zeta + \lambda(1 - C_0\eta)^k + (C_1B^{-1} + C_2)\eta^{1/2},
\]

where \( C_0 = c_0^2\rho^2/(8\beta) \), \( C_1 = 224(LR + G)^2\beta^3/2d\rho^{-1}/c_0 \), \( C_2 = 224Ld\beta^{3/2}\rho^{-1}/c_0 \) are problem-dependent constants. This completes the proof.

\( \square \)

B.2 Proof of Corollary 4.8

We first present the following technical lemma.

Lemma B.1. Under Assumption 4.3, the objective function \( f(x) \) satisfies

\[
f(x) \geq \frac{m}{4}\|x\|^2 + f(x^*) - \frac{b}{2}.
\]

Now we prove Corollary 4.8.

Proof of Corollary 4.8. The first step is to characterize the quantity of \( \lambda \). Let \( \Omega = \mathcal{B}(0, R) \), the
initial distribution $\mu_0$ takes form

$$\mu_0(dx) = \frac{e^{-\beta L|x|^2_2}dx}{\int_\Omega e^{-\beta L|y|^2_2}dy}.$$ 

Direct calculation gives

$$\frac{\mu_0(dx)}{\pi^*(dx)} \leq \frac{\int_\Omega e^{-\beta f(y)}dy}{\int_\Omega e^{-\beta L|y|^2_2}dy} \cdot e^{-\beta L|x|^2_2 + \beta f(x)}.$$ 

By Assumption 4.4, we have

$$f(x) \leq f(x^*) + \frac{L}{2} \|x - x^*\|_2^2 \leq f(x^*) + L\|x^*\|_2^2 + L\|x\|_2^2,$$

which implies that

$$e^{-\beta L|x|^2_2 + \beta f(x)} \leq e^{\beta[f(x^*) + L\|x^*\|_2^2]}.$$ 

Moreover, by Lemma B.1, we have

$$\int_\Omega e^{-\beta f(y)}dy \leq \int_{\mathbb{R}^d} e^{-\beta f(y)}dy \leq e^{-\beta[f(x^*) - b/2]}\int_{\mathbb{R}^d} e^{-m\beta|y|^2_2/4}dy = \left(\frac{4\pi}{m\beta}\right)^{d/2} e^{-\beta[f(x^*) - b/2]}.$$ 

Note that $\Omega = B(0, \bar{R}(\zeta))$ with $\zeta \leq 1/2$, it is easy to verify that

$$\int_{\Omega} e^{-\beta L|y|^2_2}dy \geq \frac{1}{2} \int_{\mathbb{R}^d} e^{-\beta L|y|^2_2}dy = \frac{1}{2} \left(\frac{\pi}{L\beta}\right)^{d/2}.$$ 

Combining the above results, we can get

$$\lambda \leq \max_{x \in \Omega} \frac{\mu_0(dx)}{\pi^*(dx)} \leq 2 \left(\frac{4L}{m}\right)^{d/2} e^{\beta[L|x^*|_2^2 + b/2]} = e^{O(d)}. \tag{B.2}$$

In order to ensure that the sampling error $\|\mu_k - \pi\|_{TV}$ is smaller than $\epsilon$, it suffices to choose $\zeta$, $\eta$ and $k$ such that

$$\lambda(1 - C_0\eta)^k = \frac{\epsilon}{3}, \quad 3\zeta = \frac{\epsilon}{3}, \quad C_1B^{-1}\eta^{1/2} + C_2\eta^{1/2} = \frac{\epsilon}{3}.$$ 

Thus we have $R = \bar{R}(\zeta) = \widetilde{O}(d^{1/2} \beta^{-1/2})$. Then it follows that $C_0 = O(\rho^2 \beta^{-1})$, $C_1 = \widetilde{O}(d^2 \rho^{-1} \beta^{1/2})$ and $C_2 = O(d^3 \rho^{-1} \beta^{1/2})$. Plugging these into the above equation immediately implies that $\zeta = O(\epsilon)$,

$$\eta = O\left(\frac{\rho^2 \epsilon^2}{d^2 \beta} \wedge \frac{B^2 \rho^2 \epsilon^2}{d^2 \beta}\right) \quad \text{and} \quad k = O\left(\frac{\log(\lambda/\epsilon)}{C_0\eta}\right) = \widetilde{O}\left(\frac{d^3 \beta^2}{\rho^4 \epsilon^2} \vee \frac{d^5 \beta^2}{B^2 \rho^4 \epsilon^2}\right),$$

which completes the proof. \qed
B.3 Proof of Corollary 4.10

Proof of Corollary 4.10. We first denote $\Omega = B(0, R)$, then it holds that,

$$
\mathbb{E}[h(x_k)] - \mathbb{E}[h(x^*)] = \int_{\Omega} h(x) \mu_k(dx) - \int_{\mathbb{R}^d} h(x) \pi(dx) \\
\leq \left| \int_{\Omega} h(x) \mu_k(dx) - \int_{\Omega} h(x) \pi(dx) \right| + \int_{\mathbb{R}^d} h(x) \pi(dx).
$$

Note that $h(x)$ is a polynomial growth function with degree $H$, thus by definition, for all $x \in \Omega$, we have

$$
h(x) \leq C(1 + \|x\|_2^H),
$$

for some absolute constant $C$. Then by Corollary 4.8, we know that $\|P(x_k) - \pi\|_{TV} \leq \epsilon$ for any $k \geq k_{\text{max}}$. Thus it follows that

$$
\left| \int_{\Omega} h(x) \mu_k(dx) - \int_{\Omega} h(x) \pi(dx) \right| \leq C(1 + R^H) \left| \int_{\Omega} \mu_k(dx) - \int_{\Omega} \pi(dx) \right| \leq C(1 + R^H)\epsilon.
$$

The rest of the proof will be proving the upper bound of $\int_{\mathbb{R}^d \setminus \Omega} h(x) \pi(dx)$. We first introduce an auxiliary distribution defined by

$$
q(x) = \frac{e^{-m\beta|x|^2/8}}{(8\pi/(m\beta))^{d/2}}.
$$

Note that the stationary distribution $\pi$ takes form

$$
\pi(dx) = \frac{e^{-\beta f(x)}}{Z} dx,
$$

where $Z = \int_{\mathbb{R}^d} e^{-f(x)} dx$ is the normalization coefficient. By Raginsky et al. (2017) ((3.21) in Section 3.5), we know that under Assumption 4.4, it holds that $Z \geq \exp(-\beta f(x^*)) \cdot [2\pi/(\beta L)]^{d/2}$. Then it is clear that if

$$
e^{-\beta \left[ f(x) + m|x|^2/8 \right]} \leq \exp \left( -\beta f(x^*) \right) \cdot \left( \frac{m}{4L} \right)^{d/2},
$$

we have $\pi^*(x) \leq q(x)$. By Lemma B.1, we know that

$$
-f(x) + \frac{m}{8} \|x\|^2_2 \leq \frac{b}{2} - f(x^*) - \frac{m}{8} \|x\|^2_2.
$$

(B.3)
Therefore, it can be guaranteed that \( \pi(x) \leq q(x)^4 \) if \( \|x\|_2^2 \geq 4m^{-1} (\beta^{-1} d \log(4L/m) + b) \). Therefore, for any \( R^2 \geq 4m^{-1} (\beta^{-1} d \log(4L/m) + b) \) it holds that,

\[
\int_{\mathbb{R}^d \setminus \Omega} h(x) \pi(dx) \leq \frac{1}{[8\pi/(m\beta)]^{d/2}} \int_{\|x\|_2^2 \geq R^2} C(1 + \|x\|_2^R) \cdot \exp\left(-m\beta\|x\|_2^2/8\right) dx \\
\leq 2C \int_{x \geq m\beta R^2/4} x^{H/2} \cdot \frac{x^{d/2-1} e^{-x/2}}{2^{d/2} \Gamma(d/2)} dx,
\]

where the second inequality follows from the probability density function of \( \chi_d^2 \) distribution and the fact that \( R \geq 1 \). Moreover, assuming \( d \geq H \), it is easy to verify that when \( x \geq 2Hd \), we have

\[
x^{H/2} \cdot \frac{x^{d/2-1} e^{-x/2}}{2^{d/2} \Gamma(d/2)} \leq \frac{(x/2)^{d/2-1} e^{-x/4}}{2^{d/2} \Gamma(d/2)}.
\]

Thus, if \( R^2 \geq 8Hd/(m\beta) \), we have

\[
\int_{x \geq m\beta R^2/4} x^{H/2} \cdot \frac{x^{d/2-1} e^{-x/2}}{2^{d/2} \Gamma(d/2)} dx \leq \int_{x \geq m\beta R^2/4} \frac{(x/2)^{d/2-1} e^{-x/4}}{2^{d/2} \Gamma(d/2)} dx = 2\mathbb{P}_{z \sim \chi_d^2}[z \geq m\beta R^2/8].
\]

By standard tail bound of \( \chi_d^2 \) distribution, we have

\[
\mathbb{P}_{z \sim \chi_d^2}[z \geq d + 2\sqrt{d \log(1/\delta) + 2 \log(1/\delta)}] \leq \delta.
\]

Therefore, set \( R = 2\tilde{R}(\epsilon) \vee \sqrt{8Hd/(m\beta)} \), we have

\[
\int_{\mathbb{R}^d \setminus \Omega} h(x) \pi(dx) \leq 4C\epsilon.
\]

Combining all previous results, we obtain

\[
\mathbb{E}[h(x_L)] - \mathbb{E}[h(x^*)] \leq C(5 + R^H)\epsilon.
\]

Plugging our choice of \( R \), we complete the proof. \( \square \)

### B.4 Proof of Theorem 5.2

The main body of the proof of Theorem 5.2 is the same as that of Theorem 4.5. The only difference/improvement is that provided Assumption 5.1, a sharper approximation error between the transition distributions \( \mathcal{T}_n^0(\cdot) \) and \( \mathcal{T}_n(\cdot) \) can be proved, implying SGLD is closer to its metropolized counterpart. We formally state this result in the following lemma.

