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Faster Sampling without Isoperimetry via Diffusion-based Monte Carlo

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Abstract

To sample from a general target distribution $p_* \propto e^{-f_*}$ beyond the isoperimetric condition, Huang et al. (2023) proposed to perform sampling through reverse diffusion, giving rise to *Diffusion-based Monte Carlo* (DMC). Specifically, DMC follows the reverse SDE of a diffusion process that transforms the target distribution to the standard Gaussian, utilizing a non-parametric score estimation. However, the original DMC algorithm encountered high gradient complexity[1], resulting in an *exponential dependency* on the error tolerance ϵ of the obtained samples. In this paper, we demonstrate that the high complexity of the original DMC algorithm originates from its redundant design of score estimation, and proposed a more efficient DMC algorithm, called RS-DMC, based on a novel recursive score estimation method. In particular, we first divide the entire diffusion process into multiple segments and then formulate the score estimation step (at any time step) as a series of interconnected mean estimation and sampling subproblems accordingly, which are correlated in a recursive manner. Importantly, we show that with a proper design of the segment decomposition, all sampling subproblems will only need to tackle a strongly log-concave distribution, which can be very efficient to solve using the standard sampler (e.g., Langevin Monte Carlo) with a provably rapid convergence rate. As a result, we prove that the gradient complexity of RS-DMC exhibits merely a *quasi-polynomial dependency* on ϵ. This finding is highly unexpected as it substantially enhances the prevailing belief of the necessity for exponential gradient complexity in all prior works such as Huang et al. (2023). Under commonly used dissipative conditions, our algorithm is provably much faster than the popular Langevin-based algorithms. Our algorithm design and theoretical framework illuminate a novel direction for addressing sampling problems, which could be of broader applicability in the community.

Keywords: Diffusion-based Monte Carlo, Quasi-polynomial complexity

1. We denote gradient complexity as the required number of gradient calculations to achieve at most ϵ sampling error.

1. Introduction

Sampling problems, i.e., generating samples from a given target distribution $p_* \propto \exp(-f_*)$, have received increasing attention in recent years. A popular approach for solving this problem is to apply gradient-based Markov chain Monte Carlo (MCMC) methods, such as Unadjusted Langevin Algorithms (ULA) (Neal, 1992; Roberts and Tweedie, 1996), Underdamped Langevin Dynamics (ULD) (Cheng et al., 2018; Ma et al., 2021; Mou et al., 2021), and Metropolis-Adjusted Langevin Algorithm (MALA) (Roberts and Stramer, 2002; Xifara et al., 2014). In particular, these algorithms can be seen as the discretization of the continuous Langevin dynamics (LD) and its variants (Ma et al., 2015), which will converge to a unique stationary distribution that follows $p_* \propto \exp(-f_*)$, under regularity conditions on the energy function $f_*(\boldsymbol{x})$ (Roberts and Tweedie, 1996).

The convergence rate of the Langevin-based algorithms heavily depends on the isoperimetric-like properties of the target distribution p_*: guaranteeing the convergence in polynomial time requires p_* to be, e.g., log-concave, satisfying log-Sobolev or Poincaré inequalities or their generalizations with well-behaving coefficients. Unfortunately, for general non-log-concave distributions, the convergence rate typically depends exponentially on the problem dimension (Raginsky et al., 2017; Holzmüller and Bach, 2023) (i.e., $\sim \exp(d)$), or even the convergence to p_* cannot be guaranteed altogether (one instead only guarantee to converge to some local stationarity (Balasubramanian et al., 2022)). This implies that the Langevin-based algorithms may not be the ideal candidate for solving such hard sampling problems. To this end, we are interested in addressing the following question:

Can we develop a new sampling algorithm that enjoys a non-exponential convergence rate for sampling general non-log-concave distributions?

To address this problem, we draw inspiration from recent studies—including Montanari (2023); Huang et al. (2023)—that attempt to design samplers based on diffusion models (Sohl-Dickstein et al., 2015; Ho et al., 2020; Vargas et al., 2023). We refer to this class of samplers as the **diffusion-based Monte Carlo** (DMC) methods. In particular, the algorithm developed in Huang et al. (2023) is based on the reverse process of the Ornstein-Uhlenbeck (OU) process, which starts from the target distribution p_* and converges to a standard Gaussian distribution. The mathematical formula of the OU process and its reverse process are given as follows (Anderson, 1982; Song et al., 2020):

$$\mathrm{d}\mathbf{x}_t = -\mathbf{x}_t \mathrm{d}t + \sqrt{2}\mathrm{d}B_t, \quad \mathbf{x}_0 \sim p_0(\boldsymbol{x}) = p_*, \qquad \text{(OU Process)}$$

$$\mathrm{d}\mathbf{x}_t^{\leftarrow} = \left[\mathbf{x}_t^{\leftarrow} + 2\nabla \log p_{T-t}(\mathbf{x}_t^{\leftarrow})\right]\mathrm{d}t + \sqrt{2}\mathrm{d}B_t, \quad \mathbf{x}_0^{\leftarrow} \sim p_T(\boldsymbol{x}) \approx \mathcal{N}(\mathbf{0}, \mathbf{I}), \qquad \text{(Reverse Process)}$$

where B_t denotes the Brownian term, $p_t(\boldsymbol{x})$ denotes the underlying distribution of the particle at time t along the OU process, T denotes the end time of the OU process, and $\nabla \log p_t(\boldsymbol{x})$ denotes the score function of the distribution $p_t(\boldsymbol{x})$. In fact, the exponentially slow convergence rate of the Langevin-based algorithms stems from the rather long mixing time of Langevin dynamics to its stationary distribution, while in contrast, the OU process exhibits a much shorter mixing time. Therefore, principally, if the reverse process of the OU process can be perfectly recovered, one can avoid suffering from the issue of slow mixing of Langevin dynamics, and develop more efficient sampling algorithms accordingly.

Then, the key to recovering (Reverse Process) is to obtain a good estimation for the score $\nabla \log p_t(\boldsymbol{x})$ for all $t \in [0, T]$. Huang et al. (2023) proposed a score estimation method called reverse diffusion sampling (RDS) based on an inner-loop ULA. However, it still suffers from the exponential dependency with respect to the target sampling error, which requires $\exp\left(\mathcal{O}(1/\epsilon)\right)$

gradient complexity to achieve the ϵ sampling error in KL divergence. The reason behind this is that RDS involves many *hard* subproblems that need to sample non-log-concave distributions with bad isoperimetric properties, which incurs huge gradient complexities in the desired Langevin algorithms.

In this work, we argue that the *hard* subproblems in Huang et al. (2023) are redundant or even unnecessary, and propose a more efficient diffusion-based Monte Carlo method, called recursive score DMC (RS-DMC), that only requires **quasi-polynomial gradient complexity** to sampling general non-log-concave distributions. At the core of RS-DMC is a novel non-parametric method for score estimation, which involves a series of interconnected mean estimation and sampling subproblems that are correlated in a recursive manner. In particular, we first divide the entire forward process into several segments starting from $0, S, \ldots, (K-1)S$, and estimate the scores $\{\nabla \log p_{kS}(\boldsymbol{x})\}_{k=0,\ldots,K-1}$ recursively. Given the segments, the score within each segment $\nabla \log p_{kS+\tau}(\boldsymbol{x})$ will be further estimated according to the reference score $\nabla \log p_{kS}(\boldsymbol{x})$, where $\tau \in [0, S]$ can be arbitrarily chosen. Importantly, given proper configuration of the segment length (i.e., S), we can show that all sampling subproblems in the developed score estimation method are *much easier*, as long as the target distribution p_* is log-smooth and has bounded second moment. Then, all intermediate target distributions are guaranteed to be strongly log-concave, which can be sampled very efficiently via standard ULA. Accordingly, based on the samples generated via ULA, the mean estimation subproblems can be then resolved very efficiently under some mild assumptions on the tail of the posterior distribution (e.g., moment bounds). We summarize the main contributions as follows:

- We propose a new Diffusion Monte Carlo algorithm, called RS-DMC, for sampling general non-log-concave distributions. At the core is a novel and efficient recursive score estimation algorithm. In particular, based on a properly designed recursive structure, we show that the hard non-log-concave sampling problem can be divided into a series of benign sampling subproblems that can be solved very efficiently via standard ULA.

- We establish the convergence guarantee of the proposed RS-DMC algorithm under very mild assumptions, which only require the target distribution to be log-smooth and to have a bounded second moment. In contrast, to obtain provable convergence (to the target distribution), the Langevin-based methods typically require additional isoperimetric conditions (e.g., Log-Sobolev inequality, Poincaré inequality, etc). This justifies that our algorithm can be applied to a broader class of distributions with rigorous theoretical convergence guarantees.

- We prove that the gradient complexity of our algorithm is $\exp\left[\mathcal{O}(\log^3(d/\epsilon))\right]$ to achieve ϵ sampling error in KL divergence, which only has a quasi-polynomial dependency on the target error ϵ and dimension d. In contrast, under even stronger conditions in our work, the gradient complexity in prior works either need exponential dependency in ϵ (i.e., $\exp\big(\mathcal{O}(1/\epsilon)\big)$) (Huang et al., 2023) or exponential dependency in d, (i.e., $\exp\big(\mathcal{O}(d)\big)$) (Raginsky et al., 2017; Xu et al., 2018)[2] (which requires the additional dissipative condition). This demonstrate the efficiency of our algorithm.

2. Preliminaries

In this section, we will first introduce the notations and problem settings that are commonly used in the following sections. We will then present some fundamental properties, such as the closed form of

2. We omit the d-dependency in Huang et al. (2023) and ϵ-dependency in Raginsky et al. (2017); Xu et al. (2018) for the ease of presentation.

the transition kernel and the expectation form of score functions along the OU process. Finally, we will specify the assumptions that the target distribution is required in our algorithms and analysis.

Notations. We use the lowercase bold symbol $\mathbf{x}$ to denote the random vector, and the lowercase italicized bold symbol $\boldsymbol{x}$ means a fixed vector. We use $\|\cdot\|$ to denote the standard Euclidean distance. We say $a_n = \mathrm{poly}(n)$ if $a_n \le \mathcal{O}(n^c)$ for some constant c and $\mathrm{pow}(a, b) = a^b$.

The segmented OU process. We define $\mathbb{N}_{a,b} = [a, b] \cap \mathbb{N}_*$ for brevity. Suppose the length of each segment is $S \in \mathbb{R}_+$, and we divide the entire forward process with length T into $K \in \mathbb{N}_+$ segments satisfying $K = T/S$. In this condition, we can reformulate the previous SDE as

$$\begin{aligned} &\mathbf{x}_{k,0} \sim p_{0,0} = p_* \text{ when } k = 0, \text{ else } \mathbf{x}_{k,0} = \mathbf{x}_{k-1,S} && k \in \mathbb{N}_{0,K-1} \\ &\mathrm{d}\mathbf{x}_{k,t} = -\mathbf{x}_{k,t}\mathrm{d}t + \sqrt{2}\mathrm{d}B_t && k \in \mathbb{N}_{0,K-1}, t \in [0, S], \end{aligned} \tag{1}$$

where $\mathbf{x}_{k,t}$ denotes the random variable of the OU process at time $(kS + t)$ with underlying density $p_{k,t}$. Besides, we define the following conditional density, i.e., $p_{(k,t)|(k',t')}(\boldsymbol{x}|\boldsymbol{x}')$, which presents the probability of obtaining $\mathbf{x}_{k,t} = \boldsymbol{x}$ when $\mathbf{x}_{k',t'} = \boldsymbol{x}'$. The diagram of SDE (1) is presented in Fig 1.

