Non-convex Learning via Replica Exchange Stochastic Gradient MCMC

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Abstract

Replica exchange Monte Carlo (reMC), also known as parallel tempering, is an important technique for accelerating the convergence of the conventional Markov Chain Monte Carlo (MCMC) algorithms. However, such a method requires the evaluation of the energy function based on the full dataset and is not scalable to big data. The naive implementation of reMC in mini-batch settings introduces large biases, which cannot be directly extended to the stochastic gradient MCMC (SGMCMC), the standard sampling method for simulating from deep neural networks (DNNs). In this paper, we propose an adaptive replica exchange SGMCMC (reSGMCMC) to automatically correct the bias and study the corresponding properties. The analysis implies an acceleration-accuracy trade-off in the numerical discretization of a Markov jump process in a stochastic environment. Empirically, we test the algorithm through extensive experiments on various setups and obtain the state-of-the-art results on CIFAR10, CIFAR100, and SVHN in both supervised learning and semi-supervised learning tasks.

1. Introduction

The increasing concern for AI safety problems draws our attention to MCMC, which is known for its asymptotic uncertainty quantification (Chen et al., 2015; Teh et al., 2016), and guarantees in non-convex optimizations (Zhang et al., 2017; Raginsky et al., 2017). Traditional MCMC methods have achieved tremendous success. However, the efficient sampling algorithm in DNNs was not well studied until the invention of stochastic gradient Langevin dynamics (SGLD) (Welling and Teh, 2011), which scales up the computation in DNNs by injecting noises to stochastic gradients. Since then, various high-order SGMCMC algorithms have been proposed, which incorporate strategies such as Hamiltonian dynamics (Chen et al., 2014; Ma et al., 2015; Ding et al., 2014), Hessian approximation (Li et al., 2016; Şimşekli et al., 2016), and high-order numerical schemes (Chen et al., 2015; Li et al., 2019) to improve the convergence.

In addition to the high-order algorithms, we can also follow traditional MCMC algorithms combined with simulated annealing (Kirkpatrick et al., 1983), simulated tempering (Marinari and Parisi, 1992), dynamical weighting (Wong and Liang, 1997) or replica exchange Monte Carlo (Swendsen and Wang, 1986; Earl and Deem, 2005). Among these advancements, simulated annealing SGMCMC (Mangoubi and Vishnoi, 2018) and simulated tempering SGMCMC (Lee et al., 2018) show how dynamical temperatures speed up the convergence. However, simulated annealing is very sensitive to the fast-decaying temperatures, and simulated tempering requires a lot on the approximation of the normalizing constant. For the latter, the replica exchange Monte Carlo is easier to analyze and implement and is suitable for parallelism. Specifically, the replica exchange Langevin diffusion utilizes multiple diffusion processes with different temperatures and proposes to swap the processes while training. Intuitively, the high-temperature process acts as a bridge to connect the various modes. As such, the acceleration effect can be theoretically quantified (Dupuis et al., 2012; Chen et al., 2019). However, despite these advantages, a proper replica exchange SGMCMC (reSGMCMC) has long been missing in the deep learning community.

A bottleneck that hinders the development of reSGMCMC is the naive extension of the acceptance-rejection criterion that fails in mini-batch settings. Various attempts (Bardenet et al., 2017; Korattikara et al., 2014) were proposed to solve this issue. However, they introduce biases even with the ideal normality assumption on the noise. Some unbiased estimators (Bhanot and Kennedy, 1985; Beskos et al., 2006) have ever been presented, but the large variance leads to inefficient inference. To remove the bias while maintaining efficiency, Ceperley and Dewing (1999) proposed a corrected criterion under normality assumptions, and Seita et al. (2017); Quiroz et al. (2019) further analyzed the model errors with the asymptotic normality assumptions. However, the above algorithms fail when the required corrections are
time-varying and much larger than the energies as shown in Fig.3(a–b). Consequently, an effective algorithm with the potential to adaptively estimate the corrections and balance between acceleration and accuracy is in great demand.

In this paper, we propose an adaptive replica exchange SGMCMC algorithm via stochastic approximation (SA) (Robbins and Monro, 1951; Liang et al., 2007; Deng et al., 2019), a standard method in adaptive sampling to estimate the latent variable: the unknown correction. The adaptive algorithm not only shows the asymptotic convergence in standard scenarios but also gives a good estimate when the corrections are time-varying and excessively large. We theoretically analyze the discretization error for reSGMCMC in mini-batch settings and show the accelerated convergence in 2-Wasserstein distance. Such analysis sheds light on the use of biased estimates of unknown corrections to obtain a trade-off between acceleration and accuracy. In summary, this algorithm has three main contributions:

1. We propose a novel reSGMCMC to speed up the computations of SGMCMC in DNNs with theoretical guarantees. The theory shows the potential of using biased corrections and a large batch size to obtain better performance.

2. We identify the problem of time-varying corrections in DNNs and propose to adaptively estimate the time-varying corrections, with potential extension to a variety of time-series prediction techniques.

3. We test the algorithm through extensive experiments using various models. It achieves the state-of-the-art results in both supervised learning and semi-supervised learning tasks on CIFAR10, CIFAR100, and SVHN datasets.

2. Preliminaries

A standard sampling algorithm is the Langevin diffusion, which is a stochastic differential equation (SDE) as follows:

\[
d\beta_t^{(1)} = -\nabla U(\beta_t^{(1)}) dt + \sqrt{2\tau_1} dW_t^{(1)},
\]

where \(\beta_t^{(1)} \in \mathbb{R}^d\), \(U(\cdot)\) is the energy function, \(W_t^{(1)} \in \mathbb{R}^d\) is the Brownian motion, and \(\tau_1 > 0\) is the temperature.

Under mild growth conditions on \(U\), the Langevin diffusion \(\{\beta_t^{(1)}\}_{t \geq 0}\) converges to the unique invariant Gibbs distribution \(\pi_{\tau_1}(\beta^{(1)}) \propto e^{-\frac{U(\beta^{(1)})}{\tau_1}}\), where the temperature \(\tau_1\) is crucial for both optimization and sampling of the non-convex energy function \(U\). On the one hand, a high-temperature \(\tau_1\) achieves the exploration effect: the convergence to the flattened Gibbs distribution of the whole domain is greatly facilitated. However, the flattened distribution is less concentrated around the global optima (Raginsky et al., 2017), and the geometric connection to the global minimum is affected (Zhang et al., 2017). On the other hand, a low-temperature \(\tau_1\) leads to the exploitation effect: the solutions explore the local geometry rapidly, but they are more likely to get trapped in local optima, leading to a slow convergence in both optimization and sampling. Therefore, the potential of using a fixed temperature is quite limited.

A powerful algorithm called replica exchange Langevin diffusion (reLD), also known as parallel tempering Langevin diffusion, has been proposed to accelerate the convergence of the SDE as shown in Fig.1. reLD proposes to simulate a high-temperature particle for exploration and a low-temperature particle for exploitation and allows them to swap simultaneously. Now consider the following coupled processes with a higher temperature \(\tau_2 > \tau_1\) and \(W^{(2)}\) independent of \(W^{(1)}\):

\[
\begin{align*}
d\beta_t^{(1)} &= -\nabla U(\beta_t^{(1)}) dt + \sqrt{2\tau_1} dW_t^{(1)} \\
d\beta_t^{(2)} &= -\nabla U(\beta_t^{(2)}) dt + \sqrt{2\tau_2} dW_t^{(2)}. 
\end{align*}
\]

Eq.(2) converges to the invariant distribution with density

\[\pi(\beta^{(1)}, \beta^{(2)}) \propto e^{-\frac{U(\beta^{(1)})}{\tau_1} - \frac{U(\beta^{(2)})}{\tau_2}}.\]

By allowing the two particles to swap, the positions are likely to change from \((\beta_t^{(1)}, \beta_t^{(2)})\) to \((\beta_{t+\Delta t}^{(2)}, \beta_{t+\Delta t}^{(1)})\) with a swapping rate \(rS(\beta_t^{(1)}, \beta_t^{(2)})dt\), where the constant \(r \geq 0\) is the swapping intensity, and \(S(\cdot, \cdot)\) satisfies

\[S(\beta_t^{(1)}, \beta_t^{(2)}) := e^{\frac{1}{\tau_1 - \tau_2} \left(U(\beta^{(1)}) - U(\beta^{(2)})\right)}.
\]

In such a case, reLD is a Markov jump process, which is reversible (Chen et al., 2019) and leads to the same invariant distribution (3).

3. Replica Exchange Stochastic Gradient Langevin Dynamics

The wide adoption of the replica exchange Monte Carlo in traditional MCMC algorithms motivates us to design replica exchange stochastic gradient Langevin dynamics for DNNs, but the straightforward extension of reLD to replica exchange stochastic gradient Langevin dynamics is highly non-trivial (Chen et al., 2014; Ma et al., 2015; Şimşekli et al., 2016). In this section, we will first show that naïve extensions of replica exchange Monte Carlo to SGD (naïve reSGLD) lead to large biases. Afterward, we will present an adaptive replica exchange stochastic gradient Langevin dynamics (reSGLD) that will automatically adjust the bias and yield a good approximation to the correct distribution.
3.1. Naïve reSGLD

We denote the entire data by $D = \{d_i\}_{i=1}^N$, where $d_i$ is a data point. Given the model parameter $\beta$, we consider the following energy function (negative log-posterior)

$$ L(\tilde{\beta}) = -\log p(\tilde{\beta}) - \sum_{i=1}^N \log P(d_i|\tilde{\beta}). \quad (5) $$

where $p(\tilde{\beta})$ is a proper prior and $\sum_{i=1}^N \log P(d_i|\tilde{\beta})$ is the complete data log-likelihood. When the number of data points $N$ is large, it is expensive to evaluate $L(\tilde{\beta})$ directly. Instead, we propose to approximate the energy function with a mini-batch of data $B = \{d_{s_i}\}_{i=1}^n$, where $s_i \in \{1, 2, ..., N\}$. We can easily check that if $B$ is sampled randomly with or without replacement, we obtain the following unbiased estimator of the energy function

$$ \tilde{L}(\tilde{\beta}) = -\log p(\tilde{\beta}) - \frac{N}{n} \sum_{i=1}^n \log P(d_{s_i}|\tilde{\beta}). \quad (6) $$

