Non-Convex Stochastic Optimization via Non-Reversible Stochastic Gradient Langevin Dynamics

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Abstract

Stochastic gradient Langevin dynamics (SGLD) is a powerful algorithm for optimizing a non-convex objective, where a controlled and properly scaled Gaussian noise is added to the stochastic gradients to steer the iterates towards a global minimum. SGLD is based on the overdamped Langevin diffusion which is reversible in time. By adding an anti-symmetric matrix to the drift term of the overdamped Langevin diffusion, one gets a non-reversible diffusion that converges to the same stationary distribution with a faster convergence rate. In this paper, we study the non-reversible stochastic gradient Langevin dynamics (NSGLD) which is based on discretization of the non-reversible Langevin diffusion. We provide finite-time performance bounds for the global convergence of NSGLD for solving stochastic non-convex optimization problems. Our results lead to non-asymptotic guarantees for both population and empirical risk minimization problems. Numerical experiments for a simple polynomial function optimization, Bayesian independent component analysis and neural network models show that NSGLD can outperform SGLD with proper choices of the anti-symmetric matrix.

1 Introduction

Considering the stochastic non-convex optimization problem:

\[
\min_{x \in \mathbb{R}^d} F(x) := \mathbb{E}_{Z \sim \mathcal{D}} [f(x, Z)], \tag{1.1}
\]

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where $f : \mathbb{R}^d \times Z \to \mathbb{R}$ is a continuous and non-convex function mapping $x \to f(x, Z)$, $Z$ is a random variable drawn from an unknown probability distribution $D$ supported on some unknown collection $Z$. Assuming we can access to an independent identical distributed (i.i.d.) samples $\hat{Z} = (Z_1, Z_2, \ldots, Z_n)$ from $D$, the goal is to compute an approximate minimizer $\hat{x}$ (possibly with a randomized algorithm) of the population risk, i.e. we want to compute $\hat{x}$ such that $\mathbb{E} F(\hat{x}) - F^* \leq \hat{\epsilon}$ for a given target accuracy $\hat{\epsilon} > 0$, where $F^* = \min_{x \in \mathbb{R}^d} F(x)$ and the expectation is taken over the random vector $\hat{Z}$ and the additional randomness for generating $\hat{x}$. This formulation arises frequently in several contexts including machine learning. Because the population distribution $D$ is typically unknown in practice, a common popular approach is to consider the empirical risk minimization problem

$$\min_{x \in \mathbb{R}^d} F_{\hat{z}}(x) := \frac{1}{n} \sum_{i=1}^{n} f(x, z_i),$$

(1.2)

based on the dataset $z = (z_1, z_2, \ldots, z_n) \in \mathcal{Z}^n$ as a proxy to the problem (1.1) and minimize the empirical risk

$$\mathbb{E} F_{\hat{z}}(x) - \min_{x \in \mathbb{R}^d} F_{\hat{z}}(x),$$

(1.3)

instead, where the expectation is taken with respect to any other randomness encountered during the algorithm to generate $x$. Many algorithms have been proposed to solve the problem (1.1) and its finite-sum version (1.3). Among these, gradient descent, stochastic gradient and their variance-reduced or momentum-based variants come with guarantees for finding a local minimizer or a stationary point for non-convex problems. In some applications, convergence to a local minimum can be satisfactory. However, in general, methods with global convergence guarantees are also desirable and preferable in many settings.

Stochastic gradient algorithms based on Langevin Monte Carlo are popular variants of stochastic gradient which admit asymptotic global convergence guarantees where a properly scaled Gaussian noise is added to the gradient estimate. Recently, Raginsky et al. [RRT17] provided a non-asymptotic analysis of Stochastic Gradient Langevin Dynamics (SGLD, see [WT11]) to find the global minimizers for both population risk and empirical risk minimization problems. The SGLD can be viewed as the analogue of stochastic gradient in the Markov Chain Monte Carlo (MCMC) literature. The SGLD iterates $\{X_k\}$ takes the following update form:

$$X_{k+1} = X_k - \eta g_k + \sqrt{2\eta\beta^{-1}}\xi_k,$$

(1.4)

where $\eta > 0$ is the step size, $\beta > 0$ is the inverse temperature, $g_k$ is a conditionally unbiased estimator of the gradient $\nabla F_{\hat{z}}$ and $\xi_k$ is a standard Gaussian random vector. The analysis of SGLD in [RRT17] is built on the continuous-time diffusion process known as the overdamped Langevin stochastic differential equation (SDE):

$$dX(t) = -\nabla F_{\hat{z}}(X(t)) \, dt + \sqrt{2\beta^{-1}} dB(t), \quad t \geq 0,$$

(1.5)

where $B(t)$ is a standard $d$-dimensional Brownian motion. The overdamped Langevin diffusion (1.5) is reversible$^1$ and admits a unique stationary (or equilibrium) distribution $\pi_{\hat{Z}}(dx) \propto e^{-\beta F_{\hat{z}}(x)} dx$

$^1$A diffusion process $X(t)$ is reversible if $X(0)$ is distributed according to the stationary measure $\pi$, then $(X(t))_{0 \leq t \leq T}$ and $(X(T - t))_{0 \leq t \leq T}$ have the same law for each $T$. 

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under some assumptions on $F$. It is well documented that (see e.g. [HHMS05]) considering non-reversible variants of (1.5) can help accelerate convergence of the diffusion to the equilibrium. Specifically, consider the following non-reversible diffusion:

$$dX(t) = -A_J(\nabla F_z(X(t))) \, dt + \sqrt{2\beta^{-1}} dB(t), \quad A_J = I + J,$$

(1.6)

where $J \neq 0$ is a $d \times d$ anti-symmetric matrix, i.e. $J^T = -J$, and $I$ is a $d \times d$ identity matrix. The stationary distribution $\pi_z$ of this non-reversible Langevin diffusion (1.6) is the same as the stationary distribution generated by the overdamped Langevin SDE (1.5). In addition, [HHMS05] showed by comparing the spectral gaps that adding $J \neq 0$, the convergence to the stationary distribution of (1.6) is at least as fast as the overdamped Langevin diffusion ($J = 0$), and is strictly faster except for some rare situations.

In this paper, we study a non-reversible stochastic gradient Langevin dynamics (NSGLD) algorithm and use it to solve the non-convex population and empirical risk minimization problems. The NSGLD algorithm is based on the Euler-discretization of (1.6) with a stochastic gradient and it has the update form:

$$X_{k+1} = X_k - \eta A_J g(X_k, U_{z,k}) + \sqrt{2\eta\beta^{-1}} \xi_k,$$

(1.7)

where $\{U_{z,k}\}_{k=0}^\infty$ is a sequence of i.i.d. random elements such that $g$ is a conditionally unbiased estimator for the gradient of $F_z$ and satisfies $E[g(x, U_{z,k})] = \nabla F_z(x)$ for any $x \in \mathbb{R}^d$. When $J = 0$, the NSGLD iterates in (1.7) reduces to the SGLD iterates in (1.4). Although asymptotic convergence guarantees for non-reversible Langevin diffusions (1.6) exists (see e.g. [HHMS93, HHMS05]), there is a lack of finite-time explicit performance bounds for solving stochastic non-convex optimization problems with NSGLD in the literature. In this paper, we establish the global convergence of NSGLD and provide finite-time guarantees of NSGLD to find approximate minimizers of both empirical and population risks. Numerical experiments are conducted to illustrate our results and showed that NSGLD can outperform SGLD in applications if the antisymmetric matrix is well chosen.

1.1 Contributions

Our contributions can be summarized as follows:

- Under Assumptions 1-5 for the component functions $f(x, z)$ and the gradient noises, we show that NSGLD converges to an $\varepsilon$-approximate global minimizer of the empirical risk minimization problem after $\text{poly} \left( \frac{1}{\lambda_{s,J}}, \beta, d, \frac{1}{\varepsilon}, \|A_J\| \right)$ iterations in expectation, where $\lambda_{s,J}$ is the uniform spectral gap of the non-reversible Langevin SDE (1.6) governing the speed of convergence of it to its stationary distribution. See Corollary 2. To our knowledge, this is the first work that provides non-asymptotic performance guarantees of NSGLD in the context of non-convex empirical risk minimization.

- For controlling the population risk during NSGLD iterations, in addition to the empirical risk, one has to control the generalization error $F(X_k) - F_z(X_k)$. By exploiting the fact that the stationary distribution for the non-reversible diffusion (1.6) is the same as the reversible SDE (1.5), we show in Corollary 3 that the generalization error is no worse than that of the available bounds for SGLD given in [RRT17].
On the technical side, in order to establish these results, we adapt the proof techniques of [RRT17] developed for SGLD to NSGLD and combine it with the analysis of [HHMS05] which quantifies the convergence rate of the non-reversible Langevin SDE to its equilibrium. We overcome several technical challenges and the key steps of our proofs are as follows. First, we show in Theorem 1 the convergence of $\mathbb{E}_{F_\mathbf{z}}(X(t))$ to $\mathbb{E}_{X \sim \pi_\mathbf{z}} F_\mathbf{z}(X)$ for the non-reversible Langevin SDE in (1.6) when $t$ is large. We build on [HHMS05] which established the convergence of $X(t)$ to equilibrium in $L^2(\pi_\mathbf{z})$ and in variational norm (see Section 2.2), not the 2-Wasserstein distance in [RRT17]. However, the results in [HHMS05] do not directly imply the convergence in the expected function value. We overcome this challenge by establishing a novel uniform $L^4$ bound of $X(t)$, apply the continuous-time convergence results from [HHMS05] on a compact set, and provide additional estimates outside the compact set. Second, we show that NSGLD iterates track the non-reversible Langevin SDE (1.6) closely with small step sizes. We use the approach in [RRT17] via relative entropy estimates, but our analysis requires to show the uniform $L^2$ bound and exponential integrability of $X(t)$ by using a different Lyapunov function from [RRT17]. In addition, our analysis on this discretization error improves the one in [RRT17] for $J = 0$, based on a tighter estimate on the exponential integrability.

We complement our theoretical results with the empirical evaluations of the performance of NSGLD on a variety of optimization tasks such as optimizing a simple double well function, Bayesian Independent Component Analysis and Deep learning problems. Our experiments suggest that NSGLD can outperform SGLD in applications with proper choices of anti-symmetric matrices $J$.

1.2 Related Literature

Langevin dynamics has been studied under simulated annealing algorithms in the optimization, physics and statistics literature and its asymptotic convergence guarantees are well known (see e.g. [Gid85, Haj85, GM91, KGV83, BT93, BLNR15, BM99]). However, finite-time performance guarantees for Langevin dynamics have not been studied until more recently. In a seminal work, [RRT17] obtained the first finite-time global convergence performance guarantees for stochastic gradient Langevin dynamics (SGLD). By directly analyzing the discrete-time SGLD iterates, [XCZG18] improved upon the complexity results from [RRT17] in the context of non-convex empirical risk minimizations. See also [ZLC17, TLR18] for related results on convergence of SGLD to local minima. A number of papers studied the non-reversible diffusion $X(t)$ in (1.6) with a quadratic objective $F_\mathbf{z}$, in which case $X(t)$ in (1.6) becomes a Gaussian process. Using the rate of convergence of the covariance of $X(t)$ as the criterion, [HHMS93] showed that $J = 0$ is the worst choice, and improvement is possible if and only if the eigenvalues of the matrix associated with the linear drift term are not identical. [LNP13] proved the existence of the optimal antisymmetric matrix $J$ such that the rate of convergence to equilibrium is maximized, and provided an easily implementable algorithm for constructing them. [WHC14] proposed two approaches to design $J$ to obtain the optimal convergence rate of Gaussian diffusion and they also compared their algorithms with the one in [LNP13]. [GM16] studied optimal linear drift for the speed of convergence in the hypoelliptic case. However, the optimal choice of $J$ is still open when the objective is non-quadratic.

Another line of related research focused on sampling and Monte Carlo methods based on the non-
reversible Langevin diffusion (1.6). As have been observed in the literature [RBS16], non-reversible Langevin sampler can outperform their reversible counterparts in terms of rate of convergence to equilibrium, asymptotic variance and large deviation functionals. For instance, [DLP16, RBS15] showed that the asymptotic variance can be reduced by using the non-reversible Langevin sampler. [DPZ17] constructed efficient sampling algorithms based on the Lie-Trotter decomposition of a nonreversible diffusion process into reversible and nonreversible components. They showed that samplers based on this scheme can significantly outperform standard MCMC methods, at the cost of introducing some controlled bias. [RBS14] used the Donsker-Varadhan large deviations theory to analyze the speed of convergence of non-reversible Langevin diffusion to the invariant measure, and showed acceleration of the convergence speed due to a larger large deviations rate function. We also refer the readers to [MCF15] which presented a general recipe for devising stochastic gradient MCMC (Markov Chain Monte Carlo) samplers based on continuous diffusions including the non-reversible SDE in (1.6). Our work is different from these studies in that we focus on optimization and analyze the expected suboptimality of NSGLD iterates, while typically one studies the convergence to equilibrium for ergodic averages in sampling.

2 Preliminaries

2.1 Assumptions

We first state the assumptions used in this paper below. Note that we do not assume $f$ to be convex or strongly convex in any region.

**Assumption 1.** The function $f$ is continuously differentiable and taking non-negative values, then there exists some constant $A, B \geq 0$, such that

$$|f(0, z)| \leq A, \quad \|\nabla f(0, z)\| \leq B, \quad \text{with any } z \in \mathcal{Z}.$$ 

**Assumption 2.** For each $z \in \mathcal{Z}$, the function $f(\cdot, z)$ is $M$-smooth: for some $M > 0$,

$$\|\nabla f(w, z) - \nabla f(v, z)\| \leq M \|w - v\|, \quad \text{for any } w, v \in \mathbb{R}^d.$$ 

**Assumption 3.** For any $z \in \mathcal{Z}$, $f(\cdot, z)$ is $(m, b)$-dissipative, that is

$$\langle x, \nabla f(x, z) \rangle \geq m\|x\|^2 - b, \quad \text{for any } x \in \mathbb{R}^d.$$ 

**Assumption 4.** There exists $\delta \in [0, 1)$, for any data set $z$, such that

$$\mathbb{E}\|g(x, U_z) - \nabla F_z(x)\|^2 \leq 2\delta \left(M^2\|x\|^2 + B^2\right), \quad \text{for any } x \in \mathbb{R}^d.$$ 

**Assumption 5.** The initial state $X(0)$ of the NSGLD algorithm satisfies $\|X(0)\| \leq R := \sqrt{b/m}$ with probability one, i.e. $X(0) \in B_R(0)$, the Euclidean ball centered at 0 with radius $R$.

The first assumption of non-negativity of $f$ can be assumed without loss of generality by subtracting a constant and shifting the coordinate system as long as $f$ is bounded below. Also the non-negative $f$ implies the non-negativity of $F_x$ by (1.1) and (1.2). The second assumption of
Lipschitz gradients is in general unavoidable for discretized Langevin algorithms to obtain convergence (see e.g. [MSH02]), and the third assumption is known as the dissipativity condition (see e.g. [Hal88]) and is standard in the literature to ensure the convergence of Langevin diffusions to the stationary distribution (see e.g. [RRT17, MSH02]). The fourth assumption is regarding the amount of noise present in the gradient estimates and allows not only constant variance noise but allows the noise variance to grow with the norm of the iterates (which is the typical situation in mini-batch methods in stochastic gradient methods). Finally, it is not hard to see from the dissipativity condition that any stationary point \( y \) of \( F_x \) satisfies \( |y| \leq R \), which naturally leads to the fifth assumption on the starting point of the NSGLD algorithm.

### 2.2 Convergence Rate to the Equilibrium of the Non-Reversible Langevin SDE

We discuss the convergence rate to the equilibrium of the non-reversible Langevin SDE in (1.6) based on Hwang et al. [HHMS05]. Write \( \pi_z \) for its stationary distribution.

Hwang et al. [HHMS05] considered the spectral gap in \( L^2(\pi_z) \) to analyze the rate of convergence of the non-reversible Langevin SDE in (1.6) to the equilibrium. Specifically, let \( \mathcal{L}_{z,J} \) be the infinitesimal generator of the SDE in (1.6). Define

\[
\lambda_{z,J} := \sup \{ \text{the real part of } \phi : \phi \text{ is in the spectrum of } \mathcal{L}_{z,J}, \phi \neq 0 \}.
\]  

(2.1)

In general, the eigenvalues of the generator \( \mathcal{L}_{z,J} \) are complex numbers, there is a simple eigenvalue 0 and all the other eigenvalues have negative real parts. The quantity \( \lambda_{z,J} \) (or sometimes \( |\lambda_{z,J}| \)) is referred to as the spectral gap of the generator \( \mathcal{L}_{z,J} \), since \( |\lambda_{z,J}| \) is the minimal gap between the zero eigenvalue and the real parts of the rest of the non-zero eigenvalues.

The existence of a spectral gap, i.e. \( \lambda_{z,J} < 0 \), implies that for any \( g \in L^2(\pi_z) \),

\[
\int_{\mathbb{R}^d} \left( \mathbb{E}_y g(X(t)) - \int_{\mathbb{R}^d} g(y) \pi_z(dy) \right)^2 \pi_z(dy) dy \\
\leq C_{z,J} \cdot \int_{\mathbb{R}^d} \left( g(y) - \int_{\mathbb{R}^d} g(y) \pi_z(dy) \right)^2 \pi_z(dy) dy \cdot e^{2\lambda_{z,J}t},
\]  

(2.2)

where \( C_{z,J} \) is a constant that may depend on \( F_x \), \( J \) and \( \beta \). That is, the non-reversible Langevin SDE in (1.6) convergences to equilibrium exponentially fast with rate \( \lambda_{z,J} \) in the following sense:

\[
\| T(t) g - \pi_z(g) \|_{L^2(\pi_z)} \leq \sqrt{C_{z,J}} \cdot \| g - \pi_z(g) \|_{L^2(\pi_z)} \cdot e^{\lambda_{z,J}t},
\]

where \( T(t) = e^{t\mathcal{L}_{x,J}} \), \( \pi_z(g) \) means the integration of \( g \) with respect to \( \pi_z \), and \( \| \cdot \|_{L^2(\pi_z)} \) denote the norm in \( L^2(\pi_z) \). Note when \( J = 0 \), the constant \( C_{z,J} \equiv 1 \). See, e.g., [RBS16, Section 3.1].