**Lemma B.2.** Under Assumptions 4.4 and 5.1, let \( G = \| \nabla f(0) \|_2 \) and set \( r = \sqrt{10\eta d/\beta} \). Then if \( \eta \leq D^2(10d\beta)^{-1} \wedge D(LR + G)^{-1} \beta^{-1} \), there exists a constant

\[
\delta = 28M d^{3/2} \beta^{-1/2} \eta^{3/2} + 10L(LR + G)d^{1/2} \beta^{1/2} \eta^{3/2} + 12\beta(LR + G)^2 d\eta/B + 2\beta^2(LR + G)^4 \eta^2/B
\]

\[\tag{4}
\]

Here we slightly abuse the notation by using \( \pi(x) \) to define the probability density function of \( \pi \) at point \( x \).
such that for any set $A \subseteq \Omega$ and any point $u \in \Omega$, it holds that

$$(1 - \delta)T_u^*(A) \leq T_u(A) \leq (1 + \delta)T_u^*(A).$$

**Proof of Theorem 5.2.** Similar to the proof of Theorem 4.5, we first characterize the feasible range of $\eta$ that satisfies all requirements in Lemmas B.2, 6.3 and 6.4. Then by Lemma B.2, we know that if $\eta \leq \left[25d\beta(LR + G)^2\right]^{-1} \wedge L^2d^{-1}M^{-2}/25$ and $\beta \geq 1$, the transition distribution $T_u(\cdot)$ can be $\delta$-close to $T_u^*(\cdot)$ with

$$\delta = 28Md^{3/2}\beta^{-1/2}\eta^{3/2} + 10(LR + G)d^{1/2}\beta^{1/2}\eta^{3/2} + 12\beta(LR + G)^2d\eta/B + 2\beta^2(LR + G)^4\eta^2/B \leq 14(LR + G)^2\beta d\eta/B + [28Md^{3/2}\beta^{-1/2} + 10(LR + G)d^{1/2}\beta^{1/2}]\eta^{3/2} \leq 14Ld\eta + 14(LR + G)^2\beta d\eta/B.$$

Then based on the requirement of $\eta$ and the lower bound of $\phi$ in Lemma 6.4, it suffices to set the step size to be

$$\eta \leq \min \left\{ \frac{1}{25\beta(LR + G)^2}, \frac{1}{35(Ld + (LR + G)^2\beta d)/B}, \left( \frac{c_0\rho}{16\sqrt{\beta}(14Ld\eta + 14(LR + G)^2\beta d\eta/B)} \right)^2 \right\}.$$

Therefore, by Lemma 6.5, set $R = R(\zeta)$, we have

$$\|\mu_k - \pi\|_{TV} \leq \|\pi - \pi^*\|_{TV} + \|\mu_k - \pi^*\|_{TV} \leq 3\zeta + \lambda (1 - \phi^2/8)k + \frac{16\delta}{\phi} \leq 3\zeta + \lambda (1 - C_0\eta)k + C_1B^{-1}\eta^{1/2} + C_2\eta,$$

where $C_0 = c_0^2\rho^2/\beta$, $C_1 = 224(LR + G)^2\beta^{3/2}d\rho^{-1}/c_0$, $C_2 = \rho^{-1}[448Md^{3/2} + 160(LR + G)d^{1/2}\beta]/c_0$ are problem-dependent constants. \hfill \Box

**B.5 Proof of Corollary 5.3**

**Proof of Corollary 5.3.** From (B.2), we know that $\mu_0$ is a $\lambda$-warm start with respect to $\pi^*$ with $\lambda = e^{O(\delta)}$. Then in order to guarantee that the sampling error $\|\mu_k - \pi\|_{TV} \leq \epsilon$, it suffices to set

$$\lambda (1 - C_0\eta)k = \epsilon/4, \ 3\zeta = \epsilon/4, C_1B^{-1}\eta^{1/2} = \epsilon/4, \ C_2\eta = \epsilon/4.$$

Therefore, we have $\zeta = O(\epsilon)$ and thus $R = R(\zeta) = O(d^{1/2}\beta^{-1/2}\log^{1/2}(\epsilon))$. Note that we have $C_0 = O(\rho^2\beta^{-1})$, $C_1 = \tilde{O}(d^2\rho^{-1}\beta^{1/2})$ and $C_2 = \tilde{O}(d^3\beta\rho^{-1} + d\beta^{1/2}\rho^{-1})$, plugging these into the above equation gives

$$\eta = \tilde{O}\left( \frac{\rho^2B^2\epsilon^2}{d^4\beta} \wedge \frac{\rho\epsilon}{d^3/2 + d\beta^{1/2}} \right)$$

and

$$k = O\left( \frac{\log(\lambda/\epsilon)}{C_0\eta} \right) = \tilde{O}\left( \frac{d^5\beta^2}{\rho^4B^2\epsilon^2} + \frac{d^5/2\beta + d^2\beta^{3/2}}{\rho^3\epsilon} \right).$$
C Proof of Lemmas in Section 6

In this section, we provide the proof of Lemmas used in Section 6.

C.1 Proof of Lemma 6.1

Before providing the detailed proof of Lemma 6.1, we first present the following useful lemma.

Lemma C.1. Let $g(x, I)$ be the stochastic gradient with mini-batch size $|I| = B < n$, then for any vector $a$ and $|x|_2 \leq R$, there exists a constant $K = LR + G$ such that

$$
\mathbb{E}_I \left[ \exp \left( \langle a, g(x, I) - \nabla f(x) \rangle \right) \right] \leq \exp(K^2|a|_2^2/B).
$$

Moreover, we have $\mathbb{E}_I \left[ \exp \left( \langle a, g(x, I) - \nabla f(x) \rangle \right) \right] = 1$ if $B = n$.

Proof of Lemma 6.1. Note that the Markov processes defined by $T_u^*(\cdot)$ and $T_u(\cdot)$ are 1/2-lazy according to (6.3). We prove the lemma by considering two cases: $u \notin A$ and $u \in A$. We first prove the lemma in the first case. Note that when $u \notin A$, we have

$$
T_u^*(A) = \int_A T_u^*(w) dw = \int_A \alpha_u(w) T_u(w) dw. \quad \text{(C.1)}
$$

By (6.2), we know that $w$ is restricted in $w \in B(u, r) \cap B(0, R) \{u\}$. For sufficiently small step size $\eta$, we can ensure $\delta \leq 1/2$. In the rest of this proof we will show that $\alpha_u(w) \geq 1 - \delta/2$ for all $w \in B(u, r) \cap B(0, R) \{u\}$, which together with (C.1) implies

$$(1 - \delta/2) T_u(A) \leq T_u^*(A) \leq T_u(A),$$

and thus (6.4) also holds since $\alpha_u(w) \geq 1 - \delta/2$. Then, it suffices to prove that

$$
\frac{T_u^*(w)}{T_u(w)} \cdot \exp(-\beta(f(w) - f(u))) \geq 1 - \delta/2. \quad \text{(C.2)}
$$

By the definition of $T_u(w)$, it is equivalent to proving

$$
\frac{\mathbb{E}_{I_1} \left[ \exp \left( -\beta f(w) - \frac{|w-u+\eta g(w, I_2)|_2^2}{4\eta/\beta} \right) \right]}{\mathbb{E}_{I_2} \left[ \exp \left( -\beta f(u) - \frac{|w-u+\eta g(u, I_2)|_2^2}{4\eta/\beta} \right) \right]} \geq 1 - \delta/2,
$$

where $I_1, I_2 \subseteq [n]$ are two independent mini-batches of data. Let $I_1$ and $I_2$ denote the numerator and denominator of the L.H.S. of the above inequality respectively. Then regarding $I_1$, by Jensen’s inequality and convexity of the function $\exp(\cdot)$, we have

$$
I_1 \geq \exp \left( -\beta f(w) - \frac{\mathbb{E}_{I_1} \|w-u+\eta g(w, I_1)||_2^2}{4\eta/\beta} \right).
$$
\[ I_1 \geq \exp \left( -\beta f(w) - \frac{\|w - w\|^2}{4\eta} + 2\eta \langle w - w, \nabla f(w) \rangle + \eta^2 \mathbb{E}_{I_1} [\|g(w, I_1)\|^2 | w] \right) \]

\[ \geq \exp \left( -\beta f(w) - \frac{\|w - w\|^2}{4\eta} + 2\eta \langle w - w, \nabla f(w) \rangle + \eta^2 \mathbb{E}_{I_1} [\|g(w, I_1)\|^2 | w] \right) \cdot \exp \left( -\frac{\beta \|\nabla f(w)\|^2}{2} \right) \]

where the last inequality is by Lemma C.1. Then we move on to upper bounding \( I_2 \),

\[ I_2 = \exp \left( -\beta f(u) \right) \cdot \mathbb{E}_{I_2} \left[ \exp \left( -\frac{\|w - w\|^2}{4\eta} + 2\eta \langle w - w, \nabla f(u) \rangle \right) \right] \]

\[ \leq \exp \left( -\frac{\beta \|\nabla f(u)\|^2}{2} \right) \cdot \exp \left( -\frac{\beta \|\nabla f(u)\|^2}{4} \right) \]

where the last inequality holds due to Lemma C.1. Then by Young’s inequality, \( I_3 \) can be further upper bounded by

\[ I_3 \leq \exp \left( \frac{\beta^2 K^2 (\|w - u\|^2 + \eta^2 \|\nabla f(u)\|^2)}{2B} - \frac{\beta \eta \|\nabla f(u)\|^2}{4} \right) \]

where the second inequality is by Lemma A.2. Combining the previous results for \( I_1 \) and \( I_2 \), we have

\[ \frac{I_1}{I_2} \geq \exp \left( -\beta (f(w) - f(u)) - \frac{\beta \langle w - w, \nabla f(w) + f(u) \rangle}{2} \right) \]

\[ \cdot \exp \left( \frac{\beta \eta (\|\nabla f(u)\|^2 - \|\nabla f(w)\|^2)}{4} - \frac{\beta^2 K^2 (\|w - u\|^2 + (LR + G)^2 \eta^2)}{2B} + \frac{\beta \eta K^2 d}{2} \right) \]

(C.4)