Let $\tilde{\beta}_k$ denote the estimate of $\tilde{\beta}$ at the $k$-th iteration. Next, SGLD proposes the following iterations:

$$ \tilde{\beta}_{k+1} = \tilde{\beta}_k - \eta_k \nabla \tilde{L}(\tilde{\beta}_k) + 2\eta_k \tau_1 \xi_k, \quad (7) $$

where $\eta_k$ is the learning rate, the stochastic gradient $\nabla \tilde{L}(\tilde{\beta}_k)$ is the unbiased estimator of the exact gradient $\nabla L(\tilde{\beta}_k)$, $\xi_k$ is a standard $d$-dimensional Gaussian vector with mean $0$ and identity covariance matrix. It is known that SGLD asymptotically converges to a unique invariant distribution $\pi(\tilde{\beta}) \propto \exp\left(-L(\tilde{\beta})/\tau_1\right)$ (Teh et al., 2016) as $\eta_k \to 0$. If we simply replace gradients with stochastic gradients in the replica exchange gradient Langevin dynamics, we have

$$ \tilde{\beta}_{k+1}^{(1)} = \tilde{\beta}_k^{(1)} - \eta_k \nabla \tilde{L}(\tilde{\beta}_k^{(1)}) + 2\eta_k \tau_1 \xi_k^{(1)} $$

$$ \tilde{\beta}_{k+1}^{(2)} = \tilde{\beta}_k^{(2)} - \eta_k \nabla \tilde{L}(\tilde{\beta}_k^{(2)}) + 2\eta_k \tau_2 \xi_k^{(2)}. \quad (8) $$

Furthermore, we swap the Markov chains in (8) with the naïve stochastic swapping rate $rS(\tilde{\beta}_{k+1}^{(1)}, \tilde{\beta}_{k+1}^{(2)})\eta_k$:

$$ S(\tilde{\beta}_{k+1}^{(1)}, \tilde{\beta}_{k+1}^{(2)}) = e^{\left(\frac{\tau_1}{\tau_2} - \frac{\tau_2}{\tau_1}\right)(\tilde{L}(\tilde{\beta}_{k+1}^{(1)}) - \tilde{L}(\tilde{\beta}_{k+1}^{(2)}))}. \quad (9) $$

Apparently, the unbiased estimators $\tilde{L}(\tilde{\beta}_{k+1}^{(1)})$ and $\tilde{L}(\tilde{\beta}_{k+1}^{(2)})$ in $S(\tilde{\beta}_{k+1}^{(1)}, \tilde{\beta}_{k+1}^{(2)})$ do not provide an unbiased estimator of $S(\tilde{\beta}_{k+1}^{(1)}, \tilde{\beta}_{k+1}^{(2)})$ after a non-linear transformation as shown in (9), which leads to a large bias.

3.2. Replica Exchange Stochastic Gradient Langevin Dynamics with Correction

A viable MCMC algorithm requires the approximately unbiased estimators of the swapping rates to “satisfy” the detailed balance property (Ceperley and Dewing, 1999; Andrieu and Roberts, 2009; Nicholls et al., 2012) and the weak solution of a Markov jump process with unbiased stochastic coefficients has also been studied in Gyöngy (1986); Bentata and Cont (2012). When we make normality assumption on the stochastic energy $\tilde{L}(\tilde{\beta}) \sim N(L(\tilde{\beta}), \sigma^2)$, it follows

$$ \tilde{L}(\tilde{\beta}^{(1)}) - \tilde{L}(\tilde{\beta}^{(2)}) = L(\tilde{\beta}^{(1)}) - L(\tilde{\beta}^{(2)}) + \sqrt{2}\sigma W_1, \quad (10) $$

where $W_1$ follows the standard normal distribution and can be viewed as a Brownian motion at $t = 1$. Consider the evolution of the stochastic swapping rate $\{\tilde{S}_t\}_t\in[0,1]$ in each swap as a geometric Brownian motion:

$$ \tilde{S}_t = e^{(\frac{\tau_1}{\tau_2} - \frac{\tau_2}{\tau_1})\left(L(\tilde{\beta}^{(1)}) - L(\tilde{\beta}^{(2)})\right) - \left(\frac{\tau_1}{\tau_2} - \frac{\tau_2}{\tau_1}\right)\sigma^2 t + \sqrt{2}\sigma W_t}, \quad (11) $$

Set $\tau_3 = \frac{1}{\tau_1} - \frac{1}{\tau_2}$ and take the partial derivatives of $\tilde{S}_t$

$$ \frac{d\tilde{S}_t}{dt} = -\tau_3^2 \sigma^2 \tilde{S}_t, \quad \frac{d\tilde{S}_t}{dW_t} = \sqrt{2}\tau_3 \sigma \tilde{S}_t, \quad \frac{d^2\tilde{S}_t}{dW_t^2} = 2\tau_3^2 \sigma^2 \tilde{S}_t. $$

Itô’s lemma shows that

$$ d\tilde{S}_t = \left(\frac{d\tilde{S}_t}{dt} + \frac{1}{2} \frac{d^2\tilde{S}_t}{dW_t^2}\right)dt + dW_t $$

$$ = -\tau_3^2 \sigma^2 \tilde{S}_t dt + \sqrt{2}\tau_3 \sigma \tilde{S}_t dW_t. $$

Notice that $\{\tilde{S}_t\}_t\in[0,1]$ is a Martingale and yields the same expectation for $\forall t \in [0, 1]$. By fixing $t = 1$ in (11), we have

$$ \tilde{S}_1 = e^{(\frac{\tau_1}{\tau_2} - \frac{\tau_2}{\tau_1})(L(\tilde{\beta}^{(1)}) - L(\tilde{\beta}^{(2)})) - \left(\frac{\tau_1}{\tau_2} - \frac{\tau_2}{\tau_1}\right)\sigma^2}, \quad (12) $$

where the stochastic swapping rate $\tilde{S}_1$ is an unbiased estimator of $\tilde{S}_0 = e^{(\frac{\tau_1}{\tau_2} - \frac{\tau_2}{\tau_1})(L(\tilde{\beta}^{(1)}) - L(\tilde{\beta}^{(2)}))}$, and the correction term $\left(\frac{\tau_1}{\tau_2} - \frac{\tau_2}{\tau_1}\right)\sigma^2$ aims to remove the bias from the swaps.

An advantage of interpreting the correction term from the perspective of geometric Brownian motion is that we can naturally extend it to geometric Lévy process (Applebaum, 2004), which is more suitable for the heavy-tailed energy (Şişmeleki et al., 2019). Admittedly, the estimation of the tail-index of extreme-value distributions and the correction under Lévy process go beyond the scope of this paper, so we leave it for future works.

3.3. Adaptive Replica Exchange Stochastic Gradient Langevin Dynamics

In reality, the exact variance $\sigma^2$ is hardly known and subject to estimation. The normality assumption may be violated and even no longer time-independent.
3.3.1. FIXED VARIANCE $\sigma^2$

We use stochastic approximation (SA) to adaptively estimate the unknown variance while sampling from the posterior. In each SA step, we obtain an unbiased sample variance $\hat{\sigma}^2$ for the true $\sigma^2$ and update the adaptive estimate $\hat{\sigma}^2_{m+1}$ through

$$
\hat{\sigma}^2_{m+1} = (1 - \gamma_m)\hat{\sigma}^2_m + \gamma_m\hat{\sigma}^2_{m+1},
$$

where $\gamma_m$ is the smoothing factor at the $m$-th SA step. The SA step is updated less frequently than the standard sampling to reduce the computational cost. When the normality assumption holds, we notice that $\hat{\sigma}^2_m = \sum_{i=1}^m \tilde{\sigma}^2_i / m$ when $\gamma_m = \frac{1}{m}$. Following central limit theorem (CLT), we have that $\hat{\sigma}^2_m - \sigma^2 = \mathcal{O}(\frac{1}{\sqrt{m}})$. Inspired by theorem 2 from Chen et al. (2015), we expect that the weak convergence of the adaptive sampling algorithm holds since the bias decreases sufficiently fast ($\frac{1}{m} \sum_{i=1}^m \mathcal{O}(\frac{1}{\sqrt{m}}) \to 0$ as $m \to \infty$).

In practice, the normality assumption is likely to be violated when we use a small batch size $n$, but the unknown distribution asymptotically approximates the normal distribution as $n \to \infty$ and yield a bias $\mathcal{O}(\frac{1}{n})$ in each SA step. Besides, the mini-batch setting usually introduces a very large noise on the estimator of the energy function, which requires a large correction term and leads to almost-zero swapping rates.

To handle this issue, we introduce a correction factor $F$ to reduce the correction term from $\left(\frac{1}{\tau_1} - \frac{1}{\tau_2}\right)\hat{\sigma}^2$ to $\left(\frac{1}{\tau_1} - \frac{1}{F}\right)\hat{\sigma}^2$.

We note that a large $F > 1$ introduces some bias, but may significantly increase the acceleration effect, giving rise to an acceleration-accuracy trade-off in finite time. Now, we show the algorithm in Alg. 1. In addition to simulations of multi-modal distributions, our algorithm can be also combined with simulated annealing (Li et al., 2009; Martino et al., 2016) to accelerate the non-convex optimization and increase the hitting probability to the global optima (Mangoubi and Vishnoi, 2018).

3.3.2. TIME-VARYING VARIANCE $\sigma^2$

In practice, the variance $\sigma^2$ usually varies with time, resulting in time-varying corrections. For example, in the optimization of residual networks on CIFAR10 and CIFAR100 datasets, we notice from Fig. 3(a-b) that the corrections are time-varying. As such, we cannot use a fixed correction anymore to deal with the bias. The treatment for the time-varying corrections includes standard methods for time-series data, and a complete recipe for modeling the data goes beyond our scope. We still adopt the method of stochastic approximation and choose a fixed smoothing factor $\gamma$ so that

$$
\hat{\sigma}^2_{m+1} = (1 - \gamma)\hat{\sigma}^2_m + \gamma\hat{\sigma}^2_{m+1},
$$

Such a method resembles the simple exponential smoothing and acts as robust filters to remove high-frequency noise.

Algorithm 1 Adaptive Replica Exchange Stochastic Gradient Langevin Dynamics Algorithm. For sampling purposes, we fix the temperatures $\tau_1$ and $\tau_2$. For optimization purposes, we keep annealing $\tau_1$ and $\tau_2$ during each epoch. Empirically, a larger $\gamma_m$ tracks the dynamics better but is less robust. The intensity $r$ and $\eta$ are omitted in the corrected swaps.

repeat

**Sampling Step**

$$
\hat{\beta}^{(1)}_{k+1} = \hat{\beta}^{(1)}_k - \eta_k^{(1)}\nabla\hat{L}(\hat{\beta}^{(1)}_k) + \sqrt{2\eta_k^{(1)}\tau_1}\xi_k^{(1)}
$$

$$
\hat{\beta}^{(2)}_{k+1} = \hat{\beta}^{(2)}_k - \eta_k^{(2)}\nabla\hat{L}(\hat{\beta}^{(2)}_k) + \sqrt{2\eta_k^{(2)}\tau_2}\xi_k^{(2)},
$$

**SA Step**

Obtain an unbiased estimate $\hat{\sigma}^2_{m+1}$ for $\sigma^2$.

$$
\hat{\sigma}^2_{m+1} = (1 - \gamma_m)\hat{\sigma}^2_m + \gamma_m\hat{\sigma}^2_{m+1}.
$$

**Swapping Step**

Generate a uniform random number $u \in [0, 1]$.

$$
\hat{S}_1 = e^{\left(\frac{1}{\tau_1} - \frac{1}{\tau_2}\right)\left(L(\hat{\beta}^{(1)}_{k+1}) - L(\hat{\beta}^{(2)}_{k+1}) - \left(\frac{1}{\tau_1} - \frac{1}{\tau_2}\right)\hat{\sigma}^2_{k+1}\right)}.
$$

if $u < \hat{S}_1$ then

Swap $\hat{\beta}^{(1)}_{k+1}$ and $\hat{\beta}^{(2)}_{k+1}$.

end if

until $k = k_{max}$

It can be viewed as a special case of autoregressive integrated moving average (ARIMA) (0,1,1) model but often outperforms the ARIMA equivalents because it is less sensitive to the model selection error (Bossons, 1966). From the regression perspective, this method can be viewed as a zero-degree local polynomial kernel model (Gijbels et al., 1999), which is robust to distributional assumptions.