Using the spectral gap as one comparison criteria, Hwang et al. [HHMS05, Section 2] showed that

- \( \lambda_{z,J} \leq \lambda_{z,J=0} < 0 \);
- The equality \( \lambda_{z,J} = \lambda_{z,J=0} \) holds in some rare situations: if \( \lambda_{z,J=0} \) is in the discrete spectrum of \( \mathcal{L}_{z,J=0} \), then \( \lambda_{z,J} = \lambda_{z,J=0} \) if and only if \( \mathcal{L}_{z,J} - \mathcal{L}_{z,J=0} \) or \( \mathcal{L}_{z,J} - \mathcal{L}_{z,J=0} \) leaves a nonzero subspace of the eigenspace corresponding to \( \lambda_{z,J=0} \) to be invariant.
In other words, generically the non-reversible Langevin SDE in (1.6) converges to the equilibrium faster than the reversible SDE in (1.5). This is a continuous time result.

Write \( p_{z,J}(t, x, y) \) for the transition probability of the SDE in (1.6) from state \( x \) to state \( y \) in \( t \) units of time. The inequality (2.2) also implies the exponential convergence of \( p_{z,J}(t, x, y) \) to \( \pi_z(dy) \) in variational norm, where the variational norm of two probability measures is the supremum of the difference between two probabilities over all events. Specifically, there exists a locally bounded function \( g_{z,J}(x) \) that may depend on \( z \) and \( J \), such that

\[
\int_{\mathbb{R}^d} |p_{z,J}(t, x, y) - \pi_z(y)| \, dy \leq g_{z,J}(x) e^{\rho_{z,J} t}.
\]

(2.3)

See [HHMS05, Theorem 4] and its proof for details.

To facilitate the presentation, we also define the uniform spectral gap by

\[
\lambda_{\ast,J} := \inf_{z \in \mathbb{Z}^n} |\lambda_{z,J}|.
\]

(2.4)

This quantity will be used in the study of performance bound for population risk minimizations. Note when \( J = 0 \), the diffusion process (1.6) reduces to the reversible Langevin diffusion (1.5), and \( \lambda_{\ast,J=0} \) becomes the uniform spectral gap \( \lambda_{\ast} \) defined in [RRT17] in the study of stochastic gradient langevin dynamics. In addition, since \( \lambda_{z,J} \leq \lambda_{z,J=0} < 0 \), we have

\[
\lambda_{\ast,J} \geq \lambda_{\ast,J=0} > 0.
\]

(2.5)

3 Main Results

3.1 Convergence to Equilibrium in Expectations

We now state our first set of results. The first result translates the convergence of the non-reversible Langevin diffusion in (1.6) in spectral gaps to equilibrium to the convergence of the expectation of the empirical risk \( F_z \). Conditional on the sample \( z \), we use \( \nu_{z,t} \) to denote the probability law of \( X(t) \) in (1.6) at time \( t \). Recall that \( B_R(0) \) denotes the Euclidean ball centered at 0 with radius \( R = \sqrt{b/m} \), and \( \lambda_{z,J} \) is defined in (2.1).

**Theorem 1.** Considering the non-reversible Langevin SDE in (1.6). If Assumptions 1 - 5 hold, then for any \( \beta \geq 3/m \) and \( \varepsilon > 0 \),

\[
|\mathbb{E}_{X \sim \nu_{z,k\eta}} F_z(X) - \mathbb{E}_{X \sim \pi_z} F_z(X)| \leq \mathcal{I}_0(z, J, \varepsilon),
\]

(3.1)

where

\[
\mathcal{I}_0(z, J, \varepsilon) := \left[ \left( \frac{M + B}{2} + \frac{B}{2} + A \right) \hat{C}_{z,J} + (M + B) c \right] \cdot \varepsilon,
\]

(3.2)

for some constant \( c \) and constant \( \hat{C}_{z,J} \) depending on data set \( z \in \mathbb{Z}^n \) and a \( d \times d \) anti-symmetric matrix \( J \), provided that

\[
k\eta \geq \max \left\{ \frac{2}{|\lambda_{z,J}|} \log \left( \frac{1}{\varepsilon} \right), 1 \right\}.
\]

(3.3)
The constant $D_c$ is defined in Lemma 4 and the constant $\hat{C}_{z,J}$ is defined in (A.22). We next consider the iterates $X_k$ of the NSGLD algorithm in (1.7), and we denote the probability law of $X_k$ by $\mu_{z,k}$ conditional on the sample $z$. Since the NSGLD algorithm is based on the Euler discretization of the non-reversible Langevin SDE in (1.6), we can control the discretization error with stochastic gradients and use Theorem 1 to obtain the following result.

**Corollary 1.** Under the setting of Theorem 1 where the Assumptions 1 - 5 hold, let $\beta \geq 3/m$, for any given $\varepsilon > 0$, the performance bound of NSGLD algorithm admits

\[
\left| \mathbb{E}_{X \sim \mu_{z,k}} F_z(X) - \mathbb{E}_{X \sim \pi_z} F_z(X) \right| \leq I_0(z, J, \varepsilon) + I_1(z, J, \varepsilon),
\]

where $I_0(z, J, \varepsilon)$ is defined in (3.2) and

\[
I_1(z, J, \varepsilon) := \left( M \sqrt{C_d} + B \right) \left( \hat{C}_0 \frac{\varepsilon}{\sqrt{|\lambda_{z,J}=0|}} + \hat{C}_1 \delta^{1/4} \frac{2 \log(1/\varepsilon)}{|\lambda_{z,J}|} \right) \left( \sqrt{2 \log \left( \frac{2 \log(1/\varepsilon)}{|\lambda_{z,J}|} \right)} \right),
\]

for some constants $C_d$, $\hat{C}_0$, $\hat{C}_1$ and $0 \leq \delta < 1$ is the gradient noise level satisfying Assumption 4, provided that the step size $\eta$ satisfies

\[
\eta \leq \min \left\{ 1, \frac{m^2}{(m^2 + 8M^2)M \| A_J \|^2}, \frac{\varepsilon^4}{4 \left( \log(1/\varepsilon) \right)^2 \| A_J \|^4 |\lambda_{z,J}=0|^2} \right\},
\]

and

\[
k\eta = \frac{2}{|\lambda_{z,J}|} \log \left( \frac{1}{\varepsilon} \right) \geq e.
\]

The expressions of constants $C_d$, $\hat{C}_0$ and $\hat{C}_1$ can be found in Lemma 1 and Lemma 3 respectively.

In the next subsections, we will show that this result combined with some basic properties of the equilibrium distribution $\pi_z$ leads to a number of results which provide performance guarantees for both the empirical risk and population risk minimization.

### 3.2 Performance Bound for the Empirical Risk Minimization

Consider using the NSGLD algorithm in (1.7) to solve the empirical risk minimization problem given in (1.2). The performance of the algorithm can be measured by the expected sub-optimality: $\mathbb{E}_{X \sim \mu_{z,k}} F_z(X) - \min_{x \in \mathbb{R}^d} F_z(x)$. To obtain performance guarantees, in light of Corollary 1, one has to control the quantity

\[
\mathbb{E}_{X \sim \pi_z} F_z(X) - \min_{x \in \mathbb{R}^d} F_z(x),
\]

which is a measure of how much the equilibrium distribution $\pi_z$ concentrates around a global minimizer of the empirical risk. For finite $\beta$, [RRT17, Proposition 11] derives an explicit bound of the form

\[
\mathbb{E}_{X \sim \pi_z} F_z(X) - \min_{x \in \mathbb{R}^d} F_z(x) \leq I_2 := \frac{d}{2\beta} \log \left( \frac{eM}{m} \left( \frac{b\beta}{d} + 1 \right) \right).
\]
Hence we can obtain the following performance bound for the empirical risk minimization. The proof is omitted.

**Corollary 2 (Empirical risk minimization).** Consider the iterates \( \{X_k\} \) of the NSGLD algorithm in (1.7). Under the setting of Corollary 1, by taking the constant \( \beta \geq 3/m \), for any given \( \varepsilon > 0 \), we have

\[
\mathbb{E} F_\mathbf{z}(X_k) - \min_{x \in \mathbb{R}^d} F_\mathbf{z}(x) = \mathbb{E} F_\mathbf{z}(X_k) - \mathbb{E}_{X \sim \pi^*_N} F_\mathbf{z}(X) + \mathbb{E}_{X \sim \pi^*_N} F_\mathbf{z}(X) - \min_{x \in \mathbb{R}^d} F_\mathbf{z}(x) \\
\leq I_0(\mathbf{z}, J, \varepsilon) + I_1(J, \varepsilon) + I_2, \tag{3.9}
\]

where \( I_0(\mathbf{z}, J, \varepsilon) \) is defined in (3.2), \( I_2 \) is taken in (3.8), and \( I_1(J, \varepsilon) \) is defined by

\[
I_1(J, \varepsilon) := (M \sqrt{C_d} + B) \left( \tilde{C}_0 \frac{\varepsilon}{\sqrt{\lambda_{*, J = 0}}} + \tilde{C}_1 \delta^{1/4} \sqrt{\frac{2 \log(1/\varepsilon)}{\lambda_{*, J}}} \right) \sqrt{\log \left( \frac{2 \log(1/\varepsilon)}{|\lambda_{*, J}|} \right)}, \tag{3.10}
\]

with \( \lambda_{*, J} = \inf_{\mathbf{z} \in \mathbb{Z}^n} |\lambda_{\mathbf{z}, J}| \) given in (2.4) and \( \delta \) is gradient noise level under the setting in Assumption 4, and \( C_0, C_1 \) are two constants defined in Lemma 3, provided that

\[
k \eta = \frac{2}{\lambda_{*, J}} \log \left( \frac{1}{\varepsilon} \right) \geq e,
\]

and

\[
\eta \leq \min \left\{ 1, \frac{m^2}{(m^2 + 8M^2)M\|A_J\|^2}, \frac{\varepsilon^4}{4(\log(1/\varepsilon))^2\|A_J\|^4 \lambda_{*, J = 0}^2} \right\}.
\]

### 3.3 Performance Bound for the Population Risk Minimization

To obtain the performance bound for the population risk minimization in (1.1), we control the expected population risk of \( X_k \) in (1.7): \( \mathbb{E} F(X_k) - F^* \). To this end, in addition to the empirical risk, one has to account for the differences between the finite sample size problem (1.2) and the original problem (1.1). In particular we have the following corollary.

**Corollary 3 (Population risk minimization).** Consider the iterates \( \{X_k\} \) of the NSGLD algorithm in (1.7). Under the setting in Corollary 1, for some constant \( \beta \geq 3/m \) and \( \varepsilon > 0 \), the upper bound for the expected population risk of \( X_k \) is given by

\[
\mathbb{E} F(X_k) - F^* \leq \overline{I}_0(J, \varepsilon) + \overline{I}_1(J, \varepsilon) + \overline{I}_2 + \overline{I}_3(n), \tag{3.11}
\]

by taking

\[
k \eta = \frac{2}{\lambda_{*, J}} \log \left( \frac{1}{\varepsilon} \right) \geq e,
\]

with step size

\[
\eta \leq \min \left\{ 1, \frac{m^2}{(m^2 + 8M^2)M\|A_J\|^2}, \frac{\varepsilon^4}{4(\log(1/\varepsilon))^2\|A_J\|^4 \lambda_{*, J = 0}^2} \right\},
\]

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and
\[ I_0(J, \varepsilon) := \left[ C_J \left( \frac{M + B}{2} + \frac{B}{2} + A \right) + (M + B)D_c \right] \cdot \varepsilon, \tag{3.12} \]
where \( C_J \) is some constant that depends on \( J \) and \( I_1(J, \varepsilon) \) and \( I_2 \) are given in Corollary 2, and \( I_3(n) \) is provided by Proposition 12, \([RRT17]\),
\[ I_3(n) := \frac{4 \left( \frac{M^2}{m} (b + d/\beta) + B^2 \right) \beta c_{LS}}{n}, \]
where \( \lambda_{*,J=0} = \lambda_* \) and \( c_{LS} \) is a constant satisfying
\[ c_{LS} \leq \frac{2m^2 + 8M^2}{m^2 M \beta} + \frac{1}{\lambda_*} \left( \frac{6M(d + \beta)}{m} + 2 \right). \]

3.4 Discussion

In this section we briefly discuss the comparison of the performance of the NSGLD algorithm with that of the SGLD algorithm (corresponding to \( J = 0 \)) in the context of the empirical risk minimization problem. Note that while adding a nonzero antisymmetric matrix \( J \) increases the rate of convergence of diffusions to the equilibrium (i.e. \( \lambda_{*,J} > \lambda_{*,J=0} \)), it will also give rise to a large discretization error and amplify the gradient noise if one runs NSGLD and SGLD with the same stepsize. Building on our theoretical results in previous sections, we give some further analysis below to show that NSGLD can outperform SGLD when the matrix \( J \) is properly chosen and the function to optimize satisfy certain spectral properties.

As in as in \([RRT17]\) and \([XCG18]\), we define an almost empirical risk minimizer as a point which is within the ball of the global minimizer with radius \( \tilde{O}(d \log(1 + \beta)/\beta) \) and we discuss the performance of NSGLD in terms of gradient complexity, i.e., the total number of stochastic gradients required to achieve an almost empirical risk minimizer in the mini-batch setting. We use the notation \( \tilde{O}(\cdot), \Omega(\cdot) \) gives explicit dependence on the parameters \( \beta, d, \lambda_{*,J}, \delta \), but hides factors that depend (at worst) polynomially on other parameters in Section 2.1. Our result in Corollary 2 together with Section J in the appendix suggests that the performance bound of NSGLD is given by (ignoring the \( \log \log(1/\varepsilon) \) term):
\[ \tilde{O} \left( \frac{\sqrt{\beta}(d + \beta)}{\lambda_{*,J=0}} \cdot \varepsilon + \frac{d \log(1 + \beta)}{\beta} \right), \tag{3.13} \]
after \( \mathcal{K}_J \) iterations with
\[ \mathcal{K}_J = \tilde{\Omega} \left( \frac{\sqrt{\beta}(d + \beta)}{\lambda_{*,J=0} \varepsilon^4} \log^3 \left( \frac{1}{\varepsilon} \right) \cdot \frac{||A_J||^4 \lambda_{*,J=0}^2}{\lambda_{*,J}^2} \right) \quad \text{and} \quad \eta \leq \frac{\varepsilon^4}{4 (\log(1/\varepsilon))^2} \frac{1}{||A_J||^2 \lambda_{*,J=0}^2}, \tag{3.14} \]
and the gradient noise \( \delta \) is set to be the same as the step size. Note here \( A_J = I + J \). For any anti-symmetric matrix \( J \), we have \( ||A_J||^2 = 1 + ||J||^2 \) (see Lemma 10). It is generally difficult to spell out the dependency of \( \tilde{C}_{*,J} \) on the matrix \( J \) for nonconvex empirical risk minimization.
problems. On the other hand, Raginsky et al. [RRT17] showed that $\hat{C}_{z,t=0} = \tilde{O}(1/\sqrt{\lambda_{s,J=0}})$, where $1/\lambda_{s,J=0} = e^{\tilde{O}(\beta+4)}$; see also [BGK05]. Hence in the following discussion we will consider reasonable matrix $J$ with norm under control and assume the first two terms in (3.13) are both of the order $\tilde{O}(1/\sqrt{\lambda_{s,J=0}})$.

In the mini-batch setting, at each iteration of NSGLD, one samples uniformly with replacement a random i.i.d. mini batch of size $\ell$. Following [RRT17] and [XCZG18], we can infer from (3.13) and (3.14) that the gradient complexity of the NSGLD algorithm with anti-symmetric matrix $J$ is given by

$$\hat{K}_J := K_J \cdot \ell = K_J/\eta = \tilde{O} \left( \frac{\sqrt{\beta}(\beta + d)}{\lambda_{s,J} \varepsilon^8} \log^5 \left( \frac{1}{\varepsilon} \right) \cdot \frac{\|A_J\|\lambda_{s,J=0}^4}{\lambda_{s,J}^4} \right)$$

Hence to compare $\hat{K}_J$ with $\hat{K}_{J=0}$, we compare $\frac{\|A_J\|\lambda_{s,J=0}^4}{\lambda_{s,J}^4}$ with $1/\lambda_{s,J=0}$ (when $J = 0$). Generally one can not compute the spectral gap $\lambda_{s,J}$ explicitly. In order to do the comparison, we consider the asymptotic setting with $\beta \to \infty$ and rely on the literature on metastability in diffusion processes to get explicit formulas of $\lambda_{s,J}$. We discuss this in the next section.

### 3.4.1 Formulas of $\lambda_{s,J=0}$ and $\lambda_{s,J}$

We summarize formulas of $\lambda_{s,J=0}$ and $\lambda_{s,J}$ in this section. We consider $F$ to be a Morse function admitting finite number of local minima, where the Hessian of $F$ are non-degenerate at all local minima and saddle points.

For the reversible SDE in (1.5), [BGK05] studied precise asymptotics for small eigenvalues of its generator $L_0 = -\nabla F \cdot \nabla + \beta^{-1} \Delta$ as $\beta \to \infty$. Assuming all the valleys of $F$ have different depths, there is one saddle point connecting two local valleys or minima, and the Hessian at the saddle points has one negative eigenvalue with other eigenvalues positive, [BGK05, Theorem 1.2] showed that the spectral gap is given by

$$\lambda_{s,J=0} = \frac{\mu^*_\sigma}{2\pi} \sqrt{\frac{\det HessF(a)}{|\det HessF(\sigma)|}} e^{-\beta |F(\sigma) - F(a)|} \cdot \left[ 1 + O \left( \beta^{-1/2} \log(1/\beta) \right) \right] .$$

In this formula, $a$ is a local minimum of $F$ with second deepest valley ($a$ is just the local, not the global, minimum of $F$ if $F$ admits two local minima), $\sigma$ is the saddle point connecting $a$ and the global minimum of $F$, and $-\mu^*_\sigma$ is the unique negative eigenvalue of the Hessian of $F$ at the saddle point $\sigma$. For precise definitions of these quantities, see [BGK05].