It is well known that the smoothness condition in Assumption 4.4 (Nesterov, 2018) is equivalent to
the following inequalities,
\[
\begin{align*}
    f(w) &\leq f(u) + \langle w - u, \nabla f(u) \rangle + \frac{L\|w - u\|^2}{2}, \\
    f(u) &\geq f(w) + \langle u - w, \nabla f(w) \rangle - \frac{L\|w - u\|^2}{2},
\end{align*}
\]
which immediately implies
\[
    \left| f(w) - f(u) - \langle w - u, \nabla f(w) + f(u) \rangle/2 \right| \leq \frac{L\|w - u\|^2}{2}. \tag{C.5}
\]
In addition, by Lemma A.2 and Assumption 4.4, it holds that
\[
    \left| \|f(u)\|^2 - \|f(w)\|^2 \right| \leq \left( \|f(u) - f(w)\| \cdot \|f(u) + f(w)\| \right)^2 / 2L \leq 2L(LR + G)\|w - u\|^2. \tag{C.6}
\]
Now, substituting (C.5) and (C.6) into (C.4) and using the fact that $\|w - u\| \leq r = \sqrt{10\eta d/\beta}$, we have
\[
    \frac{I_1}{I_2} \geq \exp \left( - \frac{L\beta\|w - u\|^2}{2} - \frac{\beta\eta L(LR + G)\|w - u\|^2}{2} - \frac{\beta^2 K^2(\|w - u\|^2 + (LR + G)^2\eta^2 + \eta d(\beta^{-1/2}))}{2B} \right)
\]
\[
    \geq \exp \left( - \frac{5Ld\eta - 5L(LR + G)d^{1/2}\beta^{1/2}\eta^{3/2} - 6\beta K^2d\eta}{B} - \frac{\beta^2 K^2(LR + G)^2\eta^2}{2B} \right)
\]
\[
    \geq 1 - 5Ld\eta - 5L(LR + G)d^{1/2}\beta^{-1/2}\eta^{3/2} - 6\beta K^2d\eta/B - \beta^2 K^2(LR + G)^2\eta^2/B
\]
\[
    = 1 - \delta/2,
\]
where we plug in the fact that $K = LR + G$ in the last equality. This completes the proof for the case $u \notin \mathcal{A}$.

In the second case that $u \in \mathcal{A}$, we can split $\mathcal{A}$ into $\{u\}$ and $\mathcal{A}\setminus\{u\}$. Note that by our result in the first case, we have $(1 - \delta)\mathcal{T}_u^*(\mathcal{A}\setminus\{u\}) \leq \mathcal{T}_u(\mathcal{A}\setminus\{u\}) \leq (1 + \delta)\mathcal{T}_u^*(\mathcal{A}\setminus\{u\})$. Therefore, it remains to prove that $(1 - \delta)\mathcal{T}_u^*(u) \leq \mathcal{T}_u(u) \leq (1 + \delta)\mathcal{T}_u^*(u)$. Note that starting from $u$, the probability of the Markov chain generated by $T^*$ stays at $u$ is
\[
    \mathcal{T}_u^*(u) = \mathcal{T}_u(u) + (1 - \mathcal{T}_u(u)) \cdot \left( 1 - \mathbb{E}_{w \sim \mathcal{T}_u(w \neq u)}[\alpha_u(w) | u] \right).
\]
By our previous results, we know that $\alpha_u(w) \geq 1 - \delta/2$ for all $w \in B(u, r) \cap \Omega\setminus\{u\}$. Therefore, we have
\[
    \mathcal{T}_u(u) \leq \mathcal{T}_u^*(u) \leq \mathcal{T}_u(u)(1 + \delta/2),
\]
where the inequality on the right hand side of $\mathcal{T}_u^*(u)$ is due to the fact that $\mathcal{T}_u(u) \geq 1/2$ and thus $\mathcal{T}_u(u) \geq (1 - \mathcal{T}_u(u))$. Then it is evident that we have $(1 - \delta)\mathcal{T}_u^*(u) \leq \mathcal{T}_u(u) \leq (1 + \delta)\mathcal{T}_u^*(u)$, which completes the proof for the second case. \qed
C.2 Proof of Lemma 6.3

Now we characterize the convergence of SGLD to the truncated target distribution \( \pi^* \). Note that Markov chains defined by \( T_u(\cdot) \) and \( T_u^*(\cdot) \) are restricted in the set \( \Omega = B(0, R) \). Let \( \mu_k \) be the distribution of iterate \( x_k \) of Algorithm 1, we define the following function

\[
h_k(p) = \sup_{A : A \subseteq \Omega, \pi^*(A) = p} \mu_k(A) - \pi^*(A), \quad \forall p \in [0, 1].
\]

Based on definition of the total variation distance between \( \mu_k \) and \( \pi^* \), we have

\[
\|\mu_k - \pi^*\|_{TV} = \sup_{A : A \subseteq \Omega} |\mu_k(A) - \pi^*(A)|
= \sup_{A : A \subseteq \Omega} \max \{\mu_k(A) - \pi^*(A), \pi^*(A) - \mu_k(A)\}
= \sup_{A : A \subseteq \Omega} \max \{\mu_k(A) - \pi^*(A), \mu_k(\Omega \setminus A) - \pi^*(\Omega \setminus A)\}
= \sup_{A : A \subseteq \Omega} \mu_k(A) - \pi^*(A).
\]

Then in order to prove the result in Lemma 6.3, it suffices to show that

\[
h_k(p) \leq \lambda(1 - \phi^2/8)^k + \frac{16\delta}{\phi},
\]

for all \( p \in (0, 1) \).

**Lemma C.2.** Let \( T_u^*(\cdot) \) be a time-reversible Markov chain with unique stationary distribution \( \pi^*(\cdot) \). Then for any approximate Markov chain \( T_u(\cdot) \) satisfying \((1 - \delta)T_u^*(\cdot) \leq T_u(\cdot) \leq (1 + \delta)T_u^*(\cdot)\) with \( \delta \leq \min\{1 - \sqrt{2}/2, \phi/16\} \), there exist three parameters \( \phi_k, \hat{\phi}_k \) and \( \tilde{\phi}_k \) depending on \( \mu_k(\cdot) \) that satisfy \( \phi_k \geq \phi \),

\[
2(1 - \delta)\phi_k \leq \tilde{\phi}_k \leq \hat{\phi}_k \leq 2(1 + \delta)\phi_k, \quad \text{and} \quad \sqrt{1 - \tilde{\phi}_k} + \sqrt{1 + \hat{\phi}_k} \leq 2(1 - \phi_k^2/8),
\]

such that the following inequality holds for all \( p \in (0, 1) \),

\[
h_k(p) \leq \frac{1}{2}h_{k-1}(p - \tilde{\phi}_k\Gamma_p) + \frac{1}{2}h_{k-1}(p + \hat{\phi}_k\Gamma_p) + 2\delta\phi_k\sqrt{\Gamma_p},
\]

where \( \Gamma_p = \min\{p, 1 - p\} \).

**Proof of Lemma 6.3.** By Lemma C.2, we know that if \( \delta \leq \min\{1 - \sqrt{2}/2, \phi/16\} \), there exist three parameters \( \phi_k, \tilde{\phi}_k \) and \( \hat{\phi}_k \) depending on \( \mu_k(\cdot) \) such that when \( p \in (0, 1/2] \),

\[
h_k(p) \leq \frac{1}{2}[h_{k-1}(p - \tilde{\phi}_k p) + h_{k-1}(p + \hat{\phi}_k p)] + 2\delta\phi_k\sqrt{p}, \quad \text{(C.7)}
\]

and when \( p \in (1/2, 1) \),

\[
h_k(p) \leq \frac{1}{2}[h_{k-1}(p - \tilde{\phi}_k (1 - p)) + h_{k-1}(p + \hat{\phi}_k (1 - p))] + 2\delta\phi_k\sqrt{1 - p}.
\]
Then, we will prove the desired result via mathematical induction. Instead of directly proving the
inequality in this lemma, we aim to prove a stronger version,
\[
h_k(p) \leq \min \{ \sqrt{p}, \sqrt{1-p} \} \cdot \left[ \lambda \left( 1 - \phi^2 / 8 \right)^k + \frac{16\delta}{\phi} \right],
\] (C.8)
We first verify the hypothesis (C.8) for the case \( k = 0\), based on the definition of \( h_0(p) \) we have that there exists a set \( A_0 \subseteq \Omega \) satisfying \( \pi^*(A_0) = p \) such that
\[
h_0(p) = \mu_0(A_0) - \pi^*(A_0).
\]
When \( p \leq 1/2 \), by the definition of \( \lambda \)-warm initialization in (4.1), it holds that
\[
h_0(p) \leq \max\{\mu_0(A_0) - \pi^*(A_0), \pi^*(A_0) - \mu_0(A_0)\} \leq \lambda p \leq \sqrt{p} \cdot \left( \lambda + \frac{16\delta}{\phi} \right).
\]
When \( p \geq 1/2 \), similarly we have
\[
h_0(p) = (1 - \mu_0(\Omega \setminus A_0)) - (1 - \pi^*(\Omega \setminus A_0))
\leq \lambda (1 - p)
\leq \sqrt{1-p} \cdot \left( \lambda + \frac{16\delta}{\phi} \right),
\]
which verifies the hypothesis for the case \( k = 0 \). Now we assume the hypothesis (C.8) holds for
\( 0, \ldots, k - 1 \). According to Lemma C.2, the following holds when \( p \in (0, 1/2] \),
\[
h_k(p) \leq \frac{1}{2} \left[ h_{k-1}(p - \tilde{\phi}_k p) + h_{k-1}(p + \tilde{\phi}_k p) \right] + 2\delta \phi_k \sqrt{p}
\leq \frac{\sqrt{p - \tilde{\phi}_k p} + \sqrt{p + \tilde{\phi}_k p}}{2} \left( \lambda \left( 1 - \phi^2 / 8 \right)^{k-1} + \frac{16\delta}{\phi} \right) + 2\delta \phi_k \sqrt{p}
\leq \frac{\sqrt{p} \left( \sqrt{1 - \tilde{\phi}_k} + \sqrt{1 + \tilde{\phi}_k} \right)}{2} \left( \lambda \left( 1 - \phi^2 / 8 \right)^{k-1} + \frac{16\delta}{\phi} \right) + 2\delta \phi_k \sqrt{p},
\]
where the second inequality is based on the hypothesis for \( k - 1 \). Again from Lemma C.2, we know that \( \sqrt{1 - \tilde{\phi}_k} + \sqrt{1 + \tilde{\phi}_k} \leq 2(1 - \phi_k^2 / 8) \), which further implies
\[
h_k(p) \leq \sqrt{p} \cdot \left( 1 - \phi_k^2 / 8 \right) \left( \lambda \left( 1 - \phi^2 / 8 \right)^{k-1} + \frac{16\delta}{\phi} \right) + 2\delta \phi_k \sqrt{p}
\leq \sqrt{p} \cdot \left( \lambda \left( 1 - \phi^2 / 8 \right)^{k} + \frac{16\delta}{\phi} - 2\delta \phi_k^2 / \phi + 2\delta \phi_k \right)
\leq \sqrt{p} \cdot \left( \lambda \left( 1 - \phi^2 / 8 \right)^{k} + \frac{16\delta}{\phi} \right),
\]
where the last inequality is due to \( \phi \leq \phi_k \). Similar result can be proved when \( p \in (1/2, 1) \) and thus we omit it here. Thus we are able to verify the hypothesis for \( k \).
C.3 Proof of Lemma 6.4