4. Convergence Analysis

We theoretically analyze the acceleration effect and the accuracy of reSGLD in terms of 2-Wasserstein distance between the Borel probability measures $\mu$ and $\nu$ on $\mathbb{R}^d$

$$
\mathcal{W}_2(\mu, \nu) := \inf_{\Gamma \in \text{Couplings}(\mu, \nu)} \left\| \int ||\beta_\mu - \beta_\nu||^2d\Gamma(\beta_\mu, \beta_\nu) \right\|,
$$

where $\| \cdot \|$ is the Euclidean norm, and the infimum is taken over all joint distributions $\Gamma(\beta_\mu, \beta_\nu)$ with $\mu$ and $\nu$ being its marginal distributions.

Our analysis begins with the fact that reSGLD in Algorithm 1 tracks the replica exchange Langevin diffusion (2). For ease of analysis, we consider a fixed learning rate $\eta$ for both chains. reSGLD can be viewed as a special discretization of the continuous-time Markov jump process. In
particular, it differs from the standard discretization of the continuous-time Langevin algorithms (Chen et al., 2019; Yin and Zhu, 2010; Raginsky et al., 2017; Sato and Naka-
gawa, 2014) in that we need to consider the discretization of the Markov jump process in a stochastic environment. To handle this issue, we follow Dupuis et al. (2012) and view the swaps of positions as swaps of the temperatures, which have been proven equivalent in distribution.

**Lemma 1** (Discretization Error). Given the smoothness and dissipativity assumptions in the appendix, and a small learning rate $\eta$, we have that

$$\mathbb{E}_{\nu_0 \leq k \leq T} \left[ \| \beta_k - \tilde{\beta}_k \|^2 \right] \leq \mathcal{O}(\eta + \max_i \mathbb{E}[\|\phi_i\|^2] + \max_i \sqrt{\mathbb{E}[\psi_i]}),$$

where $\tilde{\beta}_k$ is the continuous-time interpolation for reSGLD, $\phi := \nabla U - \nabla \tilde{U}$ is the noise in the stochastic gradient, and $\psi := S - \tilde{S}$ is the noise in the stochastic swapping rate.

Then we quantify the evolution of the 2-Wasserstein distance between $\nu_t$ and the invariant distribution $\pi$, where $\nu_t$ is the probability measure associated with reLD at time $t$. The key tool is the exponential decay of entropy when $\pi$ satisfies the log-Sobolev inequality (LSI) (Bakry et al., 2014). To justify LSI, we first verify LSI for reLD without swaps, which is a direct result (Cattiaux et al., 2010) given the Lyapunov function criterion and the Poincaré inequality (Chen et al., 2019). Then we verify LSI for reLD with swaps by analyzing the corresponding Dirichlet form, which is strictly larger than the Dirichlet form associated with reLD without swaps. Finally, the exponential decay of the 2-Wasserstein distance follows from the Otto-Villani theorem (Bakry et al., 2014) by connecting 2-Wasserstein distance with the relative entropy.

**Lemma 2** (Accelerated exponential decay of $W_2$). Under the smoothness and dissipativity assumptions, we have that the replica exchange Langevin diffusion converges exponentially fast to the invariant distribution $\pi$:

$$W_2(\nu_t, \pi) \leq D_0 e^{-k \eta(1+\delta_S)/c_{\text{LS}}} \mathcal{O}(\eta + \max_i \mathbb{E}[\|\phi_i\|^2] + \max_i \sqrt{\mathbb{E}[\psi_i]}),$$

where $\delta_S := \inf_{S \geq 0} \frac{\mathcal{E}_S(\sqrt{\frac{ds}{E}})}{E(\sqrt{\frac{ds}{E}})} - 1$ is the very acceleration effect depending on the swapping rate $S$, $E$ and $\mathcal{E}_S$ are the Dirichlet forms defined in the appendix, $c_{\text{LS}}$ is the constant in the log-Sobolev inequality, $D_0 = \sqrt{2c_{\text{LS}} D(\nu_0 || \pi)}$.

Finally, combining the definition of Wasserstein distance and the triangle inequality, we have that

**Theorem 1** (Convergence of reSGLD). Let the smoothness and dissipativity assumptions hold. For the distribution $\{\mu_k\}_{k \geq 0}$ associated with the discrete dynamics $\{\tilde{\beta}_k\}_{k \geq 1}$, we have the following estimates for $k \in \mathbb{N}^+$:

$$W_2(\mu_k, \pi) \leq \frac{D_0 e^{-k \eta(1+\delta_S)/c_{\text{LS}}}}{k} \mathcal{O}(\eta + \max_i \mathbb{E}[\|\phi_i\|^2] + \max_i \mathbb{E}[\|\psi_i\|^2]) + \mathcal{O}(\eta + \max_i \mathbb{E}[\|\phi_i\|^2] + \max_i \mathbb{E}[\|\psi_i\|^2]),$$

where $D_0 = \sqrt{2c_{\text{LS}} D(\mu_0 || \pi)}$, $\delta_S := \inf_{S \geq 0} \frac{\mathcal{E}_S(\sqrt{\frac{ds}{E}})}{E(\sqrt{\frac{ds}{E}})} - 1$.

Ideally, we want to boost the acceleration effect $\delta_S$ by using a larger swapping rate $S$ and increase the accuracy by reducing the mean squared errors $\mathbb{E}[\|\phi_i\|^2]$ and $\mathbb{E}[\|\psi_i\|^2]$. One possible way is to apply a large enough batch size, which may be yet inefficient given a large dataset. Another way is to balance between acceleration and accuracy by tuning the correction factor $F$. In practice, a larger $F$ leads to a larger acceleration effect and also injects more biases.

### 5. Experiments

#### 5.1. Simulations of Gaussian Mixture Distributions

In this group of experiments, we evaluate the acceleration effects and the biases for reSGLD on multi-modal distributions based on different assumptions on the estimators for the energy function. As a comparison, we choose SGLD and the naive reSGLD without corrections as baselines. The learning rates $\eta^{(1)}$ and $\eta^{(2)}$ are both set to 0.03, and the temperatures $T_1$ and $T_2$ are set to 1 and 10, respectively. In particular, SGLD uses the learning rate $\eta^{(1)}$ and the temperature $T_1$. We simulate 100,000 samples from each distribution and propose to estimate the correction every 100 iterations. The correction estimator is calculated based on the variance of 10 samples of $U_1(x)$. The initial correction is set to 100 and the step size $\gamma_m$ for stochastic approximation is chosen as $\frac{1}{m}$. The correction factor $F$ is 1 in the first two examples.

We first demonstrate reSGLD on a simple Gaussian mixture distribution $e^{-U_1(x)} \sim 0.4 N(-3, 0.7^2) + 0.6 N(2, 0.5^2)$, where $U_1(x)$ is the energy function. We assume we can only obtain the unbiased energy estimator $\tilde{U}_1(x) \sim N(U_1(x), 2^2)$ and the corresponding stochastic gradient at each iteration. From Fig.2(a,b), we see that SGLD suffers from the local trap problem and takes a long time to converge. The naive reSGLD algorithm alleviated the local trap problem, but is still far away from the ground truth distribution without a proper correction. The naive reSGLD converges faster than reSGLD in the early phase due to a larger swapping rate, but ends up with a large bias when the training continues. By contrast, reSGLD successfully balances the trade-off between acceleration and accuracy by tuning the correction factor $F$. In practice, a larger $F$ leads to a larger acceleration effect and also injects more biases.
Convergence of Sample Mean

We use the 20, 32, 56-layer ResNet (denoted as ResNet-20, ResNet-32, ResNet-56) and wide ResNet (WRN) as model architectures. We note that the two modes are far away from each other and maintain accuracy, we try momentum stochastic gradient descent, we use stochastic gradient Hamiltonian Monte Carlo (SGHMC) as the baseline estimator is updated each epoch based on the variance counteract the annealing effect of the temperatures. The variance estimator is updated each epoch based on the variance of 10 samples of the stochastic energies and the smoothing factor is set to $\gamma = 0.3$ in (14). Consequently, the computations only increase by less than 5%. In addition, we use a thinning factor 200 and report all the results based on Bayesian model averaging. We repeat every experiment five times to obtain the mean and 2 standard deviations.

We see from Fig.2(c) that reSGLD still gives a good approximation to the ground true distribution while the others don’t.

In the third example, we show a case when the correction factor $F$ is useful. We sample from a Gaussian mixture distribution $e^{-U_3(x)} \sim 0.4N(-6, 0.7^2) + 0.6N(4, 0.5^2)$. We note that the two modes are far away from each other and the distribution is more difficult to simulate. More interestingly, we assume $U_3(x) \sim U_3(x) + 7f(\nu = 10)$, which requires a large correction term and ends up with no swaps in the finite 100,000 iterations at $F = 1$. In such a case, the unbiased algorithm behaves like the ordinary SGLD as in Fig.2(c) and still suffers from the local trap problems. To achieve larger acceleration effects to avoid local traps and maintain accuracy, we try $F$ at 2, 4 and $\infty$ (Inf), where the latter is equivalent to the naïve reSGLD. We see from Fig.2(d) that $F = 2$ shows the best approximations, despite that the swapping rate $S$ is only 0.4%. Further increases on the acceleration effect via larger correction factors $F$ give larger swapping rates (7.1% and 46%) and potentially accelerate the convergence in the beginning. However, the biases become more significant as we increase $F$ and lead to larger errors in the end.

5.2. Optimization of Image Data

We evaluate the adaptive replica exchange Monte Carlo on CIFAR10 and CIFAR100, which consist of 50,000 32 $\times$ 32 RGB images for training and 10,000 images for testing. CIFAR10 and CIFAR100 have 10 classes and 100 classes, respectively. We adopt the well-known residual networks (ResNet) and wide ResNet (WRN) as model architectures. We use the 20, 32, 56-layer ResNet (denoted as ResNet-20, et al.), WRN-16-8 and WRN-28-10, where, for example, WRN-16-8 denotes a ResNet that has 16 layers and is 8 times wider than the original. Inspired by the popular momentum stochastic gradient descent, we use stochastic gradient Hamiltonian Monte Carlo (SGHMC) as the baseline sampling algorithm and use the numerical method proposed by Saatci and Wilson (2017) to reduce the tuning cost. We refer to the momentum stochastic gradient descent algorithm as M-SGD and the adaptive replica exchange SGHMC algorithm as reSGHMC.