For the non-reversible Langevin SDE in (1.6), Peutrec and Michel [PM19] studied the spectral asymptotics for the associated generator $L_J = -A_J \nabla F \cdot \nabla + \beta^{-1} \Delta$ as $\beta \to \infty$. Under similar assumptions on $F$, [PM19, Theorem 1.9] showed that as $\beta \to \infty$, the associated spectral gap is given by

$$\lambda_{s,J} = \frac{\mu^*_\sigma}{2\pi} \sqrt{\frac{\det HessF(a)}{|\det HessF(\sigma)|}} e^{-\beta |F(\sigma) - F(a)|} \cdot \left[ 1 + O \left( \beta^{-1/2} \right) \right] ,$$

where $-\mu^*_\sigma$ is the unique negative eigenvalue of $A_J \cdot \nabla$, where $\nabla \sigma$ is the Hessian of $F$ at the saddle point $\sigma$, i.e. $\nabla \sigma = HessF(\sigma)$. 

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3.4.2 Comparison of gradient complexity: \( \hat{K}_{J} \) vs \( \hat{K}_{J=0} \)

We are now ready to compare the gradient complexity \( \hat{K}_J \) of the NSGLD algorithm with \( \hat{K}_{J=0} \) of the SGLD algorithm. It is clear from (3.15) that for a nonzero antisymmetric matrix \( J \), we have 

\[
\hat{K}_J < \hat{K}_{J=0} \text{ if } \|A_J\|_{\lambda^*,J=0}^4 \frac{\lambda^5_{*,J=0}}{\lambda^5_{*,J} < 1}. 
\]

From (3.16) and (3.17) and using \( \|A_J\|^2 = 1 + \|J\|^2 \), we obtain

\[
\frac{\|A_J\|^4}{\lambda^5_{*,J}} = (1 + \|J\|^2)^4 \left( \frac{\mu^*(\sigma)}{\mu_J^*(\sigma)} \right)^5. 
\]

We want to study when the quantity in (3.18) is smaller than one so that NSGLD can perform better than SGLD with \( J = 0 \) in terms of gradient complexity. Without loss of generality, we consider a diagonal Hessian matrix \( \mathbb{L}^\sigma \) at the saddle point where \( \mathbb{L}^\sigma = D := \text{diag}\{-1, \lambda_1, \lambda_2, \ldots, \lambda_{d-1}\} \) with \( \lambda_i > 0 \) and \( \mu^*(\sigma) = 1 \). We next compute \( \mu_J^*(\sigma) \) and \( \|J\|^2 \) for a particular class of anti-symmetric matrices \( J \), where \( -\mu_J^*(\sigma) \) is the unique negative eigenvalue of \((I + J) \cdot D\). Before we proceed, we remark that the general case can be handled similarly. The Hessian matrix \( \mathbb{L}^\sigma \) is symmetric and diagonalizable, so that \( \mathbb{L}^\sigma = Q D Q^T \) (up to permutations) for some orthogonal matrix \( Q \). The eigenvalues of \((I + QJQ^T)\mathbb{L}^\sigma = Q((I + J)D)Q^T \) are the same as the eigenvalues of \((I + J)D\). In addition, \( QJQ^T \) remains to be an antisymmetric matrix when \( J \) is anti-symmetric.

We consider the anti-symmetric matrix \( J \) has a block diagonal structure that allows explicit computations. Suppose the dimension \( d \) is an even number (the case of \( d \) is odd can be handled similarly by removing the last row and the last column of the \( J \) matrix in (3.19)). We consider an anti-symmetric matrix \( J \) in the following form:

\[
J = \begin{bmatrix}
0 & a_1 & & \\
-a_1 & 0 & a_2 & \\
& -a_2 & 0 & \\
& & \ddots & \\
& & & 0 & a_{d/2} \\
& & & -a_{d/2} & 0
\end{bmatrix} 
\]

where \( a_i \in \mathbb{R} \). It is straightforward to verify that the unique negative eigenvalue of \( A_J \cdot \mathbb{L}^\sigma = (I+J)D \) is given by

\[
\mu_0 = \frac{(\lambda_1 - 1) - \sqrt{(\lambda_1 - 1)^2 + 4(a_1^2 + 1)\lambda_1}}{2} < 0. 
\]

Hence, we have \( \mu_J^*(\sigma) = -\mu_0 \). Since \( \mu^*(\sigma) = 1 \), it follows that

\[
\frac{\mu^*(\sigma)}{\mu_J^*(\sigma)} = \frac{2}{\sqrt{(\lambda_1 - 1)^2 + 4(a_1^2 + 1)\lambda_1} - (\lambda_1 - 1)}. 
\]
Since \(\|J\|^2 = \max_{1 \leq i \leq d/2} a_i^2\), if we choose \(a_i\) such that \(a_i^2 \geq a_1^2\) for each \(i = 2, \ldots, d/2\), we infer that

\[
\frac{\|A_J\|^8_{\lambda^5, J=0}}{\lambda^5_{\lambda, J}} = (1 + \|J\|^2)^4 \cdot \left(\frac{\mu^*(\sigma)}{\mu^*_J(\sigma)}\right)^5
\]

\[
= (1 + a_1^2)^4 \cdot \left(\frac{2}{\sqrt{(\lambda_1 - 1)^2 + 4(a_1^2 + 1)\lambda_1 - (\lambda_1 - 1)}}\right)^5. \tag{3.22}
\]

This quantity (3.22) is smaller than one if and only if

\[
2 (1 + a_1^2)^{4/5} + (\lambda_1 - 1) < \sqrt{(\lambda_1 - 1)^2 + 4(a_1^2 + 1)\lambda_1}, \tag{3.23}
\]

which is equivalent to

\[
(1 + a_1^2)^{3/5} + (\lambda_1 - 1) (1 + a_1^2)^{-1/5} < \lambda_1, \tag{3.24}
\]

which is equivalent to

\[
\lambda_1 > \frac{(1 + a_1^2)^{3/5} - (1 + a_1^2)^{-1/5}}{1 - (1 + a_1^2)^{-1/5}} = \frac{(1 + a_1^2)^{4/5} - 1}{(1 + a_1^2)^{1/5} - 1} = \left(1 + (1 + a_1^2)^{2/5}\right) \cdot \left(1 + (1 + a_1^2)^{1/5}\right). \tag{3.25}
\]

Hence when \(\lambda_1 > 4\), we can choose \(a_1 > 0\) small so that \(\hat{\mathcal{K}}_J < \hat{\mathcal{K}}_{J=0}\).

## 4 Numerical Experiments

In this section we present numerical results. We conduct several experiments to assess the performance of Non-Reversible Stochastic Gradient Langevin Dynamics (NSGLD) algorithm and compare it with Stochastic Gradient Langevin Dynamics (SGLD) algorithm. We focus on three examples: a simple polynomial function optimization, Bayesian Independent Component Analysis and Neural Network models.

### 4.1 Simple Demonstration

We first demonstrate the performance of the NSGLD algorithm on a simple example, which is a two-dimensional non-convex piecewise function optimization. Through this simple example we can learn how the NSGLD algorithm works on a non-convex optimization problem, and how it may outperform the SGLD method. We take the objective function as:

\[
f(x) = \begin{cases} 
\frac{1}{4} x_1^2 + \alpha x_1 & \text{if } \|x\| \leq \frac{1}{2} \\
\frac{1}{2} (\|x\| - 1)^2 + \alpha x & \text{if } \|x\| > \frac{1}{2}
\end{cases} \quad \text{where } x \in \mathbb{R}^2, \ \alpha = (0.2, 0.2). \tag{4.1}
\]

In this example, since the function lives on \(\mathbb{R}^2\), the \(2 \times 2\) anti-symmetric matrix \(J\) must be of the following form:

\[
J = \begin{bmatrix} 0 & \tau \\ -\tau & 0 \end{bmatrix}, \quad \tau \in \mathbb{R}. \tag{4.2}
\]
For this function in (4.1), it is non-convex and has two minima. One is the local minimum \((\frac{1}{5}, \frac{1}{5})\) and function value is 0.29. The other is the global minimum \((-\frac{\sqrt{2}}{2}, -\frac{1}{5})\) and minimal value is -0.3228. The contour plot of the function is given in Figure 1(a) with two minima shown on the plot. In the experiments, the initial point of the NSGLD algorithm is assigned to \((1, 1)\) with corresponding function value 0.4858, and this starting point is near the local minimum. We tuned the SGLD method and found the optimal step size is 1. We also used the same step size in the NSGLD method. We compare the SGLD method and NSGLD method with different \(\tau\) values in (4.2). To see the expectation of the convergence speed, we use 50 samples and calculate the average over these samples. Since both SGLD and NSGLD method include the random noise \(\xi\) in the iteration, we use the same random source for both methods in each sample.

The results are shown in Figure 1(b), which shows the expected function value of SGLD and NSGLD iterates with different \(\tau\)'s. We observe that NSGLD can outperform SGLD with proper choices of \(\tau\), and one can tune \(\tau\) to achieve faster convergence in this experiment. On the other hand, we also observe that \(\tau\) cannot be too big. In Figure 1(b), when \(\tau = 1.612\) the function will not converge to the global minimum; when \(\tau\) increases further, the objective function will go to infinity.

### 4.2 Bayesian Independent Component Analysis

In the following experiments, we use the random \(d \times d\) anti-symmetric matrix \(J\).

\[
J = \begin{bmatrix}
0 & j_{1,2} & \cdots & j_{1,d} \\
-j_{1,2} & 0 & \cdots & j_{2,d} \\
\vdots & \vdots & \ddots & \vdots \\
-j_{1,d} & -j_{2,d} & \cdots & 0
\end{bmatrix}, \quad \text{where } j_{m,n} \sim \mathcal{N}\left(0, \frac{\tau^2}{d^2}\right) \text{ for } m \neq n. \quad (4.3)
\]

In the next experiment, we will compare SGLD with NSGLD for the Bayesian ICA problem, which is commonly used in machine learning field such as signal processing and face recognition. The Bayesian ICA attempts to decompose a multivariate signal into independent non-Gaussian signals. In the following we will briefly review the Bayesian ICA model. Given the data set \(\{x_i; i = 1, 2, ..., m\}\) and \(x_i \in \mathbb{R}^n\), our goal is to recover the independent sources \(s = Wx\), where
\( s \in \mathbb{R}^n \) and \( W \in \mathbb{R}^{n \times n} \). We assume that the distribution of each independent component source \( s_i \) is given by the density \( p_s \). The joint distribution of the sources \( s \) is given by:

\[
p(s) = \prod_{i=1}^{n} p_s(s_i).
\]

Then the log likelihood is given by:

\[
\ell(W) = \sum_{i=1}^{m} \left( \sum_{j=1}^{n} \log g'(w^T_j x^i) + \log \|W\| \right),
\]

where \( w_j \) is the \( j \)-th column of matrix \( W \).

The goal then becomes finding the optimal unmixing matrix \( W \) which maximizes the log likelihood.

For the Bayesian ICA problem, we used two datasets: one is the Iris plants dataset\(^1\) the other one is the Diabetes dataset\(^2\). The Iris plants dataset consists of 3 different types of irises (Setosa, Versicolour, and Virginica) petal and sepal length. The Diabetes dataset consists of 10 baseline variables, age, sex, body mass index, average blood pressure, and six blood serum measurements for each diabetes patient. The Bayesian ICA model can extract the features from the original data and help to separate data, and thus can improve subsequent tasks such as classification and regression.

In both experiments, we let the distribution \( s_i \) follow the sigmoid function, such that \( p_s(s) = g'(s) \), where \( g(s) = 1/(1 + \exp(-s)) \). To see the expectation of the convergence speed, we use 20 samples and calculate the average over these samples. Since both SGLD and NSGLD methods include the random noise \( \xi \) in the iteration, we use the same random source for both methods in each sample. In the Iris plants dataset, we tuned the SGLD method and set the decaying step size equal to \( 0.01/(1 + 0.1t) \), where \( t = 1, 2, ..., T \) is the iteration number. We set \( \tau \) in (4.3) to be 0.02 and the same stepsize in NSGLD method. The result of Iris is shown in Figure 2(a). In the Diabetes dataset, we tuned the decaying stepsize to be \( 0.1/(1 + 0.1t) \), where \( t = 1, 2, ..., T \) is the iteration number. We set \( \tau \) in (4.3) to be 7 and the same stepsize in NSGLD method. The result of Diabetes is shown in Figure 2(b). In both experiments, we can observe that the NSGLD algorithm converges faster than the SGLD method in the ICA task.

### 4.3 Neural Network Model

In the next set of experiments, we focus on applying the methods on the Neural Network model. All the experiments are based on the IMDB dataset\(^3\). The IMDB dataset contains 25,000 movies reviews, and reviews are labeled by sentiment (positive/negative). The purpose of the Neural Network model is to do the classification based on the IMDB dataset. We will test our NSGLD algorithm and compare it with stochastic gradient descent (SGD) and SGLD.

We test three Neural Network structures on this dataset. The first one is the Fully-connected Neural Network, which has one hidden layer, and the result is shown in Figure 3(a). The second one is the Long Short-Term Memory (LSTM) Neural Network, and the result is shown in Figure 3(b). The third one is the Convolutional Neural Network and Long Short-Term Memory (CNN LSTM) Neural Network, and the result is shown in Figure 3(c). In all these experiments, the step size

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1. The dataset is available [https://archive.ics.uci.edu/ml/datasets/Iris](https://archive.ics.uci.edu/ml/datasets/Iris).
2. The dataset is available [https://archive.ics.uci.edu/ml/datasets/diabetes](https://archive.ics.uci.edu/ml/datasets/diabetes).
is 0.1, the batch size is 1000, and we use the antisymmetric matrix $J$ in (4.3) with $\tau = 0.5$ for Fully-connected Neural Network, $\tau = 2$ for LSTM Network, and $\tau = 0.1$ for CNN LSTM Network. We again observe that NSGLD can outperform SGLD and SGD in different model architectures.

5 Conclusion

In our paper, we studied a non-reversible stochastic gradient Langevin dynamics (NSGLD) by adding an anti-symmetric matrix to the drift term of the Langevin dynamics. We provided finite-time performance bounds for the global convergence of NSGLD for solving stochastic non-convex optimization problems. Our results led to non-asymptotic guarantees for both population and empirical risk minimization problems. We conducted numerical experiments for several problems including a simple polynomial function optimization, Bayesian independent component analysis and neural network models, and we showed that NSGLD can outperform SGLD with proper choices of the anti-symmetric matrix.

3 The dataset is available https://datasets.imdbws.com/.
 Constants

\[
C_c = \frac{3MR^2 + 3BR + 3B + 6A + 3b \log 3}{2m} + \frac{3b(M + B)}{m^2} + \frac{6M\beta^{-1}d(M + B)}{m^3} \tag{A.1}
\]

\[
C_d = \frac{3MR^2 + 6BR + 3B + 6A + 3b \log 3}{2m} + \frac{6\delta(2bM^2 + B^2m)(M + B)}{m^4}
+ \frac{12M\beta^{-1}d(M + B)}{m^3} + \frac{3b(M + B)}{m^2} \tag{A.2}
\]

\[
D_c = \frac{9}{m^2} \left( \frac{M}{2} R^2 + BR + A \right)^2 + \frac{9U + 9b(M + B)C_c}{m^2} + \frac{9M(B + 2A)}{m^2} \beta^{-1}d \tag{A.10}
\]

\[
U = \frac{(B + 2A)^2}{2} + \frac{18(M + B)^2}{m^2} \left( b + \beta^{-1} + \frac{2(M + B)\beta^{-1}}{m^2} \right)^2
+ \frac{24\beta^{-1}(2bM^2 + mB^2)(M + B)^2}{m^4} + 2bB + 2A + b^2 \tag{A.11}
\]

\[
\hat{C}_0 = \left( 16 \log (L_0 + L_1) \left( C_0 + \sqrt{C_0} \right) \right)^{1/2} \tag{A.7}
\]

\[
\hat{C}_1 = \left( 16 \log (L_0 + L_1) \left( C_1 + \sqrt{C_1} \right) \right)^{1/2} \tag{A.8}
\]

\[
C_0 = 2\beta M^2 \left( M^2 C_d + B^2 + \frac{d}{\beta} \right), \quad C_1 = (1 + 2M^2)\beta \left( M^2 C_d + B^2 \right) \tag{A.9}
\]

\[
L_0 = \exp \left( \frac{MR^2}{2} + BR + A + \frac{3b}{2m} \log 3 \right) \tag{A.4}
\]

\[
L_1 = \frac{(3m - 9\beta^{-1})(B/2 + A) + 3b(M + B)}{2(M + B)}
+ \frac{6\beta^{-1}Md - 9b\beta^{-1}}{2m} \exp \left\{ \frac{3}{m} \left( \frac{B}{2} + A + \frac{M + B}{m - 3\beta^{-1}} \left( b + \frac{\beta^{-1}(2Md - 3b)}{m} \right) \right) \right\} \tag{A.5}
\]

Table 1: Summary of the constants used in the paper and where they are defined.
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A Proof of Theorem 1 and Corollary 1

A.1 Technical Lemmas

We first state a few technical lemmas and corollaries that will be used in the proofs of Theorem 1 and Corollary 1. Their proofs are deferred to the appendix.

To prove Corollary 1, we need the following results.