In order to prove a lower bound of the conductance of $\mathcal{T}_u^*(\cdot)$, we follow the same idea used in Lee and Vempala (2018); Mangoubi and Vishnoi (2019), which is basically built upon the following lemma.

Lemma C.3 (Lemma 13 in Lee and Vempala (2018)). Let $\mathcal{T}_u^*(\cdot)$ be a time-reversible Markov chain on $\Omega$ with stationary distribution $\pi^*$. Fix any $\Delta > 0$, suppose for any $u, v \in \Omega$ with $\|u - v\|_2 \leq \Delta$ we have $\|\mathcal{T}_u^*(\cdot) - \mathcal{T}_v^*(\cdot)\|_{TV} \leq 0.99$, then the conductance of $\mathcal{T}_u^*(\cdot)$ satisfies $\phi \geq C \rho \Delta$ for some absolute constant $C$, where $\rho$ is the Cheeger constant of $\pi^*$.

Similar results have been shown in Dwivedi et al. (2018); Ma et al. (2018) for bounding the $s$-conductance of Markov chains. In order to apply Lemma C.3, we need to verify the corresponding conditions, i.e., proving that as long as $\|u - v\|_2 \leq \Delta$ we have $\|\mathcal{T}_u^*(\cdot) - \mathcal{T}_v^*(\cdot)\|_{TV} \leq 0.99$ for some $\Delta$.

Before moving on to the detailed proof, we first recall some definitions. Recalling (6.1), we define

$$P(z|u) = \mathbb{E}_T[P(z|u, T)] = \mathbb{E}_T \left[ \frac{1}{(4\pi \eta/\beta)^d/2} \exp \left( -\frac{\|z - u + \eta g(u, T)\|_2^2}{4\eta/\beta} \right) | u \right]$$

as the distribution after one-step standard SGLD step (i.e., without the accept/reject step). Note that Algorithm 1 only accepts the candidate iterate in the region $\Omega \cap B(u, r)$, we can compute the acceptance probability as follows,

$$p(u) = \mathbb{P}_{z \sim P(\cdot|u)} [z \in \Omega \cap B(u, r)].$$

Therefore, for any $z \in \Omega \cap B(u, r)$, the transition probability $\mathcal{T}_u^*(z)$ takes form

$$\mathcal{T}_u^*(z) = \frac{2 - p(u) + p(u)(1 - \alpha_u(z))}{2} \delta_u(z) + \frac{\alpha_u(z)}{2} P(z|u) \cdot I[z \in \Omega \cap B(u, r)].$$

Then the rest proof will be proving the upper bound of $\|\mathcal{T}_u^*(\cdot) - \mathcal{T}_v^*(\cdot)\|_{TV}$, and we state another two useful lemmas as follows.

Lemma C.4. If the step size satisfies $\eta \leq [40d^{-1}(LR + G)^2 \beta]^{-1}$, for any $u \in \Omega$, the acceptance probability $p(u)$ satisfies $p(u) \geq 0.4$.

Lemma C.5. Under Assumption 4.4, for any two points $u, v \in \mathbb{R}^d$, it holds that

$$\|P(\cdot|u) - P(\cdot|v)\|_{TV} \leq \frac{(1 + L \eta)\|u - v\|_2}{\sqrt{2\eta/\beta}}.$$
\[
\begin{align*}
&\leq \max_{u, z} \left[ \frac{2 - p(u) + p(u)(1 - \alpha_u(z))}{2} \right]_{I_1} \\
&+ \frac{1}{2} \left[ \int_{z \in A} \alpha_u(z) P(z|u) \mathbb{1}(z \in S_u) - \alpha_v(z) P(z|v) \mathbb{1}(z \in S_v) \, dz \right]_{I_2}.
\end{align*}
\]

Then we aim to upper bound the quantities \( I_1 \) and \( I_2 \) separately. In terms of \( I_1 \), Lemma 6.1 combined with (C.2) implies that

\[
\max_{u, z} \alpha_u(z) \geq 1 - \delta/2,
\]

where \( \delta \) is the approximation factor between \( T_u(\cdot) \) and \( T_u^*(\cdot) \) defined in Lemma 6.1. By Lemma C.4, we know that \( p(u) \geq 0.4 \) for any \( \mathcal{I} \) and \( u \in \mathcal{K} \). Then combining with (C.9), \( I_1 \) can be upper bounded by

\[
I_1 \leq 0.8 + 0.1\delta.
\]

Regarding \( I_2 \), by triangle inequality we have

\[
I_2 \leq \int_{z \in A} (1 - \alpha_u(z)) P(z|u) \mathbb{1}(z \in S_u) \, dz + \int_{z \in A} (1 - \alpha_v(z)) P(z|v) \mathbb{1}(z \in S_v) \, dz \\
+ \left[ \int_{z \in A} p(u) P(z|u) - p(v) P(z|v) \, dz \right]_{I_3} \\
\leq \delta + \left[ \int_{z \in A} P(z|u) \mathbb{1}(z \in S_u) - P(z|v) \mathbb{1}(z \in S_v) \, dz \right]_{I_3},
\]

where the last inequality is by (C.9). Regarding \( I_3 \), we further have,

\[
I_3 \leq \left[ \int_{z \in A} \mathbb{1}(z \in S_v)(P(z|u) - P(z|v)) \, dz \right] + \left[ \int_{z \in A} \left[ \mathbb{1}(z \in S_u) - \mathbb{1}(z \in S_v) \right] P(z|u) \, dz \right] \\
\leq \|P(\cdot|u) - P(\cdot|v)\|_{TV} + \max \left\{ \int_{z \in S_v \setminus S_u} P(z|u) \, dz, \int_{z \in S_v \setminus S_u} P(z|v) \, dz \right\} \\
\leq \|P(\cdot|u) - P(\cdot|v)\|_{TV} + \max \left\{ \int_{z \in \mathbb{R}^d \setminus S_u} P(z|u) \, dz, \int_{z \in \mathbb{R}^d \setminus S_v} P(z|v) \, dz \right\}.
\]

For any \( \mathcal{I} \), note that \( P(z|u, \mathcal{I}) \) is a Gaussian distribution with mean \( u - \eta g(u, \mathcal{I}) \) and covariance matrix \( 2\eta I/\beta \), thus we have

\[
\int_{\mathbb{R}^d \setminus S_u} P(z|u, \mathcal{I}) \, dz \leq \mathbb{P}_{z \sim \chi_d^2}(z \geq 0.5\beta(r - \eta \|g(u, \mathcal{I})\|_2)^2/\eta) \\
\int_{\mathbb{R}^d \setminus S_v} P(z|u, \mathcal{I}) \, dz \leq \mathbb{P}_{z \sim \chi_d^2}(z \geq 0.5\beta(r - \eta \|g(u, \mathcal{I})\|_2 - \|u - v\|_2)^2/\eta).
\]
Note that the above inequalities hold for any choice of $I$. Thus, if $\|u - v\|_2 \leq 0.1r$ and $\eta \leq 0.1d\beta^{-1}/(LR + G)^2$, by Lemma A.2, we have $r - \eta\|g(u, I)\|_2 - \|u - v\|_2 \geq \sqrt{6.4\eta d/\beta}$, and then
\[
\max \left\{ \int_{z \in \mathbb{R}^d \setminus S_u} P(z|u)dz, \int_{z \in \mathbb{R}^d \setminus S_v} P(z|u)dz \right\} \leq \mathbb{P}_{z \sim \chi^2_d}(z \leq 3.2d) \leq 0.1.
\]

Then combining the above results and apply Lemma C.5, assume $\eta \leq 1/L$, we have
\[
I_3 \leq 0.1 + \|P(\cdot|u) - P(\cdot|v)\|_{TV} \leq 0.1 + \sqrt{2\beta}\|u - v\|_2/\sqrt{\eta}.
\]

This immediately implies that $I_2 \leq \delta + \sqrt{2\beta}\|u - v\|_2/\sqrt{\eta} + 0.1$ and finally
\[
\|T_u(\cdot) - T_v(\cdot)\|_{TV} \leq I_1 + I_2/2 \leq 0.85 + 0.1\delta + \frac{\sqrt{\beta}\|u - v\|_2}{\sqrt{2\eta}}.
\]

By Lemma 6.1, we know that if $\eta \leq [25\beta(LR + G)^2]^{-1}$, we have
\[
\delta = 10Ld\eta + 10L(LR + G)d^{1/2}\beta^{1/2}\eta^{3/2} + 12\beta(LR + G)^2d\eta/B + 2\beta^2(LR + G)^4\eta^2/B
\]
\[
\leq 14Ld\eta + 14(LR + G)^2\beta d\eta/B.
\]

Thus if
\[
\eta \leq \frac{1}{25\beta(LR + G)^2} \wedge \frac{1}{35(Ld + (LR + G)^2\beta d/B)} \quad \text{and} \quad \|u - v\|_2 \leq \frac{\sqrt{2\eta}}{10\sqrt{\beta}} \leq 0.1r,
\]
we have $\|T_u(\cdot) - T_v(\cdot)\|_{TV} \leq 0.99$. Then by Lemma C.3, we have the following lower bound on the conductance of $T_u^{-}(\cdot)$
\[
\phi \geq c_0\rho\sqrt{\eta/\beta},
\]
where $c_0$ is an absolute constant. This completes the proof. \qed

### C.4 Proof of Lemma 6.5

We present the following useful lemma that characterizes the probability measure of the region $B(0, R(\zeta))$ under the target distribution $\pi$.