We first run several experiments to study the ideal corrections for the optimization of deep neural networks based on the fixed temperatures $\tau_1 = 0.01$ and $\tau_2 = 0.05$. We observe from Fig.(3)(a, b) that the corrections are thousands of times larger than the energy losses, which implies that an exact correction leads to no swaps in practice and no acceleration can be achieved. The desire to obtain more acceleration effects drives us to manually shrink the corrections by increasing $F$ to increase the swapping rates, although we have to suffer from some model bias.

We study the model performance by applying different correction factors $F$. We choose batch-size 256 and run the experiments within 500 epochs. We first tune the optimal hyperparameters for M-SGD, SGHMC and the low-temperature chain of reSGHMC: we set the learning rate $\eta_k^{(1)}$ to 2e-6 in the first 200 epochs and decay it afterward by a factor of 0.984 every epoch; the low temperature follows an annealing schedule $\tau_1 = 0.01$, to accelerate the optimization; the weight decay is set to 25. Then, as to the high-temperature chain of reSGHMC, we use a larger learning rate $\eta_k^{(2)} = 1.5\eta_k^{(1)}$ and a higher temperature $\tau_2 = 5\tau_1$. We set $F$ as $F_0$ in the beginning and then adapt the value to counteract the annealing effect of the temperatures. We use a thinning factor 200 and report all the results based on Bayesian model averaging. We repeat every experiment five times to obtain the mean and 2 standard deviations.
thus a larger acceleration effect, however, the performance still decreases as we increase $F_0$, implying that the biases start to dominate the error and the diminishing marginal improvement on the acceleration effect is no longer significant. We note that there is only one extra hyper-parameter, namely, the correction factor $F$, required to tune, and it is independent of the standard SGHMC. This shows that the tuning cost is acceptable.

| Model   | CIFAR10 | CIFAR100 |
|---------|---------|----------|
|         | M-SGD   | SGHMC    | reSGHMC  | M-SGD   | SGHMC    | reSGHMC  |
| RESNet-20  | 94.21±0.16 | 94.22±0.12 | 94.62±0.18 | 72.45±0.20 | 72.49±0.18 | 74.14±0.22 |
| RESNet-32  | 95.15±0.08 | 95.18±0.06 | 95.35±0.08 | 75.01±0.22 | 75.14±0.28 | 76.55±0.30 |
| RESNet-56  | 96.01±0.08 | 95.95±0.10 | 96.12±0.06 | 78.96±0.32 | 79.04±0.30 | 80.14±0.34 |
| WRN-16-8   | 96.71±0.06 | 96.73±0.08 | 96.87±0.06 | 81.70±0.26 | 82.07±0.22 | 82.95±0.30 |
| WRN-28-10  | 97.33±0.08 | 97.32±0.06 | 97.42±0.06 | 83.79±0.18 | 83.76±0.14 | 84.38±0.18 |

To obtain a comprehensive evaluation of reSGHMC, we use the optimal correction factor for reSGHMC and test it on ResNet20, 32, 56, WRN-16-8 and WRN-28-10. From Table.1, we see that reSGHMC consistently outperforms SGHMC and M-SGD on both datasets, showing the robustness of reSGHMC to various model architectures. For CIFAR10, our method works better with ResNet-20 and ResNet-32 and improves the prediction accuracy by 0.4% and 0.2%, respectively. Regarding the other model architectures, it still slightly outperforms the baselines by roughly 0.1%-0.2%, although this dataset is highly optimized. Specifically, reSGHMC achieves the state-of-the-art 97.42% accuracy with WRN-28-10 model. For CIFAR100, reSGHMC works particularly well based on various model architectures. It outperforms the baseline by as high as 1.5% using ResNet-20 and ResNet-32, and around 1% based on the other architectures. It also achieves the state-of-the-art 84.38% based on WRN-28-10 on CIFAR100.

We also conduct the experiments using larger batch sizes with ResNet-20 and report the results in Table.2. We run the same iterations and keep the other setups the same. We find that a larger batch size significantly boosts the performance of reSGHMC by as much as 0.4% accuracies on CIFAR10 and 1% on CIFAR100, which shows the potential of using a large batch size in the future.

### 5.3. Bayesian GANs for Semi-supervised Learning

Semi-supervised learning (SSL) is an economic machine learning task because it doesn’t require all the data to have pricey labels and still shows promising results. However, the multi-modal problem is more severe in the training of SSLs, such as Bayesian GANs (Saatci and Wilson, 2017), which motivates us to utilize a more powerful algorithm for multi-modal sampling. Therefore, we further evaluate reSGHMC in SSL on CIFAR10, CIFAR100 and the StreetView House Numbers dataset (SVHN)\(^1\) using Bayesian GANs and study how swaps boost the performance.

Regarding the Bayesian GANs used for SSLs, we transform the ordinary discriminator into a K+1-class classifier, where $K$ is the number of classes in each dataset, and $K = 10$ for CIFAR10 and SVHN and $K = 100$ for CIFAR100. During training, a five-layer Bayesian deconvolutional GAN is used as the generator to increase the performance of the

\(^1\)SVHN consists of 73,257 10-class images for training and 26,032 images for testing.
Table 3. Semi-supervised learning on CIFAR10, CIFAR100 and SVHN based on different number of labels.

| $N_s$ | CIFAR10 | CIFAR100 | SVHN  |
|-------|---------|----------|-------|
|       | SGHMC   | reSGHMC  | SGHMC | reSGHMC | SGHMC | reSGHMC |
| 2000  | 74.72±0.39 | 77.73±0.31 | 50.76±0.71 | 55.53±0.64 | 88.75±0.44 | 91.59±0.38 |
| 3000  | 77.96±0.32 | 80.85±0.23 | 53.07±0.71 | 57.09±0.77 | 91.32±0.41 | 94.03±0.36 |
| 4000  | 79.06±0.29 | 81.61±0.24 | 57.05±0.59 | 62.23±0.69 | 91.92±0.41 | 94.25±0.31 |
| 5000  | 81.74±0.36 | 84.67±0.28 | 59.34±0.64 | 64.83±0.72 | 92.63±0.46 | 94.33±0.34 |

Figure 4. reSGHMC versus SGHMC on benchmark datasets in semi-supervised learning.

6. Conclusion and Future Work

We propose the adaptive replica exchange SGMCMC algorithm and prove the accelerated convergence in terms of 2-Wasserstein distance. The theory implies an accuracy-acceleration trade-off and guides us to tune the correction factor $F$ to obtain the optimal performance. We support our theory with extensive experiments and obtain significant improvements over the vanilla SGMCMC algorithms on CIFAR10, CIFAR100, and SVHN.

For future works, it is promising to relax the asymptotic normality assumption to the heavy-tailed generalization of Lévy-stable distribution (Şimşekli et al., 2019) and apply Itô’s lemma to geometric Lévy process to analyze the bias from fat-tailed noises with small batch sizes. Besides, variance reduction (Xu et al., 2018) of the stochastic noise to obtain a larger acceleration effect is also appealing in both theory and practice. From the computational perspective, it is also interesting to study parallel multi-chain reSGMCMC in larger machine learning tasks.
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Supplementary Material for “Non-convex Learning via Replica Exchange Stochastic Gradient MCMC”

In this supplementary material, we prove the convergence in §A and show the experimental setup in §B.

A. Convergence Analysis

A.1. Background

The continuous-time replica exchange Langevin diffusion (reLD) \( \{ \beta_t \}_{t \geq 0} := \left\{ \left( \beta_t^{(1)}, \beta_t^{(2)} \right) \right\} \) is a Markov process compounded with a Poisson jump process. In particular, the Markov process follows the stochastic differential equations

\[
\begin{align*}
\frac{d\beta_t^{(1)}}{dt} &= -\nabla U(\beta_t^{(1)}) dt + \sqrt{2\tau_1} dW_t^{(1)}, \\
\frac{d\beta_t^{(2)}}{dt} &= -\nabla U(\beta_t^{(2)}) dt + \sqrt{2\tau_2} dW_t^{(2)},
\end{align*}
\]

(16)

where \( \beta_t^{(1)}, \beta_t^{(2)} \) are the particles (parameters) at time \( t \) in \( \mathbb{R}^d \), \( W^{(1)}, W^{(2)} \in \mathbb{R}^d \) are two independent Brownian motions, \( U : \mathbb{R}^d \to \mathbb{R} \) is the energy function, \( \tau_1 < \tau_2 \) are the temperatures. The jumps originate from the swaps of particles \( \beta_t^{(1)} \) and \( \beta_t^{(2)} \) and follow a Poisson process where the jump rate is specified as the Metropolis form \( rS(\beta_t^{(1)}, \beta_t^{(2)}) dt \). Here \( r \geq 0 \) is a constant, and \( S \)

\[ S(\beta_t^{(1)}, \beta_t^{(2)}) = e^\left( \frac{1}{\tau_1} - \frac{1}{\tau_2} \right) \left( U(\beta_t^{(1)}) - U(\beta_t^{(2)}) \right). \]

Under such a swapping rate, the probability \( \nu_t \) associated with reLD at time \( t \) is known to converge to the invariant measure (Gibbs distribution) with density

\[ \pi(\beta^{(1)}, \beta^{(2)}) \propto e^{-\frac{\nu(\beta^{(1)})}{\tau_1} - \frac{\nu(\beta^{(2)})}{\tau_2}}. \]

In practice, obtaining the exact energy and gradient for reLD (16) in a large dataset is quite expensive. We consider the replica exchange stochastic gradient Langevin dynamics (reSGLD), which generates iterates \( \{ \tilde{\beta}^{(k)} \}_{k \geq 1} \) as follows

\[
\begin{align*}
\tilde{\beta}^{(1)}(k + 1) &= \tilde{\beta}^{(1)}(k) - \eta \nabla U(\tilde{\beta}^{(1)}(k)) + \sqrt{2\eta \tau_1} \xi^{(1)}_k, \\
\tilde{\beta}^{(2)}(k + 1) &= \tilde{\beta}^{(2)}(k) - \eta \nabla U(\tilde{\beta}^{(2)}(k)) + \sqrt{2\eta \tau_2} \xi^{(2)}_k,
\end{align*}
\]

(17)

where \( \eta \) is considered to be a fixed learning rate for ease of analysis, and \( \xi^{(1)}_k \) and \( \xi^{(2)}_k \) are independent Gaussian random vectors in \( \mathbb{R}^d \). Moreover, the positions of the particles swap based on the stochastic swapping rate. In particular, \( \tilde{S}(\beta^{(1)}, \beta^{(2)}) := S(\beta^{(1)}, \beta^{(2)}) + \psi \), and the stochastic gradient \( \nabla U(\cdot) + \psi \) can be written as \( \nabla U(\cdot) + \phi \), where both \( \psi \) and \( \phi \) are random variables with mean not necessarily zero. We also denote \( \mu_k \) as the probability measure associated with \( \{ \tilde{\beta}^{(k)}(k) \}_{k \geq 1} \) in reSGLD (17) at step \( k \), which is close to \( \nu_{k\eta} \) in a suitable sense.