**Lemma 1** (Uniform $L^2$ bounds on NSGLD [GGZ18a] and non-reversible Langevin SDE). Under Assumptions 1, 2, 3 and 5. For any data set $z \in \mathcal{Z}^n$,

$$
\sup_{t>0} \mathbb{E}_z \|X(t)\|^2 \leq C_c := \frac{3MR^2 + 3BR + 3B + 6A + 3b \log 3}{2m} + \frac{3b(M + B)}{m^2} + \frac{6M\beta^{-1}d(M + B)}{m^3}.
$$

Moreover, for $\eta \leq \frac{m^2}{(m^2 + 8M^2)M\|A\|^2} \wedge 1$, we have

$$
\sup_{k>0} \mathbb{E}_z \|X_k\|^2 \leq C_d := \frac{3MR^2 + 6BR + 3B + 6A + 3b \log 3}{2m} + \frac{6\beta(2bM^2 + B^2m)(M + B)}{m^4}
$$

$$
+ \frac{12M\beta^{-1}d(M + B)}{m^3} + \frac{3b(M + B)}{m^2}.
$$

**Lemma 2** (Exponential integrability of non-reversible Langevin SDE). If Assumptions 1, 2, 3 and 5 hold, given $\beta \geq 3/m$, for any $t \geq 0$, the exponential integrability of non-reversible SDE admits,

$$
\mathbb{E}_z \left[e^{\|X(t)\|^2}\right] \leq L_0 + L_1 \cdot t < \infty,
$$

where

$$
L_0 := \exp \left(\frac{MR^2}{2} + BR + A + \frac{3b}{2m}\log 3\right),
$$

$$
L_1 := \frac{(3m - 9\beta^{-1})(B/2 + A) + 3b(M + B)}{2(M + B)} + \frac{6\beta^{-1}Md - 9b\beta^{-1}}{2m} \exp \left\{\frac{3}{m} \left(\frac{B}{2} + A + \frac{M + B}{m - 3\beta^{-1}} \left(b + \frac{\beta^{-1}(2Md - 3b)}{m}\right)\right)\right\}.
$$

Before we state the next lemma, let us first introduce the definition of the 2-Wasserstein distance, which is a common choice measuring the distance between two probability measures. For any two probability measures $\mu$, $\nu$, the 2-Wasserstein distance is defined as:

$$
W_2(\mu, \nu) = \left(\inf_{U \sim \mu, V \sim \nu} \mathbb{E}\|U - V\|^2\right)^{\frac{1}{2}},
$$

where the infimum is taken over all random couplings of $U \sim \mu$ and $V \sim \nu$, with the marginal distributions being $\mu$ and $\nu$. 

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Lemma 3 (Diffusion approximation). Suppose Assumptions 1-5 hold, let \( \mu_{z,k} \) be the probability law of \( X_k \) in (1.7) and \( \nu_{z,k\eta} \) be the probability law of \( X(k\eta) \) in (1.6). For any \( \eta \leq \frac{m^2}{(m^2+8M^2)M\|A_J\|^2} \land 1 \) such that \( k\eta \geq e \), the diffusion approximation under 2-Wasserstein metric is
\[
W_2(\mu_{z,k},\nu_{z,k\eta}) \leq \left( \hat{C}_0 \eta^{1/4} + \hat{C}_1 \delta^{1/4} \right) \sqrt{k\eta\sqrt{\log(k\eta)}}\|A_J\|, \tag{A.6}
\]
where
\[
\hat{C}_0 := \left( 16 \log (L_0 + L_1) \left( C_0 + \sqrt{C_0} \right) \right)^{1/2}, \tag{A.7}
\]
\[
\hat{C}_1 := \left( 16 \log (L_0 + L_1) \left( C_1 + \sqrt{C_1} \right) \right)^{1/2}, \tag{A.8}
\]
with
\[
C_0 := 2\beta M^2 \left( M^2 C_d + B^2 + d\beta^{-1} \right), \quad C_1 := (1 + 2M^2)\beta \left( M^2 C_d + B^2 \right), \tag{A.9}
\]
where \( L_0, L_1 \) are constants defined in Lemma 2, and \( C_d \) is defined in (A.2).

Lemma 3 states that NSGLD recursion (1.7) tracks the continuous-time non-reversible Langevin SDE (1.6) in 2-Wasserstein distance. This lemma is the key ingredient in the proof of Corollary 1, and its proof relies on Lemmas 1 and 2.

To prove Theorem 1, we need the following three results.

Lemma 4 (Uniform \( L^4 \) bound on non-reversible Langevin SDE). With Assumptions 1, 2, 3 and 5, we have
\[
\sup_{t>0} \mathbb{E}\|X(t)\|^4 \leq D_c := \frac{9}{m^2} \left( \frac{M^2}{2} R^2 + BR + A \right)^2 + \frac{9U + 9b(M + B)C_c}{m^2} \times \nonumber
\]
\[
+ \frac{6M(M + B)^2}{m^3} \left( B + 2B\sqrt{2b/m} + \frac{2bM}{m} + 4A \right) \beta^{-1}d, \tag{A.10}
\]
where \( C_c \) is given in Lemma 1 and
\[
U := \frac{(B + 2A)^2}{2} + \frac{18(M + B)^2}{m^2} \left( b + \beta^{-1} + \frac{2(M + B)\beta^{-1}}{m^2} \right)^2 \nonumber
\]
\[
+ \frac{24\beta^{-1}(2bM^2 + MB^2)(M + B)^2}{m^4} + 2bB + 2A + b^2. \tag{A.11}
\]

Hwang [HHMS05] derived the following Lemma 5 as their Theorem 4 without specifying \( g_{z,J}(\|x\|) \) which comes from a local Harnack inequality (see e.g. [Tru68]). In the following Lemma 5, we build upon Hwang [HHMS05, Theorem 4] and discuss the dependence of \( g_{z,J}(x) \) on \( z \) and \( J \) by applying a Harnack inequality with a more transparent Harnack constant in [BRS08]. We have the following result.
Lemma 5. Suppose Assumption 1 and 2 hold, then
\[
\int_{\mathbb{R}^d} |p_{z,J}(t,x,y) - \pi_z(y)| \, dy \leq C_{z,J}(x) \cdot g_{z,J}(\|x\|) \cdot e^{\lambda_{z,J} t},
\] (A.12)
where \(C_{z,J}\) is from the spectral gap inequality in (2.2) and
\[
g_{z,J}(\|x\|) = e^{\lambda_{z,J} \frac{\|x\|}{\|x\|_\infty}} \left( \frac{16 \Gamma(d/2 + 1)}{3} \frac{d \cdot (\beta + (1/2 + \beta) \left( \frac{1}{2} \|A_J\| (\|x\| + M + B) + \sqrt{\beta - 1} \right)^2}{(2M/\beta)} + 1 \right),
\] (A.13)
where \(\tilde{C} > 0\) is some universal constant. It follows that uniformly in \(z\), we have
\[
\int_{\mathbb{R}^d} |p_{z,J}(t,x,y) - \pi_z(y)| \, dy \leq C_{*,J} \cdot g_J(\|x\|) \cdot e^{\lambda_{*,J} t},
\] (A.14)
where \(C_{*,J} := \sup_{z \in \mathbb{Z}^d} C_{z,J}\) and
\[
g_J(\|x\|) = e^{\lambda_{*,J} \frac{\|x\|}{\|x\|_\infty}} \left( \frac{16 \Gamma(d/2 + 1)}{3} \frac{d \cdot (\beta + (1/2 + \beta) \left( \frac{1}{2} \|A_J\| (\|x\| + M + B) + \sqrt{\beta - 1} \right)^2}{(2M/\beta)} + 1 \right).\] (A.15)

Lemma 6. Under Assumptions 1, 2, 3 and 5, taking \(\beta > 3/m\) and \(k\eta \geq 1\). For \(x \in \mathbb{R}^d\), we have the following estimate:
\[
\int_{\mathbb{R}^d} \int_{\|x\| > K} \|x\|^2 |p_{z,J}(k\eta, w, x) - \pi_x(x)| \, dx dv_{z,0}(dw) \leq 2D_c e^{\lambda_{z,J} k\eta/2},
\] (A.16)
where \(K\) is defined as
\[
K := e^{\lambda_{z,J} k\eta/4},
\] (A.17)
and \(\lambda_{z,J} < 0\) is defined in (2.1), \(D_c\) is a constant in (A.10).

A.2 Proof of Theorem 1

Proof. We can compute
\[
|\mathbb{E}_{X \sim \nu_{z,k\eta}} F_z(X) - \mathbb{E}_{X \sim \pi_z} F_z(X)| = \left| \int_{\mathbb{R}^d} F_z(x) \nu_{z,k\eta}(dx) - \int_{\mathbb{R}^d} F_z(x) \pi_z(dx) \right|
\]
\[
= \left| \int_{\mathbb{R}^d} F_z(x) \left( \int_{\mathbb{R}^d} p_{z,J}(t, w, x) \nu_{z,0}(dw) - \int_{\mathbb{R}^d} \nu_{z,0}(dw) \pi_z(x) \right) dx \right|
\]
\[
\leq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} F_z(x) |p_{z,J}(t, w, x) - \pi_z(x)| \, dx dv_{z,0}(dw),
\] (A.18)
where in the last inequality we have used the Fubini’s Theorem. From the result of the quadratic bound (I.3) for the function $F_z$ in Lemma 7, we obtain

$$
\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} F_z(x) |p_{z,t}(t, w, x) - \pi_z(x)| \, dx \nu_{z,0}(dw)
$$

$$\leq \int_{\mathbb{R}^d} \nu_{z,0}(w) \int_{\mathbb{R}^d} \left( \frac{M + B}{2} \|x\|^2 + \frac{B}{2} + A \right) \|p_{z,t}(t, w, x) - \pi_z(x)\| \, dx \, dw
$$

$$= \frac{M + B}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \|x\|^2 \|p_{z,t}(t, w, x) - \pi_z(x)\| \, dx \nu_{z,0}(dw)
$$

$$+ \left( \frac{B}{2} + A \right) \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \|p_{z,t}(t, w, x) - \pi_z(x)\| \, dx \nu_{z,0}(dw).
$$

(A.19)

To bound the first term, we use the constant $K > 0$ defined in (A.17) to break the integral into two parts and consider the bounds for each term,

$$
\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \|x\|^2 \|p_{z,t}(t, w, x) - \pi_z(x)\| \, dx \nu_{z,0}(dw)
$$

$$= \int_{\mathbb{R}^d} \int_{\|x\| \leq K} \|x\|^2 \|p_{z,t}(t, w, x) - \pi_z(x)\| \, dx \nu_{z,0}(dw)
$$

$$+ \int_{\mathbb{R}^d} \int_{\|x\| > K} \|x\|^2 \|p_{z,t}(t, w, x) - \pi_z(x)\| \, dx \nu_{z,0}(dw).
$$

(A.20)

By Lemma 5 and $K = e^{\lambda_{z,t}|k\eta/4}$, we have

$$
\int_{\mathbb{R}^d} \int_{\|x\| \leq K} \|x\|^2 \|p_{z,t}(k\eta, w, x) - \pi_z(x)\| \, dx \nu_{z,0}(dw)
$$

$$\leq \int_{\mathbb{R}^d} K^2 C_{z,t} \cdot g_{z,t}(\|w\|) \cdot e^{\lambda_{z,t}|k\eta|} \nu_{z,0}(dw) = e^{\lambda_{z,t}|k\eta/2} C_{z,t} \int_{\|w\| \leq R} g_{z,t}(\|w\|) \nu_{z,0}(dw),
$$

(A.21)

where $\nu_{z,0}$ is supported on an Euclidean ball with radius $R$ by Assumption 5. The definition of $g_{z,t}(\|w\|)$ implies that it is increasing in $\|w\|$. It follows from (A.21) that

$$
\int_{\mathbb{R}^d} \int_{\|x\| \leq K} \|x\|^2 \|p_{z,t}(k\eta, w, x) - \pi_z(x)\| \, dx \nu_{z,0}(dw) \leq C_{z,t} e^{\lambda_{z,t}|k\eta/2},
$$

(A.22)

where $C_{z,t} := C_{z,t} g_{z,t}(R)$. $g_{z,t}$ function is defined in (A.13) from Lemma 5. In addition, Lemma 6 implies:

$$
\int_{\mathbb{R}^d} \int_{\|x\| > K} \|x\|^2 \|p_{z,t}(t, w, x) - \pi_z(x)\| \, dx \nu_{z,0}(dw) \leq 2D e^{\lambda_{z,t}|k\eta/2}.
$$

(A.23)

As a result, the first term in (A.19) is bounded by (A.21) and (A.23).

To bound the second term in (A.19), we apply Lemma 5 directly with $\nu_{z,0}$ is supported on
\[ \|X(0)\| \leq R \text{ by Assumption 5} \]

\[ \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |p_{z,j}(t, w, x) - \pi_x(x)| \, dx \nu_{z,0}(dw) \leq C_{z,j} \cdot g_{z,j}(R) e^{\lambda_{z,j}k\eta} = \tilde{C}_{z,j} e^{\lambda_{z,j}k\eta}. \quad (A.24) \]

Hence, we infer from (A.21), (A.23) and (A.24) to get the bound in (A.19) that

\[ \left| \mathbb{E}_{X \sim \nu_{z,k\eta}} F_z(X) - \mathbb{E}_{X \sim \pi_x} F_z(X) \right| \leq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} F_z(x) |p_{z,j}(k\eta, w, x) - \pi_x(x)| \, dx \nu_{z,0}(dw) \]

\[ \leq \frac{M + B}{2} \left( \tilde{C}_{z,j} + 2D_c \right) e^{\lambda_{z,j}k\eta/2} + \left( \frac{B}{2} + A \right) \cdot \tilde{C}_{z,j} e^{\lambda_{z,j}k\eta} \]

\[ < \left[ \tilde{C}_{z,j} \left( \frac{M + B}{2} + \frac{B}{2} + A \right) + (M + B)D_c \right] e^{\lambda_{z,j}k\eta/2}, \quad (A.25) \]

where we used the condition \( k\eta \geq 1 \) with \( \lambda_{z,j} < 0 \), which implies \( e^{\lambda_{z,j}k\eta} < e^{\lambda_{z,j}k\eta/2} \), that was used to infer the strict inequality above. Therefore, for \( \beta \geq 3/m \), we obtain

\[ \left| \mathbb{E}_{X \sim \nu_{z,k\eta}} F_z(X) - \mathbb{E}_{X \sim \pi_x} F_z(X) \right| \leq I_0(z, J, \varepsilon), \quad (A.26) \]

with any given \( \varepsilon > 0 \),

\[ I_0(z, J, \varepsilon) := \left[ \tilde{C}_{z,j} \left( \frac{M + B}{2} + \frac{B}{2} + A \right) + (M + B)D_c \right] \cdot \varepsilon, \quad (A.27) \]

provided that

\[ k\eta \geq \max \left\{ \frac{2}{|\lambda_{z,j}|} \log \left( \frac{1}{\varepsilon} \right), 1 \right\}. \]

The proof is complete. \( \square \)

### A.3 Proof of Corollary 1

**Proof.** Recall the two probability measures \( \mu_{z,k} = \mathcal{L}(X_k | Z = z) \) and \( \nu_{z,k\eta} = \mathcal{L}(X(t) | Z = z) \). Then we can use the triangular inequality and obtain

\[ \left| \mathbb{E}_{X \sim \mu_{z,k}} F_z(X) - \mathbb{E}_{X \sim \pi_x} F_z(X) \right| \]

\[ \leq \left| \mathbb{E}_{X \sim \mu_{z,k}} F_z(X) - \mathbb{E}_{X \sim \nu_{z,k\eta}} F_z(X) \right| + \left| \mathbb{E}_{X \sim \nu_{z,k\eta}} F_z(X) - \mathbb{E}_{X \sim \pi_x} F_z(X) \right|. \quad (A.28) \]

First, we consider the first term, inferring from the 2-Wasserstein continuity for functions of quadratic growth in Lemma 8,

\[ \left| \mathbb{E}_{X \sim \mu_{z,k}} F_z(X) - \mathbb{E}_{X \sim \nu_{z,k\eta}} F_z(X) \right| \]

\[ = \left| \int_{\mathbb{R}^d} F_z(x) \mu_{z,k}(dx) - \int_{\mathbb{R}^d} F_z(x) \nu_{z,k\eta}(dx) \right| \leq (M\sigma + B) W_2(\mu_{z,k}, \nu_{z,k\eta}), \quad (A.29) \]
where the constant $\sigma = \sqrt{C_d}$ with $C_d$ defined in Lemma 1. Applying the diffusion approximation in Lemma 3, we have

$$
\left| \mathbb{E}_{X \sim \nu_{z,k}} F_z(X) - \mathbb{E}_{X \sim \pi_{z,k}} F_z(X) \right| 
\leq (M \sqrt{C_d} + B) \left( \hat{C}_0 \eta^{1/4} + \hat{C}_1 \delta^{1/4} \right) \sqrt{k \eta} \sqrt{\log(k \eta)} \|A_J\|. 
$$

(A.30)

Next, we consider the upper bound term in the above inequality where it requires

$$
k \eta = \frac{2}{|\lambda_{z,J}|} \log(1/\epsilon) \geq \epsilon,
$$

(A.31)

By choosing

$$
\eta \leq \min \left\{ 1, \frac{m^2}{(m^2 + 8M^2)M \|A_J\|^2}, \frac{\epsilon^4}{4(\log(1/\epsilon))^2 \|A_J\|^4} |\lambda_{z,J}|^2 \right\}.
$$

Then we get

$$
\left| \mathbb{E}_{X \sim \mu_{z,k}} F_z(X) - \mathbb{E}_{X \sim \nu_{z,k}} F_z(X) \right| 
\leq I_1(z, J, \epsilon) = (M \sqrt{C_d} + B) \left( \hat{C}_0 \frac{\epsilon}{|\lambda_{z,J}|} + \hat{C}_1 \delta^{1/4} \sqrt{2 \log(1/\epsilon)} \|A_J\| \right) \sqrt{\log \left( \frac{2 \log(1/\epsilon)}{|\lambda_{z,J}|} \right)}.
$$

Next, the upper bound for the second term in (A.28) can be found in Theorem 1 as the following

$$
\left| \mathbb{E}_{X \sim \nu_{z,k}} F_z(X) - \mathbb{E}_{X \sim \pi_{z,k}} F_z(X) \right| \leq I_0(z, J, \epsilon),
$$