**Lemma C.6.** Under Assumptions 4.3 and 4.4, let $\Omega = B(0, R(\zeta))$, it holds that
\[
\pi(\Omega) \geq 1 - \zeta.
\]

**Proof of Lemma 6.5.** According to the definition of total variation distance, we know that there exists a set $A \in \mathbb{R}^d$ such that
\[
\|\pi^* - \pi\|_{TV} = |\pi^*(A) - \pi(A)| \leq |\pi^*(A \cap \Omega) - \pi(A \cap \Omega)| + \pi(A \setminus \Omega)
\]
\[
\leq |\pi^*(A \cap \Omega) - \pi(A \cap \Omega)| + \pi(\mathbb{R}^d \setminus \Omega),
\]
where the first inequality is by triangle inequality. By Lemma C.6, we have $\pi(\mathbb{R}^d \setminus \Omega) \leq \zeta$. For the
first term on the R.H.S. of the above inequality, we have

$$|\pi^*(A \cap \Omega) - \pi(A \cap \Omega)| = \left| \int_{A \cap \Omega} \pi^*(du) - \int_{A \cap \Omega} \pi(du) \right|. \tag{C.10}$$

Recall the definition of the truncated distribution $\pi^*$, for any $u \in \Omega$, we have

$$\pi(du) = \frac{e^{-\beta f(u)}du}{\int_{\mathbb{R}^d} e^{-\beta f(x)}dx}, \quad \text{and} \quad \pi^*(du) = \frac{e^{-\beta f(u)}du}{\int_{\Omega} e^{-\beta f(x)}dx} = \frac{\pi(du)}{\pi(\Omega)},$$

which immediately implies

$$\pi^*(du) - \pi(du) = \left( \frac{1}{\pi(\Omega)} - 1 \right) \pi(du) \leq \frac{\zeta}{1 - \zeta} \pi(du).$$

Plugging this into (C.10) yields

$$|\pi^*(A \cap \Omega) - \pi(A \cap \Omega)| \leq \frac{\zeta}{1 - \zeta} \int_{A \cap \Omega} \pi(u) du \leq \frac{\zeta}{1 - \zeta}.$$

Combining the above results, we have for any $\zeta \leq 1/2$ that

$$\|\pi^* - \pi\|_{TV} \leq \zeta + \frac{\zeta}{1 - \zeta} \leq 3\zeta,$$

which completes the proof. \hfill \square

## D Proof of Lemmas in Appendices B and C

### D.1 Proof of Lemma B.1

**Proof of Lemma B.1.** We will prove this for two cases: 1) $\|x\|_2 \leq \sqrt{2b/m}$ and 2) $\|x\|_2 \geq \sqrt{2b/m}$. For the first case, it is evident that

$$f(x) \geq f(x^*) \geq f(x^*) + \frac{m}{4}\|x\|^2_2 - \frac{b}{2},$$

where the last inequality is due to the fact that $\|x\|^2_2 \leq \sqrt{2b/m}$. For the second case, based on Assumption 4.3, define $g(x) = f(x) - m\|x\|^2_2/4$, it is clear that

$$\langle \nabla g(x), x \rangle = \langle \nabla f(x), x \rangle - \frac{m}{2}\|x\|^2_2 \geq \frac{m}{2}\|x\|^2_2 - b.$$

Therefore, if $\|x\|_2 \geq \sqrt{2b/m}$, we have $\langle \nabla g(x), x \rangle \geq 0$ and thus we have $\langle \nabla g(x), \alpha x \rangle \geq 0$ for any $\alpha \geq 0$. Then, for any $x$ with $\|x\|_2 > \sqrt{2b/m}$, let $y = \sqrt{2b/m}x/\|x\|_2$, we have

$$g(x) = g(y) + \int_0^1 \langle \nabla g(y + t(x - y)), x - y \rangle dt \geq g(y), \tag{D.1}$$
where the inequality is due to the facts that $\|y + t(x - y)\|_2 \geq \sqrt{2b/m}$ and $y + t(x - y) = \alpha(x - y)$ with $\alpha = t + \sqrt{2b/m/(\|x\|_2 - \sqrt{2b/m})}$. By the definition of function $g(\cdot)$, we have that for any $y$ with $\|y\|_2 \leq \sqrt{2b/m}$,

$$g(y) = f(y) - m\|y\|_2^2/4 \geq f(x^*) - b/2. \quad \text{(D.2)}$$

Plugging (D.2) into (D.1) gives

$$g(x) \geq g(y) \geq f(x^*) - b/2.$$ 

thus it follows that

$$f(x) \geq \frac{m}{4}\|x\|_2^2 + f(x^*) - \frac{b}{2}, \quad \text{(D.3)}$$

which completes the proof. \hfill \square

### D.2 Proof of Lemma B.2

**Proof of Lemma B.2.** Similar to the proof of Lemma 6.1, the essential part is to prove that $\alpha_u(w) \geq 1 - \delta/2$ for all $w \in B(u, r) \cap \Omega \setminus \{u\}$. We will prove that under Assumption 5.1, the first term on the R.H.S. of (C.4) can be improved. By Assumption 5.1 and Nesterov (2018), we know

$$f(w) - f(u) \leq \langle w - u, \nabla f(u) \rangle + \frac{1}{2}(w - u)\top \nabla^2 f(u)(w - u) + \frac{M}{6}\|w - u\|_2^3,$$

$$f(u) - f(w) \geq \langle u - w, \nabla f(w) \rangle + \frac{1}{2}(u - w)\top \nabla^2 f(w)(u - w) - \frac{M}{6}\|u - w\|_2^3.$$

Thus it follows that

$$|2f(w) - 2f(u) - \langle w - u, \nabla f(u) + f(w) \rangle|,$$

$$\leq \frac{1}{2}|(w - u)\top (\nabla^2 f(u) - \nabla^2 f(w))(w - u)| + \frac{M}{3}\|w - u\|_2^3,$$

$$\leq \frac{5M}{6}\|w - u\|_2^3,$$

where the second inequality is by Assumption 5.1 as well. Then combining with (C.6), let $I_1$ and $I_2$ be the same as those in the proof of Lemma 6.1, we can derive the following by (C.4),

$$\frac{I_1}{I_2} \geq \exp \left( - \frac{5M\beta\|w - u\|_2^3}{12} - \frac{\beta\eta L(LR + G)\|w - u\|_2}{2} - \frac{\beta^2K^2(\|w - u\|_2^2 + (LR + G)^2\eta^2 + \beta^{-1}\eta d/2)}{2B} \right)$$

$$\geq \exp \left( - \frac{14Md^{3/2}\beta^{-1/2}\eta^{3/2} - 5L(LR + G)d^{1/2}\beta^{1/2}\eta^{3/2}}{2B} - \frac{6\beta K^2 d\eta}{B} - \frac{\beta^2 K^2(LR + G)^2\eta^2}{2B} \right)$$

$$\geq 1 - \frac{14Md^{3/2}\beta^{-1/2}\eta^{3/2} - 5L(LR + G)d^{1/2}\beta^{1/2}\eta^{3/2} - 6\beta(LR + G)^2d\eta/B - \beta^2(LR + G)^4\eta^2/B}{B}$$

$$= 1 - \delta/2,$$

31
where we use the fact that $K = LR + G$ in the last inequality. Then following the same procedure as in the proof of Lemma 6.1, we are able to complete the proof.

### D.3 Proof of Lemma C.1

**Proof of Lemma C.1.** Note that we have $\|x\|_2 \leq R$, then by Lemma A.2 we know that

$$\|g(x, I_1) - \nabla f(x)\|_2 - \|g(x, I_2) - \nabla f(x)\|_2 \leq \|g(x, I_1) - g(x, I_2)\|_2 \leq 2LR + 2G,$$

for all $x$. Then by Hoeffding’s lemma, we have that there exists a constant $K = LR + G$ such that

$$E_I \left[ \exp \left( \langle a, g(x, I) - \nabla f(x) \rangle \right) \right] \leq \exp(K^2\|a\|_2^2)$$

for any $a \in \mathbb{R}^d$. Moreover, note that $I$ is uniformly sampled from $[n]$ without replacement. Let $I'$ be the stochastic mini-batch sampled from $[n]$ with replacement, by Lemma 1.1 in Bardenet et al. (2015) and the convexity of function $\exp(\cdot)$, we have

$$E_I \left[ \exp \left( \langle a, g(x, I) - \nabla f(x) \rangle \right) \right] \leq E_I \left[ \exp \left( \langle a, g(x, I') - \nabla f(x) \rangle \right) \right].$$

Then based on the fact that each element in $I'$ is independently drawn from $[n]$, we have

$$E_{I'} \left[ \exp \left( \langle a, g(x, I') - \nabla f(x) \rangle \right) \right] = E_{I'} \left[ \prod_{i \in I'} \exp \left( \frac{1}{B} \langle a, g(x, \{i\}) - \nabla f(x) \rangle \right) \right]$$

$$= \prod_{i \in I'} E_i \left[ \exp \left( \frac{1}{B} \langle a, g(x, \{i\}) - \nabla f(x) \rangle \right) \right]$$

$$\leq \prod_{i \in I'} \exp \left( K^2\|a\|_2^2/B^2 \right)$$

$$= \exp \left( K^2\|a\|_2^2/B \right).$$

Furthermore, note that if $B = n$, we have $E_I \left[ \exp \left( \langle a, g(x, I) - \nabla f(x) \rangle \right) \right] = 1$. This completes the proof.