The reverse segmented OU process. According to (Reverse Process), the reverse process of the segmented SDE (1) can be presented as

$$\begin{aligned} &\mathbf{x}^{\leftarrow}_{k,0} \sim p_{K-1,S} \text{ when } k = K-1, \text{ else } \mathbf{x}^{\leftarrow}_{k,0} = \mathbf{x}^{\leftarrow}_{k+1,S} && k \in \mathbb{N}_{0,K-1} \\ &\mathrm{d}\mathbf{x}^{\leftarrow}_{k,t} = \left[\mathbf{x}^{\leftarrow}_{k,t} + 2\nabla \log p_{k,S-t}(\mathbf{x}^{\leftarrow}_{k,t})\right] \mathrm{d}t + \sqrt{2}\mathrm{d}B_t && k \in \mathbb{N}_{0,K-1}, t \in [0, S] \end{aligned}$$

where particles satisfy $\mathbf{x}^{\leftarrow}_{k,t} = \mathbf{x}_{k,S-t}$ with underlying density $p^{\leftarrow}_{k,t} = p_{k,S-t}$ for any $k \in \mathbb{N}_{0,K-1}$ and $t \in [0, S]$. To approximately solve the SDE with numerical methods, we first split each segment into R intervals $\{[(r-1)\eta, r\eta]\}_{r=1,\ldots,R}$, where η is the interval length and $R = S/\eta$. Then we can replace the score function $\nabla \log p_{k,S-t}$ as $\mathbf{v}^{\leftarrow}_{k,t}$, and for $t \in [r\eta, (r+1)\eta]$, we freeze the value of this coefficient in the SDE at time $(k, r\eta)$. Then starting from the standard Gaussian distribution, we consider the following new SDE:

$$\begin{aligned} &\mathbf{x}^{\leftarrow}_{k,0} \sim p_\infty = \mathcal{N}(\mathbf{0}, \boldsymbol{I}) \text{ when } k = K-1, \text{ else } \mathbf{x}^{\leftarrow}_{k,0} = \mathbf{x}^{\leftarrow}_{k+1,S} && k \in \mathbb{N}_{0,K-1} \\ &\mathrm{d}\mathbf{x}^{\leftarrow}_{k,t} = \left[\mathbf{x}^{\leftarrow}_{k,t} + 2\mathbf{v}^{\leftarrow}_{k,\lfloor t/\eta \rfloor \eta}\left(\mathbf{x}^{\leftarrow}_{k,\lfloor t/\eta \rfloor \eta}\right)\right] \mathrm{d}t + \sqrt{2}\mathrm{d}B_t && k \in \mathbb{N}_{0,K-1}, t \in [0, S] \end{aligned} \tag{2}$$

where p_∞ denotes the stationary distribution of the forward process. Similar to the segmented OU process, we define the following conditional density, i.e., $p^{\leftarrow}_{k,t|t'}(\boldsymbol{x}|\boldsymbol{x}')$, which presents the probability of obtaining $\mathbf{x}^{\leftarrow}_{k,t} = \boldsymbol{x}$ when $\mathbf{x}^{\leftarrow}_{k,t'} = \boldsymbol{x}'$. The diagram of SDE (2) is presented in Fig 1.

Basic properties of the OU process. Previously, we have demonstrated that SDE (1) is an alternative presentation of the OU process. Therefore, the properties in the OU process can be directly introduced for this segmented version. First, the transition kernel in the k-th segment satisfies

$$p_{k,t|0}(\boldsymbol{x}|\boldsymbol{x}_0) = \left(2\pi\left(1 - e^{-2t}\right)\right)^{-d/2} \cdot \exp\left[\frac{-\left\|\boldsymbol{x} - e^{-t}\boldsymbol{x}_0\right\|^2}{2\left(1 - e^{-2t}\right)}\right], \quad \forall\, 0 < t \le S.$$

Plugging the transition kernel into Tweedie's formula, the score function can be reformulated as the following lemma whose proof is deferred in Appendix E.

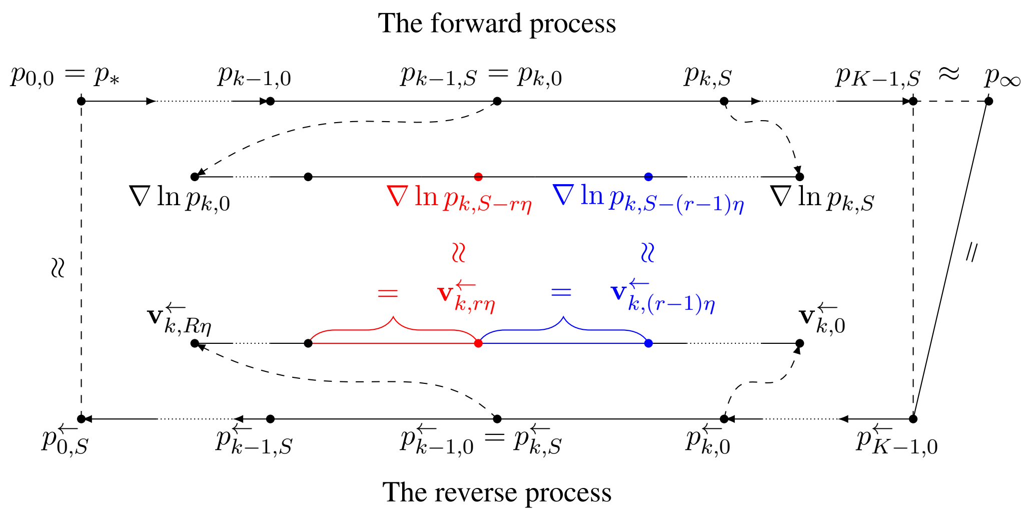

Figure 1: The illustration of SDE (1) and (2) with the definitions in Section 2. The top of the figure describes the underlying distribution of the segmented OU process, SDE (1), and the bottom presents the corresponding distribution in the reverse segmented OU process, SDE (2). For the intermediate part, the upper half describes the gradients of the log densities along the forward SDE (1), while the lower half describes approximated scores used to update particles in the reverse SDE (2).

Lemma 1 (Lemma 1 of Huang et al. (2023)) *For any $k \in \mathbb{N}_{0,K-1}$ and $t \in [0, S]$, the score function can be written as*

$$\nabla \log p_{k,S-t}(\boldsymbol{x}) = \mathbb{E}_{\mathbf{x}_0 \sim q_{k,S-t}(\cdot|\boldsymbol{x})}\left[-\frac{\boldsymbol{x} - e^{-(S-t)}\boldsymbol{x}_0}{\left(1 - e^{-2(S-t)}\right)}\right]$$

where the conditional density function $q_{k,S-t}(\cdot|\boldsymbol{x})$ is defined as

$$q_{k,S-t}(\boldsymbol{x}_0|\boldsymbol{x}) \propto \exp\left(\log p_{k,0}(\boldsymbol{x}_0) - \frac{\left\|\boldsymbol{x} - e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1 - e^{-2(S-t)}\right)}\right).$$

Therefore, to approximate the score $\nabla \log p_{k,S-r\eta}(\boldsymbol{x})$ with an estimator $\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})$, we can draw samples from $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$ and calculate their empirical mean.

Assumptions. To guarantee the convergence in KL divergence, the Langevin-based methods require the target distribution to satisfy certain isoperimetric properties such as Log-Sobolev inequality (LSI) and Poincaré inequality (PI) or even strong log-concavity (Vempala and Wibisono, 2019; Cheng and Bartlett, 2018; Dwivedi et al., 2018; Ma et al., 2019; Zou et al., 2019, 2021; Dong et al., 2022) (the formal definitions of these conditions are deferred to Appendix A). Some other works consider milder assumptions such as modified LSI (Erdogdu and Hosseinzadeh, 2021) and weak Poincaré inequality (Mousavi-Hosseini et al., 2023), but they are only the analytical continuation of LSI and PI, which still exhibit a huge gap with the general non-log-concave distributions. Huang et al. (2023) requires the target distribution p_* to have a heavier tail than that of the Gaussian distribution.

Remarkably, our algorithm does not require any isoperimetric condition or condition on the tail properties of p_* to establish the convergence guarantee. We only require the following mild conditions on the target distribution.

[A1] For any $k \in \mathbb{N}_{0,K-1}$ and $t \in [0, S]$, the score $\nabla \log p_{k,t}$ is L-Lipschitz.

[A2] The target distribution has a bounded second moment, i.e., $M := \mathbb{E}_{p_*}[\|\cdot\|^2] < \infty$.

Assumption **[A1]** corresponds to the L-smoothness condition of the log density f_* in traditional ULA analysis, which has been widely made in prior works (Chen et al., 2023b,c; Huang et al., 2023). It is often used to ensure that numerical discretization is feasible. We emphasize that Assumption **[A1]** may be relaxed only to assume the target distribution is smooth rather than the entire OU process (based on Lemmas 12 and 14 in Chen et al. (2023a)) or even only the second moment bounded and identity data covariance matrix (in the counterpart of Benton et al. (2023)). We do not include this additional relaxation in this paper to make our analysis clearer. Assumption **[A2]** is one of the weakest assumptions being adopted for the analysis of posterior sampling.

3. Proposed Methods

In this section, we introduce a new approach called Recursive Score Estimation (RSE) and describe the proposed Recursive Score Diffusion-based Monte Carlo (RS-DMC) method. We start by discussing the motivations and intuitions behind the use of recursion. Next, we provide implementation details for the RSE process and emphasize the importance of selecting an appropriate segment length. Finally, we present the RS-DMC method based on the RSE approach.

3.1. Difficulties of the vanilla DMC

We consider the reverse segmented OU process, i.e., SDE 2 and begin with the original version of DMC in Huang et al. (2023), which can be seen as a special case of the reverse segmented OU process with a large segment length $S = T$ and a small number of segments $K = 1$. According to the reverse SDE 2, for the r-th iteration within one single segment, we need to estimate $\nabla \log p_{0,S-r\eta}$ to update the particles. Specifically, by Lemma 1, we have

$$\nabla \log p_{0,S-r\eta}(\boldsymbol{x}) = \mathbb{E}_{\mathbf{x}_0 \sim q_{0,S-r\eta}(\cdot|\boldsymbol{x})}\left[-\frac{\boldsymbol{x} - e^{-(S-r\eta)}\boldsymbol{x}_0}{\left(1 - e^{-2(S-r\eta)}\right)}\right]$$

for any $\boldsymbol{x} \in \mathbb{R}^d$, where the conditional distribution is

$$q_{0,S-r\eta}(\boldsymbol{x}_0|\boldsymbol{x}) \propto \exp\left(\log p_{0,0}(\boldsymbol{x}_0) - \frac{\left\|\boldsymbol{x} - e^{-(S-r\eta)}\boldsymbol{x}_0\right\|^2}{2\left(1 - e^{-2(S-r\eta)}\right)}\right). \tag{3}$$

Since the analytic form $\nabla \log p_{0,0} = -\nabla f_*$ exists, we can use the ULA to draw samples from $q_{0,S-r\eta}(\cdot|\boldsymbol{x})$ and calculate the empirical mean to estimate $\nabla \log p_{0,S-r\eta}(\boldsymbol{x})$.

However, sampling from $q_{0,S-r\eta}(\cdot|\boldsymbol{x})$ is not trivial. When r is small, sampling $q_{0,S-r\eta}(\cdot|\boldsymbol{x})$ via ULA is almost as difficult as sampling $p_{0,0}(\boldsymbol{x}_0)$ via ULA (see (3)), since the additive quadratic term, whose coefficient is $e^{-2(S-r\eta)}/2(1 - e^{-2(S-r\eta)})$, will be nearly negligible in this case. This is because that $S = T$ is large and then $e^{-2(S-r\eta)}/2(1 - e^{-2(S-r\eta)}) \sim \exp(-2T)$ becomes extremely

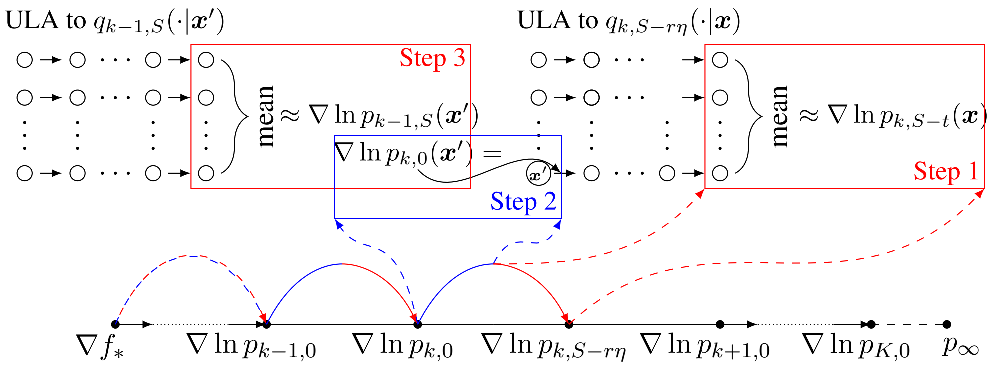

Figure 2: The illustration of recursive score estimation (RSE). The upper half presents RSE locally, which shows how to utilize the former score, $\nabla \log p_{k,0}(\boldsymbol{x}')$ to update particles by ULA in the sampling subproblem formulated by the latter score, $\nabla \log p_{k,S-t}(\boldsymbol{x})$. The lower half presents RSE globally, which is a series of interconnected mean estimation and sampling subproblems accordingly.

small when $r\eta = O(T)$. Specifically, in Huang et al. (2023), when $e^{-2(S-r\eta)} \leq 2L/(1+2L)$, the LSI parameter of $q_{0,S-r\eta}(\cdot|\boldsymbol{x})$ can be as worse as $\exp\big(-\mathcal{O}(1/\epsilon)\big)$. Then applying ULA for sampling this distribution needs a dramatically high gradient complexity that is exponential in $1/\epsilon$.