Therefore, inferring from (A.28),

$$
\left| \mathbb{E}_{X \sim \mu_{z,k}} F_z(X) - \mathbb{E}_{X \sim \pi_{z,k}} F_z(X) \right| \leq I_0(z, J, \epsilon) + I_1(z, J, \epsilon).
$$

The proof is complete.

\[ \square \]

**B Proof of Lemma 1**

Proof. The uniform $L^2$ bound on non-reversible Langevin SDE follows [GGZ18a], and we will prove uniform $L^2$ bound on NSGLD algorithm (1.7). Recall the dynamics for NSGLD algorithm follows:

$$
X_{k+1} = X_k - \eta A_J g(X_k, U_{z,k}) + \sqrt{2\eta \beta^{-1}} \xi_k, 
$$

(B.1)

with stochastic gradient $g(x, U_{z,k})$ which is a conditionally unbiased estimator for $F_z(x)$,

$$
\mathbb{E} [g(x, U_{z,k})] = \nabla F_z(x), \quad x \in \mathbb{R}^d.
$$

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We have a quadratic bound in Lemma 7:

\[ \|x\|^2 \leq \frac{3}{m} F_x(x) + \frac{3b}{2m} \log 3. \]

Our aim is to find an uniform bound for \( \mathbb{E} F_x(X_k) \). Inferring the proof in \cite[Lemma 30]{GGZ18b}, suppose we can establish

\[ \frac{\mathbb{E} F_x(X_{k+1}) - \mathbb{E} F_x(X_k)}{\eta} \leq -\varepsilon \mathbb{E} F_x(X_k) + b\varepsilon, \]  

uniformly for small \( \eta \) and \( \varepsilon, b \) are positive constants which are independent of \( \eta \), then we have

\[ \mathbb{E} F_x(X_{k+1}) \leq \mathbb{E} F_x(X_0) + b. \]  

Note that \( \nabla F \) is Lipschitz continuous with Lipschitz constant \( M \). We have

\[ F(y) \leq F(x) + \nabla F(x)(y - x) + \frac{M}{2} \|y - x\|^2. \]

We can compute that

\[ \frac{\mathbb{E} F_x(X_{k+1}) - \mathbb{E} F_x(X_k)}{\eta} \]

\[ = \frac{1}{\eta} \left( \mathbb{E} \left[ F_x \left( X_k - \eta A_J g(X_k, U_{z,k}) + \sqrt{2\eta \beta^{-1} \xi_k} \right) \right] - \mathbb{E} F_x(X_k) \right) \]

\[ \leq -\mathbb{E} [\nabla F_x(X_k)] A_J \nabla F_x(X_k) \]

\[ + \frac{M}{2\eta} \mathbb{E} \left\| \eta A_J g(X_k, U_{z,k}) - \nabla F_x(X_k) - \eta A_J \nabla F_x(X_k) + \sqrt{2\eta \beta^{-1} \xi_k} \right\|^2 \]

\[ \leq -\mathbb{E} \|\nabla F_x(X_k)\|^2 \]

\[ + \frac{M}{2\eta} \left( \eta^2 \|A_J\|^2 \mathbb{E} \|g(X_k, U_{z,k}) - \nabla F_x(X_k)\|^2 + \eta^2 \|A_J\|^2 \mathbb{E} \|\nabla F_x(X_k)\|^2 + 2\eta \beta^{-1} \mathbb{E} \|\xi_k\|^2 \right), \]  

(B.5)

where the first inequality is using \( \mathbb{E}[g(x, U_{z,k})] = \nabla F_x(x) \) for \( x \in \mathbb{R}^d \), and the last equality is due to the fact that the inner product of independent random vectors is 0. Then using Assumption 4, we have

\[ \frac{\mathbb{E} F_x(X_{k+1}) - \mathbb{E} F_x(X_k)}{\eta} \]

\[ \leq -\mathbb{E} \|\nabla F_x(X_k)\|^2 + M\eta\delta \|A_J\|^2 \left( M^2 \mathbb{E} \|X_k\|^2 + B^2 \right) + \frac{M}{2} \eta \|A_J\|^2 \mathbb{E} \|\nabla F_x(X_k)\|^2 + M\beta^{-1} d \]

\[ = -\left( 1 - \frac{M}{2} \eta \|A_J\|^2 \right) \mathbb{E} \|\nabla F_x(X_k)\|^2 + M^2 \eta\delta \|A_J\|^2 \mathbb{E} \|X_k\|^2 + M \left( \eta\delta \|A_J\|^2 B^2 + \beta^{-1} d \right). \]  

(B.6)
If $\|x\| \geq \sqrt{2b/m}$, $(m,b)$-dissipative in Assumption 3 implies,

$$\|\nabla F(x)\| \geq m\|x\| - \frac{b}{\|x\|} \geq \frac{m}{2}\|x\|. \tag{B.7}$$

Then (B.6) implies

$$\frac{\mathbb{E}F_z(X_{k+1}) - \mathbb{E}F_z(X_k)}{\eta} \leq -\left(1 - \frac{M\|A_J\|^2}{2} - \frac{4M^3\delta\|A_J\|^2}{m^2}\eta\right)\mathbb{E}\|\nabla F_z(X_k)\|^2 + \mathbb{E}\|X_k\|^2 + M(\eta\delta\|A_J\|^2B^2 + \beta^{-1}d).$$

According to Assumption 4, $0 \leq \delta < 1$, and under the assumption for the stepsize $\eta$, we have

$$\eta \leq \frac{m^2}{Mm^2\|A_J\|^2 + 8M^3\|A_J\|^2} \leq \frac{m^2}{Mm^2\|A_J\|^2 + 8M^3\delta\|A_J\|^2},$$

it implies

$$1 - \frac{M\|A_J\|^2}{2}\eta - \frac{4M^3\delta\|A_J\|^2}{m^2}\eta \geq \frac{1}{2}.$$ 

By applying (B.7) again, we can compute that

$$\frac{\mathbb{E}F_z(X_{k+1}) - \mathbb{E}F_z(X_k)}{\eta} \leq -\frac{m^2}{8}\mathbb{E}\|X_k\|^2 + M(\eta\delta\|A_J\|^2B^2 + \beta^{-1}d).$$

If $\|x\| < \sqrt{2b/m}$, under the assumption for the stepsize $\eta$, we have

$$\eta \leq \frac{m^2}{Mm^2\|A_J\|^2 + 8M^3\|A_J\|^2} < \frac{2}{M\|A_J\|^2},$$

so that

$$1 - \frac{M\|A_J\|^2}{2}\eta > 0.$$ 

Hence, (B.6) implies,

$$\frac{\mathbb{E}F_z(X_{k+1}) - \mathbb{E}F_z(X_k)}{\eta} \leq M^3\eta\delta\|A_J\|^2(2b/m) + M(\eta\delta\|A_J\|^2B^2 + \beta^{-1}d).$$

Overall, for all $x \in \mathbb{R}^d$, we have

$$\frac{\mathbb{E}F_z(X_{k+1}) - \mathbb{E}F_z(X_k)}{\eta} \leq -\frac{m^2}{8}\mathbb{E}\|X_k\|^2 + \frac{2bM^3}{m}\eta\delta\|A_J\|^2 + M(\eta\delta\|A_J\|^2B^2 + \beta^{-1}d) + \frac{mb}{4} \leq -\frac{m^2}{8}\mathbb{E}\|X_k\|^2 + \delta \left(\frac{bM^3}{m} + \frac{B^2}{2}\right) + M\beta^{-1}d + \frac{mb}{4}, \tag{B.8}$$
where we used $\eta < 1/(2M\|A_j\|^2)$ to get the strict inequality. We recall the quadratic bound for objective function:

$$F_z(x) \leq \frac{M + B}{2} \|x\|^2 + \frac{B}{2} + A.$$ 

Hence, we get

$$\frac{\mathbb{E}F_z(X_{k+1}) - \mathbb{E}F_z(X_k)}{\eta} \leq -\frac{m^2}{4(M + B)} F_z(X_k) + \frac{m^2(B + 2A)}{8(M + B)} + \delta \left(\frac{bM^2}{m} + \frac{B^2}{2}\right) + M\beta^{-1}d + \frac{mb}{4}.$$ 

Therefore, for $\eta \leq \frac{m^2}{(m^2 + 8M^2)\|A_j\|^2}$, we have the following inequality by (B.3),

$$\mathbb{E}F_z(X_{k+1}) \leq \mathbb{E}F_z(X_0) + \frac{2\delta(2bM^2/m + B^2)(M + B)}{m^2} + \frac{4M\beta^{-1}d(M + B)}{m^2} + \frac{b(M + B)}{m} + \frac{B}{2} + A.$$ 

With $\|X(0)\| \leq R$, $F_z(X_0)$ is bounded by

$$F_z(X_0) \leq \frac{M}{2} \|X_0\|^2 + B\|X_0\| + A \leq \frac{M}{2}R^2 + BR + A.$$ 

In addition, we recall that

$$\|x\|^2 \leq \frac{3}{m} F_z(x) + \frac{3b}{2m} \log 3.$$ 

Therefore, we obtain the uniform $L^2$ bound for $\|X_k\|$:

$$\sup_{k \geq 0} \mathbb{E}\|X_k\|^2 \leq \frac{3}{m} \mathbb{E}F_z(X_k) + \frac{3b}{2m} \log 3$$

$$\leq \frac{3MR^2 + 6BR + 3B + 6A + 3b \log 3}{2m} + \frac{6\delta(2bM^2 + B^2m)(M + B)}{m^4}$$

$$+ \frac{12M\beta^{-1}d(M + B)}{m^3} + \frac{3b(M + B)}{m^2}. \quad (B.9)$$

The proof is complete.

\[C\] Proof of Lemma 2

Proof. First, notice that the quadratic bound in Lemma 7 gives that uniformly in $z \in \mathcal{Z}^n$,

$$\frac{3}{m} F_z(x) \geq \|x\|^2 - \frac{3b}{2m} \log 3.$$ 

Thus it suffices for us to get a uniform bound for $\mathbb{E} \left[ e^{\frac{3}{m} F_z(X(t))} \right]$. We recall that the non-reversible Langevin SDE is given by

$$dX(t) = -A_j (\nabla F_z(X(t))) dt + \sqrt{2\beta^{-1}} dB(t), \quad (C.1)$$
whose infinitesimal generator for this system is
\[ \mathcal{L}_J = -A_J \nabla F_z \cdot \nabla + \beta^{-1} \Delta. \]

For any \( x \in \mathbb{R}^d \), we can compute that
\[ \mathcal{L}_J F_z(x) = -A_J \nabla F_z(x) \cdot \nabla F_z(x) + \beta^{-1} \Delta F_z(x) = -\| \nabla F_z(x) \|^2 + \beta^{-1} \Delta F_z(x). \quad (C.2) \]

where \( J \) is an anti-symmetric matrix and \( \langle J \nabla F, \nabla F \rangle = 0 \). For any constant \( \alpha > 0 \), we get
\[ \mathcal{L}_J (e^{\alpha F_z}) = (\alpha \mathcal{L}_J F_z + \alpha^2 \beta^{-1} \| \nabla F \|^2) e^{\alpha F_z} = \left( (\alpha - \alpha^2 \beta^{-1}) \mathcal{L}_J F_z + \alpha^2 \beta^{-2} \Delta F_z \right) e^{\alpha F_z}, \]
\[ = \left( - (\alpha - \alpha^2 \beta^{-1}) \| \nabla F_z \|^2 + \alpha \beta^{-1} \Delta F_z \right) e^{\alpha F_z}. \quad (C.3) \]

where we used the property of the anti-symmetric matrix \( J \), such that \( \langle \nabla F_z, J \nabla F_z \rangle = 0 \). Recall \( F_z \) is \( M \)-smooth, then \( \Delta F \leq Md \). In addition, by assuming \( \beta > \alpha > 0 \), then \( \alpha - \alpha^2 \beta^{-1} > 0 \), and the relation \((C.3)\) implies
\[ \mathcal{L}_J (e^{\alpha F_z}) \leq (\alpha \beta^{-1} \Delta F_z) e^{\alpha F_z} \leq (\alpha \beta^{-1} Md) e^{\alpha F_z}. \]

Recall that the initial condition satisfies \( \| X(0) \| \leq R \), and the quadratic bound Lemma 7 for function \( F_z \):
\[ F_z(x) \leq \frac{M}{2} \| x \|^2 + B \| x \| + A. \]

Then it follows from Corollary 2.4 [CHJ13] that we have the exponential integrability:
\[ \mathbb{E} \left[ e^{\alpha F_z(X(t))} \right] \leq \mathbb{E} \left[ e^{\alpha F_z(X(0))} \right] e^{\alpha \beta^{-1} M dt} \leq e^{\alpha \left( \frac{MR^2}{2} + BR + A + \beta^{-1} M dt \right)} < \infty. \quad (C.4) \]

Next, by applying Itô’s formula to \( e^{\left(3/m\right) F_z} \), we get:
\[ e^{\frac{3}{m} F_z(X(t))} = e^{\frac{3}{m} F_z(X(0))} + \int_0^t \mathcal{L}_J \left( e^{\frac{3}{m} F_z(X(s))} \right) ds + \int_0^t \frac{3 \sqrt{2 \beta^{-1}}}{m} \nabla F_z(X(s)) e^{\frac{3}{m} F_z(X(s))} dB(s). \quad (C.5) \]
We can check that the square integrability condition holds for the diffusion term in (C.5). That is, for any $t > 0$,

$$\int_0^t \frac{18\beta^{-1}}{m} E \left[ \left\| \nabla F_\alpha(X(s)) e_{\frac{m}{m}} F_\alpha(X(s)) \right\|^2 \right] ds$$

$$\leq \int_0^t \frac{18\beta^{-1}}{m} E \left[ (2M^2 \|X(s)\|^2 + 2B^2) e_{\frac{m}{m}} F_\alpha(X(s)) \right] ds$$

$$\leq \int_0^t \frac{18\beta^{-1}}{m} E \left[ (2M^2 \left( \frac{3}{m} \left( F_\alpha(X(s)) + \frac{b}{2} \log 3 \right) \right) + 2B^2 \right) e_{\frac{m}{m}} F_\alpha(X(s)) \right] ds$$

$$\leq \int_0^t \frac{18\beta^{-1}}{m} E \left[ M^2 e_{\frac{m}{m}} F_\alpha(X(s)) + \left( \frac{3bM^2 \log 3}{m} + 2B^2 \right) e_{\frac{m}{m}} F_\alpha(X(s)) \right] ds < \infty. \quad (C.6)$$

The first and second inequalities above are due to the quadratic bounds in Lemma 7, (I.1) and (I.3) and the third inequality above is due to the fact that $x \leq e^x, x > 0$ and the exponential integrability property in (C.4) with $\alpha = 6/m$. As a result, we know $\int_0^t \frac{3\sqrt{2\beta^{-1}}}{m} \nabla F_\alpha(X(s)) e_{\frac{m}{m}} F_\alpha(X(s)) dB(s)$ is a martingale, then we can take the expectation in (C.5) and obtain:

$$E \left[ e_{\frac{m}{m}} F_\alpha(X(t)) \right] = E \left[ e_{\frac{m}{m}} F_\alpha(X(0)) \right] + \int_0^t E \left[ \mathcal{L}_J \left( e_{\frac{m}{m}} F_\alpha(X(s)) \right) \right] ds.$$

Next, we compute an upper bound for $E \left[ \mathcal{L}_J \left( e_{\frac{m}{m}} F_\alpha(X(s)) \right) \right]$ in the above equation. Lemma 28 in [GGZ18a] gives the Lyapunov condition for $F_\alpha(x)$ such that

$$\mathcal{L}_J F_\alpha(x) \leq - \frac{m^2}{2(M + B)} F_\alpha(x) + \frac{m^2(B/2 + A)}{2(M + B)} + \frac{mb}{2} + \beta^{-1} Md. \quad (C.7)$$

Then by applying (C.3) and $\beta > 3/m$, we have

$$\mathcal{L}_J \left( e_{\frac{m}{m}} F \right) \leq \left[ - \left( \frac{3m - 9\beta^{-1}}{2(M + B)} \right) F \right.$$

$$+ \left( \frac{(3m - 9\beta^{-1})(B/2 + A) + 3b(M + B)}{2(M + B)} \right) + \frac{6\beta^{-1} Md - 9b\beta^{-1}}{2m} \right] e_{\frac{m}{m}} F. \quad (C.8)$$

If

$$- \left( \frac{3m - 9\beta^{-1}}{2(M + B)} \right) F_\alpha + \left( \frac{(3m - 9\beta^{-1})(B/2 + A) + 3b(M + B)}{2(M + B)} \right) + \frac{6\beta^{-1} Md - 9b\beta^{-1}}{2m} < 0,$$

then we have $\mathcal{L}_J \left( e_{\frac{m}{m}} F_\alpha \right) < 0$. Otherwise,

$$- \left( \frac{3m - 9\beta^{-1}}{2(M + B)} \right) F_\alpha + \left( \frac{(3m - 9\beta^{-1})(B/2 + A) + 3b(M + B)}{2(M + B)} \right) + \frac{6\beta^{-1} Md - 9b\beta^{-1}}{2m} \geq 0,$$

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which implies
\[ F_* \leq \frac{B}{2} + A + \frac{M + B}{m - 3\beta^{-1}} \left( b + \frac{\beta^{-1}(2Md - 3b)}{m} \right). \]  
(C.9)

Since the objective function \( F_* \) is non-negative, it follows from (C.8) that
\[ \mathcal{L}_J \left( e^{\frac{3}{m}F_*} \right) \leq \left( \frac{(3m - 9\beta^{-1})(B/2 + A) + 3b(M + B)}{2(M + B)} + \frac{6\beta^{-1}Md - 9b\beta^{-1}}{2m} \right) e^{\frac{3}{m}F_*}. \]  
(C.10)

Using the upper bound of \( F_* \) in the previous calculation, we get, for \( \beta > \frac{3}{m} \),
\[ \mathcal{L}_J \left( e^{\frac{3}{m}F_*} \right) \leq l_1 e^{l_2}, \]  
(C.11)

with
\[ l_1 := \frac{(3m - 9\beta^{-1})(B/2 + A) + 3b(M + B) + 6\beta^{-1}Md - 9b\beta^{-1}}{2m}, \]  
(C.12)

and
\[ l_2 := \frac{3}{m} \left( \frac{B}{2} + A + \frac{M + B}{m - 3\beta^{-1}} \left( b + \frac{\beta^{-1}(2Md - 3b)}{m} \right) \right). \]  
(C.13)