### D.4 Proof of Lemma C.2

**Lemma D.1** (Lemma 1.2 in Lovász and Simonovits (1993)). For any atom-free distributions $\mu$ and $\nu$ on $\Omega$, define function

$$l(p) = \sup_{g: \Omega \to [0,1]} \int \Omega g(x) \mu(dx) \text{ s.t. } \int \Omega g(x) \nu(dx) = p.$$  

Then there exists a set $A \in \Omega$ with $\nu(A) = p$ such that $l(p) = \mu(A)$.

**Proof of Lemma C.2.** Similar to the proof of Lemma 1.3 in Lovász and Simonovits (1993), we first define the following functions for all $u, A \in \Omega$, 

$$g_1(u, A) = \begin{cases} 2T_u(A) - 1, & u \in A \\ 0, & u \notin A \end{cases} \quad g_2(u, A) = \begin{cases} 1, & u \in A \\ 2T_u(A), & u \notin A \end{cases}$$

32
It is easy to verify that \( g_1(u, A) + g_2(u, A) = 2T_u(A) \) for all \( u \in \Omega \). In addition, for a 1/2-lazy Markov process \( T_u(\cdot) \) defined as in (6.3), we have \( g_1(\cdot, \cdot), g_2(\cdot, \cdot) \in [0, 1] \). Based on the above definitions, we can further derive that

\[
\int_{\Omega} g_1(u, A)\pi^*(du) = \int_A [2T_u(A) - 1]\pi^*(du) \\
= \int_A [1 - 2T_u(\Omega \setminus A)]\pi^*(du) \\
= \pi^*(A) - 2\int_A T_u^*(\Omega \setminus A)\pi^*(du) - 2\left[ \int_A [T_u(\Omega \setminus A) - T_u^*(\Omega \setminus A)]\pi^*(du) \right]_{r_1}, \tag{D.4}
\]

and

\[
\int_{\Omega} g_2(u, A)\pi^*(du) = \pi^*(A) + \int_{\Omega \setminus A} 2T_u(A)\pi^*(du) \\
= \pi^*(A) + 2\int_{\Omega \setminus A} T_u^*(A)\pi^*(du) + 2\int_{\Omega \setminus A} [T_u(A) - T_u^*(A)]\pi^*(du) \\
= \pi^*(A) + 2\int_A T_u^*(\Omega \setminus A)\pi^*(du) + 2\left[ \int_A [T_u(A) - T_u^*(A)]\pi^*(du) \right]_{r_2}, \tag{D.5}
\]

where the last equality is by the fact that \( T_u^*(\cdot) \) is a time-reversible Markov chain with stationary distribution \( \pi^*(\cdot) \). Note that we have \( (1 - \delta)T_u^* (A) \leq T_u(A) \leq (1 + \delta)T_u^*(A) \), the approximation error terms \( r_1 \) and \( r_2 \) can be upper bounded as follows,

\[
|r_1| \leq \delta \int_A T_u^*(\Omega \setminus A)\pi^*(du) \\
|r_2| \leq \delta \int_{\Omega \setminus A} T_u^*(A)\pi^*(du) = \delta \int_A T_u^*(\Omega \setminus A)\pi^*(du).
\]

Then, combining (D.4) and (D.5) gives

\[
\int_{\Omega} [g_1(u, A) + g_2(u, A)]\pi^*(du) = 2\pi^*(A) - 2r_1 + 2r_2. \tag{D.6}
\]

Based on the definition of \( h_k(p) \), we know that there exists a set \( A_k \) satisfying \( \pi^*(A_k) = p \) such that

\[
h_k(p) = \mu_k(A_k) - \pi^*(A_k). \tag{D.7}
\]

Moreover, note that the distribution \( \mu_k(\cdot) \) is generated by conducting one-step transition (based on transition distribution \( T_u(\cdot) \)) from distribution \( \mu_{k-1}(\cdot) \), we have

\[
\mu_k(A_k) = \int_{A_k} \mu_k(du) = \int_{\Omega} T_u(A_k)\mu_{k-1}(du).
\]
Based on the definitions of functions $g_1$ and $g_2$, the above equation can be reformulated as

$$
\mu_k(A_k) = \frac{1}{2} \int_\Omega [g_1(u, A_k) + g_2(u, A_k)] \mu_{k-1}(du). 
$$

(D.8)

By (D.6), we know that

$$
\int_\Omega [g_1(u, A_k) + g_2(u, A_k)] \pi^*(du) = 2\pi^*(A_k) - 2r_1 + 2r_2,
$$

(D.9)

where $r_1$ and $r_2$ are two approximation error terms satisfying

$$
|r_1|, |r_2| \leq \delta \int_{A_k} T_{u}^*(\Omega \setminus A_k) \pi^*(du).
$$

(D.10)

Then based on Lemma D.1, we know that there exist two sets $A_{k-1}^1, A_{k-1}^2 \subseteq \Omega$ satisfying

$$
p_1 := \pi^*(A_{k-1}^1) = \int_\Omega g_1(u, A_k) \pi^*(du) \quad \text{and} \quad p_2 := \pi^*(A_{k-1}^2) = \int_\Omega g_2(u, A_k) \pi^*(du),
$$

(D.11)

such that

$$
\int_\Omega g_1(u, A_k) \mu_{k-1}(du) \leq \mu_{k-1}(A_{k-1}^1) \quad \text{and} \quad \int_\Omega g_2(u, A_k) \mu_{k-1}(du) \leq \mu_{k-1}(A_{k-1}^2).
$$

Therefore, based on (D.8) and (D.9), we have

$$
h_k(p) = \mu_k(A_k) - \pi^*(A_k)
= \frac{1}{2} \int_\Omega [g_1(u, A_k) + g_2(u, A_k)] \mu_{k-1}(du) - \frac{1}{2} \int_\Omega [g_1(u, A_k) + g_2(u, A_k)] \pi^*(du)
- r_1 + r_2
\leq \frac{1}{2} \left[ \mu_{k-1}(A_{k-1}^1) + \mu_{k-1}(A_{k-1}^2) - \pi^*(A_{k-1}^1) - \pi^*(A_{k-1}^2) \right] + |r_1 - r_2|
\leq \frac{1}{2} \left[ h_{k-1}(p_1) + h_{k-1}(p_2) \right] + |r_1 - r_2|,
$$

where the first inequality is by (D.9) and (D.11) and triangle inequality, and the last equality is by the definition of function $h_{k-1}(\cdot)$. Recalling (D.4), (D.5), and (D.11) the probabilities $p_1$ and $p_2$ can be reformulate as

$$
p_1 = p - \tilde{\varphi}_k \min\{p, 1-p\} \quad \text{and} \quad p_2 = p + \tilde{\varphi}_k \min\{p, 1-p\},
$$

where

$$
\tilde{\varphi}_k = \frac{2 \int_{A_k} T_{u}^*(\Omega \setminus A_k) \pi^*(du) - 2r_1}{\min\{p, 1-p\}} \quad \text{and} \quad \tilde{\varphi}_k = \frac{2 \int_{A_k} T_{u}^*(\Omega \setminus A_k) \pi^*(du) + 2r_2}{\min\{p, 1-p\}}.
$$

34
We further define
\[ \phi_k = \frac{\int_{A_k} T_u^*(\Omega \setminus A_k) \pi^*(du)}{\min\{p, 1 - p\}}. \]

Apparently, according to Definition 6.2, it holds that \( \phi_k \geq \phi_s \). In addition, by (D.10) and our definitions of \( \phi_k \) and \( \phi' \), it can be also derived that
\[ 2(1 - \delta)\phi_k \leq \phi_k' \leq \phi_k \leq 2(1 + \delta)\phi_k. \]

Since the transition kernel \( T_u(\cdot) \) is 1/2-lazy, we have \( \tilde{\phi}_k \leq 1 \). Then, if \( \delta \leq \min\{1 - \sqrt{2}/2, \phi/16\} \), we have \( \tilde{\phi}_k \geq \sqrt{2}\phi_k \) and \( \hat{\phi}_k - \phi_k \leq 4\delta\phi_k \leq \phi_k^2/4 \). Moreover, note that \( \sqrt{1 - x} \leq 1 - x/2 - x^2/8 \) for all \( x \in (0, 1) \), we have
\[ \sqrt{1 - \tilde{\phi}_k} + \sqrt{1 + \hat{\phi}_k} = \sqrt{1 - \tilde{\phi}_k} + \sqrt{1 + \hat{\phi}_k + \phi_k - \hat{\phi}_k} \]
\[ \leq 1 - \frac{\tilde{\phi}_k}{2} - \frac{\phi_k^2}{8} + 1 + \frac{\hat{\phi}_k}{2} \]
\[ \leq 2 - \frac{\phi_k^2}{4}. \]

Moreover, (D.10) also implies that
\[ |r_1 - r_2| \leq 2\delta \int_{A_k} T_u^*(\Omega \setminus A_k) \pi^*(du) = 2\delta\phi_k \min\{p, 1 - p\} \leq 2\delta\phi_k \min\{\sqrt{p}, \sqrt{1 - p}\}. \]

Therefore, we can finally upper bound \( h_k(p) \) as follows,
\[ h_k(p) \leq \frac{1}{2} [h_{k-1}(p - \tilde{\phi}_k \min\{p, 1 - p\}) + h_{k-1}(p + \hat{\phi}_k \min\{p, 1 - p\})] \]
\[ + 2\delta\phi_k \min\{\sqrt{p}, \sqrt{1 - p}\}, \]
which completes the proof. \( \square \)

D.5 Proof of Lemma C.4

Proof of Lemma C.4. For any \( \mathcal{I} \), we have
\[ \int_{\Omega \setminus \mathcal{B}(u, r)} P(z | u, \mathcal{I}) dz = \int_{\mathcal{B}(u, r)} P(z | u, \mathcal{I}) dz - \int_{\mathcal{B}(u, r) \setminus \Omega} P(z | u, \mathcal{I}) dz \]
\[ \geq \int_{\mathcal{B}(u, r)} P(z | u, \mathcal{I}) dz - \int_{\mathcal{R}^d \setminus \Omega} P(z | u, \mathcal{I}) dz. \quad (D.12) \]