3.2. Intuition of the recursion

Therefore, the key to avoiding sampling such a hard distribution is to restrict the segment length. By Lemma 1, it can be straightforwardly verified that if the segment length satisfies $S \leq \frac{1}{2}\log\left(\frac{2L+1}{2L}\right)$,

$$-\nabla^2_{\boldsymbol{x}_0} \log q_{k,S-r\eta}(\boldsymbol{x}_0|\boldsymbol{x}) \succeq -\nabla^2_{\boldsymbol{x}_0} \log p_{k,0}(\boldsymbol{x}_0) + \frac{e^{-2S}}{1-e^{-2S}} \cdot \boldsymbol{I} \succeq \frac{e^{-2S}}{2(1-e^{-2S})} \cdot \boldsymbol{I} \tag{4}$$

where the last inequality follows from Assumption **[A1]**. This implies that $q_{k,S-r\eta}(\boldsymbol{x}_0|\boldsymbol{x})$ is strongly log-concave for all $r \leq \lfloor S/\eta \rfloor$, which can be efficiently sampled via the standard ULA. However, ULA requires to calculate the score function $\nabla_{\boldsymbol{x}_0} \log q_{k,S-r\eta}(\boldsymbol{x}_0|\boldsymbol{x})$, which further needs to calculate $\nabla \log p_{k,0}(\boldsymbol{x})$ according to Lemma 1. Different from the vanilla DMC where the formula of $\nabla \log p_{0,0}(\boldsymbol{x})$ is known, the score $\nabla \log p_{k,0}(\boldsymbol{x})$ in (4) is an unknown quantity, which also requires to be estimated. In fact, based on our definition, we can rewrite $p_{k,0}(\boldsymbol{x})$ as $p_{k-1,S}(\boldsymbol{x})$ (see Figure 1), then applying Lemma 1, we can again decompose the problem of estimating $\nabla \log p_{k-1,S}(\boldsymbol{x})$ into the subproblems of sampling $q_{k-1,S}(\cdot|\boldsymbol{x})$ and the estimation of $\nabla \log p_{k-1,0}(\boldsymbol{x})$, which is naturally organized in a recursive manner. Therefore, by recursively adopting this subproblem decomposition, we summarize the recursive process for approximating $\nabla \log p_{k,S-r\eta}(\boldsymbol{x})$ as follows and illustrate the diagram in Figure 2:

- **Step 1:** We approximate the score $\nabla \log p_{k,S-r\eta}(\boldsymbol{x})$ by a mean estimation with samples generated by running ULA over the intermediate target distribution $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$.
- **Step 2:** When running ULA for $q_{k,S-t}(\cdot|\boldsymbol{x})$, we estimate the score $\nabla \log p_{k,0} = \nabla \log p_{k-1,S}$.

- **Step 3:** We jump to Step 1 to approximate the score $\nabla \log p_{k-1,S}(\boldsymbol{x})$ via drawing samples from $q_{k-1,S}(\cdot|\boldsymbol{x})$, and continue the recursion.

3.3. Recursive Score Estimation and Reverse Diffusion Sampling

Recursive Score Estimation. We have already explained the rough intuition behind introducing recursion. By conducting the recursion, we need to solve a series of sampling and mean estimation subproblems. Then, it is demanding to control the error propagation between these subproblems in order to finally ensure small sampling errors. In particular, this amounts to the adaptive adjustment of the sample numbers for mean estimation and iteration numbers for ULA in solving sampling subproblems. Specifically, if we require score estimation $\mathbf{v}^{\leftarrow}_{k,r\eta}\colon \mathbb{R}^d \to \mathbb{R}^d$ to satisfy

$$\left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})\right\|^2 \le \epsilon,\ \forall \boldsymbol{x}\in\mathbb{R}^d \tag{5}$$

with a high probability, then the sample number in Step 1 and the number of calls of Step 2 (the iteration number of ULA) in Fig 2 will be two functions with respected to the target error ϵ, denoted as $n_{k,r}(\epsilon)$ and $m_{k,r}(\epsilon)$ respectively. Furthermore, when Step 2 is introduced to update ULA, we rely on an approximation of $\nabla \log p_{k,0}$ instead of the exact score. To ensure (5) is met, the error resulting from estimating $\nabla \log p_{k,0}$ should be typically smaller than ϵ. We express this requirement as:

$$\left\|\nabla \log p_{k,0}(\boldsymbol{x}) - \mathbf{v}^{\leftarrow}_{k,0}(\boldsymbol{x})\right\|^2 \le l_{k,r}(\epsilon),\ \forall \boldsymbol{x}\in\mathbb{R}^d.$$

where $l_{k,r}(\epsilon)$ is a function of ϵ that satisfies $l_{k,r}(\epsilon)\le\epsilon$. Under this condition, we provide Alg 1, i.e., RSE, to calculate the score function for the r-th iteration at the k-th segment, i.e., $\nabla \log p_{k,S-r\eta}(\boldsymbol{x})$. Note that the initial distribution q_0' and the step size τ_r in Line 4 and 9 should be chosen carefully to guarantee the convergence of inner ULA, i.e.,

$$q_0'(\boldsymbol{x}') \propto \exp\left(-\frac{\left\|\boldsymbol{x} - e^{-(S-r\eta)}\boldsymbol{x}'\right\|^2}{2(1-e^{-2(S-r\eta)})}\right) \quad \text{and} \quad \tau_r = \mathcal{O}\left(e^{2(S-r\eta)}\left(1-e^{-2(S-r\eta)}\right)^2\cdot d^{-1}\epsilon\right).$$

Quasi-polynomial Complexity. We consider the ideal case for interpreting the complexity of our score estimation method. In particular, since the benign error propagation, i.e., $l_{k,r}(\epsilon)=\epsilon$, is almost proven in Lemma 20, we suppose the number of calls to the recursive function, $\mathsf{RSE}(k-1,0,\boldsymbol{x}',l_{k,r}(\epsilon))$, is uniformly bounded by $m_{k,r}(\epsilon)\cdot n_{k,r}(\epsilon)$ for all feasible (k,r) pairs when the RSE algorithm is executed with input $(k,r,\boldsymbol{x},\epsilon)$. Then, recall that we will conduct the recursion in at most K rounds. The total gradient complexity for estimating one score will be

$$\left[m_{k,r}(\epsilon)\cdot n_{k,r}(\epsilon)\right]^{\mathcal{O}(K)} = \left[m_{k,r}(\epsilon)\cdot n_{k,r}(\epsilon)\right]^{\mathcal{O}(T/S)}.$$

This formula highlights the importance of selecting a sufficiently large segment with length S to reduce the number of recursive function calls and improve gradient complexity. In our analysis, we set $S=\frac{1}{2}\log\left(\frac{2L+1}{2L}\right)$, which is "just" small enough to ensure that all intermediate target distributions in the sampling subproblems are strongly log-concave. Due to the choice of T is $\mathcal{O}(\log(d/\epsilon))$ in general cases and $m_{k,r}(\cdot)$ and $n_{k,r}(\cdot)$ are typically polynomial w.r.t. the target sampling error ϵ and dimension d (Theorem 5 in Appendix B), we expect a quasi-polynomial gradient complexity.

Algorithm 1 Recursive Score Estimation (approximate $\nabla \log p_{k,S-r\eta}(\boldsymbol{x})$): $\mathsf{RSE}(k, r, \boldsymbol{x}, \epsilon)$

Input : The segment number $k \in \mathbb{N}_{0,K-1}$, the iteration number $r \in \mathbb{N}_{0,R-1}$, variable $\boldsymbol{x}$ requiring the score function, error tolerance ϵ.

if $k \equiv -1$ **then**
  return $-\nabla f_*(\boldsymbol{x})$
Initial the returned vector $\boldsymbol{v}' \leftarrow \boldsymbol{0}$
for $i = 1$ *to* $n_{k,r}(\epsilon)$ **do**
  Draw $\boldsymbol{x}'_0$ from an initial distribution q'_0
  for $j = 0$ *to* $m_{k,r}(\epsilon, \boldsymbol{x}) - 1$ **do**
    $\boldsymbol{v}'_j \leftarrow \mathsf{RSE}\left(k-1, 0, \boldsymbol{x}'_j, l_{k,r}(\epsilon)\right)$ /* Recursive score estimation $\nabla \log p_{k-1,S}(\boldsymbol{x}'_j)$ */
    if $r \not\equiv 0$ **then** $t' \leftarrow S - r\eta$ **else** $t' \leftarrow S$;
    /* The gap of time since the last call */
    Update the particle

$$\boldsymbol{x}'_{j+1} := \boldsymbol{x}'_j + \tau_r \cdot \underbrace{\left(\boldsymbol{v}'_j + \frac{e^{-t'}\boldsymbol{x} - e^{-2t'}\boldsymbol{x}'_j}{1 - e^{-2t'}}\right)}_{\approx \nabla \log q_{k,S-r\eta}(\boldsymbol{x}'_j|\boldsymbol{x})} + \sqrt{2\tau_r} \cdot \xi$$

    where ξ is sampled from $\mathcal{N}\left(0, \boldsymbol{I}_d\right)$
  end
  Update the score estimation of $\boldsymbol{v}' \approx \nabla \log p_{k,S-r\eta}(\boldsymbol{x})$ with empirical mean as

$$\boldsymbol{v}' := \boldsymbol{v}' + \frac{1}{n_{k,r}(\epsilon)}\left(-\frac{\boldsymbol{x} - e^{-t'}\boldsymbol{x}'_{m_{k,r}(\epsilon)}}{1 - e^{-2t'}}\right)$$

end
Return : $\boldsymbol{v}'$ /* As the approximation of $\nabla \log p_{k,S-r\eta}(\boldsymbol{x})$ */

Algorithm 2 Recursive Score Diffusion-based Monte Carlo (RS-DMC)

Input : Initial particle $\mathbf{x}^{\leftarrow}_{K,S}$ sampled from p_∞, Terminal time T, Step size η, required convergence accuracy ϵ.

for $k = K-1$ *down to* 0 **do**
  Initialize the particle as $\boldsymbol{x}^{\leftarrow}_{k,0} \leftarrow \boldsymbol{x}^{\leftarrow}_{k+1,S}$
  for $r = 0$ *to* $R-1$ **do**
    Approximate the score, i.e., $\nabla \log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})$ by $\boldsymbol{v}' \leftarrow \mathsf{RSE}(k, r, \boldsymbol{x}^{\leftarrow}_{k,r\eta}, l(\epsilon))$
    $\boldsymbol{x}^{\leftarrow}_{k,(r+1)\eta} \leftarrow e^{\eta}\boldsymbol{x}^{\leftarrow}_{k,r\eta} + \left(e^{\eta} - 1\right)\boldsymbol{v}' + \xi$ where ξ is sampled from $\mathcal{N}\left(0, \left(e^{2\eta} - 1\right)\boldsymbol{I}_d\right)$
  end
end
Return : $\boldsymbol{x}^{\leftarrow}_{0,S}$

Diffusion-based Monte Carlo with Recursive Score Estimation. Based on Alg 1, we can directly apply the DDPM (Ho et al., 2020) based method to perform the sampling, giving rise to the Recursive

Score Diffusion-based Monte Carlo (RS-DMC) method. We summarize the algorithm in Alg 2 (the detailed setup of $m_{k,r}(\cdot)$, $n_{k,r}(\cdot)$, $l_{k,r}(\cdot)$ are provided in Theorem 5 in Appendix B).