Therefore, it follows from (C.5) that
\[
\begin{align*}
\mathbb{E} \left[ e^{\frac{3}{m}F_*(X(t))} \right] & = \mathbb{E} \left[ e^{\frac{3}{m}F_*(X(0))} \right] + \int_0^t \mathbb{E} \left[ \mathcal{L}_J \left( e^{\frac{3}{m}F_*(X(s))} \right) \right] ds \\
& \leq \mathbb{E} \left[ e^{\frac{3}{m}F_*(X(0))} \right] + \int_0^t l_1 e^{l_2} ds = \mathbb{E} \left[ e^{\frac{3}{m}F_*(X(0))} \right] + l_1 e^{l_2} \cdot t.
\end{align*}
\]  
(C.14)

With the initial condition satisfying \( \|X(0)\| \leq R \), we can bound \( F_*(X(0)) \) by the quadratic bound (I.3) in Lemma 7, that is,
\[ F_*(X(0)) \leq \frac{M}{2} \|X(0)\|^2 + B\|X(0)\| + A \leq \frac{MR^2}{2} + BR + A. \]

As a result, for any \( t > 0 \), with \( \beta > 3/m \) and \( \|X(0)\| \leq R \), we get
\[ \mathbb{E} \left[ e^{\frac{3}{m}F_*(X(t))} \right] \leq e^{\frac{MR^2}{2} + BR + A} + l_1 e^{l_2} (t). \]

Moreover, the quadratic bound in (I.1) from Lemma 7 gives
\[ \frac{3}{m} F_*(x) \geq \|x\|^2 - \frac{3b}{2m} \log 3, \]
which implies
\[ \mathbb{E} \left[ e^{\|X(t)\|^2} \right] \leq e^{\frac{MR^2}{2} + BR + A + \frac{3b}{2m} \log 3 + l_1 e^{l_2} (t)} < \infty. \]

The proof is complete.  
\[ \square \]
\section{Proof of Corollary 3}

\textit{Proof.} Let $X_k$ follow the probability law $\mathcal{L}(X_k | Z = z) = \mu_{z,k}$ and the samples drawn by Gibbs algorithm $\pi_z = \mathcal{L}(\hat{X}^* | Z = z)$ with $Z = (Z_1, Z_2, ..., Z_n)$ being a random variable from an unknown distribution and $z = (z_1, z_2, ..., z_n)$ being a deterministic data sample. The decomposition for population risk minimization problem admits the following inequality,

$$E F(X_k) - F^* = \left( E F(X_k) - E F(\hat{X}^*) \right) + \left( E F(\hat{X}^*) - E F_Z(\hat{X}^*) \right) + \left( E F_Z(\hat{X}^*) - F^* \right). \quad (D.1)$$

We can write the first term in (D.1) as the following identity over all possible training data set $z$ in $Z^n$.

$$E F(X_k) - E F(\hat{X}^*) = \int_{Z^n} P^\otimes n(dz) \left( \int_{\mathbb{R}^d} F_z(x) \mu_{z,k}(dx) - \int_{\mathbb{R}^d} F_z(x) \pi_z(dx) \right), \quad (D.2)$$

where $P^\otimes n$ is the product measures over the independent and identically distributed random variables $Z_1, Z_2, ..., Z_n$ supported on $Z^n$. To find an upper bound for the first term, we can consider an uniform bound over $z \in Z^n$ by using Corollary 1. For a deterministic $z \in Z^n$, Corollary 1 states that,

$$\left| E_{X \sim \mu_{z,k}} F_z(X) - E_{X \sim \pi_z} F_z(X) \right| \leq I_0(z, J, \varepsilon) + I_1(z, J, \varepsilon).$$

Recall we define $I_0(z, J, \varepsilon)$ in (3.2) and we have

$$\sup_{z \in Z^n} C_{z,J} = \sup_{z \in Z^n} C_{z,J} g_{z,J}(R) \leq \sup_{z \in Z^n} C_{z,J} g_{z,J}(R) =: C_J,$$

where $g_{z,J}(R) = \sup_{z \in Z^n} g_{z,J}(R)$. Therefore, we can bound $\sup_{z \in Z^n} I_0(z, J, \varepsilon)$ by:

$$\overline{I}_0(J, \varepsilon) := \left[ C_J \left( \frac{M + B}{2} + \frac{B}{2} + A \right) + (M + B) D_c \right] \cdot \varepsilon. \quad (D.3)$$

It follows that we can bound the first term in (D.1) as

$$\left| E F(X_k) - E F(\hat{X}^*) \right| \leq \overline{I}_0(J, \varepsilon) + I_1(J, \varepsilon),$$

where $I_1(J, \varepsilon)$ is given in Corollary 2, which uniformly bounds $I_1(z, J, \varepsilon)$.

The second term in (D.1) is the generalization error of Gibbs algorithm that bounded in Lemma 9, also see Proposition 12 in Raginsky et al. \cite{RRT17}. In our notation, this part is bounded by $I_3(n)$ where $n$ is the size of training set,

$$\left| E F(\hat{X}^*) - E F_Z(\hat{X}^*) \right| \leq \frac{4 \left( \frac{M^2 (b + d/\beta) + B^2}{m} \right) \beta_{CLS}}{n} = I_3(n),$$
The third term in (D.1) is bounded by:

\[
\mathbb{E} F_Z(\hat{X}^*) - F^* = \mathbb{E} \left[ F_Z(\hat{X}^*) - \min_{x \in \mathbb{R}^d} F_Z(x) \right] + \mathbb{E} \left[ \min_{x \in \mathbb{R}^d} F_Z(x) - F_Z(x^\pi) \right] \\
\leq \mathbb{E} \left[ F_Z(X^\pi) - \min_{x \in \mathbb{R}^d} F_Z(x) \right] \leq I_2 = \frac{d}{2\beta} \log \left( \frac{eM}{m} \left( \frac{b\beta}{d} + 1 \right) \right) ,
\]

where \( I_2 \) is defined in (3.8) from Proposition 11, Raginsky et al. [RRT17]. The proof is complete.

\[\blacksquare\]

E  Proof of Lemma 3

Proof. The proof closely follows from the proof of Lemma 7 in Raginsky et al. [RRT17]. Defining the continuous-time interpolation for \( X_k \),

\[
\bar{X}(t) = X_0 - \int_0^t A_J g(\bar{X}(\lfloor s/\eta \rfloor \eta), \bar{U}_z(s)) \, ds + \sqrt{2\beta^{-1}} \int_0^t dB(s) , \tag{E.1}
\]

where \( \bar{U}_z(t) := U_{z,k} \) for all \( t \in [k\eta, (k+1)\eta) \). Here \( \bar{X}(k\eta) \) and \( X_k \) follow the same probability law \( \mu_{z,k} \). The result from Gyöngy [Gyö86] implies \( \bar{X} \) has the same marginals as \( \tilde{X} \) which is a Markov process:

\[
\tilde{X}(t) = X_0 - \int_0^t A_J g_{z,s}(X(s)) \, ds + \sqrt{2\beta^{-1}} \int_0^t dB(s) , \tag{E.2}
\]

with

\[
g_{z,s}(x) := \mathbb{E}_z \left[ g \left( \bar{X}(\lfloor s/\eta \rfloor \eta), \bar{U}_z(s) \right) \mid \bar{X}(t) = x \right] . \tag{E.3}
\]

Suppose the non-reversible Langevin diffusion \( X(t) \) follows the probability measure \( \mathbb{P} \), and \( \tilde{X}(t) \) follows the probability measure \( \mathbb{\tilde{P}} \). The Radon-Nikodym derivative is represented by the Girsanov formula under the filtration \( \mathcal{F}_t \) for \( t > 0 \)

\[
\frac{d\mathbb{\tilde{P}}}{d\mathbb{P}} \bigg|_{\mathcal{F}_t} = e^{\sqrt{\frac{2}{\beta}} \int_0^t A_J (\nabla F_\xi(\tilde{X}(s)) - g_{z,s}(\tilde{X}(s))) \, dB(s) - \frac{\beta}{2} \int_0^t \| A_J (\nabla F_\xi(\tilde{X}(s)) - g_{z,s}(\tilde{X}(s))) \|^2 \, ds} . \tag{E.4}
\]
Since the probability law of $\bar{X}(t)$ and $\tilde{X}(t)$ are the same for each $t > 0$, we can use the martingale property of Ito integral and compute the relative entropy as follows:

$$D \left( \tilde{P}_t \parallel P_t \right) := - \int d\tilde{P}_t \log \frac{dP_t}{d\tilde{P}_t}$$

$$= \frac{\beta}{4} \| A_J \|^2 \int_0^t \mathbb{E}_z \| \nabla F_z(\bar{X}(s)) - g_{z,s}(\bar{X}(s)) \|^2 ds$$

$$= \frac{\beta}{4} \| A_J \|^2 \int_0^t \mathbb{E}_z \| \nabla F_z(\bar{X}(s)) - g_{z,s}(\bar{X}(s)) \|^2 ds \ . \quad \text{(E.5)}$$

It follows that

$$D \left( \tilde{P}_{k\eta} \parallel P_{k\eta} \right) = \frac{\beta}{4} \| A_J \|^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E}_z \| \nabla F_z(\bar{X}(s)) - g_{z,s}(\bar{X}(s)) \|^2 ds$$

$$\leq \frac{\beta}{4} \| A_J \|^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E}_z \| \nabla F_z(\bar{X}(s)) - g(\bar{X}([s/\eta]\eta), U_z(s)) \|^2 ds$$

$$\leq \frac{\beta}{2} \| A_J \|^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E}_z \| \nabla F_z(\bar{X}(s)) - \nabla F_z(\bar{X}([s/\eta]\eta)) \|^2 ds$$

$$+ \frac{\beta}{2} \| A_J \|^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E}_z \| \nabla F_z(\bar{X}([s/\eta]\eta)) - g(\bar{X}([s/\eta]\eta), U_z(s)) \|^2 ds \ . \quad \text{(E.6)}$$

With Assumption 2, we can infer that the first term in (E.6) is bounded as follows,

$$\frac{\beta}{2} \| A_J \|^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E}_z \| \nabla F_z(\bar{X}(s)) - \nabla F_z(\bar{X}([s/\eta]\eta)) \|^2 ds$$

$$\leq \frac{\beta}{2} M^2 \| A_J \|^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E}_z \| \bar{X}(s) - \bar{X}([s/\eta]\eta) \|^2 ds \ . \quad \text{(E.7)}$$

In addition, for some $s > 0$, $j\eta \leq s < (j+1)\eta$,

$$\bar{X}(s) - \bar{X}(j\eta) = -(s - j\eta)g(X_j, U_{z,j}) + \sqrt{2\beta^{-1}}(B_s - B_{j\eta}) \ .$$
Then, we can get
\[
\mathbb{E}_z \left\| X(s) - X \left(\lfloor s/\eta \rfloor \eta \right) \right\|^2 = (s - j\eta)^2 \mathbb{E}_z \left\| g(X_j, U_{z,j}) \right\|^2 + 2\beta^{-1}(s - j\eta)^2 d
\]
\[
\leq (s - j\eta)^2 \mathbb{E}_z \left\| g(X_j, U_{z,j}) - \nabla F_z(X_j) \right\|^2 + (s - j\eta)^2 \mathbb{E}_z \left\| \nabla F_z(X_j) \right\|^2 + 2\beta^{-1}(s - j\eta)^2 d
\]
\[
\leq 2(s - j\eta)^2(1 + \delta) \left( M^2 \sup_{j > 0} \mathbb{E}_z \|X_j\|^2 + B^2 \right) + 2\beta^{-1}(s - j\eta)^2 d. \tag{E.8}
\]

The last inequality is from Assumption 4 and the quadratic bound for $\nabla F_z$ in Lemma 7, such that $\mathbb{E}_z \left\| \nabla F_z(X_j) \right\|^2 \leq 2 \left( M^2 \sup_{j > 0} \mathbb{E}_z \|X_j\|^2 + B^2 \right)$. For some $s - j\eta < \eta < 1$ and $\delta < 1$, the bound for the first term in (E.6) can be computed as,
\[
\frac{\beta}{2} M^2 \|A_j\|^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E}_z \left\| X(s) - X \left(\lfloor s/\eta \rfloor \eta \right) \right\|^2 ds
\]
\[
\leq \beta M^2 \|A_j\|^2 k\eta \left( 2\eta(1 + \delta) \left( M^2 \sup_{j > 0} \mathbb{E}_z \|X_j\|^2 + B^2 \right) + 2\beta^{-1} d\eta \right). \tag{E.9}
\]

With Assumption 4, for $j\eta \leq s < (j + 1)\eta$, we can rewrite the second term in (E.6) as
\[
\frac{\beta}{2} \|A_j\|^2 \sum_{j=0}^{k-1} \int_{j\eta}^{(j+1)\eta} \mathbb{E}_z \left\| \nabla F_z(X_j) - g(X_j, U_{z,j}) \right\|^2 ds
\]
\[
\leq \beta \|A_j\|^2 \left( M^2 \sup_{j > 0} \mathbb{E}_z \|X_j\|^2 + B^2 \right) k\eta\delta. \tag{E.10}
\]

Combining these two inequality, we can have an upper bound for the relative entropy in (E.6),
\[
D \left( \mathbb{P}_{k\eta} \left\| \mathbb{P}_{k\eta} \right\| \right) \leq \beta M^2 \|A_j\|^2 k\eta \left( 2\eta(1 + \delta) \left( M^2 \sup_{j > 0} \mathbb{E}_z \|X_j\|^2 + B^2 \right) + 2\beta^{-1} d\eta \right)
\]
\[
+ \beta \|A_j\|^2 \left( M^2 \sup_{j > 0} \mathbb{E}_z \|X_j\|^2 + B^2 \right) k\eta\delta. \tag{E.11}
\]

From Lemma 1, we conclude that, for any $\eta \leq \frac{m^2}{(m^2 + 8M^2) \|A_j\|^2} \wedge 1$,
\[
D \left( \mu_{z,k} \left\| \nu_{z,k\eta} \right\| \right) \leq 2M^2 \beta \left( M^2 C_d + B^2 + \beta^{-1} d \right) \|A_j\|^2 k\eta^2 + (1 + 2M^2)\beta \left( M^2 C_d + B^2 \right) \|A_j\|^2 k\eta\delta
\]
\[
= (C_0\eta + C_1\delta) \|A_j\|^2 (k\eta), \tag{E.12}
\]

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where

\[ C_0 = 2\beta M^2 \left( M^2 C_d + B^2 + \frac{d}{\beta} \right), \quad C_1 = (1 + 2M^2)\beta (M^2 C_d + B^2). \] (E.13)

With \( k\eta \geq e, \eta \leq \sqrt{\eta} \leq 1 \) and \( \delta < \sqrt{\delta} < 1 \), then we can also compute

\[
D(\mu_{z,k} \| \nu_{z,k\eta}) + \sqrt{D(\mu_{z,k} \| \nu_{z,k\eta})} = (C_0\eta + C_1\delta)\|A_J\|^2k\eta + (\sqrt{C_0\eta} + \sqrt{C_1\delta})\|A_J\|k\eta
\leq \left( (C_0 + \sqrt{C_0})\sqrt{\eta} + (C_1 + \sqrt{C_1})\sqrt{\delta} \right) \|A_J\|^2k\eta
\] (E.14)

The result from Bolley and Villani \[BV05\] states that for any two Borel probability measures \( \mu, \nu \) on \( \mathbb{R}^d \) with finite second moment,

\[
W_2^2(\mu, \nu) \leq C_\nu \left[ \sqrt{D(\mu \| \nu)} + \left( \frac{D(\mu \| \nu)}{2} \right)^{1/4} \right].
\]

with

\[
C_\nu = 2 \inf_{\lambda > 0} \left( \frac{1}{\lambda} \left( \frac{3}{2} + \log \int_{\mathbb{R}^d} e^{\lambda \|x\|^2} \nu(dx) \right) \right)^{1/2}.
\]

Let \( \mu = \mu_{z,k}, \nu = \nu_{z,k\eta} \) and take \( \lambda = 1 \), inferring from Lemma 2, \( k\eta \geq 1 \), we can compute

\[
W_2^2(\mu_{z,k}, \nu_{z,k\eta}) \leq 4 \log(L_0 + L_1(k\eta)) \left[ \sqrt{D(\mu_{z,k} \| \nu_{z,k\eta})} + \left( \frac{D(\mu_{z,k} \| \nu_{z,k\eta})}{2} \right)^{1/4} \right]^2
\leq 8(\log(L_0 + L_1) + \log(k\eta)) \left[ D(\mu_{z,k} \| \nu_{z,k\eta}) + \sqrt{D(\mu_{z,k} \| \nu_{z,k\eta})} \right],
\] (E.15)

where \( \|X(0)\| \leq R = \sqrt{b/m} \). Additionally, let \( k\eta \geq e \), we have \( (k\eta) \log(k\eta) > k\eta \), hence

\[
W_2^2(\mu_{z,k}, \nu_{z,k\eta}) \leq \left( \hat{C}_0^2 \sqrt{\eta} + \hat{C}_1^2 \sqrt{\delta} \right) (k\eta) \log(k\eta) \|A_J\|^2,
\]

with

\[
\hat{C}_0 = \left( 16 \log(L_0 + L_1) \left( C_0 + \sqrt{C_0} \right) \right)^{1/2}, \quad \hat{C}_1 = \left( 16 \log(L_0 + L_1) \left( C_1 + \sqrt{C_1} \right) \right)^{1/2},
\]

where \( C_0 = \tilde{O}(\beta + d) \) and \( C_1 = \tilde{O}(\beta) \) are in (A.9), \( L_0 = \tilde{O}(1) \) in (A.4) and \( L_1 = e^{\tilde{O}(\beta)} \) in (A.5). The proof is complete. \( \square \)
Proof of Lemma 4

Proof. To prove the uniform $L^4$ bound for the non-reversible Langevin SDE (1.6), we first recall the quadratic bound for $F_z$ in (I.3),

$$\frac{m}{3} \|x\|^2 - b < \frac{m}{3} \|x\|^2 - \frac{b}{2} \log 3 \leq F_z(x),$$

which implies the following:

$$\|x\|^4 \leq \left( \frac{3}{m} F_z(x) + \frac{3b}{m} \right)^2 \leq \frac{9}{m^2} F_z^2(x) + \frac{9b(M + B)}{m^2} \|x\|^2 + \frac{18b}{m^2} \left( \frac{B}{2} + A \right) + \frac{9b^2}{m^2}. \quad (F.1)$$

For $X(0) = x_0 \in \mathbb{R}^d$ with $\|x_0\| \leq R = \sqrt{b/m}$, there is a uniform bound for $\mathbb{E}\|X(t)\|^2$, i.e. $\mathbb{E}\|X(t)\|^2 \leq C_c$ where $C_c$ is a constant in (A.1) from Lemma 1. Next, we focus on computing an upper bound for $\mathbb{E}F^2_z(X(t))$.