Thus the remaining part is to prove that the R.H.S. of the above inequality is greater than 0.4. Regarding \( I_1 \), note that \( P(z | u, \mathcal{I}) \) is a Gaussian distribution with mean \( u - \eta g(u, \mathcal{I}) \) and covariance
matrix $2\eta I/\beta$, thus we have

$$
\int_{B(u,r)} P(z|u, I) dz \geq \mathbb{P}_{z \sim \chi^2_d}(z \leq 0.5\beta(r - \eta \|g(u, I)\|_2)^2/\eta).
$$

By Lemma A.2, we know that $\|g(u, I)\|_2 \leq LR + G$. Therefore, based on our choice $r = \sqrt{10\eta d/\beta}$, it is clear that if

$$
\eta \leq \frac{0.1d}{\beta(LR + G)^2},
$$

we have $r - \eta \|g(u, I)\|_2 \geq \sqrt{8\eta d/\beta}$ and thus

$$
\int_{B(u,r)} P(z|u, I) dz \geq \mathbb{P}_{z \sim \chi^2_d}(z \leq 4d) \geq 0.95. \quad (D.13)
$$

Then we will prove the upper bound of $I_2$. Note that the set $\Omega$ is a ball centered at the origin and $u \in \Omega$, we can construct a point $w$ as follows,

$$
w = u - \frac{(R - \sqrt{R^2 - r^2})u}{\|u\|_2}.
$$

It is easy to verify that a half space of $B(w, r)$ is contained by the set $\Omega$. Let $Q(z|w) = N(w, 2\eta I/\beta)$, it follows that

$$
\int_{\Omega} Q(z|w) dz \geq \int_{\Omega \cap B(w, r)} Q(z|w) dz \geq \frac{1}{2} \int_{B(w, r)} Q(z|w) dz.
$$

Note that $Q(z|w)$ is a Gaussian distribution with mean $w$ and covariance matrix $2\eta I/\beta$, thus we have

$$
\int_{\Omega} Q(z|w) dz \geq \frac{1}{2} \mathbb{P}_{z \sim \chi^2_d}(z \leq 5d) \geq 0.475.
$$

Moreover, by Pinsker’s inequality (Cover and Thomas, 2012), we have

$$
\left| \int_{\Omega} P(z|u, I) dz - \int_{\Omega} Q(z|w) dz \right| \leq \|P(-|u, I) - Q(-|w)\|_{TV} \leq \sqrt{2D_{KL}(P(-|u, I), Q(-|w))}.
$$

Note that $P(-|u, I)$ and $Q(-|w)$ are Gaussian distributions with the same covariance matrices, we have $D_{KL}(P(-|u, I), Q(-|w)) = \beta\|u - v\|_2^2/(4\eta)$. Therefore, it follows that

$$
\left| \int_{\Omega} P(z|u, I) dz - \int_{\Omega} Q(z|w) dz \right| \leq \mathbb{E}\|w - (u - \eta g(u, I))\|_2 \leq \sqrt{\beta/2\eta \cdot (\|w - u\|_2 + \eta \|g(u, I)\|_2)}.
$$

By our construction of $w$, we have

$$
\|w - u\|_2 = R - \sqrt{R^2 - r^2} = R(1 - \sqrt{1 - r^2/R^2}) \leq r^2/R = \frac{10\eta d}{\beta R}.
$$

36
By Lemma A.2, we know that $\|g(u, I)\|_2 \leq LR + G$. Therefore, if the step size satisfies
\[ \eta \leq \frac{1}{40} \left( d\beta^{-1} R^{-1} + (LR + G) \beta^{1/2} \right)^{-1}, \]
we have $\|P(\cdot|u, I) - Q(\cdot|w)\|_{TV} \leq 0.025$, and thus
\[ \int_{\Omega} P(z|u, I)dz = 1 - \int_{\Omega} P(z|u, I)dz \leq 1 - \int_{\Omega} Q(z|w)dz = 0.025 = 0.55. \]
Combining with (D.13), we have the following by (D.12),
\[ \int_{\Omega \cap B(u, r)} P(z|u, I)dz \geq \int_{B(u, r)} P(z|u, I)dz - \int_{\Omega \cap B(u, r)} P(z|u, I)dz \geq 0.95 - 0.55 = 0.4. \]
This completes the proof.

D.6 Proof of Lemma C.5

Proof of Lemma C.5. By the definition of total variation distance, we know there exists a set $A \in \mathbb{R}^d$ such that
\[
\|P(\cdot|u) - P(\cdot|v)\|_{TV} = |P(A|u) - P(A|v)| = \left| \int_A P(z|u) - P(z|v)dz \right| = \left| \mathbb{E}_I \left[ \int_A P(z|u, I) - P(z|v, I)dz \right] \right| \leq \mathbb{E}_I[\|P(z|u, I) - P(z|v, I)\|_{TV}],
\]
where the last inequality is by triangle inequality and the definition of total variation distance. By Pinsker’s inequality, we have
\[
\|P(z|u, I) - P(z|v, I)\|_{TV} \leq \sqrt{2D_{KL}(P(\cdot|u, I), P(\cdot|v, I))} = \frac{\|u - \eta g(u, I) - (v - \eta g(v, I))\|_2}{\sqrt{2\eta/\beta}},
\]
where the last equality follows from the fact that $P(\cdot|u, I)$ and $P(\cdot|v, I)$ are two Gaussian distributions with different means and same covariance matrices. By triangle inequality, we have
\[
\|u - \eta g(u, I) - (v - \eta g(v, I))\|_2 \leq \|u - v\|_2 + \eta \|g(u, I) - g(v, I)\|_2 \leq (1 + L\eta)\|u - v\|_2,
\]
where the second inequality is by Assumption 4.4. Therefore, we have
\[
\|P(\cdot|u) - P(\cdot|v)\|_{TV} \leq \mathbb{E}_I[\|P(z|u, I) - P(z|v, I)\|_{TV}] \leq \frac{(1 + L\eta)\|u - v\|_2}{\sqrt{2\eta/\beta}}.
\]
This completes the proof. \qed
D.7 Proof of Lemma C.6

Proof of Lemma C.6. Define a Gaussian distribution $q(x) = e^{-m\beta \|x\|^2/2}/(8\pi/(m\beta))^{d/2}$. Then by (B.3) and proof of Corollary 4.10, we have $q(x) \geq \pi(x)$ if $\|x\|^2 \geq 4m^{-1}(\beta^{-1}d \log(4L/m) + b)$. Thus, for any $\alpha \geq 4m^{-1}(\beta^{-1}d \log(4L/m) + b)$, we have

$$\int_{\|x\|^2 \geq \alpha} \pi(dx) \leq \int_{\|x\|^2 \geq \alpha} q(x)dx = \mathbb{P}_{z \sim \chi^2_d}[z \geq m\beta\alpha/4],$$

where the last equality is due to the fact that $q(x)$ is a Gaussian distribution with mean 0 and covariance matrix $4I/(m\beta)$. By standard tail bound of Chi-Square distribution, for any $\delta \in (0, 1)$ we have

$$\mathbb{P}_{z \sim \chi^2_d}[z \geq d + 2\sqrt{d \log(1/\delta) + 2 \log(1/\delta)}] \leq \delta.$$

Therefore, define by $\Omega = \mathcal{B}(0, \overline{R}(\zeta))$ with

$$\overline{R}(\zeta) = \left[\max\left\{\frac{4d \log(4L/m) + 4\beta b}{m\beta}, \frac{4d + 8\sqrt{d \log(1/\delta)} + 8 \log(1/\delta)}{m\beta}\right\}\right]^{1/2},$$

we have

$$\pi(\Omega) = \int_{\|x\|^2 \leq \overline{R}(\zeta)} \pi(dx) = 1 - \int_{\|x\|^2 \geq \overline{R}(\zeta)} \pi(dx) \geq 1 - \mathbb{P}_{z \sim \chi^2_d}[z \geq m\beta\overline{R}(\zeta)/4] \geq 1 - \zeta,$$

which completes the proof.

References

Bakry, D., Barthe, F., Cattiaux, P., Guillin, A. et al. (2008). A simple proof of the poincaré inequality for a large class of probability measures. Electronic Communications in Probability 13 60–66.

Bardenet, R., Maillard, O.-A. et al. (2015). Concentration inequalities for sampling without replacement. Bernoulli 21 1361–1385.

Bou-Rabee, N., Eberle, A. and Zimmer, R. (2018). Coupling and convergence for Hamiltonian monte carlo. arXiv preprint arXiv:1805.00452.

Bou-Rabee, N. and Hairer, M. (2013). Nonasymptotic mixing of the mala algorithm. IMA Journal of Numerical Analysis 33 80–110.
BUSER, P. (1982). A note on the isoperimetric constant. In *Annales scientifiques de l’École Normale Supérieure*, vol. 15.

CHAU, N. H., MOULINES, É., RÁSONYI, M., SABANIS, S. and ZHANG, Y. (2019). On stochastic gradient Langevin dynamics with dependent data streams: the fully non-convex case. *arXiv preprint arXiv:1905.13142*.

CHEN, C., DING, N. and CARIN, L. (2015). On the convergence of stochastic gradient mcmc algorithms with high-order integrators. In *Advances in Neural Information Processing Systems*.

CHEN, C., WANG, W., ZHANG, Y., SU, Q. and CARIN, L. (2017). A convergence analysis for a class of practical variance-reduction stochastic gradient mcmc. *arXiv preprint arXiv:1709.01180*.

CHEN, T., FOX, E. and GUESTRIN, C. (2014). Stochastic gradient Hamiltonian monte carlo. In *International Conference on Machine Learning*.

CHEN, X., DU, S. S. and TONG, X. T. (2020). On stationary-point hitting time and ergodicity of stochastic gradient Langevin dynamics. *Journal of Machine Learning Research* **21** 1–41.