4. Analysis of RS-DMC

In this section, we will establish the convergence guarantee for RS-DMC and reveal how the gradient complexity depends on the problem dimension and the target sampling error. We will also compare the gradient complexity of RS-DMC with other sampling methods to justify its strength. Additionally, we will provide a proof roadmap that briefly summarizes the critical theoretical techniques.

4.1. Theoretical Results

The following theorem states that RS-DMC can provably converge to the target distribution in KL-divergence with quasi-polynomial gradient complexity.

Theorem 2 (Gradient complexity of RS-DMC, informal) *Under Assumptions* **[A1]**-**[A2]**, *let* $p^{\leftarrow}_{0,S}$ *be the distribution of the samples generated by RS-DMC, then there exists a collection of appropriate hyperparameters* $n_{k,r}, m_{k,r}, \tau_r, \eta, l_{k,r}$ *and* l *such that with probability at least* $1-\epsilon$, *it holds that* $\mathrm{KL}\left(p_*\|p^{\leftarrow}_{0,S}\right) = \tilde{O}(\epsilon)$. *Besides, the gradient complexity of RS-DMC is*

$$\exp\left[\mathcal{O}\left(L^3 \cdot \log^3\left((Ld+M)/\epsilon\right) \cdot \max\left\{\log\log Z^2, 1\right\}\right)\right], \tag{6}$$

where Z *denotes the maximum norm of particles which appears in Alg 2.*

We defer the detailed configurations of $n_{k,r}, m_{k,r}, \tau_r, \eta, l_{k,r}$, l and relative constants in the formal version of this theorem, i.e., Theorem 5 Appendix B and Table 2 in Appendix A, respectively. From this theorem, we note the gradient complexity will be exponentially dependent on the smoothness L. Actually, such an exponential dependence may be inevitable under Assumption **[A1]** and **[A2]**. Considering the sampling problem with the target distribution $\exp(-\beta U)$, when the temperature β increases to $\tilde{\mathcal{O}}(d/\epsilon)$ level (e.g., the smoothness is also $\tilde{\mathcal{O}}(d/\epsilon)$), the sampling problem can be very close to an optimization problem. Then, if the gradient complexity of RS-DMC does not have an exponential dependency on the smoothness, it can be used to solve the optimization problem with potentially quasi-polynomial gradient calculations. This contradicts the $\tilde{\Omega}((LR^2/\epsilon)^{d/2})$ lower bound results proved in Ma et al. (2019). In the following, we compare our theoretical results with those of other previous work.

Comparison with ULA. The gradient complexity of ULA has been well studied for sampling the non-log-concave distribution. However, in order to prove the convergence in KL divergence or TV distance, they typically require additional isoperimetric conditions, such as Log-Soboleve and Poincaré inequality (see Definitions 3 and 4). In particular, when p_* satisfies LSI with parameter α, Vempala and Wibisono (2019) proved the $\mathcal{O}\left(d\epsilon^{-1}\alpha^{-2}\right)$ in KL convergence. However, for general non-log-concave distributions, α is not dimension-free. For instance, under the Dissipative condition (Hale, 2010), α can be as worse as $\exp(-\mathcal{O}(d))$ (Raginsky et al., 2017), leading to a $\exp(\mathcal{O}(d))$ gradient complexity results (Xu et al., 2018).

When the isoperimetric condition is absent, Balasubramanian et al. (2022) proved the convergence of ULA based on the Fisher information measure, i.e., $\mathrm{FI}\left(p\|p_*\right) := \mathbb{E}_p[\|\nabla\log(p/p_*)\|^2]$, they showed that ULA can generate the samples that satisfy $\mathrm{FI}\left(p\|p_*\right) \le \epsilon$ for some small error tolerance

ϵ. However, it may be unclear what can be entailed by such a guarantee $\mathrm{FI}\left(p\|p_*\right) \le \epsilon$. It has demonstrated that, in some cases, even if the Fisher information $\mathrm{FI}\left(p\|p_*\right)$ is very small, the total variation distance/KL divergence remains bounded away from zero (Balasubramanian et al. (2022)). This suggests that the convergence guarantee in Fisher information might be weaker than that in KL divergence (i.e., our convergence guarantee).

Comparison with DMC. Then we make a detailed comparison with DMC in (Huang et al., 2023), which is the most similar algorithm compared to ours. Firstly, we would like to strengthen again that our convergence results are obtained on a milder assumption, while Huang et al. (2023) additionally requires the target distribution to have a heavier tail. Besides, as discussed in the introduction section, DMC has a much worse gradient complexity since it performs all score estimation straightforwardly, while RS-DMC is based on a recursive structure. Consequently, DMC involves many hard sampling subproblems that take exponential time to solve, while RS-DMC only involves strongly log-concave subsampling problems that can be efficiently solved within polynomial time. As a result, the gradient complexity of RDS is proved to be $\mathrm{poly}(d)\cdot \mathrm{poly}(1/\epsilon)\cdot \exp\left(\mathcal{O}(1/\epsilon)\right)$, which is significantly worse than the quasi-polynomial gradient complexity of RS-DMC.

4.2. Proof Sketch

In this section, we aim to highlight the technical innovations by presenting the roadmap of our analysis. Due to space constraints, we have included the technical details in the Appendix.

Firstly, by requiring Novikov's conditions, we can establish an upper bound on the KL divergence gap between the target distribution p_* and the underlying distribution of output particles, i.e., $p^{\leftarrow}_{0,S}$, by Girsanov's Theorem which demonstrates

$$
\begin{aligned}
\mathrm{KL}\left(p_*\|p^{\leftarrow}_{0,S}\right) \le & \underbrace{\mathrm{KL}\left(p_{K-1,S}\|p^{\leftarrow}_{K-1,0}\right)}_{\text{Term 1}} + \underbrace{2\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{\mathbf{x}^{\leftarrow}_{k,r\eta}}\left[\left\|\nabla\log p_{k,S-r\eta}(\mathbf{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\mathbf{x}^{\leftarrow}_{k,r\eta})\right\|^2\right]\mathrm{d}t}_{\text{Term 3}} \\
& + \underbrace{2\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{(\mathbf{x}^{\leftarrow}_{k,t+r\eta},\mathbf{x}^{\leftarrow}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\mathbf{x}^{\leftarrow}_{k,t+r\eta}) - \nabla\log p_{k,S-r\eta}(\mathbf{x}^{\leftarrow}_{k,r\eta})\right\|^2\right]\mathrm{d}t}_{\text{Term 2}}.
\end{aligned}
$$

Although Novikov's condition may not be met in general, we employ techniques in Chen et al. (2023a) and sidestep this issue by utilizing a differential inequality argument as shown in Lemma 27.

Upper bound Term 1. Intuitively, Term 1 appears since we utilize the standard Gaussian to initialize the reverse OU process (SDE (2)) rather than $p_{K-1,S}$ which can hardly be sampled from directly in practice. Therefore, the first term can be bounded using exponential mixing of the forward (Ornstein-Uhlenbeck) process towards the standard Gaussian in Lemma 9, i.e.,

$$
\mathrm{KL}\left(p_{K-1,S}\|p^{\leftarrow}_{K-1,0}\right) \le \mathrm{KL}\left(p_*\|p^{\leftarrow}_{K-1,0}\right)\exp(-KS) \le (Ld+M)\exp(-KS),
$$

where $p^{\leftarrow}_{K-1,0} = \mathcal{N}(\mathbf{0},\boldsymbol{I})$ as shown SDE (2).

Upper bound Term 2. Term 2 corresponds to the discretization error, which has been successfully addressed in previous work Chen et al. (2023b,a). By utilizing the unique structure of the Ornstein-Uhlenbeck process, they managed to limit both the time and space discretization errors, which decrease as η becomes smaller. To ensure the completeness of our proof, we have included it in Lemma 13, utilizing the segmented notation.

Upper bound Term 3. Term 3 represents the accuracy of the score estimation. In diffusion models, due to the parameterization of the target density, this term is trained by a neural network and assumed to be less than ϵ to ensure the convergence of the reverse process. However, in RS-DMC, the score estimation is obtained using a non-parametric approach, i.e., Alg 1. To this end, we can provide rigorous high probability bound for this term under Alg 1, which is stated in Lemma 23. Roughly speaking, for Alg 1 with input each $(k, r, \boldsymbol{x}, \epsilon)$, suppose the score estimation of $\nabla \log p_{k,0}$ is given as $\mathbf{v}^{\leftarrow}_{k-1,0}$ satisfying the following event

$$\bigcap_{\boldsymbol{x}' \in \mathbb{S}_{k,r}(\boldsymbol{x},\epsilon)} \left\|\nabla \log p_{k,0}(\boldsymbol{x}') - \mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2 \le l_{k,r}(\epsilon)$$

where $\mathbb{S}_{k,r}(\boldsymbol{x},\epsilon)$ denotes the set of particles appear in Alg 1 except for the recursion. In this condition, Lemma 20 provides the upper bound of score estimation error as:

$$\begin{aligned} \left\|\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}) - \nabla \log p_{k,S-r\eta}(\boldsymbol{x})\right\|^2 \le & \frac{2e^{-2(S-r\eta)}}{\left(1-e^{-2(S-r\eta)}\right)^2} \cdot \underbrace{\left\| -\frac{1}{n_{r,k}(\epsilon)} \sum_{i=1}^{n_{r,k}(\epsilon)} \mathbf{x}'_i + \mathbb{E}_{\mathbf{x}' \sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right] \right\|^2}_{\text{Term 3.1}} \\ & + \frac{2e^{-2(S-r\eta)}}{\left(1-e^{-2(S-r\eta)}\right)^2} \cdot \underbrace{\left\| -\mathbb{E}_{\mathbf{x}' \sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right] + \mathbb{E}_{\mathbf{x}' \sim q_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right] \right\|^2}_{\text{Term 3.2}} \end{aligned}$$

where $q'_{k,S-r\eta}(\cdot|\boldsymbol{x})$ is the underlying distribution of output particles, i.e., $\mathbf{x}'_{m_{k,r}(l_{k,r}(\epsilon))}$ in Alg 1. Considering that the distribution $q_{k,S-r\eta}$ is strongly log-concave (given in Eq. 4) and we can get a lower bound on the strongly log-concave constant (see Lemma 15). Therefore, $q'_{k,S-r\eta}$ also satisfies the log-Sobolev inequality due to Lemma 32, which can imply the variance upper bound (see Lemma 35). Then, in our proof, we directly make use of the Sobolev inequality to derive the high-probability bound (or concentration results) for estimating the mean of $q'_{k,S-r\eta}(\cdot|\boldsymbol{x})$ in Term 3.1 with Lemma 20 by selecting sufficiently large $n_{k,r}(\epsilon)$. Besides, Term 3.2 can be upper bounded by $\mathrm{KL}\big(q'_{k,S-r\eta}(\cdot|\boldsymbol{x})\|q_{k,S-r\eta}(\cdot|\boldsymbol{x})\big)$, which can be well controlled by conducting the ULA with a sufficiently large iteration number $m_{k,r}(\epsilon)$. Therefore, by conducting the following decomposition

$$\begin{aligned} & \mathbb{P}\left[\left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le \epsilon\right] \\ & \ge (1-\delta)\mathbb{P}\left[\bigcap_{\boldsymbol{x}' \in \mathbb{S}_{k,r}(\boldsymbol{x},\epsilon)} \left\|\nabla \log p_{k,0}(\boldsymbol{x}') - \mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2 \le l_{k,r}(\epsilon)\right]. \end{aligned}$$

We only need to use this proof process recursively with a proper choice of δ (δ as a function of ϵ) to get the bound:

$$\mathbb{P}\left[\left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le \epsilon\right] \ge 1-\epsilon,$$

which implies Term 3 $\le \tilde{O}(\epsilon)$ with a probability at least $1-\epsilon$. Due to the large amount of computation, we defer the details of the recursive proof procedure and the choice of δ to the Appendix E.3.