Recall the infinitesimal generator of the SDE in (1.6):

$$\mathcal{L}_J = -A_J \nabla F_z \cdot \nabla + \beta^{-1} \Delta.$$ 

Then, we can compute that

$$\mathcal{L}_J F_z(x) = -A_J \nabla F_z(x) \cdot \nabla F_z(x) + \beta^{-1} \Delta F_z(x) = -\|\nabla F_z(x)\|^2 + \beta^{-1} \Delta F_z(x),$$

where $J$ is an $d \times d$ anti-symmetric matrix so that $\langle J \nabla F_z, \nabla F_z \rangle = 0$. Moreover, we can compute that

$$\mathcal{L}_J F^2_z(x) = (2F_z \mathcal{L}_J F_z + 2\beta^{-1}\|\nabla F_z\|^2)$$

$$= -2(F_z(x) - \beta^{-1})\|\nabla F_z(x)\|^2 + 2\beta^{-1} F_z(x) \Delta F_z(x). \quad (F.2)$$

By $(m, b)$-dispassive property, we have

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

so that for any $\|x\| \geq \sqrt{2b/m}$, we have

$$\|\nabla F_z(x)\| \geq m\|x\| - \frac{b}{\|x\|} \geq \frac{m}{2} \|x\|,$$

which yields $\|\nabla F_z(x)\|^2 \geq (m^2/4)\|x\|^2$. Moreover, the objective function $F_z$ is $M$-smooth, so that $\Delta F_z(x) \leq Md$.

For any $\|x\| \geq \sqrt{2b/m}$, under the assumption that $\beta \geq 3/m$, the quadratic bound for $F_z$ in
equation (I.3) shows that

\[ \frac{m}{3} \|x\|^2 - b < F_k(x) \leq \frac{M + B}{2} \|x\|^2 + \frac{B}{2} + A, \]  

(F.3)

Then it follows from (F.2), for \( \|x\| \geq \sqrt{2b/m} \), we have

\[
\begin{align*}
\mathcal{L}_J F_k^2(x) &\leq -2 \left( \frac{m}{3} \|x\|^2 - b - \beta^{-1} \right) \cdot \frac{m^2}{4} \|x\|^2 + 2\beta^{-1} \left( \frac{M + B}{2} \|x\|^2 + \frac{B}{2} + A \right) Md \\
&= -\frac{m^2}{2} \|x\|^2 \left( \frac{m}{3} \|x\|^2 - b - \beta^{-1} - \frac{2(M + B)\beta^{-1}}{m^2} \right) + 2\beta^{-1} \left( \frac{B}{2} + A \right) Md. \\
\end{align*}
\]

(F.4)

Let

\[ S := \left( \frac{6b}{m} + \frac{6\beta^{-1}}{m} + \frac{12(M + B)\beta^{-1}}{m^3} \right)^{1/2} > \sqrt{2b/m}. \]

Then (F.4) is equivalent to

\[
\mathcal{L}_J F_k^2(x) \leq -\frac{m^2}{2} \|x\|^2 \left( \frac{m}{3} \|x\|^2 - \frac{m}{6} S^2 \right) + 2\beta^{-1} \left( \frac{B}{2} + A \right) Md. \]

(F.5)

Therefore, if \( \|x\| > S \), for (F.5), we have

\[
\begin{align*}
\mathcal{L}_J F_k^2(x) &\leq -\frac{m^3}{12} \|x\|^4 + (B + 2A) \beta^{-1} Md. \\
\end{align*}
\]

(F.6)

On the other hand, if \( \sqrt{2b/m} < \|x\| \leq S \), we obtain from (F.5) that

\[
\begin{align*}
\mathcal{L}_J F_k^2(x) &\leq -\frac{m^3}{6} \|x\|^4 + \frac{m^3}{12} \|x\|^2 S^2 + (B + 2A) \beta^{-1} Md \\
&\leq -\frac{m^3}{12} \|x\|^4 + \frac{m^3}{12} S^4 + (B + 2A) \beta^{-1} Md. \\
\end{align*}
\]

To summarize, for any \( \|x\| \geq \sqrt{2b/m} \), we have,

\[
\begin{align*}
\mathcal{L}_J F_k^2(x) &\leq -\frac{m^3}{12} \|x\|^4 + \frac{m^3}{12} S^4 + (B + 2A) \beta^{-1} Md \\
&\leq -\frac{m^3}{12} \|x\|^4 + 3m \left( b + \beta^{-1} + \frac{2(M + B)\beta^{-1}}{m^2} \right)^2 + (B + 2A) \beta^{-1} Md. \\
\end{align*}
\]

(F.7)
Next we consider the case \( \|x\| \leq \sqrt{2b/m} \) and obtain from the equation (F.2) that,

\[
\mathcal{L}_J F^2_x(x) = -2F_x(x)\|\nabla F_x(x)\|^2 + 2\beta^{-1}\|\nabla F_x(x)\|^2 + 2\beta^{-1}F_x(x)\Delta F_x(x) \\
\leq 2\beta^{-1}\|\nabla F_x(x)\|^2 + 2\beta^{-1}F_x(x)\Delta F_x(x),
\]

where we use the fact \( F_x \) function is non-negative in Assumption 1. By applying the quadratic bounds in Lemma 7 that

\[
\|\nabla F_x(x)\| \leq M \|x\| + B, \\
F_x(x) \leq \frac{M}{2} \|x\|^2 + B\|x\| + A,
\]

and \( M \)-smoothness of \( F_x \) so that \( \Delta F_x \leq M d \), we get

\[
\mathcal{L}_J F^2_x(x) \leq 2\beta^{-1} \left( 2M^2 \|x\|^2 + 2B^2 \right) + 2\beta^{-1} \left( \frac{M}{2} \|x\|^2 + B\|x\| + A \right) Md \\
\leq \frac{8b\beta^{-1}M^2}{m} + 4\beta^{-1}B^2 + \left( \frac{2b\beta^{-1}M}{m} + 2\beta^{-1}B\sqrt{2b/m} + 2\beta^{-1}A \right) Md. 
\tag{F.8}
\]

Hence, for any \( x \in \mathbb{R}^d \), we can compute from (F.7) and (F.8),

\[
\mathcal{L}_J F^2_x(x) \leq -\frac{m^3}{12} \|x\|^4 + \frac{m^3}{12}S^4 + (B + 2A) \beta^{-1}Md \\
+ \frac{8b\beta^{-1}M^2}{m} + 4\beta^{-1}B^2 + \left( \frac{2b\beta^{-1}M}{m} + 2\beta^{-1}B\sqrt{2b/m} + 2\beta^{-1}A \right) Md \\
\leq -\frac{m^3}{12} \|x\|^4 + 3m \left( b + \beta^{-1} + \frac{2(M + B)\beta^{-1}}{m^2} \right)^2 + \frac{8b\beta^{-1}M^2}{m} + 4\beta^{-1}B^2 \\
+ \beta^{-1} \left( B + 2B\sqrt{2b/m} + \frac{2bM}{m} + 4A \right) Md. 
\tag{F.9}
\]

Then using the quadratic bounds for \( F_x \) in (F.3):

\[
\frac{2}{M + B} \left( F_x(x) - \frac{B}{2} - A \right) \leq \|x\|^2 \leq \frac{3}{m} F_x(x) + \frac{3b}{m}. 
\tag{F.10}
\]

we get

\[
2\|x\|^4 + \frac{8(B/2 + A)^2}{(M + B)^2} \geq \left( \|x\|^2 + \frac{2(B/2 + A)}{M + B} \right)^2 \geq \frac{4}{(M + B)^2} F^2_x(x).
\]

Hence, we have

\[
\|x\|^4 \geq \frac{2}{(M + B)^2} F^2_x(x) - \frac{(B + 2A)^2}{(M + B)^2}.
\]

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Then by (F.9), we can compute,

$$
\mathcal{L}_j F^2_z(x) \leq -\frac{m^3}{6(M+B)^2} F^2_z(x) + \frac{m^3(B + 2A)^2}{12(M+B)^2} + 3m \left( b + \beta^{-1} + \frac{2(M+B)\beta^{-1}}{m^2} \right)^2 \\
+ \frac{8b\beta^{-1}M^2}{m} + 4\beta^{-1}B^2 + \beta^{-1} \left( B + 2B\sqrt{2b/m} + \frac{2bM}{m} + 4A \right) Md. \quad (F.11)
$$

Let

$$
\mathcal{L}_j F^2_z(x) \leq -c_1 F^2_z(x) + K_1.
$$

By Itô’s formula, we get

$$
e^{c_1 t} F^2_z(X(t)) = F^2_z(X(0)) + \int_0^t e^{c_1 s} \mathcal{L}_j F^2_z(X(s))ds + \int_0^t e^{c_1 s} F_z(X(s))\nabla F_z(X(s))\sqrt{2\beta^{-1}}dB(s),
$$

(F.12)

By using Corollary 2.4 [CHJ13] in (C.4) and the similar argument in (C.6), we can show

$$
\mathbb{E} \int_0^t \left\| e^{c_1 s} F_z(X(s))\nabla F_z(X(s))\sqrt{2\beta^{-1}} \right\|^2 ds \leq \mathbb{E} \int_0^t e^{2c_1 s} \left\| e^{F_z(X(s))\nabla F_z(X(s))} \right\|^2 2\beta^{-1} ds < \infty.
$$

Hence, the last term in (F.12) is a martingale. Taking expectation for both side, we have

$$
e^{c_1 t} \mathbb{E} F^2_z(X(t)) \leq \mathbb{E} F^2_z(X(0)) + \int_0^t e^{c_1 s} K_1 ds. \quad (F.13)
$$

It implies,

$$
\mathbb{E} F^2_z(X(t)) \leq e^{-c_1 t} \mathbb{E} F^2_z(X(0)) + \frac{K_1(1 - e^{-c_1 t})}{c_1},
$$

taking $t \rightarrow \infty$, we have

$$
\mathbb{E} F^2_z(X(t)) \leq \mathbb{E} F^2_z(X(0)) + \frac{K_1}{c_1}.
$$

Therefore, we have

$$
\mathbb{E} F^2_z(X(t)) \leq F^2_z(x_0) + \frac{(B + 2A)^2}{2} + \frac{18(M + B)^2}{m^2} \left( b + \beta^{-1} + \frac{2(M+B)\beta^{-1}}{m^2} \right)^2 \\
+ \frac{24\beta^{-1}(2bM^2 + mB^2)(M + B)^2}{m^4} + \frac{6\beta^{-1}(M + B)^2}{m^3} \left( B + 2B\sqrt{2b/m} + \frac{2bM}{m} + 4A \right) Md, \quad (F.14)
$$

where $X(0) = x_0 \in \mathbb{R}^d$. Furthermore, we can use the quadratic bound for $F_z$ in (I.3) to get the bound for the first term:

$$
F^2_z(x_0) \leq \left( \frac{M}{2} \| x_0 \|^2 + B\| x_0 \| + A \right)^2 \leq \left( \frac{M}{2} R^2 + BR + A \right)^2.
$$
As a result, we can compute the uniform $L^4$ bound $\mathbb{E}\|X(t)\|^4$ by using the relations in (F.1) and (F.14):

$$\mathbb{E}\|X(t)\|^4 \leq \frac{9}{m^2} \mathbb{E}F_z^2(X(t)) + \frac{9b(M + B)}{m^2} \mathbb{E}\|X(t)\|^2 + \frac{18b}{m^2} \left(\frac{B}{2} + A\right) + \frac{9b^2}{m^2}.$$ 

Hence, we conclude that

$$\mathbb{E}\|X(t)\|^4 \leq \mathcal{D}_c = \frac{9}{m^2} \left(\frac{M}{2} R^2 + BR + A\right)^2 + \frac{9U + 9b(M + B)\mathcal{C}_c}{m^2} + \frac{6M(M + B)^2}{m^3} \left(B + 2B \sqrt{2b/m} + \frac{2bM}{m} + 4A\right) \beta^{-1} d,$$

where

$$U = \frac{(B + 2A)^2}{2} + \frac{18(M + B)^2}{m^2} \left(b + \beta^{-1} + \frac{2(M + B)\beta^{-1}}{m^2}\right)^2 + \frac{24\beta^{-1}(2bM^2 + MB^2)(M + B)^2}{m^4} + 2bB + 2A + b^2.$$

The proof is complete. 

\section{Proof of Lemma 5}

\textbf{Proof.} By following the same arguments as in the proof of Theorem 4 in [HHMS05], we have

\[ \int_{\mathbb{R}^d} |p_{z,J}(t, x, y) - \pi_z(y)| dy \]
\[ \leq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (p_{s,z,J}(x, z)p_{t-s,z,J}(z, y) - 1) \pi_z(z) dz \bigg| \pi_z(y) dy \]
\[ = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (p_{s,z,J}(x, z)p_{t-s,z,J}(y, z) - 1) \pi_z(z) dz \bigg| \pi_z(y) dy \]
\[ = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left\| p_{t-s,z,J}(y, z) p_{s,z,J}(x, z) \pi_z(z) dz - \int_{\mathbb{R}^d} p_{s,z,J}(x, z) \pi_z(z) dz \right\| \pi_z(y) dy \]
\[ \leq \int_{\mathbb{R}^d} \left( \int_{\mathbb{R}^d} |T_{z,J}(t-s)(p_{s,z,J}(x, \cdot))(y) - \pi_z(p_{s,z,J}(x, \cdot))| \pi_z(y) dy \right)^{1/2} \]
\[ \leq C_{z,J} \cdot e^{\|z\| \|T_{z,J}(t-s)(p_{s,z,J}(x, \cdot))(y) - \pi_z(p_{s,z,J}(x, \cdot))\|_2^2} \]
\[ \leq C_{z,J} \cdot e^{\|z\| \|p_{s,z,J}(x, \cdot) - 1\|_2^2} \]

for any given $0 < s < t$, where $C_{z,J}$ is from the spectral inequality (2.2) and $p_{s,z,J}(x, y) := p_{z,J}(s, x, y)/\pi_z(y)$, where $T_{z,J}$ is the adjoint of the semigroup $T_{z,J}$, that is defined as for any $x \in \mathbb{R}^d$ and $s \in \mathbb{R}^+$,

\[ T_{z,J}(s)f(x) = \int_{\mathbb{R}^d} p_{z,J}(s, x, y)f(y) dy. \]
where $T_{z,J}(s) = e^{sL_J}$ and $L_J$ is the corresponding infinitesimal generator.

According to the proof of Theorem 4 in [HHMS05],

$$\|p_{s,z,J}(x,\cdot) - 1\| \leq \|p_{s,z,J}(x,\cdot)\| + 1 \leq \frac{C_{z,J}(N,x)}{\pi_2(B(x,N/2))} + 1,$$

where $C_{z,J}(N,x)$ is the Harnack constant in the following Harnack inequality:

$$\sup_{y \in B(x,N/2)} T_{z,J}(s)f(y) \leq C_{z,J}(N,x) \inf_{y \in B(x,N/2)} T_{z,J}(2s)f(y),$$

for any $x \in \mathbb{R}^d$, $N > 0$, and any $f$ with $\pi_z(f) = 1$ and $f \geq 0$.