CHEN, Y., CHEN, J., DONG, J., PENG, J. and WANG, Z. (2019a). Accelerating nonconvex learning via replica exchange Langevin diffusion. In *International Conference on Learning Representations*.

CHEN, Y., DWIVEDI, R., WAINWRIGHT, M. J. and YU, B. (2019b). Fast mixing of metropolized hamiltonian monte carlo: Benefits of multi-step gradients. *arXiv preprint arXiv:1905.12247*.

CHENG, X., CHATTERJI, N. S., ABBASI-YADKORI, Y., BARTLETT, P. L. and JORDAN, M. I. (2018a). Sharp convergence rates for Langevin dynamics in the nonconvex setting. *arXiv preprint arXiv:1805.01648*.

CHENG, X., CHATTERJI, N. S., BARTLETT, P. L. and JORDAN, M. I. (2018b). Underdamped Langevin mcmc: A non-asymptotic analysis. In *Proceedings of the 31st Conference On Learning Theory*, vol. 75.

CHIANG, T.-S., HWANG, C.-R. and SHEU, S. J. (1987). Diffusion for global optimization in $\mathbb{R}^n$. *SIAM Journal on Control and Optimization* **25** 737–753.

COUSINS, B. and VEMPALA, S. (2014). A cubic algorithm for computing gaussian volume. In *Proceedings of the twenty-fifth annual ACM-SIAM symposium on Discrete algorithms*. SIAM.

COVER, T. M. and THOMAS, J. A. (2012). *Elements of information theory*. John Wiley & Sons.

DALALYAN, A. S. (2017a). Further and stronger analogy between sampling and optimization: Langevin Monte Carlo and gradient descent. In *Conference on Learning Theory*.

DALALYAN, A. S. (2017b). Theoretical guarantees for approximate sampling from smooth and log-concave densities. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **79** 651–676.

DALALYAN, A. S. and KARAGULYAN, A. (2019). User-friendly guarantees for the Langevin monte carlo with inaccurate gradient. *Stochastic Processes and their Applications* **129** 5278–5311.
DALALYAN, A. S. and RIOU-DURAND, L. (2018). On sampling from a log-concave density using kinetic Langevin diffusions. *arXiv preprint arXiv:1807.09382*.

DENG, W., FENG, Q., GAO, L., LIANG, F. and LIN, G. (2020). Non-convex learning via replica exchange stochastic gradient mcmc. In *International Conference on Machine Learning*.

DURMUS, A. and MOULINES, E. (2016). Sampling from strongly log-concave distributions with the unadjusted Langevin algorithm.

DURMUS, A., MOULINES, E. and SAKSMAN, E. (2017a). On the convergence of hamiltonian monte carlo. *arXiv preprint arXiv:1705.00166*.

DURMUS, A., MOULINES, E. et al. (2017b). Nonasymptotic convergence analysis for the unadjusted Langevin algorithm. *The Annals of Applied Probability* **27** 1551–1587.

Dwivedi, R., Chen, Y., Wainwright, M. J. and Yu, B. (2018). Log-concave sampling: Metropolis-hastings algorithms are fast! In *Proceedings of the 31st Conference On Learning Theory*.

EBERLE, A. (2016). Reflection couplings and contraction rates for diffusions. *Probability theory and related fields* **166** 851–886.

EBERLE, A., GUILLIN, A. and ZIMMER, R. (2017). Couplings and quantitative contraction rates for Langevin dynamics. *arXiv preprint arXiv:1703.01617*.

ERDOGDU, M. A., MACKEY, L. and SHAMIR, O. (2018). Global non-convex optimization with discretized diffusions. In *Advances in Neural Information Processing Systems*.

GAO, X., GÜRBÜZBALABAN, M. and ZHU, L. (2018a). Breaking reversibility accelerates Langevin dynamics for global non-convex optimization. *arXiv preprint arXiv:1812.07725*.

GAO, X., GÜRBÜZBALABAN, M. and ZHU, L. (2018b). Global convergence of stochastic gradient Hamiltonian monte carlo for non-convex stochastic optimization: Non-asymptotic performance bounds and momentum-based acceleration. *arXiv preprint arXiv:1809.04618*.

LANGEVIN, P. (1908). On the theory of brownian motion. *CR Acad. Sci. Paris* **146** 530–533.

LEDOUX, M. (1994). A simple analytic proof of an inequality by p. buser. *Proceedings of the American mathematical society* **121** 951–959.

LEE, H., RISTESKI, A. and GE, R. (2018). Beyond log-concavity: Provable guarantees for sampling multi-modal distributions using simulated tempering Langevin monte carlo. In *Advances in Neural Information Processing Systems*.

LEE, Y. T. and VEMPALA, S. S. (2017). Eldan’s stochastic localization and the kls hyperplane conjecture: An improved lower bound for expansion. In *2017 IEEE 58th Annual Symposium on Foundations of Computer Science (FOCS)*. IEEE.
Lee, Y. T. and Vempala, S. S. (2018). Convergence rate of riemannian hamiltonian monte carlo and faster polytope volume computation. In Proceedings of the 50th Annual ACM SIGACT Symposium on Theory of Computing.

Lovász, L. and Simonovits, M. (1990). The mixing rate of markov chains, an isoperimetric inequality, and computing the volume. In Proceedings [1990] 31st annual symposium on foundations of computer science. IEEE.

Lovász, L. and Simonovits, M. (1993). Random walks in a convex body and an improved volume algorithm. Random structures & algorithms 4 359–412.

Ma, Y.-A., Chen, Y., Jin, C., Flammarion, N. and Jordan, M. I. (2018). Sampling can be faster than optimization. arXiv preprint arXiv:1811.08413.

Mangoubi, O. and Vishnoi, N. (2018). Dimensionally tight bounds for second-order hamiltonian monte carlo. In Advances in neural information processing systems.

Mangoubi, O. and Vishnoi, N. K. (2019). Nonconvex sampling with the metropolis-adjusted Langevin algorithm. In Conference on Learning Theory.

Mengersen, K. L., Tweedie, R. L. et al. (1996). Rates of convergence of the hastings and metropolis algorithms. The annals of Statistics 24 101–121.

Mou, W., Flammarion, N., Wainwright, M. J. and Bartlett, P. L. (2019). Improved bounds for discretization of Langevin diffusions: Near-optimal rates without convexity. arXiv preprint arXiv:1907.11331.

Neal, R. M. et al. (2011). MCMC using Hamiltonian dynamics. Handbook of Markov Chain Monte Carlo 2 113–162.

Nesterov, Y. (2018). Lectures on convex optimization, vol. 137. Springer.

Nguyen, T. H., Simsekli, U. and Richard, G. (2019). Non-asymptotic analysis of fractional Langevin monte carlo for non-convex optimization. In International Conference on Machine Learning.

Parisi, G. (1981). Correlation functions and computer simulations. Nuclear Physics B 180 378–384.

Raginsky, M., Rakhlin, A. and Telgarsky, M. (2017). Non-convex learning via stochastic gradient Langevin dynamics: a nonasymptotic analysis. In Conference on Learning Theory.

Roberts, G. O. and Tweedie, R. L. (1996). Exponential convergence of Langevin distributions and their discrete approximations. Bernoulli 341–363.

Rossky, P. J., Doll, J. and Friedman, H. (1978). Brownian dynamics as smart monte carlo simulation. The Journal of Chemical Physics 69 4628–4633.

Sato, I. and Nakagawa, H. (2014). Approximation analysis of stochastic gradient Langevin dynamics by using fokker-planck equation and ito process. In Proceedings of the 31st International Conference on Machine Learning (ICML-14).
Shamir, O. (2011). A variant of azuma’s inequality for martingales with subgaussian tails. arXiv preprint arXiv:1110.2392.

Smith, R. L. (1984). Efficient monte carlo procedures for generating points uniformly distributed over bounded regions. Operations Research 32 1296–1308.

Teh, Y. W., Thiery, A. H. and Vollmer, S. J. (2016). Consistency and fluctuations for stochastic gradient Langevin dynamics. The Journal of Machine Learning Research 17 193–225.

Vempala, S. (2007). Geometric random walks: a survey. In Combinatorial and Computational Geometry. Cambridge University Press.

Vempala, S. S. and Wibisono, A. (2019). Rapid convergence of the unadjusted Langevin algorithm: Log-sobolev suffices. arXiv preprint arXiv:1903.08568.

Vollmer, S. J., Zygalakis, K. C. and Teh, Y. W. (2016). Exploration of the (non-) asymptotic bias and variance of stochastic gradient Langevin dynamics. The Journal of Machine Learning Research 17 5504–5548.

Wang, B., Zou, D., Gu, Q. and Osher, S. (2019). Laplacian smoothing stochastic gradient markov chain monte carlo. arXiv preprint arXiv:1911.00782.

Welling, M. and Teh, Y. W. (2011). Bayesian learning via stochastic gradient Langevin dynamics. In Proceedings of the 28th International Conference on Machine Learning.

Xu, P., Chen, J., Zou, D. and Gu, Q. (2018). Global convergence of Langevin dynamics based algorithms for nonconvex optimization. In Advances in Neural Information Processing Systems.

Zhang, R., Li, C., Zhang, J., Chen, C. and Wilson, A. G. (2019a). Cyclical stochastic gradient mcmc for bayesian deep learning. arXiv preprint arXiv:1902.03932.

Zhang, Y., Akyildiz, Ö. D., Damoulas, T. and Sabanis, S. (2019b). Nonasymptotic estimates for stochastic gradient Langevin dynamics under local conditions in nonconvex optimization. arXiv preprint arXiv:1910.02008.

Zhang, Y., Liang, P. and Charikar, M. (2017). A hitting time analysis of stochastic gradient Langevin dynamics. In Conference on Learning Theory.

Zou, D., Xu, P. and Gu, Q. (2019a). Sampling from non-log-concave distributions via variance-reduced gradient Langevin dynamics. In Artificial Intelligence and Statistics, vol. 89 of Proceedings of Machine Learning Research. PMLR.

Zou, D., Xu, P. and Gu, Q. (2019b). Stochastic gradient hamiltonian monte carlo methods with recursive variance reduction. In Advances in Neural Information Processing Systems.