5. Empirical Results

We consider the target distribution defined on $\mathbb{R}^2$ to be a mixture of Gaussian distributions with 6 modes. Meanwhile, we draw $1,000$ particles from the target distribution, presented as blue nodes

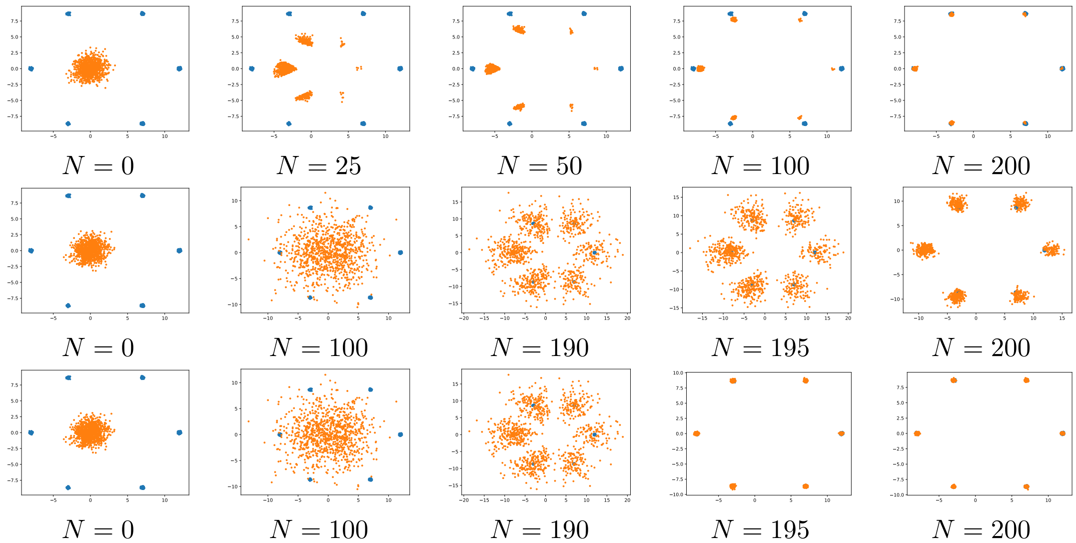

Figure 3: Illustration of the returned particles for ULA, RS-DMC-v1 and RS-DMC-v2 shown with orange particles and the blue ones sampled from the ground truth. The first row is returned by ULA, the second is RS-DMC-v1 and the last is from RS-DMC-v2. $N = \text{grad num}$.

shown in Fig. 3. We fix the random seed and initialize particles with the standard Gaussian. Then, update particles with the following three settings:

ULA. We choose ULA Neal (1992); Roberts and Tweedie (1996) as the sampler, setting the step size and the iteration number as $2 \cdot 10^{-4}$ and 200 respectively.

RS-DMC-v1. We choose RS-DMC as the sampler, setting the outer step size and the inner step size as $\eta = 0.05$ and $\tau_r = 0.01$, respectively. For inner loops, the # of samples and iterations, i.e., $n_{k,r}$ and $m_{k,r}$, are 1. For outer loops, the # of iterations is 200, and we divide the entire process into two segments, i.e., $K = 2$, and each segment contains 100 iterations, i.e., $R = 100$.

RS-DMC-v2. We choose the same hyper-parameter settings as that in RS-DMC-v1, but replace the mean estimation by the ULA's update for the last 10 iterations since when $p_t^{\leftarrow}$ is closed to p_*, i.e.,

$$\lim_{t \to T} \nabla \log p_t^{\leftarrow}(\boldsymbol{x}) = \nabla \log p_0(\boldsymbol{x}) + \mathcal{O}\left((T-t)\right) \approx -\nabla f_*(\boldsymbol{x}),$$

which follows from Lemma 10 and means $-\nabla f_*(\boldsymbol{x})$ can approximate the score.

Experimental results. To compare the behaviors of the three methods, we illustrate the particles when the algorithms return for different gradient complexity in Fig 3. We note that (1) ULA will quickly fall into some specific modes, and most steps are used to improve the mean estimation of each mode. However, the number of particles belonging to each mode is unbalanced and almost determined at the very beginning of the entire process. This is because the drift force of different modes at the origin varies greatly. (2) RS-DMC-v1 quickly covers the different modes and converges to their means. Besides, the number of particles belonging to each mode is much more balanced than that in ULA. However, since we only choose $n_{k,r} = m_{k,r} = 1$, and the score $\nabla \log p_{k,t}(\boldsymbol{x})$ does not be approximated accurately, the convergence to specific modes will be relatively slow, which causes the variance of RS-DMC-v1 larger than the target distribution. (3) RS-DMC-v2 takes the advantage of RS-DMC-v1 and estimate the the score $\nabla \log p_{k,t}(\boldsymbol{x})$, when $p_{k,t}(\boldsymbol{x})$ approaches p_*, with $-f_*(\boldsymbol{x})$ directly rather than a inner-loop mean estimation. From another perspective, RS-DMC-v2 covers the different modes by RS-DMC-v1 and achieves local convergence by ULA. Hence, it has a balanced particle distribution for each mode and shares a variance almost identical to the ground truth.

6. Conclusion

In this paper, we propose a novel non-parametric score estimation algorithm, i.e., RSE, presented in Alg 1 and derive its corresponding reverse diffusion sampling algorithm, i.e., RS-DMC, and outlined in Alg 2. By introducing the segment length S to balance the challenges of score estimation and recursive calls, RS-DMC exhibits several advantages over Langevin-based MCMC, e.g., ULA, ULD, and MALA. It can achieve KL convergence beyond isoperimetric target distributions with a quasi-polynomial gradient complexity, i.e., $\exp\left[\mathcal{O}(L^3 \cdot \log^3(d/\epsilon) \cdot \max\left\{\log\log Z^2, 1\right\})\right]$. Additionally, the theoretical result also demonstrates the efficiency of RS-DMC in challenging sampling tasks. To the best of our knowledge, this is the first work that eliminates the exponential dependence with only smoothness and the second moment bounded assumptions.

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Contents

Appendix A. Notations

Symbols	Description
φ_{σ^2}	The density function of the centered Gaussian distribution, i.e., $\mathcal{N}\left(\mathbf{0}, \sigma^2 \boldsymbol{I}\right)$.
$p_*, p_{0,0}$	The target density function (initial distribution of the forward process)
$\{\mathbf{x}_{k,t}\}_{k\in\mathbb{N}_{0,K-1}, t\in[0,S]}$	The forward process, i.e., SDE 1
$p_{k,t}$	The density function of $\mathbf{x}_{k,t}$, i.e., $\mathbf{x}_{k,t} \sim p_{k,t}$
p_∞	The density function of the stationary distribution of the forward process
$\{\mathbf{x}^{\leftarrow}_{k,t}\}_{k\in\mathbb{N}_{0,K-1}, t\in[0,S]}$	The practical reverse process following from SDE 2 with initial distribution p_∞
$p^{\leftarrow}_{k,t}$	The density function of $\mathbf{x}^{\leftarrow}_{k,t}$, i.e., $\mathbf{x}^{\leftarrow}_{k,t} \sim p^{\leftarrow}_{k,t}$

Table 1: The list of notations defined in Section 2, where $\mathbb{N}_{a,b}$ is denoted as the set of natural numbers from $a \in \mathbb{N}_*$ to any $b \in \mathbb{N}_+$.

In this section, we summarize the notations defined in Section 2 in Table 1 for easy reference and cross-checking. Additionally, another important notation is the score estimation, denoted as $\mathbf{v}^{\leftarrow}_{k,r\eta}$, which is used to approximate $\nabla \log p_{k,S-r\eta}$. When $r = 0$, $\mathbf{v}^{\leftarrow}_{k,0}$ is expected to approximate $\nabla \log p_{k,S}$ which is not explicitly defined in SDE 1. However, sine $\mathbf{x}_{k,S} = \mathbf{x}_{k+1,0}$ in Eq 1, the underlying distributions, i.e., $p_{k,S}$ and $p_{k+1,0}$, are equal, and $\tilde{\mathbf{v}}_{k,0}$ can be considered as the score estimation of $\nabla \log p_{k+1,0}$. For $\nabla \log p_{0,0}$, which can be calculated exactly as ∇f_*, we define

$$\mathbf{v}^{\leftarrow}_{-1,0}(\boldsymbol{x}) = \nabla \log p_{0,0}(\boldsymbol{x}) = -\nabla f_*(\boldsymbol{x}) \tag{7}$$

as a complement.

Isoperimetric conditions and assumptions. According to the classical theory of Markov chains and diffusion processes, some conditions can lead to fast convergence over time without being as strict as log concavity. Isoperimetric inequalities, such as the log-Sobolev inequality (LSI) or the Poincaré inequality (PI), are examples of these conditions defined as follows.

Definition 3 (Logarithmic Sobolev inequality) *A distribution with density function p satisfies the log-Sobolev inequality with a constant $\mu > 0$ if for all smooth function $g\colon \mathbb{R}^d \to \mathbb{R}$ with $\mathbb{E}_p[g^2] \le \infty$,*

$$\mathbb{E}_p\left[g^2 \log g^2\right] - \mathbb{E}_p\left[g^2\right] \log \mathbb{E}_p\left[g^2\right] \le 2\alpha^{-1}\mathbb{E}_p\left[\left\|\nabla g\right\|^2\right].$$

Constant symbol	Value	Constant symbol	Value
C_η	$2^{-14}L^{-2}$	$C_{m,1}$	$\log\left(2M \cdot 3^2 \cdot 5L\right) + M \cdot 3L$
C_n	$2^6 \cdot 5^2 \cdot C_\eta^{-1}$	C_m	$2^9 \cdot 3^2 \cdot 5^3 \cdot C_{m,1} C_\eta^{-1.5}$
$C_{u,1}$	$\log\left(\frac{5C_nC_m}{10^4}\right) + \log\left(2\max\left\{\log Z, \frac{1}{2}\right\}\right)$	$C_{u,2}$	$70/S^2 + 10/S$
$C_{u,3}$	$2C_{u,1}/S$	S	$1/2\log((2L+1)/2L)$

Table 2: Constant List independent with ϵ and d.

By supposing $g = 1 + \epsilon\hat{g}$ with $\epsilon \to 0$, a weaker isoperimetric inequality, i.e., PI can be defined Menz and Schlichting (2014).

Definition 4 (Poincaré inequality) *A distribution with density function p satisfies the Poincaré inequality with a constant $\mu > 0$ if for all smooth function $\hat{g}\colon \mathbb{R}^d \to \mathbb{R}$,*

$$\mathrm{Var}(\hat{g}) \le \alpha^{-1}\mathbb{E}_p\left[\left\|\nabla\hat{g}\right\|^2\right].$$

We also provide a list of constants used in our following proof in Table 2 to prevent confusion.