By applying Theorem 2.4. in [BRS08], we have

$$\sup_{(y,t) \in Q^*(r)} T_{z,J}(t)f(y) \leq C(d, \alpha, \gamma, \tilde{B}, r) \inf_{(y,t) \in Q(r)} T_{z,J}(t)f(y),$$

where

$$C(d, \alpha, \gamma, \tilde{B}, r) = \exp \left\{ c(d) \left( 1 + \alpha^{-1} + (\alpha^{-1/2} + \alpha^{-1})(\tilde{B}r + \gamma) \right)^2 \right\},$$

for some constant $c(d)$ depending only on $d$, with

$$\alpha = \beta^{-1}, \quad \gamma = \sqrt{\beta^{-1}d}, \quad \tilde{B} = \sup_{y \in Q} \|A_J \nabla F_z(y)\|,$$

where

$$Q(r) = B(x,r) \times (t_0, t_0 + r^2), \quad Q^*(r) = B(x,r) \times (t_0 + 7r^2, t_0 + 8r^2),$$

provided that $x \in Q(3r) \subset Q$, and $Q(r), Q^*(r) \subset Q$, where $Q := B(x,4r) \times (0,1)$, where

$$r = N/2, \quad t_0 = 6r^2,$$

so that

$$s \in (t_0, t_0 + r^2) = (6r^2, 7r^2), \quad 2s \in (t_0 + 7r^2, t_0 + 8r^2) = (13r^2, 14r^2),$$

and we can take

$$s = \frac{27}{4} r^2,$$

and $r = 1/4$ so that $Q(3r), Q(r), Q^*(r) \subset Q$.

\[2\] In [BRS08], it is backward in time, and by taking $t \mapsto -t$, we can apply their result forward in time.
Therefore, we have
\[ C_z,B(N,x) \leq \exp \left\{ c(d) \left( 1 + \beta + (\beta^{1/2} + \beta) \left( \frac{1}{4} \sup_{y \in B(x,1)} \| A_{f_{x}} \| + \sqrt{\beta^{-1}d} \right) \right)^2 \right\} \]
\[ \leq \exp \left\{ c(d) \left( 1 + \beta + (\beta^{1/2} + \beta) \left( \frac{1}{4} \| A_{f_{x}} \| \sup_{y \in B(x,1)} (M\|y\| + B + \sqrt{\beta^{-1}d}) \right) \right)^2 \right\} \]
\[ \leq \exp \left\{ c(d) \left( 1 + \beta + (\beta^{1/2} + \beta) \left( \frac{1}{4} \| A_{f} \| (M\|x\| + M + B) + \sqrt{\beta^{-1}d} \right) \right)^2 \right\}, \quad (G.10) \]

with
\[ N = 2r = \frac{1}{2}. \quad (G.11) \]

Next, let us provide a lower bound for \( \pi_z(B(x,N/2)) \), where \( B(x,r) \) is an \( \mathbb{R}^d \) Euclidean ball centered at \( x \) with radius equals to \( r \). For a fixed \( x \in \mathbb{R}^d \), we can compute
\[ \pi_z(B(x,N/2)) = \frac{1}{\Lambda_z} \int_{\|y-x\| \leq N/2} e^{-\beta F_x(y)} dy = \frac{1}{\Lambda_z} \int_{\|w\| \leq N/2} e^{-\beta F_x(w+x)} dw, \]

In addition, \( F_x \) function has quadratic bounds in Lemma 7,
\[ \frac{m}{3}\|w+x\|^2 - \frac{b}{2}\log 3 \leq F_x(w+x) \leq \frac{M+B}{2}\|w+x\|^2 + \frac{B}{2} + A \leq (M + B) \left(\|w\|^2 + \|x\|^2\right) + \frac{B}{2} + A. \]

It then follows that
\[ \pi_z(B(x,N/2)) \geq \frac{e^{-\beta(M+B)\left(\|x\|^2 + \frac{B}{2} + A\right)}}{\Lambda_z} \int_{\|w\| \leq N/2} e^{-\beta(M+B)\|w\|^2} dw \]
\[ \geq \frac{e^{-\beta(M+B)\left(\|x\|^2 + \frac{B}{2} + A + \frac{N^2}{4}\right)}}{\Lambda_z} \frac{(2\pi)^{d/2}}{\Gamma(d/2 + 1)} \left(\frac{N}{2}\right)^2. \]

The normalized constant \( \Lambda_z \) is bounded by using Gaussian integral and the quadratic bounds for \( F \) in Lemma 7,
\[ \Lambda_z = \int_{\mathbb{R}^d} e^{-\beta F_x(y)} dy \leq e^{\beta b(\log 3)/2} \int_{\mathbb{R}^d} e^{-\frac{m \beta}{2} \|y\|^2} dy \leq \left(\frac{3\pi}{m \beta}\right)^{d/2} e^{\beta b(\log 3)/2}. \]

Therefore, we have
\[ \pi_z(B(x,N/2)) \geq \left(\frac{3\pi}{m \beta}\right)^{-d/2} e^{-\beta b(\log 3)/2} e^{-\beta(M+B)\left(\|x\|^2 + \frac{B}{2} + A + \frac{N^2}{4}\right)} \frac{(2\pi)^{d/2}}{\Gamma(d/2 + 1)} \left(\frac{N}{2}\right)^2. \quad (G.12) \]
Therefore, with \( N = \frac{1}{2}, \ s = \frac{27}{64}, \) we have
\[
\int_{\mathbb{R}^d} |p_{z,J}(t, x, y) - \pi_z(y)|\,dy \leq C_{z,J} \cdot g_{z,J}(|x|) \cdot e^{\lambda_{z,J}t},
\]
(G.13)

where
\[
e^{\lambda_{z,J}|s|}||p_{z,J}(x, \cdot)|| - 1 \leq e^{\lambda_{z,J}\frac{27}{64}} \left( \frac{c(d)(1+\beta+(\beta^{1/2}+\beta)(\frac{1}{2}\|A_J\|(|M\|x|+M+B)+\sqrt{\beta^{-1}d}))^2}{(3\pi/m^3)^{-d/2}e^{-\beta(\log 3)/2}e^{-\beta(M+B)}(||x||^2+\frac{d}{2}+A+\frac{B}{16})} \right)^2 + 1).
\]
(G.14)

Next, let us compute constant \( c(d) \) in \( g_{z,J}(|x|). \) Inferring from the proof of Theorem 2.4 in [BRS08],
\[
c(d) = \tilde{c}(d)C^2(d) = \frac{\log(3 \cdot 2^{d+1})C^2(d)}{\tilde{\lambda}(d)},
\]
where \( C(d) \) is defined in Lemma 2.4 [BRS08], and the last equation from the proof given in section 6 of [AS67] gives the relation between \( C(d) \) and \( d \) as follows:
\[
C(d) = 4\sqrt{2} \cdot 2^{-3d/2}.
\]
(G.15)

Then \( \tilde{\lambda}(d) = \frac{B^2(d, \beta)}{\tilde{\lambda}(d)} \) in Corollary 2.2 [BRS08] follows the well-known Moser lemma in [Mos64]. Inferring from Main Lemma in [Mos64] \(^3\), we get
\[
\tilde{\lambda}(d) = -\log \left( \frac{8\Phi(1)}{1 + M^{2+d}} \right), \quad \text{with} \quad M \geq 2.
\]

And \( \Phi(s) \) is a continuous function which is equal to zero for any \( s \leq 0 \) and it is strictly increasing for any positive \( s. \) For example, [Mos64] takes \( \Phi(s) = \sqrt{s} \) and \( \Phi(s) = \log(1 + s) \) in their proofs. Therefore, we have
\[
\tilde{\lambda}(d) = \log \left( \frac{1 + \tilde{M}^{2+d}}{8\Phi(1)} \right) \geq \tilde{C}_0d,
\]
(G.16)

for some universal constant \( \tilde{C}_0 > 0. \) Therefore, we have
\[
c(d) = \frac{\log(3 \cdot 2^{d+1})C^2(d)}{\tilde{\lambda}(d)} \leq \frac{\log(3 \cdot 2^{d+1})32 \cdot 2^{-3d}}{\tilde{C}_0d} \leq \tilde{C}2^{-3d},
\]
(G.17)

for some universal constant \( \tilde{C} > 0. \)

\(^3\)The discussions from Page 128 to Page 130 [Mos64] indicate that \( 2\varepsilon < \frac{1}{3} \) and \( 0 < \varepsilon < \frac{1}{1 + M^{2+d}} \) with \( \tilde{M} \geq 2. \) We take \( \varepsilon = \frac{1}{4} \) and \( \varepsilon = \frac{1}{2^{d+1}M^{2+d}2} \) here. Also, we can see from Main Lemma and the proof of Theorem 4 in Page 124 [Mos64] that \( \tilde{\lambda}(d) \) in [BRS08] equals to \( \alpha \) in [Mos64] and it follows that \( \Phi(s) = e^{-\lambda(d)s}. \)
Hence, with $N = \frac{1}{2}$ and $s = \frac{27}{64}$, we conclude that

$$
\int \mathbb{R}^d |p_{z,J}(t, x, y) - \pi_z(y)| dy \leq C_{z,J} \cdot g_{z,J}(\| x \|) \cdot e^{\lambda_{z,J} t},
$$

with

$$
g_{z,J}(\| x \|) = e^{\lambda_{z,J} \frac{27}{64}} \left( \frac{16\Gamma\left( \frac{d}{2} + 1 \right) C^2}{\left( \frac{3}{2m^3} \right)^{-d/2} e^{-\beta b (\log^3/2)} e^{-\beta (M+B)(\| x \|^2 + \frac{B}{2} + A + \frac{1}{16})}} + 1 \right),
$$

for some universal constant $\tilde{C} > 0$. The proof is complete.

---

### H Proof of Lemma 6

**Proof.** First, we have the following estimate:

$$
\int \mathbb{R}^d \int_{\| x \| > K} \| x \|^2 |p_{z,J}(t, w, x) - \pi_z(x)| dx \nu_{z,0}(dw)
\leq \int_{\| x \| > K} \| x \|^2 \int \mathbb{R}^d p_{z,J}(t, w, x) \nu_{z,0}(dw) dx + \int_{\| x \| > K} \| x \|^2 \pi_z(dx)
= \int_{\| x \| > K} \| x \|^2 \nu_{z,k\eta}(dx) + \int_{\| x \| > K} \| x \|^2 \pi_z(dx)
\leq \frac{\mathbb{E}_z\| X(k\eta) \|^4}{K^2} + \frac{\mathbb{E}_z\| X(\infty) \|^4}{K^2}
\leq \frac{\mathbb{E}_z\| X(k\eta) \|^4}{K^2} + \limsup_{t \to \infty} \frac{\mathbb{E}_z\| X(t) \|^4}{K^2}
$$

where the first inequality is due the fact that $|a - b| \leq a + b, a, b > 0$, and the second inequality is a result of Chebyshev’s inequality and the stationary distribution of $X(t)$ process is $\pi_z$, and the third inequality follows from Fatou’s lemma. By the uniform $L^4$ bound in Lemma 4, we get

$$
\int \mathbb{R}^d \int_{\| x \| > K} \| x \|^2 |p_{z,J}(t, w, x) - \pi_z(x)| dx \nu_{z,0}(dw) \leq \frac{2D_c}{K^2},
$$

with $D_c$ being a constant for the uniform $L^4$ bound defined in (A.10). Next, we take

$$
K = e^{\lambda_{z,J} |k\eta|/4},
$$

so that

$$
\int \mathbb{R}^d \int_{\| x \| > K} \| x \|^2 |p_{z,J}(t, w, x) - \pi_z(x)| dx \nu_{z,0}(dw) \leq 2D_c e^{-\lambda_{z,J} |k\eta|/2}.
$$
The proof is complete. □

I Supporting Lemmas

This lemma shows that the object function can be upper and lower bounded by the quadratic function.

Lemma 7 (Quadratic bounds, Lemma 2 in [RRT17]). If Assumptions 1 and 2 hold, for all \( x \in \mathbb{R}^d \) and \( z \in \mathcal{Z} \), for some constant \( c \in [0, 1) \),

\[
\|\nabla f(x, z)\| \leq M\|x\| + B, \quad (I.1)
\]

and

\[
\frac{m(1 - c^2)}{2} \|x\|^2 + b \log c \leq f(x, z) \leq \frac{M}{2} \|x\|^2 + B\|x\| + A. \quad (I.2)
\]

For example, if we let \( c = 1/\sqrt{3} \), we can have the quadratic bounds for the object function \( f(x, z) \) as

\[
\frac{m}{3} \|x\|^2 - \frac{b}{2} \log 3 \leq f(x, z) \leq \frac{M}{2} \|x\|^2 + B\|x\| + A. \quad (I.3)
\]

The next lemma implies the equivalence of 2-Wasserstein continuity for functions to weak convergence with the finite second moments.

Lemma 8 (2-Wasserstein continuity for functions of quadratic growth, [PW16]). Let \( \mu, \nu \) be two probability measures on \( \mathbb{R}^d \) with finite second moments, and let \( g := \mathbb{R}^d \to \mathbb{R} \) be a \( C^1 \) function obeying

\[
\|\nabla g(w)\| \leq c_1 \|w\| + c_2, \quad \text{for any} \quad w \in \mathbb{R}^d,
\]

for some constants \( c_1 > 0 \) and \( c_2 > 0 \). Then

\[
\left| \int_{\mathbb{R}^d} gd\mu - \int_{\mathbb{R}^d} gd\nu \right| \leq (c_1 \sigma + c_2)W_2(\mu, \nu),
\]

where

\[
\sigma^2 := \int_{\mathbb{R}^d} \|w\|^2 \mu(dw) \vee \int_{\mathbb{R}^d} \|w\|^2 \nu(dw).
\]

The last lemma shows the uniform stability of the Gibbs measure \( \pi_z \). Fix two \( n \)-truples \( z = (z_1, ..., z_n), \tilde{z} = (\tilde{z}_1, ..., \tilde{z}_n) \) with card \( \{|i : z_i \neq \tilde{z}_i\}| = 1 \) which differ only in a single coordinate. It also implies that for any two different dataset \( z \) and \( \tilde{z} \), the difference between the minimizer of \( F \) for these two datasets can be bounded by selecting the size of the datasets.

Lemma 9 (Uniform stability, see Proposition 12 [RRT17]). For any two \( z, \tilde{z} \in \mathcal{Z}^n \) that differ only in a single coordinate, then

\[
\sup_{z \in \mathcal{Z}} \left| \int_{\mathbb{R}^d} f(x, z)\pi_z(dx) - \int_{\mathbb{R}^d} f(x, z)\pi_{\tilde{z}}(dx) \right| \leq 4 \left( \frac{M^2}{m} (b + d/\beta) + B^2 \right) \beta_{LS} \frac{1}{n},
\]

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with
\[ c_{LS} \leq \frac{2m^2 + 8M^2}{m^2 M \beta} + \frac{1}{\lambda_*} \left( \frac{6M(d + \beta)}{m} + 2 \right), \]
where \( \lambda_* = \lambda_{*, J=0} \) is defined as the uniform spectral gap for the reversible Langevin SDE in (1.5), such that
\[
\lambda_* = \inf_{z \in \mathbb{Z}^n} \inf \left\{ \frac{1}{\lambda_{*, J=0}} \int_{\mathbb{R}^d} \left| \nabla h \right|^2 d\pi_z : h \in C^1(\mathbb{R}^d) \cap L^2(\pi_z), h \neq 0, \int_{\mathbb{R}^d} h d\pi_z = 0 \right\}. \tag{I.4}
\]

Lemma 10. Let \( A_J = I + J \) where \( J \) is a \( d \)-dimensional anti-symmetric matrix, \( J^T = -J \), then
\[
\|A_J\|^2 = 1 + \|J\|^2 \geq 1. \tag{I.5}
\]

Proof. For any \( x \in \mathbb{R}^d \), then we have
\[
\langle A_J x, A_J x \rangle = \langle (I + J)x, (I + J)x \rangle = \|x\|^2 + \|Jx\|^2. \tag{I.6}
\]
where we use the fact \( \langle x, Jx \rangle = \langle -Jx, x \rangle \). Since it holds for any \( x \in \mathbb{R}^d \), we conclude that \( \|A_J\|^2 = 1 + \|J\|^2 \). \qed

\section{J Explicit Dependence of Constants on Key Parameters}

In this section, we discuss explicit dependence of the performance bound of the empirical risk minimization of NSGLD on the parameters \( \beta, d, J, \lambda_{*, J} \) that is summarized in in Section 3.4.

Recall the performance bound of the empirical risk minimization of NSGLD is based on \( I_0(z, J, \varepsilon) + I_1(J, \varepsilon) + I_2 \) from Corollary 2,
\[
I_0(z, J, \varepsilon) := \left[ \left( \frac{M + B}{2} + \frac{B}{2} + A \right) \hat{C}_{z,J} + (M + B)D_{\varepsilon} \right] \cdot \varepsilon,
\]
where \( \hat{C}_{z,J} \) is a constant depending on data set \( z \in \mathbb{Z}^n \) and a \( d \times d \) anti-symmetric matrix \( J \). Then it follows
\[
I_0(z, J, \varepsilon) = \mathcal{O} \left( \hat{C}_{z,J} \varepsilon \right). \tag{J.1}
\]

And
\[
I_1(J, \varepsilon) := \left( M \sqrt{C_d} + B \right) \left( \hat{C}_0 \frac{\varepsilon}{\lambda_{*, J=0}} + \hat{C}_1 \delta^{1/4} \sqrt{2 \log(1/\varepsilon) \|A_J\|} \right) \sqrt{\log \left( \frac{2 \log(1/\varepsilon)}{\lambda_{*, J}} \right)},
\]
with
\[
\hat{C}_0 = \mathcal{O}(\sqrt{\beta} \sqrt{\beta + d}), \quad \hat{C}_1 = \mathcal{O}(\sqrt{\beta}).
\]

\footnote{In [RRT17], their formula for \( \lambda_* \) missed \( \beta^{-1} \) factor.}
By setting the gradient noise \( \delta \) equal to the step size \( \eta \), we get

\[
\mathcal{I}_1(J, \varepsilon) = \tilde{O}\left(\left(\sqrt{\beta} + d \frac{\varepsilon}{\sqrt{\lambda_{*J=0}}}\right) \sqrt{\log\left(\frac{\log(1/\varepsilon)}{\lambda_{*J}}\right)}\right)
\]

\[
= \tilde{O}\left(\sqrt{\beta} + d \frac{\varepsilon}{\sqrt{\lambda_{*J=0}}} \left(\log \log(\varepsilon^{-1}) + \log\left(\frac{1}{\lambda_{*J}}\right)\right)^{1/2}\right)
\]

\[
\leq \tilde{O}\left(\frac{\sqrt{\beta} (\beta + d)}{\sqrt{\lambda_{*J=0}}} \varepsilon\right), \tag{J.2}
\]

where the factor \( \sqrt{\log \log(\varepsilon^{-1})} \) is negligible comparing to other factors, we also used \( \lambda_{*J} > \lambda_{*J=0} \) and \( 1/\lambda_{*J=0} = e^{\tilde{O}(\beta + d)} \) according to [RRT17]. Moreover, for \( \mathcal{I}_2 \), we have

\[
\mathcal{I}_2 = \frac{d}{2\beta} \log\left(\frac{eM}{m} \left(\frac{b\beta}{d} + 1\right)\right) = \tilde{O}\left(\frac{d \log(1 + \beta)}{\beta}\right). \tag{J.3}
\]

Hence, the performance bound for empirical risk minimization of NSGLD is

\[
\tilde{O}\left(\hat{C}_{\vec{x}, J} \varepsilon + \frac{\sqrt{\beta} (\beta + d)}{\sqrt{\lambda_{*J=0}}} \varepsilon + \frac{d \log(1 + \beta)}{\beta}\right). \tag{J.4}
\]