A.2. Overview of the analysis

We aim to study the convergence analysis of the probability measure \( \mu_k \) to the invariant measure \( \pi \) in terms of 2-Wasserstein distance,

\[ W_2(\mu, \nu) := \inf_{\Gamma \in \text{Couplings}(\mu, \nu)} \int \| \beta_\mu - \beta_\nu \|^2 d\Gamma(\beta_\mu, \beta_\nu), \]

(18)

where \( \| \cdot \| \) is the Euclidean norm, and the infimum is taken over all joint distributions \( \Gamma(\beta_\mu, \beta_\nu) \) with \( \mu \) and \( \nu \) being the marginals distributions.

By the triangle inequality, we easily obtain that for any \( k \in \mathbb{N} \) and \( t = k\eta \), we have

\[ W_2(\mu_k, \pi) \leq W_2(\mu_k, \nu_k) + W_2(\nu_k, \pi). \]

Discretization error Exponential decay
We start with the discretization error first by analyzing how reSGLD (17) tracks the reLD (16) in 2-Wasserstein distance. The critical part is to study the discretization of the Poisson jump process in mini-batch settings. To handle this issue, we follow Dupuis et al. (2012) and view the swaps of positions as swaps of temperatures. Then we apply standard techniques in stochastic calculus (Chen et al., 2019; Yin and Zhu, 2010; Sato and Nakagawa, 2014; Raginsky et al., 2017) to discretize the Langevin diffusion and derive the corresponding discretization error.

Next, we quantify the evolution of the 2-Wasserstein distance between \( \nu_t \) and \( \pi \). The key tool is the exponential decay of entropy (Kullback-Leibler divergence) when \( \pi \) satisfies the log-Sobolev inequality (LSI) (Bakry et al., 2014). To justify LSI, we first verify LSI for reSGLD without swaps, which is a direct result given a proper Lyapunov function criterion (Cattiaux et al., 2010) and the Poincaré inequality (Chen et al., 2019). Then we follow Chen et al. (2019) and verify LSI for reLD with swaps by analyzing the Dirichlet form. Finally, the exponential decay of the 2-Wasserstein distance follows from the Otto-Villani theorem by connecting the 2-Wasserstein distance with the entropy (Bakry et al., 2014).

Before we move forward, we first lay out the following assumptions:

**Assumption 1 (Smoothness).** The energy function \( U(\cdot) \) is \( C \)-smoothness, which implies that there exists a Lipschitz constant \( C \) > 0, such that for every \( x, y \in \mathbb{R}^d \), we have \( \| \nabla U(x) - \nabla U(y) \| \leq C \| x - y \| \). * 

**Assumption 2 (Dissipativity).** The energy function \( U(\cdot) \) is \( (a, b) \)-dissipative, i.e. there exist constants \( a > 0 \) and \( b \geq 0 \) such that \( \forall x \in \mathbb{R}^d, \langle x, \nabla U(x) \rangle \geq a \| x \|^2 - b \). 

Here the smoothness assumption is quite standard in studying the convergence of SGLD, and the dissipativity condition is widely used in proving the geometric ergodicity of dynamic systems (Raginsky et al., 2017; Xu et al., 2018). Moreover, the convexity assumption is not required in our theory.

### A.3. Analysis of discretization error

The key to deriving the discretization error is to view the swaps of positions as swaps of the temperatures, which has been proven equivalent in distribution (Dupuis et al., 2012). Therefore, we model reLD using the following SDE,

\[
d\beta_t = -\nabla G(\beta_t) dt + \Sigma_t dW_t,
\]

where \( G(\beta_t) = \begin{pmatrix} U(\beta_t^{(1)}) \\ U(\beta_t^{(2)}) \end{pmatrix} \), \( W \in \mathbb{R}^{2d} \) is a Brownian motion, \( \Sigma_t \) is a random matrix in continuous-time that swaps between the diagonal matrices \( M_1 = \begin{pmatrix} \sqrt{2\tau_1} I_d & 0 \\ 0 & \sqrt{2\tau_2} I_d \end{pmatrix} \) and \( M_2 = \begin{pmatrix} \sqrt{2\tau_2} I_d & 0 \\ 0 & \sqrt{2\tau_1} I_d \end{pmatrix} \) with probability \( rS(\beta_t^{(1)}, \beta_t^{(2)}) dt \), and \( I_d \in \mathbb{R}^{d \times d} \) is denoted as the identity matrix.

Moreover, the corresponding discretization of replica exchange SGLD (reSGLD) follows:

\[
\tilde{\beta}^n(k + 1) = \tilde{\beta}^n(k) - \eta \nabla G(\tilde{\beta}^n(k)) + \sqrt{\eta} \tilde{\Sigma}^n(k) \xi_k,
\]

where \( \xi_k \) is a standard Gaussian distribution in \( \mathbb{R}^{2d} \), and \( \tilde{\Sigma}^n(k) \) is a random matrix in discrete-time that swaps between \( M_1 \) and \( M_2 \) with probability \( rS(\tilde{\beta}^{(1)}(k), \tilde{\beta}^{(2)}(k)) \). We denote \( \{ \tilde{\beta}^n_t \}_{t \geq 0} \) as the continuous-time interpolation of \( \{ \tilde{\beta}^n(k) \}_{k \geq 1} \), which satisfies the following SDE,

\[
\tilde{\beta}^n_t = \tilde{\beta}_0 - \int_0^t \nabla G(\tilde{\beta}^n_{s/\eta}) ds + \int_0^t \tilde{\Sigma}^n_{s/\eta} dW_s.
\]

Here the random matrix \( \tilde{\Sigma}^n_{s/\eta} \) follows a similar trajectory as \( \tilde{\Sigma}^n(s/\eta) \). For \( k \in \mathbb{N}^+ \) with \( t = k\eta \), the relation \( \tilde{\beta}^n_t = \tilde{\beta}^n_{k\eta} = \tilde{\beta}^n(k) \) follows.

**Lemma 3 (Discretization error).** Given the smoothness and dissipativity assumptions (1) and (2), and the learning rate \( \eta \) satisfying \( 0 < \eta < 1 \land a/C^2 \), there exist constants \( D_1, D_2 \) and \( D_3 \) such that

\[
\mathbb{E}[ \sup_{0 \leq t \leq T} \| \beta_t - \tilde{\beta}^n_t \|^2 ] \leq D_1 \eta + D_2 \max_k \mathbb{E}[ \| \phi_k \|^2 ] + D_3 \max_k \sqrt{\mathbb{E}[ \| \psi_k \|^2 ]},
\]

where \( D_1 \) depends on \( \tau_1, \tau_2, d, T, C, a, b; D_2 \) depends on \( T \) and \( C; D_3 \) depends on \( r, d, T \) and \( C \).
Non-convex Learning via Replica Exchange Stochastic Gradient MCMC

**Proof** Based on the replica exchange Langevin diffusion \( \{\beta_t\}_{t \geq 0} \) and the continuous-time interpolation of the stochastic gradient Langevin diffusion \( \{\tilde{\beta}_t^n\}_{t \geq 0} \), we have the following SDE for the difference \( \beta_t - \tilde{\beta}_t^n \). For any \( t \in [0, T] \), we have

\[
\beta_t - \tilde{\beta}_t^n = -\int_0^t (\nabla G(\beta_s) - \nabla G(\tilde{\beta}_s^n))ds + \int_0^t (\Sigma_s - \Sigma_{[s/\eta]}^n)dW_s
\]

Indeed, note that

\[
\sup_{0 \leq t \leq T} \|\beta_t - \tilde{\beta}_t^n\| \leq \int_0^T \|\nabla G(\beta_s) - \nabla G(\tilde{\beta}_s^n)\|ds + \sup_{0 \leq t \leq T} \|\int_0^t (\Sigma_s - \Sigma_{[s/\eta]}^n)dW_s\|
\]

We first square both sides and take expectation, then apply the Burkholder-Davis-Gundy inequality and Cauchy-Schwarz inequality, we have

\[
\mathbb{E}[\sup_{0 \leq t \leq T} \|\beta_t - \tilde{\beta}_t^n\|^2] \leq 2\mathbb{E} \left[ \left( \int_0^T \|\nabla G(\beta_s) - \nabla G(\tilde{\beta}_s^n)\|ds \right)^2 + \sup_{0 \leq t \leq T} \|\int_0^t (\Sigma_s - \Sigma_{[s/\eta]}^n)dW_s\|^2 \right] 
\]

\[
\leq 2T \mathbb{E} \left[ \int_0^T \|\nabla G(\beta_s) - \nabla G(\tilde{\beta}_s^n)\|^2 ds \right] + 8\mathbb{E} \left[ \int_0^T \|\Sigma_s - \Sigma_{[s/\eta]}^n\|^2 ds \right] 
\]

(23)

**Estimate of stochastic gradient:** For the first term \( I \), by using the inequality

\[
\|a + b + c\|^2 \leq 3(\|a\|^2 + \|b\|^2 + \|c\|^2),
\]

we get

\[
I = 2T \mathbb{E} \left[ \int_0^T \left( \|\nabla G(\beta_s) - \nabla G(\tilde{\beta}_s^n)\| + \|\nabla G(\tilde{\beta}_s^n) - \nabla G(\tilde{\beta}_{[s/\eta]}^n)\| \right)^2 ds \right] 
\]

\[
\leq 6T \mathbb{E} \left[ \int_0^T \|\nabla G(\beta_s) - \nabla G(\tilde{\beta}_s^n)\|^2 ds \right] + 6T \mathbb{E} \left[ \int_0^T \|\nabla G(\tilde{\beta}_s^n) - \nabla G(\tilde{\beta}_{[s/\eta]}^n)\|^2 ds \right] 
\]

\[
+ 6T \mathbb{E} \left[ \int_0^T \|\nabla G(\tilde{\beta}_{[s/\eta]}^n) - \nabla G(\tilde{\beta}_{1/\eta}^n)\|^2 ds \right] 
\]

\[
\leq I_1 + I_2 + I_3. 
\]

(24)

By using the smoothness assumption 1, we first estimate

\[
I_1 \leq 6T C^2 \mathbb{E} \left[ \int_0^T \|\beta_s - \tilde{\beta}_s^n\|^2 ds \right]
\]