Appendix B. Proof of Theorem 2

Theorem 5 *The formal version of Theorem 2 In Alg 2, suppose we set*

$$\begin{aligned}
&S = 1/2\cdot\log(1+1/2L),\quad K = 2\log[(Ld+M)/\epsilon]\cdot S^{-1},\\
&\eta = C_\eta(M+d)^{-1}\epsilon,\quad R = S/\eta,\\
&l(\epsilon) = 10\epsilon,\quad l_{k,r}(\epsilon) = \epsilon/960,\\
&n_{k,r}(\epsilon) = C_n\cdot(d+M)\epsilon^{-2}\cdot\max\{d, -2\log\delta\},\\
&m_{k,r}(\epsilon,\boldsymbol{x}) = C_m\cdot(d+M)^3\epsilon^{-3}\cdot\max\{\log\|\boldsymbol{x}\|^2, 1\},\\
&\tau_r = 2^{-5}\cdot 3^{-2}\cdot e^{2(S-r\eta)}\left(1-e^{-2(S-r\eta)}\right)^2\cdot d^{-1}\epsilon
\end{aligned}$$

where δ satisfies

$$\begin{aligned}
\delta =&\mathrm{pow}\left(2, -\frac{2}{S}\log\frac{Ld+M}{\epsilon}\right)\cdot\mathrm{pow}\left(\frac{C_\eta S\epsilon^2}{4(d+M)}\cdot\log^{-2}\left(\frac{Ld+M}{\epsilon}\right)\cdot\mathrm{pow}\left(\left(\frac{Ld+M}{\epsilon}\right),\right.\right.\\
&\left.\left.-C_{u,2}\log\frac{Ld+M}{\epsilon} - C_{u,3}\right), \frac{2}{S}\log\frac{Ld+M}{\epsilon}+1\right),
\end{aligned}$$

and the initial underlying distribution q_0' of the Alg 1 with input $(k, r, \boldsymbol{x}, \epsilon)$ satisfies

$$q_0'(\boldsymbol{x}') \propto \exp\left(-\frac{\left\|\boldsymbol{x} - e^{-(S-r\eta)}\boldsymbol{x}'\right\|^2}{2(1-e^{-2(S-r\eta)})}\right),$$

we have

$$\mathbb{P}\left[\mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right) = \tilde{O}(\epsilon)\right] \ge 1-\epsilon.$$

In this condition, the gradient complexity will be

$$\exp\left[\mathcal{O}\left(L^3\cdot\log^3\left((Ld+M)/\epsilon\right)\cdot\max\left\{\log\log Z^2, 1\right\}\right)\right]$$

where Z is the maximal norm of particles appeared in Alg 2.

Proof [Proof of Theorem 5] According to Lemma 27, suppose $\hat{\mathbf{x}}_{k,t} = \mathbf{x}_{k,S-t}$ whose SDE can be presented as

$$\begin{aligned}
&\mathbf{x}^{\leftarrow}_{k,0} \sim p_{K-1,S} \text{ when } k = K-1,\ \text{else } \mathbf{x}^{\leftarrow}_{k,0} = \mathbf{x}^{\leftarrow}_{k+1,S} && k\in\mathbb{N}_{0,K-1}\\
&\mathrm{d}\mathbf{x}^{\leftarrow}_{k,t} = \left[\mathbf{x}^{\leftarrow}_{k,t} + 2\nabla\log p_{k,S-t}(\mathbf{x}^{\leftarrow}_{k,t})\right]\mathrm{d}t + \sqrt{2}\mathrm{d}B_t && k\in\mathbb{N}_{0,K-1}, t\in[0,S]
\end{aligned}$$

due to Chen et al. (2023b). Then, we have $\mathrm{KL}\left(p_*\|p^{\leftarrow}_{0,S}\right) = \mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right)$ which satisfies

$$\begin{aligned}\mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right) \leq & \underbrace{\mathrm{KL}\left(\hat{p}_{K-1,0}\|p^{\leftarrow}_{K-1,0}\right)}_{\text{Term 1}} \\ & + \sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{(\hat{\mathbf{x}}_{k,t+r\eta},\hat{\mathbf{x}}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t.\end{aligned} \tag{8}$$

Upper bound Term 1. Term 1 can be upper-bounded as

$$\text{Term 1} = \mathrm{KL}\left(p_{K-1,S}\|p^{\leftarrow}_{K-1,0}\right) \leq (Ld+M)\cdot\exp\left(-KS/2\right)$$

with Lemma 9 when $p^{\leftarrow}_{K-1,0}$ is chosen as the standard Gaussian. Therefore, we choose

$$S = \frac{1}{2}\log\frac{2L+1}{2L}, \quad K = 2\log\frac{Ld+M}{\epsilon}\cdot\left(\frac{1}{2}\log\frac{2L+1}{2L}\right)^{-1}, \quad \text{and} \quad KS \geq 2\log\frac{Ld+M}{\epsilon},$$

which make the inequality Term $1 \leq \epsilon$ establish.

For the remaining term of RHS of Eq 8, it can be decomposed as follows:

$$\begin{aligned}&\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{(\hat{\mathbf{x}}_{k,t+r\eta},\hat{\mathbf{x}}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t \\ &\leq \underbrace{2\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \nabla\log p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t}_{\text{Term 2}} \\ &\quad \underbrace{+ 2\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{(\hat{\mathbf{x}}_{k,t+r\eta},\hat{\mathbf{x}}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t}_{\text{Term 3}}\end{aligned} \tag{9}$$

Upper bound Term 2. This term is mainly from the discretization error in the reverse process. Therefore, its analysis is highly related to Chen et al. (2023b,a). To ensure the completeness of our proof, we have included it in our analysis, utilizing the segmented notation presented in Section A. Specifically, we have

$$\begin{aligned}\text{Term 2} \leq & 4\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right] \\ & + 4\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}\left[\left\|\nabla\log\frac{p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,r\eta})}{p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta})}\right\|^2\right]\mathrm{d}t \\ \leq & 4\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \left(\mathbb{E}\left[L^2\left\|\hat{\mathbf{x}}_{k,t+r\eta} - \hat{\mathbf{x}}_{k,r\eta}\right\|^2\right] + \mathbb{E}\left[\left\|\nabla\log\frac{p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta})}{p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,r\eta})}\right\|^2\right]\right)\mathrm{d}t\end{aligned}$$

where the last inequality follows from Assumption **[A1]**. Combining this result with Lemma 13, when the stepsize, i.e., η of the reverse process is $\eta = C_\eta(M+d)^{-1}\epsilon$, then it has Term $2 \leq \epsilon$.

Upper bound Term 3. Due to the randomness of $\mathbf{v}^{\leftarrow}_{k,r\eta}$, we consider a high probability bound, which is formulated as

$$\mathbb{P}\left[\bigcap_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}} \left\|\nabla\log p_{k,S-r\eta}(\mathbf{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\mathbf{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right] \ge 1-\epsilon, \tag{10}$$

which means we choose $l(\epsilon)=10\epsilon$. Lemma 23 demonstrate that under the following settings, i.e.,

$$\begin{aligned}
&l_{k,r}(\epsilon) = \epsilon/960,\\
&n_{k,r}(\epsilon) = C_n\cdot (d+M)\epsilon^{-2}\cdot \max\{d, -2\log\delta\},\\
&m_{k,r}(\epsilon,\boldsymbol{x}) = C_m\cdot (d+M)^3\epsilon^{-3}\cdot\max\{\log\|\boldsymbol{x}\|^2, 1\},
\end{aligned}$$

where δ satisfies

$$\begin{aligned}
\delta :=& \mathrm{pow}\left(2, -\frac{2}{S}\log\frac{Ld+M}{\epsilon}\right)\cdot \mathrm{pow}\left(\frac{C_\eta S\epsilon^2}{4(d+M)}\cdot\log^{-2}\left(\frac{Ld+M}{\epsilon}\right)\cdot \mathrm{pow}\left(\left(\frac{Ld+M}{\epsilon}\right),\right.\right.\\
&\left.\left.-C_{u,2}\log\frac{Ld+M}{\epsilon} - C_{u,3}\right), \frac{2}{S}\log\frac{Ld+M}{\epsilon}+1\right),
\end{aligned}$$

Eq 10 can be achieved with a gradient complexity:

$$\exp\left[\mathcal{O}\left(L^3\cdot\log^3\left((Ld+M)/\epsilon\right)\cdot\max\left\{\log\log Z^2, 1\right\}\right)\right]$$

where Z is the maximal norm of particles appeared in Alg 2. All constants can be found in Table 2. In this condition, we have

$$\text{Term 3} \le 4\cdot\frac{T}{\eta}\cdot(\eta\cdot 10\epsilon)\le 40\epsilon\log\frac{Ld+M}{\epsilon} = \tilde{O}(\epsilon).$$

Combining the upper bound of Term 1, Term 2 and Term 3, we have

$$\mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right) = \tilde{O}(\epsilon).$$

The proof is completed. ■

Corollary 6 *Suppose we set all parameters except for δ to be the same as that in Theorem 5, and define*

$$\begin{aligned}
\delta =& \mathrm{pow}\left(2, -\frac{2}{S}\log\frac{Ld+M}{\epsilon}\right)\cdot \mathrm{pow}\left(\frac{C_\eta S\epsilon\delta'}{4(d+M)}\cdot\log^{-2}\left(\frac{Ld+M}{\epsilon}\right)\cdot \mathrm{pow}\left(\left(\frac{Ld+M}{\epsilon}\right),\right.\right.\\
&\left.\left.-C_{u,2}\log\frac{Ld+M}{\epsilon} - C_{u,3}\right), \frac{2}{S}\log\frac{Ld+M}{\epsilon}+1\right),
\end{aligned}$$

we have

$$\mathbb{P}\left[\mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right) = \tilde{O}(\epsilon)\right]\ge 1-\delta'.$$

In this condition, the gradient complexity will be

$$\exp\left[\mathcal{O}\left(L^3\cdot\max\left\{\left(\log\frac{Ld+M}{\epsilon}\right)^3, \log\frac{Ld+M}{\epsilon}\cdot\log\frac{1}{\delta'}\right\}\cdot\max\left\{\log\log Z^2, 1\right\}\right)\right]$$

where Z is the maximal norm of particles appeared in Alg 2.

Proof In this corollary, we follow the same proof roadmap as that shown in Theorem 5. Combining Eq 8 and Eq 9, we have

$$\begin{aligned}\mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right) \le & \underbrace{\mathrm{KL}\left(\hat{p}_{K-1,0}\|p^{\leftarrow}_{K-1,0}\right)}_{\text{Term 1}}\\ & \underbrace{\le 2\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \nabla\log p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t}_{\text{Term 2}} \\ & \underbrace{+ 2\sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{(\hat{\mathbf{x}}_{k,t+r\eta},\hat{\mathbf{x}}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t}_{\text{Term 3}}\end{aligned} \tag{11}$$

It should be noted that the techniques for upper-bounding $\mathrm{Term}\ 1$ and $\mathrm{Term}\ 2$ are the same as that in Theorem 5.