By applying the smoothness assumption 1 and discretization scheme, we can further estimate

\[
I_2 \leq 6T C^2 \mathbb{E} \sum_{k=0}^{[T/\eta]} \int_{k\eta}^{(k+1)\eta} \|\tilde{\beta}_s^n - \tilde{\beta}_{[s/\eta]}^n\|^2 ds 
\]

\[
\leq 6T C^2 \sum_{k=0}^{[T/\eta]} \mathbb{E} \int_{k\eta}^{(k+1)\eta} \|\tilde{\beta}_s^n - \tilde{\beta}_{[s/\eta]}^n\|^2 ds 
\]

\[
\leq 6T C^2 \sum_{k=0}^{[T/\eta]} \int_{k\eta}^{(k+1)\eta} \mathbb{E} \left[ \sup_{k\eta \leq s < (k+1)\eta} \|\tilde{\beta}_s^n - \tilde{\beta}_{[s/\eta]}^n\|^2 \right] ds 
\]

(25)
For $\forall k \in \mathbb{N}$ and $s \in [k\eta, (k+1)\eta)$, we have

$$\tilde{\beta}_s^\eta - \tilde{\beta}_{(s/\eta)\eta}^\eta = \tilde{\beta}_s^\eta - \tilde{\beta}_{k\eta}^\eta = -\nabla \tilde{G}(\tilde{\beta}_{k\eta}^\eta) \cdot (s - k\eta) + \tilde{\Sigma}_{k\eta}^\eta \int_{k\eta}^s dW_r$$

which indeed implies

$$\sup_{k\eta \leq s \leq (k+1)\eta} \|\tilde{\beta}_s^\eta - \tilde{\beta}_{(s/\eta)\eta}^\eta\| \leq \|\nabla \tilde{G}(\tilde{\beta}_{k\eta}^\eta)\|(s - k\eta) + \sup_{k\eta \leq s \leq (k+1)\eta} \|\tilde{\Sigma}_{k\eta}^\eta \int_{k\eta}^s dW_r\|$$

Similar to the estimate (23), square both sides and take expectation, then apply the Burkholder-Davis-Gundy inequality, we have

$$\mathbb{E}\left[\sup_{k\eta \leq s \leq (k+1)\eta} \|\tilde{\beta}_s^\eta - \tilde{\beta}_{(s/\eta)\eta}^\eta\|^2\right] \leq 2\mathbb{E}\|\nabla \tilde{G}(\tilde{\beta}_{k\eta}^\eta)\|^2(s - k\eta)^2 + 8\sum_{j=1}^{2d}\mathbb{E}\left[\|\tilde{\Sigma}_{k\eta}^\eta(j)\|\int_{k\eta}^1 dW_r\|^2\right]$$

$$\leq 2(s - k\eta)^2\mathbb{E}\|\nabla \tilde{G}(\tilde{\beta}_{k\eta}^\eta)\|^2 + 32d\tau_2(s - k\eta),$$

where the last inequality follows from the fact that $\tilde{\Sigma}_{k\eta}^\eta$ is a diagonal matrix with diagonal elements $\sqrt{2\tau_1}$ or $\sqrt{2\tau_2}$. For the first term in the above inequality, we further have

$$2(s - k\eta)^2\mathbb{E}\|\nabla \tilde{G}(\tilde{\beta}_{k\eta}^\eta)\|^2 = 2(s - k\eta)^2\mathbb{E}\|\nabla G(\tilde{\beta}_{k\eta}^\eta) + \phi_k\|^2$$

$$\leq 4\eta^2\mathbb{E}\|\nabla G(\tilde{\beta}_{k\eta}^\eta) - \nabla G(\beta^*)\|^2 + \|\phi_k\|^2$$

$$\leq 8C^2\eta^2\mathbb{E}\|\tilde{\beta}_{k\eta}^\eta\|^2 + \|\beta^*\|^2 + 4\eta^2\mathbb{E}\|\phi_k\|^2,$$

where the first inequality follows from the separation of the noise from the stochastic gradient and the choice of stationary point $\beta^*$ of $G(\cdot)$ with $\nabla G(\beta^*) = 0$, and $\phi_k$ is the stochastic noise in the gradient at step $k$. Thus, combining the above two parts and integrate $\mathbb{E}\left[\sup_{k\eta \leq s \leq (k+1)\eta} \|\tilde{\beta}_s^\eta - \tilde{\beta}_{(s/\eta)\eta}^\eta\|^2\right]$ on the time interval $[k\eta, (k+1)\eta)$, we obtain the following bound

$$\int_{k\eta}^{(k+1)\eta} \mathbb{E}\left[\sup_{k\eta \leq s \leq (k+1)\eta} \|\tilde{\beta}_s^\eta - \tilde{\beta}_{(s/\eta)\eta}^\eta\|^2\right] ds \leq 8C^2\eta^3 \left(\sup_{k\geq 0} \mathbb{E}\|\tilde{\beta}_{k\eta}^\eta\|^2 + \|\beta^*\|^2\right) + 4\eta^3\max_k \mathbb{E}\|\phi_k\|^2 + 32d\tau_2\eta^2$$

(26)

By plugging the estimate (26) into estimate (25), we obtain the following estimates when $\eta \leq 1$,

$$\mathcal{I}_2 \leq 6TC^2 (1 + T/\eta) \left[8C^2\eta^3 \left(\sup_{k\geq 0} \mathbb{E}\|\tilde{\beta}_{k\eta}^\eta\|^2 + \|\beta^*\|^2\right) + 4\eta^3\max_k \mathbb{E}\|\phi_k\|^2 + 32d\tau_2\eta^2\right]$$

$$\leq \hat{d}_1(\tau_2, T, C, a, b)\eta + 24TC^2 (1 + T) \max_k \mathbb{E}\|\phi_k\|^2,$$

(27)

where $\hat{d}_1(\tau_2, T, C, a, b)$ is a constant depending on $d, \tau_2, T, C, a$ and $b$. Note that the above inequality requires a result on the bounded second moment of $\sup_{k>0} \mathbb{E}\|\tilde{\beta}_{k\eta}^\eta\|^2$, and this is majority proved in Lemma C.2 in Chen et al. (2019) when we choose the stepsize $\eta \in (0, a/C^2)$. We are now left to estimate the term $\mathcal{I}_3$ and we have

$$\mathcal{I}_3 \leq 6T \sum_{k=0}^{\lfloor T/\eta\rfloor} \mathbb{E}\left[\int_{k\eta}^{(k+1)\eta} \|\nabla \tilde{G}(\tilde{\beta}_{k\eta}^\eta) - \nabla \tilde{G}(\tilde{\beta}_{k\eta}^\eta)\|^2 ds\right]$$

$$\leq 6T(1 + T/\eta) \max_k \mathbb{E}\|\phi_k\|^2 \eta$$

$$\leq 6T(1 + T) \max_k \mathbb{E}\|\phi_k\|^2.$$

1The slight difference is that the constant in the RHS of (C.38) Chen et al. (2019) is changed to account for the stochastic noise.
We estimate $\hat{J}$ noise generated from mini-batch settings and is defined as below

$$
\hat{J} = \frac{1}{2} \sum_{s=1}^{T} \sum_{k=0}^{T/\eta} \mathbb{E} \left[ \left\| \Sigma_s(j) - \Sigma_{[s/\eta]}(j) \right\|^2 \right] ds
$$

Combing all the estimates of $I_1, I_2$ and $I_3$, we obtain

$$
I \leq 6TC^2 \int_0^T \mathbb{E} \left[ \sup_{0 \leq s \leq T} \left\| \beta_s - \beta_s^\eta \right\|^2 \right] ds + \hat{J}_1(d, \tau_2, T, C, a, b)\eta + 24TC^2(1 + T) \max_k \mathbb{E}[\|\phi_k\|^2]
$$

$$
+ 6T(1 + T) \max_k \mathbb{E}[\|\phi_k\|^2].
$$

Estimate of stochastic diffusion: For the second term $\mathcal{J}$, we have

$$
\mathcal{J} = 8\mathbb{E} \left[ \int_0^T \left\| \Sigma_s(j) - \Sigma_{[s/\eta]}(j) \right\|^2 ds \right]
$$

$$
\leq 8 \sum_{j=1}^{2d} \sum_{k=0}^{[T/\eta]} \int_{k\eta}^{(k+1)\eta} \mathbb{E} \left[ \left\| \Sigma_s(j) - \Sigma_{k\eta}(j) \right\|^2 \right] ds
$$

$$
\leq 8 \sum_{j=1}^{2d} \sum_{k=0}^{[T/\eta]} \int_{k\eta}^{(k+1)\eta} \mathbb{E} \left[ \left\| \Sigma_s(j) - \Sigma_{k\eta}(j) + \Sigma_{k\eta}(j) - \Sigma_{k\eta}(j) \right\|^2 \right] ds
$$

$$
\leq 16 \sum_{j=1}^{2d} \sum_{k=0}^{[T/\eta]} \int_{k\eta}^{(k+1)\eta} \mathbb{E} \left[ \left\| \Sigma_s(j) - \Sigma_{k\eta}(j) \right\|^2 \right] ds + \int_{k\eta}^{(k+1)\eta} \mathbb{E} \left[ \left\| \Sigma_{k\eta}(j) - \Sigma_{k\eta}(j) \right\|^2 \right] ds
$$

where $\Sigma_{k\eta}$ is the temperature matrix for the continuous-time interpolation of $\{\beta^n(k)\}_{k \geq 1}$, which is similar to (21) without noise generated from mini-batch settings and is defined as below

$$
\beta^n = \beta_0 - \int_0^t \nabla G(\beta^n_k)ds + \int_0^t \Sigma_{k\eta}W_k.
$$

We estimate $\mathcal{J}_1$ first, considering that $\Sigma_s$ and $\Sigma_{[s/\eta]}$ are both diagonal matrices, we have

$$
\mathcal{J}_1 = 4(\sqrt{T_2} - \sqrt{T_1})^2 \int_{k\eta}^{(k+1)\eta} \mathbb{P}(\Sigma_s(j) \neq \Sigma_{k\eta}(j)) ds
$$

$$
= 4(\sqrt{T_2} - \sqrt{T_1})^2 \mathbb{E} \left[ \int_{k\eta}^{(k+1)\eta} \mathbb{P}(\Sigma_s(j) \neq \Sigma_{k\eta}(j)|\beta_{k\eta}) ds \right]
$$

$$
= 4(\sqrt{T_2} - \sqrt{T_1})^2 r \int_{k\eta}^{(k+1)\eta} [(s - k\eta) + R(s - k\eta)] ds
$$

$$
\leq \delta_2(r, \tau_1, \tau_2)\eta^2,
$$

where $\delta_2(r, \tau_1, \tau_2) = 4(\sqrt{T_2} - \sqrt{T_1})^2 r$, and the equality follows from the fact that the conditional probability $\mathbb{P}(\Sigma_s(j) \neq \Sigma_{k\eta}(j)|\beta_{k\eta}) = rS(\beta_{k\eta}^{(1)}, \beta_{k\eta}^{(2)}) \cdot (s - \eta) + R(s - k\eta)$. Here $R(s - k\eta)$ denotes the higher remainder with respect to $s - k\eta$. The estimate of $\mathcal{J}_1$ without stochastic gradient for the Langevin diffusion is first obtained in Chen et al. (2019), we however present here again for reader’s convenience. As for the second term $\mathcal{J}_2$, it follows that

$$
\mathcal{J}_2 = 4(\sqrt{T_2} - \sqrt{T_1})^2 \int_{k\eta}^{(k+1)\eta} \mathbb{P}(\Sigma_{k\eta}(j) \neq \Sigma_{k\eta}(j)) ds
$$

$$
= 4(\sqrt{T_2} - \sqrt{T_1})^2 \mathbb{E} \left[ \left| S(\beta_{k\eta}^{(1)}, \beta_{k\eta}^{(2)}) - S(\beta_{k\eta}^{(1)}, \beta_{k\eta}^{(2)}) \right| \right]
$$

$$
\leq \delta_2(r, \tau_1, \tau_2)\eta \mathbb{E} \left[ \left| S(\beta_{k\eta}^{(1)}, \beta_{k\eta}^{(2)}) - S(\beta_{k\eta}^{(1)}, \beta_{k\eta}^{(2)}) \right|^2 \right]
$$

$$
\leq \delta_2(r, \tau_1, \tau_2)\eta \mathbb{E} \left[ \|\phi_k\|^2 \right],
$$

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where $\psi_k$ is the noise in the swapping rate. Thus, one concludes the following estimates combing $I$ and $J$.

\[
\mathbb{E}[\sup_{0 \leq t \leq T} \|\beta_t - \tilde{\beta}_t^q\|_2^2] \leq 6TC^2 \int_0^T \mathbb{E} \left[ \sup_{0 \leq s \leq T} \|\beta_s - \tilde{\beta}_s^q\|_2^2 \right] ds + \tilde{\delta}_1(t, \tau_2, T, C, a, b) \eta + 24TC^2(\eta + T) \max_k \mathbb{E}[\|\phi_k\|_2^2]
\]

\[+ 6T(1 + T)\mathbb{E}[\|\phi_k\|_2^2] + 32d(1 + T)\tilde{\delta}_2(r, \tau_1, \tau_2) \left( \eta + \max_k \sqrt{\mathbb{E}[\|\psi_k\|_2^2]} \right). \]

(33)

Apply Gronwall’s inequality to the function

\[t \mapsto \mathbb{E} \left[ \sup_{0 \leq u \leq t} \|\beta_u - \tilde{\beta}_u^q\|_2^2 \right],\]

and deduce that

\[
\mathbb{E}[\sup_{0 \leq t \leq T} \|\beta_t - \tilde{\beta}_t^q\|_2^2] \leq D_1 \eta + D_2 \max_k \mathbb{E}[\|\phi_k\|_2^2] + D_3 \max_k \sqrt{\mathbb{E}[\|\psi_k\|_2^2]},
\]

(34)

where $D_1$ is a constant depending on $\tau_1, \tau_2, d, T, C, a, b$; $D_2$ depends on $T$ and $C$; $D_3$ depends on $r, d, T$ and $C$.

\[\square\]

A.4. Exponential decay of Wasserstein distance in continuous-time

We proceed to quantify the evolution of the 2-Wasserstein distance between $\nu_t$ and $\pi$. We first consider the ordinary Langevin diffusion without swaps and derive the log-Sobolev inequality (LSI). Then we extend LSI to reLD and obtain the exponential decay of the relative entropy. Finally, we derive the exponential decay of the 2-Wasserstein distance.

In order to distinguish from the replica exchange Langevin diffusion $\beta_t$ defined in (19), we call it $\hat{\beta}_t$ which follows,

\[
d\hat{\beta}_t = -\nabla G(\hat{\beta}_t) dt + \Sigma_t dW_t.
\]

(35)

where $\Sigma_t \in \mathbb{R}^{2d \times 2d}$ is a diagonal matrix with the form $\begin{pmatrix} \sqrt{2\tau_1}I_d & 0 \\ 0 & \sqrt{2\tau_2}I_d \end{pmatrix}$. The process $\hat{\beta}_t$ is a Markov diffusion process with infinitesimal generator $\mathcal{L}$ in the following form, for $x_1 \in \mathbb{R}^d$ and $x_2 \in \mathbb{R}^d$,

\[
\mathcal{L} = -\langle \nabla_{x_1} f(x_1, x_2), \nabla U(x_1) \rangle + \tau_1 \Delta_{x_1} f(x_1, x_2) - \langle \nabla_{x_2} f(x_1, x_2), \nabla U(x_2) \rangle + \tau_2 \Delta_{x_2} f(x_1, x_2)
\]

Note that since matrix $\Sigma_t$ is a non-degenerate diagonal matrix, operator $\mathcal{L}$ is an elliptic diffusion operator. According to the smoothness assumption (1), we have that $\nabla^2 G \geq -C I_{2d}$, where $C > 0$, the unique invariant measure $\pi$ associate with the underlying diffusion process satisfies the Poincare inequality and LSI with the Dirichlet form given as follows,

\[
\mathcal{E}(f) = \int \left( \tau_1 \|\nabla_{x_1} f\|^2 + \tau_2 \|\nabla_{x_2} f\|^2 \right) d\pi(x_1, x_2), \quad f \in C_0^2(\mathbb{R}^{2d}).
\]

(36)

In this elliptic case with $G$ being convex, the proof for LSI follows from standard Bakry-Émery calculus (Bakry and Émery, 1985). Since, we are dealing with the non-convex function $G$, we are particularly interested in the case of $\nabla^2 G \geq -C I_{2d}$. To obtain a Poincaré inequality for invariant measure $\pi$, Chen et al. (2019) adapted an argument from Bakry et al. (2008) and Raginsky et al. (2017) by constructing an appropriate Lyapunov function for the replica exchange diffusion without swapping $\hat{\beta}_t$. Denote $\nu_t$ as the distribution associated with the diffusion process $\{\beta_t\}_{t \geq 0}$, which is absolutely continuous with respect to $\pi$. It is a direct consequence of the aforementioned results that the following log-Sobolev inequality holds.

**Lemma 4** (LSI for Langevin Diffusion). Under assumptions (1) and (2), we have the following log-Sobolev inequality for invariant measure $\pi$, for some constant $c_{LS} > 0$,

\[
D(\nu_t||\pi) \leq 2c_{LS} \mathcal{E}(\sqrt{\frac{d\nu_t}{d\pi}}).
\]

where $D(\nu_t||\pi) = \int d\nu_t \log \frac{d\nu_t}{d\pi}$ denotes the relative entropy and the Dirichlet form $\mathcal{E}(\cdot)$ is defined in (36).
We are now ready to prove the log-Sobolev inequality for invariant measure associated with the replica exchange Langevin diffusion (19) under the invariant measure \( \pi \). According to Theorem 3.3 (Chen et al., 2019), the Dirichlet form associated with operator \( \mathcal{L} \) has the form
\[
\mathcal{L}(f) = \mathcal{L}_{\mathcal{S}}(f) + \frac{r}{2} \int S(x_1, x_2) \cdot (f(x_2, x_1) - f(x_1, x_2))^2 d\pi(x_1, x_2), \quad f \in C_0^2(\mathbb{R}^{2d}),
\]
where \( \mathcal{L}_{\mathcal{S}} \) is the Dirichlet form associated with the replica exchange Langevin diffusion converges exponentially fast to the invariant distribution \( \pi \). 

According to Theorem 3.3 (Chen et al., 2019), the sufficient conditions to establish LSI are:

1. There exists some constant \( C \geq 0 \), such that \( \nabla^2 G \succeq -C I_{2d} \).

2. \( \pi \) satisfies a Poincaré inequality with constant \( c_p \), namely, for all probability measures \( \nu \ll \pi \), \( \chi^2(\nu \| \pi) \leq c_p \mathcal{E}(\sqrt{\frac{d\nu}{d\pi}}) \), where \( \chi^2(\nu \| \pi) := \| \frac{d\nu}{d\pi} - 1 \|^2 \) is the \( \chi^2 \) divergence between \( \nu \) and \( \pi \).

3. There exists a \( C^2 \) Lyapunov function \( V : \mathbb{R}^{2d} \to [1, \infty) \) such that \( \mathcal{E}_{\mathcal{S}}(x, x) \leq \kappa - \gamma (\| x_1 \|^2 + \| x_2 \|^2) \) for all \( (x_1, x_2) \in \mathbb{R}^{2d} \) and some \( \kappa, \gamma > 0 \).

Note that the first condition on the Hessian is obtained from the smoothness assumption (1). Moreover, the Poincaré inequality in the second condition is derived from Lemma C.1 in Chen et al. (2019) given assumptions (1) and (2).

Finally, to verify the third condition, we follow Raginsky et al. (2017) and construct the Lyapunov function \( V(x_1, x_2) := \exp \left\{ a/4 \cdot \left( \frac{\| x_1 \|^2}{\tau^2_1} + \frac{\| x_2 \|^2}{\tau^2_2} \right) \right\} \). From the dissipative assumption 2, \( V(x_1, x_2) \) satisfies the third condition because
\[
\mathcal{L}(V(x_1, x_2)) = \left( \frac{a}{2\tau_1} + \frac{a}{2\tau_2} + \frac{a^2}{4\tau_1^2} \| x_1 \|^2 + \frac{a^2}{4\tau_2^2} \| x_2 \|^2 - \frac{a}{2\tau_1} \langle x_1, \nabla G(x_1) \rangle - \frac{a}{2\tau_2} \langle x_1, \nabla G(x_2) \rangle \right) V(x_1, x_2)
\leq \left( \frac{a}{2\tau_1} + \frac{a}{2\tau_2} + \frac{ab}{2\tau_1} + \frac{ab}{2\tau_2} - \frac{a^2}{4\tau_1^2} \| x_1 \|^2 - \frac{a^2}{4\tau_2^2} \| x_2 \|^2 \right) V(x_1, x_2)
\leq (\kappa - \gamma (\| x_1 \|^2 + \| x_2 \|^2)) V(x_1, x_2),
\]
where \( \kappa = \frac{a}{2\tau_1} + \frac{a}{2\tau_2} + \frac{ab}{2\tau_1} + \frac{ab}{2\tau_2} \) and \( \gamma = \frac{a^2}{4\tau_1^2} \wedge \frac{a^2}{4\tau_2^2} \).

Therefore, the invariant measure \( \pi \) satisfies a LSI with the constant
\[
c_{LS} = c_1 + (c_2 + 2) c_p,
\]
where \( c_1 = \frac{2C}{\gamma} + \frac{\gamma}{2} \) and \( c_2 = \frac{2C}{\gamma} \left( \kappa + \gamma \int_{\mathbb{R}^{2d}} (\| x_1 \|^2 + \| x_2 \|^2) \pi(dx_1 dx_2) \right) \).