Upper bound Term 3. Due to the randomness of $\mathbf{v}^{\leftarrow}_{k,r\eta}$, we consider a high probability bound, which is formulated as

$$\mathbb{P}\left[\bigcap_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}} \left\|\nabla\log p_{k,S-r\eta}(\mathbf{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\mathbf{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right] \ge 1-\delta', \tag{12}$$

which means we choose $l(\epsilon)=10\epsilon$. Lemma 24 demonstrate that under the following settings, i.e.,

$$\begin{aligned} & l_{k,r}(\epsilon) = \epsilon/960,\\ & n_{k,r}(\epsilon) = C_n\cdot(d+M)\epsilon^{-2}\cdot\max\{d,-2\log\delta\},\\ & m_{k,r}(\epsilon,\boldsymbol{x}) = C_m\cdot(d+M)^3\epsilon^{-3}\cdot\max\{\log\|\boldsymbol{x}\|^2,1\},\end{aligned}$$

where δ satisfies

$$\begin{aligned}\delta := & \mathrm{pow}\left(2, -\frac{2}{S}\log\frac{Ld+M}{\epsilon}\right)\cdot\mathrm{pow}\left(\frac{C_\eta S\epsilon\delta'}{4(d+M)}\cdot\log^{-2}\left(\frac{Ld+M}{\epsilon}\right)\cdot\mathrm{pow}\left(\left(\frac{Ld+M}{\epsilon}\right),\right.\right.\\ & \left.\left. -C_{u,2}\log\frac{Ld+M}{\epsilon} - C_{u,3}\right), \frac{2}{S}\log\frac{Ld+M}{\epsilon}+1\right),\end{aligned}$$

Eq 12 can be achieved with a gradient complexity:

$$\exp\left[\mathcal{O}\left(L^3\cdot\max\left\{\left(\log\frac{Ld+M}{\epsilon}\right)^3, \log\frac{Ld+M}{\epsilon}\cdot\log\frac{1}{\delta'}\right\}\cdot\max\left\{\log\log Z^2, 1\right\}\right)\right]$$

where Z is the maximal norm of particles appeared in Alg 2. All constants can be found in Table 2. In this condition, we have

$$\mathrm{Term}\ 3 \le 4\cdot\frac{T}{\eta}\cdot(\eta\cdot 10\epsilon) \le 40\epsilon\log\frac{Ld+M}{\epsilon} = \tilde{O}(\epsilon).$$

Combining the upper bound of $\mathrm{Term}\ 1$, $\mathrm{Term}\ 2$ and $\mathrm{Term}\ 3$, we have

$$\mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right) = \tilde{O}(\epsilon).$$

The proof is completed. ■

Appendix C. Lemmas for Bounding Initialization Error

Lemma 7 (Lemma 11 in Vempala and Wibisono (2019)) *Suppose $p \propto \exp(-f)$ and $f\colon \mathbb{R}^d \to \mathbb{R}$ is L-gradient Lipschitz continuous function. Then, we have*

$$\mathbb{E}_{\mathbf{x}\sim p}\left[\|\nabla f(\mathbf{x})\|^2\right] \le Ld$$

Lemma 8 *Under the notation in Section A, suppose $p \propto \exp(-f)$ satisfies Assumption **[A1]** and **[A2]**, then we have*

$$\mathrm{KL}\left(p\|\varphi_1\right) \le Ld + M$$

Proof From the analytic form of the standard Gaussian, we have $\nabla^2 \log \varphi_1 = \boldsymbol{I}$. Combining this fact with Lemma 28, we have

$$\begin{aligned}\mathrm{KL}\left(p\|\varphi_1\right) \le & \frac{1}{2}\int p(\boldsymbol{x})\left\|\nabla \log \frac{p(\boldsymbol{x})}{\varphi_1(\boldsymbol{x})}\right\|^2 \mathrm{d}\boldsymbol{x}\\ \le & \int p(\boldsymbol{x})\left\|\nabla f(\boldsymbol{x})\right\|^2 \mathrm{d}\boldsymbol{x} + \int p(\boldsymbol{x})\left\|\boldsymbol{x}\right\|^2 \mathrm{d}\boldsymbol{x} \le Ld + M.\end{aligned}$$

where the last inequality follows from Lemma 7 and Assumption **[A2]**. Hence, the proof is completed. ■

Lemma 9 (Variant of Theorem 4 in Vempala and Wibisono (2019)) *Under the notation in Section A, suppose $\tilde{p}_{K-1,0}$ is chosen as the standard Gaussian distribution. Then, we have*

$$\mathrm{KL}\left(p_{K-1,S}\|p_\infty\right) \le (Ld+M)\cdot \exp\left(-KS/2\right).$$

Proof Suppose another random variable $\mathbf{z}_t \coloneqq \mathbf{x}_{\lfloor t/S\rfloor, t-\lfloor t/S\rfloor\cdot S}$ where $\mathbf{x}_{k,t}$ is shown in SDE 1, we have

$$\mathrm{d}\mathbf{z}_t = -\mathbf{z}_t\mathrm{d}t + \sqrt{2}\mathrm{d}B_t,\quad \mathbf{z}_0 = \mathbf{x}_{0,0},$$

where the underlying distribution of $\mathbf{x}_{0,0}$ satisfies $p_{0,0} = p_* \propto \exp(-f_*)$. If we denote $\mathbf{z}_t \sim p_t^{(z)}$, then Fokker-Planck equation of the previous SDE will be

$$\partial_t p_t^{(z)}(\boldsymbol{z}) = \nabla\cdot\left(p_t^{(z)}(\boldsymbol{z})\boldsymbol{z}\right) + \Delta p_t^{(z)}(\boldsymbol{z}) = \nabla\cdot\left(p_t^{(z)}(\boldsymbol{z})\nabla\log\frac{p_t^{(z)}(\boldsymbol{z})}{\exp\left(-\frac{1}{2}\|\boldsymbol{z}\|^2\right)}\right).$$

It implies that the stationary distribution is standard Gaussian, i.e., $p_\infty^{(z)} \propto \exp(-1/2\cdot\|\boldsymbol{z}\|^2)$. Then, we consider the KL convergence of $(\mathbf{z}_t)_{t\ge 0}$, and have

$$\begin{aligned}\frac{\mathrm{dKL}\left(p_t^{(z)}\|p_\infty^{(z)}\right)}{\mathrm{d}t} = & \frac{\mathrm{d}}{\mathrm{d}t}\int p_t^{(z)}(\boldsymbol{z})\log\frac{p_t^{(z)}(\boldsymbol{z})}{p_\infty^{(z)}(\boldsymbol{z})}\mathrm{d}\boldsymbol{z} = \int \partial_t p_t^{(z)}(\boldsymbol{z})\log\frac{p_t^{(z)}(\boldsymbol{z})}{p_\infty^{(z)}(\boldsymbol{z})}\mathrm{d}\boldsymbol{z}\\ = & \int \nabla\cdot\left(p_t^{(z)}(\boldsymbol{z})\nabla\log\frac{p_t^{(z)}(\boldsymbol{z})}{p_\infty^{(z)}(\boldsymbol{z})}\right)\cdot\log\frac{p_t^{(z)}(\boldsymbol{z})}{p_\infty^{(z)}(\boldsymbol{z})}\mathrm{d}\boldsymbol{z} = -\int p_t^{(z)}(\boldsymbol{z})\left\|\nabla\log\frac{p_t^{(z)}(\boldsymbol{z})}{p_\infty^{(z)}(\boldsymbol{z})}\right\|^2\mathrm{d}\boldsymbol{z}.\end{aligned} \tag{13}$$

Combining the fact $\nabla^2(-\log p_\infty^{(z)}) = \boldsymbol{I}$ and Lemma 28, we have

$$\mathrm{KL}\left(p_t^{(z)} \| p_\infty^{(z)}\right) \le 2 \int p_t^{(z)}(\boldsymbol{z}) \left\| \nabla \log \frac{p_t^{(z)}(\boldsymbol{z})}{p_\infty^{(z)}(\boldsymbol{z})} \right\|^2 \mathrm{d}\boldsymbol{z}.$$

Plugging this inequality into Eq 13, we have

$$\frac{\mathrm{dKL}\left(p_t^{(z)} \| p_\infty^{(z)}\right)}{\mathrm{d}t} = -\int p_t^{(z)}(\boldsymbol{z}) \left\| \nabla \log \frac{p_t^{(z)}(\boldsymbol{z})}{p_\infty^{(z)}(\boldsymbol{z})} \right\|^2 \mathrm{d}\boldsymbol{z} \le -\frac{1}{2}\mathrm{KL}\left(p_t^{(z)} \| p_\infty^{(z)}\right).$$

Integrating implies the desired bound,i.e.,

$$\mathrm{KL}\left(p_t^{(z)} \| p_\infty^{(z)}\right) \le \exp\left(-t/2\right) \cdot \mathrm{KL}\left(p_0^{(z)} \| p_\infty^{(z)}\right) \le \left(Ld + M\right) \cdot \exp\left(-t/2\right)$$

where the last inequality follows from Lemma 8. It implies KL divergence between the underlying distribution of $\mathbf{x}_{K-1,S}$ and p_∞ is

$$\mathrm{KL}\left(p_{K-1,S} \| p_\infty\right) = \mathrm{KL}\left(p_{KS}^{(z)} \| p_\infty^{(z)}\right) \le \left(Ld + M\right) \cdot \exp\left(-KS/2\right)$$

Hence, the proof is completed. ■

Appendix D. Lemmas for Bounding Discretization Error.

Lemma 10 (Lemma C.11 in Lee et al. (2022)) *Suppose that $p(\boldsymbol{x}) \propto e^{-f(\boldsymbol{x})}$ is a probability density function on $\mathbb{R}^d$, where $f(\boldsymbol{x})$ is L-smooth, and let $\varphi_{\sigma^2}(\boldsymbol{x})$ be the density function of $\mathcal{N}(\mathbf{0}, \sigma^2\boldsymbol{I}_d)$. Then for $L \le \frac{1}{2\sigma^2}$, it has*

$$\left\| \nabla \log \frac{p(\boldsymbol{x})}{\left(p * \varphi_{\sigma^2}\right)(\boldsymbol{x})} \right\| \le 6L\sigma d^{1/2} + 2L\sigma^2 \left\|\nabla f(\boldsymbol{x})\right\|.$$

Lemma 11 (Lemma 9 in Chen et al. (2023b)) *Under the notation in Section A, suppose that Assumption **[A1]** and **[A2]** hold. For any $k \in \mathbb{N}_{0,K-1}$ and $t \in [0, S]$, we have*

1. *Moment bound, i.e.,*
$$\mathbb{E}\left[\left\|\mathbf{x}_{k,t}\right\|^2\right] \le d \vee M.$$
2. *Score function bound, i.e.,*
$$\mathbb{E}\left[\left\|\nabla \log p_{k,t}(\mathbf{x}_{k,t})\right\|^2\right] \le Ld.$$

Lemma 12 (Variant of Lemma 10 in Chen et al. (2023b)) *Under the notation in Section A,Suppose that Assumption **[A2]** holds. For any $k \in \{0, 1, \ldots, K-1\}$ and $0 \le s \le t \le S$, we have*

$$\mathbb{E}\left[\left\|\mathbf{x}_{k,t} - \mathbf{x}_{k,s}\right\|^2\right] \le 2\left(M + d\right) \cdot \left(t - s\right)^2 + 4d \cdot \left(t - s\right)$$

Proof According to the forward process, we have

$$\begin{aligned}\mathbb{E}\left[\left\|\mathbf{x}_{k,t}-\mathbf{x}_{k,s}\right\|^2\right] =&\mathbb{E}\left[\left\|\int_s^t -\mathbf{x}_{k,r}\mathrm{d}r+\sqrt{2}\left(B_t-B_s\right)\right\|^2\right] \le \mathbb{E}\left[2\left\|\int_s^t \mathbf{x}_{k,r}\mathrm{d}r\right\|^2+4\left\|B_t-B_s\right\|^2\right]\\ \le& 2\mathbb{E}\left[\left(\int_s^t \left\|\mathbf{x}_{k,r}\right\|\mathrm{d}r\right)^2\right]+4d\cdot(t-s)\le 2\int_s^t \mathbb{E}\left[\left\|\mathbf{x}_{k,r}\right\|^2\right]\mathrm{d}r\cdot(t-s)+4d\cdot(t-s)\\ \le& 2\left(M+d\right)\cdot(t-s)^2+4d\cdot(t-s),\end{aligned}$$

where the third inequality follows from Holder's inequality and the last one follows from Lemma 11. Hence, the proof is completed. ■

Lemma 13 (Errors from the discretization) *Under the notation in Section A, if the step size of the outer loops satisfies*

$$\eta\le C_1(d+M)^{-1}\epsilon,$$

then, for any $k\in\{0,1,\ldots,K-1\}$*,* $r\in\{0,1,\ldots,R-1\}$ *and* $t\in[0,\eta]$*, we have*

$$\mathbb{E}\left[L^2\left\|\hat{\mathbf{x}}_{k,t+r\eta}-\hat{\mathbf{x}}_{k,r\eta}\right\|^2\right]+\mathbb{E}\left[\left\|\nabla\log\frac{p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta})}{p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,r\eta})}\right\|^2\right]\le 4\epsilon.$$

Proof We consider the following formulation with any $t\in[0,\eta]$,

$$\text{Term 2}=\underbrace{\mathbb{E}\left[\left\|\nabla\log\frac{p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta})}{p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,r\eta})}\right\|^2\right]}_{\text{Term 2.1}}+\mathbb{E}\left[L^2\left\|\hat{\mathbf{x}}_{k,t+r\eta}-\hat{\mathbf{x}}_{k,r\eta}\right\|^2\right]. \tag{14}$$