We are now ready to prove the log-Sobolev inequality for invariant measure associated with the replica exchange Langevin diffusion (19). We use a similar idea from Chen et al. (2019) where they prove the Poincaré inequality for the invariant measure associated with the replica exchange Langevin diffusion (19) by analyzing the corresponding Dirichlet form. In particular, a larger Dirichlet form ensures a smaller log-Sobolev constant and hence results in a faster convergence in the relative entropy and Wasserstein distance.

**Lemma 5** (Accelerated exponential decay of \( \mathcal{W}_2 \)). Under assumptions (1) and (2), we have that the replica exchange Langevin diffusion converges exponentially fast to the invariant distribution \( \pi \):
\[
\mathcal{W}_2(\nu_0, \pi) \leq D_0 e^{-k_n(1 + \delta_S)/c_{LS}},
\]
where \( D_0 = \sqrt{2c_{LS} D(\nu_0 \| \pi)} \), \( \delta_S := \inf_{t > 0} \frac{\mathcal{E}_S\left(\sqrt{\frac{d\nu}{d\pi}}\right)}{\mathcal{E}\left(\sqrt{\frac{d\nu}{d\pi}}\right)} - 1 \) is a non-negative constant depending on the swapping rate \( S(\cdot, \cdot) \) and obtains 0 only if \( S(\cdot, \cdot) = 0 \).

**Proof** Consider the infinitesimal generator associated with the diffusion process (19), denoted as \( \mathcal{L}_S \), contains an extra term arising from the temperature swapping. The operator \( \mathcal{L}_S \) in this particular case, indeed, has the following form
\[
\mathcal{L}_S = \mathcal{L} + r S(x_1, x_2) \cdot (f(x_2, x_1) - f(x_1, x_2)).
\]
According to Theorem 3.3 (Chen et al., 2019), the Dirichlet form associated with operator \( \mathcal{L}_S \) under the invariant measure \( \pi \) has the form
\[
\mathcal{E}_S(f) = \mathcal{E}(f) + \frac{r}{2} \int S(x_1, x_2) \cdot (f(x_2, x_1) - f(x_1, x_2))^2 d\pi(x_1, x_2), \quad f \in C_0^2(\mathbb{R}^{2d}),
\]
\[\footnote{a \wedge b \text{ denotes } \min\{a, b\}}\]
where $f$ corresponds to $\frac{d\mu}{d\pi(x_1, x_2)}$, and the asymmetry of $\frac{\nu}{\pi(x_1, x_2)}$ is critical in the acceleration effect (Chen et al., 2019). Given two different temperatures $\tau_1$ and $\tau_2$, a non-trivial distribution $\pi$ and function $f$, the swapping rate $S(x_1, x_2)$ is positive for almost any $x_1, x_2 \in \mathbb{R}^d$. As a result, the Dirichlet form associated with $L_S$ is strictly larger than $\mathcal{E}$. Therefore, there exists a constant $\delta_S > 0$ depending on $S(x_1, x_2)$, such that $\delta_S = \inf_{t > 0} \frac{\mathcal{E}_S(\sqrt{\frac{d\nu}{d\pi}})}{\mathcal{E}(\sqrt{\frac{d\nu}{d\pi}})} - 1$. From Lemma 4, we have

$$D(\nu_t||\pi) \leq 2c_{LS} \mathcal{E}(\sqrt{\frac{d\nu}{d\pi}}) \leq 2c_{LS} \sup_t \mathcal{E}(\sqrt{\frac{d\nu}{d\pi}}) \mathcal{E}_S(\sqrt{\frac{d\nu}{d\pi}}) = 2 \frac{c_{LS}}{1 + \delta_S} \mathcal{E}_S(\sqrt{\frac{d\nu}{d\pi}}).$$

Thus, we obtain the following log-Sobolev inequality for the unique invariant measure $\pi$ associated with replica exchange Langevin diffusion $\{\beta_t\}_{t \geq 1}$ and its corresponding Dirichlet form $\mathcal{E}_S(\cdot)$. In particular, the LSI constant $\frac{c_{LS}}{1 + \delta_S}$ in replica exchange Langevin diffusion with swapping rate $S(\cdot, \cdot) > 0$ is strictly smaller than the LSI constant $c_{LS}$ in the replica exchange Langevin diffusion with swapping rate $S(\cdot, \cdot) = 0$. By the exponential decay in entropy (Bakry et al., 2014)[Theorem 5.2.1] and the tight log-Sobolev inequality in Lemma 4, we get that, for any $t \in [k\eta, (k + 1)\eta)$,

$$D(\nu_t||\pi) \leq D(\nu_0||\pi)e^{-2t(1+\delta_S)/c_{LS}} \leq D(\mu_0||\pi)e^{-2k\eta(1+\delta_S)/c_{LS}}.$$  

Finally, we can estimate the term $\mathcal{W}_2(\nu_t, \pi)$ by the Otto-Villani theorem (Bakry et al., 2014)[Theorem 9.6.1],

$$\mathcal{W}_2(\nu_t, \pi) \leq \sqrt{2c_{LS}D(\nu_t||\pi)} \leq \sqrt{2c_{LS}D(\mu_0||\pi)}e^{-k\eta(1+\delta_S)/c_{LS}}.$$  

\[\square\]

### A.5. Summary: Convergence of reSGLD

Now that we have all the necessary ingredients in place, we are ready to derive the convergence of the distribution $\mu_k$ to the invariant measure $\mu$ in terms of 2-Wasserstein distance, 

**Theorem 2 (Convergence of reSGLD).** Let the assumptions (1) and (2) hold. For the unique invariant measure $\pi$ associated with the Markov diffusion process (19) and the distribution $\{\mu_k\}_{k \geq 0}$ associated with the discrete dynamics $\{\beta^k\}_{k \geq 1}$, we have the following estimates, for $0 \leq k \in \mathbb{N}^+$ and the learning rate $\eta$ satisfying $0 < \eta < 1 \land \alpha/C^2$,

$$\mathcal{W}_2(\mu_k, \pi) \leq D_0 e^{-k(1+\delta_S)/c_{LS}} + \delta_1 \eta + \delta_2 \max_k \mathbb{E}[\|\phi_k\|^2] + \delta_3 \max_k \sqrt{\mathbb{E}[\|\psi_k\|^2]}$$

where $D_0 = \sqrt{2c_{LS}D(\mu_0||\pi)}$, $\delta_S := \min_k \frac{\mathcal{E}_S(\sqrt{\frac{d\nu}{d\pi}})}{\mathcal{E}(\sqrt{\frac{d\nu}{d\pi}})} - 1$ is a non-negative constant depending on the swapping rate $S(\cdot, \cdot)$ and obtains the minimum zero only if $S(\cdot, \cdot) = 0$.

**Proof** We reduce the estimates into the following two terms by using the triangle inequality,

$$\mathcal{W}_2(\mu_k, \pi) \leq \mathcal{W}_2(\mu_k, \nu_t) + \mathcal{W}_2(\nu_t, \pi), \quad t \in [k\eta, (k + 1)\eta).$$

The first term $\mathcal{W}_2(\mu_k, \nu_t)$ follows from the analysis of discretization error in Lemma 3. Recall the very definition of the $\mathcal{W}_2(\cdot, \cdot)$ distance defined in (18). Thus, in order to control the distance $\mathcal{W}_2(\mu_k, \nu_t)$, $t \in [k\eta, (k + 1)\eta)$, we need to consider the diffusion process whose law give $\mu_k$ and $\nu_t$, respectively. Indeed, it is obvious that $\nu_t = \mathcal{L}(\beta_t)$ for $t \in [k\eta, (k + 1)\eta)$. For the other measure $\mu_k$, it follows that $\mu_k = \tilde{\nu}_{k\eta}$ for $t = k\eta$, where $\tilde{\nu}_{k\eta} = \mathcal{L}(\tilde{\beta}^k)$ is the probability measure associated with the continuous interpolation of reSGLD (20). By Lemma 3, we have that for $k \in \mathbb{N}$ and $t \in [k\eta, (k + 1)\eta)$,

$$\mathcal{W}_2(\mu_k, \nu_t) = \mathcal{W}_2(\tilde{\nu}_{k\eta}, \nu_t) \leq \sqrt{\mathbb{E}[\sup_0 \leq s \leq t \|\beta_s - \tilde{\beta}^k_s\|^2]} \leq \delta_1 \eta + \delta_2 \max_k \mathbb{E}[\|\phi_k\|^2] + \delta_3 \max_k \sqrt{\mathbb{E}[\|\psi_k\|^2]}.$$  

Recall from the accelerated exponential decay of replica exchange Langevin diffusion in Lemma 5, we have

$$\mathcal{W}_2(\nu_t, \pi) \leq \sqrt{2c_{LS}D(\nu_0||\pi)e^{-k\eta(1+\delta_S)/c_{LS}}} = \sqrt{2c_{LS}D(\mu_0||\pi)e^{-k\eta(1+\delta_S)/c_{LS}}}.$$  

Combing the above two estimates completes the proof.  

\[\square\]
B. Hyper-parameter Setting for Bayesian GANs

In the semi-supervised learning tasks, we fine-tune the hyper-parameters for Bayesian GANs and report them in Table 4. In particular, $N_s$ is the number of labeled data; $\eta^{(1)}$ and $\eta^{(2)}$ are the learning rates for the low-temperature chain and high-temperature chain, respectively; $\tau_1$ and $\tau_2$ are the temperatures; $\hat{F}$ is the correction factor, which often yields several swaps. In addition, the learning rates also follow a truncated exponential decay, for example, $\eta_k^{(1)} = \left(0.05 \lor e^{-\frac{k}{800}}\right) \eta^{(1)}$ and $\eta_k^{(2)} = \left(0.05 \lor e^{-\frac{k}{800}}\right) \eta^{(2)}$, where $k$ is the number of iterations.

| Dataset  | $N_s$       | $\eta^{(1)}$ | $\eta^{(2)}$ | $\tau_1$ | $\tau_2$ | $\hat{F}$ |
|----------|-------------|---------------|---------------|-----------|-----------|-----------|
| CIFAR10  | 2000 ~ 3500 | 4.5e-4        | 7.0e-4        | 0.01      | 1         | 3.0e5     |
|          | 4000 ~ 5000 | 4.5e-4        | 7.0e-4        | 0.01      | 1         | 2.0e5     |
| CIFAR100 | 2000 ~ 2500 | 5.0e-4        | 7.5e-4        | 0.04      | 1         | 1.0e4     |
|          | 3000 ~ 3500 | 5.0e-4        | 7.5e-4        | 0.02      | 1         | 2.5e4     |
|          | 4000 ~ 5000 | 5.0e-4        | 7.5e-4        | 0.01      | 1         | 5.0e4     |
| SVHN     | 2000 ~ 4000 | 4.5e-3        | 5.0e-3        | 0.01      | 1         | 8.0e4     |
|          | 4500 ~ 5000 | 4.5e-3        | 7.0e-3        | 0.01      | 1         | 8.0e4     |

Table 4. Hyper-parameter setting of Bayesian GANs for Semi-Supervised Learning experiments.