Upper bound Term 2.1. To establish the connection between $p_{k,S-r\eta}$ and $p_{k,S-(t+r\eta)}$, due to the transition kernel of the forward process (OU process), we have

$$\begin{aligned}p_{k,S-r\eta}(\boldsymbol{x})=&\int p_{k,S-(r\eta+t)}(\boldsymbol{y})\cdot\mathbb{P}\left[\boldsymbol{x},(k,S-r\eta)|\boldsymbol{y},(S-(r\eta+t))\right]\mathrm{d}\boldsymbol{y}\\ =&\int p_{k,S-(r\eta+t)}(\boldsymbol{y})\cdot\left(2\pi\left(1-e^{-2t}\right)\right)^{-\frac{d}{2}}\cdot\exp\left[\frac{-\left\|\boldsymbol{x}-e^{-t}\boldsymbol{y}\right\|^2}{2(1-e^{-2t})}\right]\mathrm{d}\boldsymbol{y}\\ =&\int e^{td}p_{k,S-(r\eta+t)}(e^t\boldsymbol{z})\cdot\left(2\pi\left(1-e^{-2t}\right)\right)^{-\frac{d}{2}}\cdot\exp\left[\frac{-\left\|\boldsymbol{x}-\boldsymbol{z}\right\|^2}{2(1-e^{-2t})}\right]\mathrm{d}\boldsymbol{z}\end{aligned} \tag{15}$$

where the last equation follows from setting $\boldsymbol{z}:=e^{-t}\boldsymbol{y}$. We define

$$p'_{k,S-(r\eta+t)}(\boldsymbol{z}):=e^{td}p_{k,S-(r\eta+t)}(e^t\boldsymbol{z})$$

which is also a density function. Therefore, for each element $\hat{\mathbf{x}}_{k,r\eta}=\boldsymbol{x}$, we have

$$\begin{aligned}\left\|\nabla\log\frac{p_{k,S-(r\eta+t)}(\boldsymbol{x})}{p_{k,S-r\eta}(\boldsymbol{x})}\right\|^2\le&2\left\|\nabla\log\frac{p_{k,S-(r\eta+t)}(\boldsymbol{x})}{p'_{k,S-(r\eta+t)}(\boldsymbol{x})}\right\|^2+2\left\|\nabla\log\frac{p'_{k,S-(r\eta+t)}(\boldsymbol{x})}{p_{k,S-r\eta}(\boldsymbol{x})}\right\|^2\\ =&2\left\|\nabla\log\frac{p_{k,S-(r\eta+t)}(\boldsymbol{x})}{p'_{k,S-(r\eta+t)}(\boldsymbol{x})}\right\|^2+2\left\|\nabla\log\frac{p'_{k,S-(r\eta+t)}(\boldsymbol{x})}{p'_{k,S-(r\eta+t)}\ast\varphi_{(1-e^{-2t})}(\boldsymbol{x})}\right\|^2\end{aligned}$$

where the last inequality follows from Eq 15. For the first term, we have

$$\begin{aligned}
&\left\|\nabla \log \frac{p_{k,S-(r\eta+t)}(\boldsymbol{x})}{p'_{k,S-(r\eta+t)}(\boldsymbol{x})}\right\| = \left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x}) - e^t \cdot \nabla \log p_{k,S-(r\eta+t)}(e^t\boldsymbol{x})\right\| \\
&\le \left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x}) - e^t \nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\| \\
&\quad + e^t \cdot \left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x}) - \nabla \log p_{k,S-(r\eta+t)}(e^t\boldsymbol{x})\right\| \\
&= (e^t - 1) \cdot \left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\| + e^t \cdot (e^t - 1) L \left\|\boldsymbol{x}\right\|.
\end{aligned} \tag{16}$$

To upper bound the latter term, we expect to employ Lemma 10. However, it requires a specific condition which denotes the smoothness of $-\nabla \log p'_{k,S-(r\eta+t)}$ should be upper bounded with the variance of $\varphi_{(1-e^{-2t})}$ as

$$\left\|-\nabla^2 \log p'_{k,S-(r\eta+t)}\right\| \le \frac{1}{2(1-e^{-2t})},$$

which can be achieved by setting

$$\eta \le \min\left\{\frac{1}{4L}, \frac{1}{2}\right\}.$$

Since the smoothness of $-\nabla \log p_{k,S-(r\eta+t)}$, i.e., Assumption **[A1]**, implies $-\nabla \log p'_{k,S-(r\eta+t)}$ is $e^{2t}L$-smooth. Besides, there are

$$t \le \eta \le \min\left\{\frac{1}{4L}, \frac{1}{2}\right\} \le \log\left(1 + \frac{1}{2L}\right) \quad \text{and} \quad e^{2t}L \le \frac{1}{2(1-e^{-2t})}.$$

Therefore, we have

$$\begin{aligned}
&\left\|\nabla \log p'_{k,S-(r\eta+t)}(\boldsymbol{x}) - \nabla \log \left(p'_{k,S-(r\eta+t)} * \varphi_{(1-e^{-2t})}\right)(\boldsymbol{x})\right\| \\
\le& 6e^{2t}L\sqrt{1-e^{-2t}}d^{1/2} + 2e^{3t}L(1-e^{-2t})\left\|\nabla \log p_{k,S-(r\eta+t)}(e^t\boldsymbol{x})\right\| \\
\le& 6e^{2t}L\sqrt{1-e^{-2t}}d^{1/2} + 2L \cdot e^t(e^{2t}-1)\left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\| \\
&+ 2L \cdot e^t(e^{2t}-1)\left\|\nabla \log p_{k,S-(r\eta+t)}(e^t\boldsymbol{x}) - \nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\| \\
\le& 6e^{2t}L\sqrt{1-e^{-2t}}d^{1/2} + 2L \cdot e^t(e^{2t}-1)\left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\| \\
&+ 2L^2 \cdot e^t(e^{2t}-1)(e^t-1)\left\|\boldsymbol{x}\right\|,
\end{aligned} \tag{17}$$

where the first inequality follows from Lemma 10, the last inequality follows from Assumption **[A1]**. Due to the range, i.e., $\eta \le 1/2$, we have the following inequalities

$$e^{2t} \le e^{2\eta} \le 1 + 4\eta \le 3, \quad 1 - e^{-2t} \le 2t \le 2\eta \quad \text{and} \quad e^t \le e^\eta \le 1 + \frac{3}{2}\cdot\eta.$$

In this condition, Eq 16 can be reformulated as

$$\begin{aligned}
\left\|\nabla \log \frac{p_{k,S-(r\eta+t)}(\boldsymbol{x})}{p'_{k,S-(r\eta+t)}(\boldsymbol{x})}\right\|^2 \le& 2\left[(e^t-1)^2 \cdot \left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\|^2 + e^{2t} \cdot (e^t-1)^2 L^2 \left\|\boldsymbol{x}\right\|^2\right] \\
\le& 5\eta^2 \left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\|^2 + 14L^2\eta^2\left\|\boldsymbol{x}\right\|^2,
\end{aligned}$$

and Eq 17 implies

$$
\begin{aligned}
&\left\|\nabla \log p'_{k,S-(r\eta+t)}(\boldsymbol{x}) - \nabla \log\left(p'_{k,S-(r\eta+t)} * \phi_{(1-e^{-2t})}\right)(\boldsymbol{x})\right\|^2\\
\le& 3\cdot\left[6^2 e^{4t}L^2(1-e^{-2t})d + 4L^2 e^{2t}(e^{2t}-1)^2\left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\|^2 + 4L^4 e^{2t}(e^{2t}-1)^2(e^t-1)^2\left\|\boldsymbol{x}\right\|^2\right]\\
\le& 3\cdot\left[2^3\cdot 3^4 L^2\eta d + 2^6\cdot 3L^2\eta^2\left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\|^2 + 3^3\cdot 2^4 L^4\eta^4\left\|\boldsymbol{x}\right\|^2\right]\\
\le& 2^3\cdot 3^5 L^2\eta d + 2^6\cdot 3^2 L^2\eta^2\left\|\nabla \log p_{k,S-(r\eta+t)}(\boldsymbol{x})\right\|^2 + 3^4\cdot L^2\eta^2\left\|\boldsymbol{x}\right\|^2,
\end{aligned}
$$

where the last inequality follows from $\eta L \le 1/4$. Hence, suppose $L \ge 1$ without loss of generality, we have

$$
\begin{aligned}
\text{Term 2.1} \le& 2\cdot\left(\mathbb{E}\left[\left\|\nabla \log \frac{p_{k,S-(r\eta+t)}(\hat{\mathbf{x}}_{k,r\eta})}{p'_{k,S-(r\eta+t)}(\hat{\mathbf{x}}_{k,r\eta})}\right\|^2\right] + \mathbb{E}\left[\left\|\nabla \log \frac{p'_{k,S-(r\eta+t)}(\hat{\mathbf{x}}_{k,r\eta})}{p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta})}\right\|^2\right]\right)\\
\le& 2^4\cdot 3^5 L^2\eta d + 2^8\cdot 3^2 L^2\eta^2\mathbb{E}\left[\left\|\nabla \log p_{k,S-(r\eta+t)}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right] + 2^2\cdot 3^4 L^2\eta^2\mathbb{E}\left[\left\|\hat{\mathbf{x}}_{k,r\eta}\right\|^2\right]\\
\le& 2^{14}L^2\eta d + 2^{13}L^2\eta^2\mathbb{E}\left[\left\|\nabla \log p_{k,S-(r\eta+t)}(\hat{\mathbf{x}}_{k,r\eta+t})\right\|^2\right] + 2^{13}L^4\eta^2\mathbb{E}\left[\left\|\hat{\mathbf{x}}_{k,r\eta+t} - \hat{\mathbf{x}}_{k,r\eta}\right\|^2\right]\\
&+ 2^{10}L^2\eta^2\mathbb{E}\left[\left\|\hat{\mathbf{x}}_{k,r\eta}\right\|^2\right].
\end{aligned}
$$

Therefore, we have

$$
\begin{aligned}
\text{Term 2} \le& 2^{14}L^2\eta d + 2^{10}L^2\eta^2\mathbb{E}\left[\left\|\hat{\mathbf{x}}_{k,r\eta}\right\|^2\right] + 2^{13}L^2\eta^2\mathbb{E}\left[\left\|\nabla \log p_{k,S-(r\eta+t)}(\hat{\mathbf{x}}_{k,r\eta+t})\right\|^2\right]\\
&+ \left(2^{13}L^2\eta^2 + 1\right)L^2\mathbb{E}\left[\left\|\hat{\mathbf{x}}_{k,r\eta+t} - \hat{\mathbf{x}}_{k,r\eta}\right\|^2\right]\\
\le& 2^{14}L^2\eta d + 2^{10}L^2\eta^2(M+d) + 2^{13}L^3\eta^2 d + 2^{10}L^2\left(2(M+d)\eta^2 + 4d\eta\right)
\end{aligned}
$$

where the last inequality follows from Lemma 11 and Lemma 12. To diminish the discretization error, we require the step size of backward sampling, i.e., η satisfies

$$
\begin{cases}
2^{14}L^2\eta d \le \epsilon\\
2^{10}\cdot L^2\eta^2(d+M) \le \epsilon\\
2^{13}\cdot L^3\eta^2 d \le \epsilon\\
2^{10}\cdot L^2\left(2(M+d)\eta^2 + 4d\eta\right) \le \epsilon
\end{cases}
\quad \Leftarrow \quad
\begin{cases}
\eta \le 2^{-14}L^{-2}d^{-1}\epsilon\\
\eta \le 2^{-5}\cdot L^{-1}(d+M)^{-0.5}\epsilon^{0.5}\\
\eta \le 2^{-6.5}\cdot L^{-1.5}d^{-0.5}\epsilon^{0.5}\\
\eta \le 2^{-6}L^{-0.5}(d+M)^{-0.5}\epsilon^{0.5}\\
\eta \le 2^{-13}L^{-2}d^{-1}\epsilon.
\end{cases}
$$

Specifically, if we choose

$$
\eta \le 2^{-14}L^{-2}(d+M)^{-1}\epsilon = C_\eta (d+M)^{-1}\epsilon,
$$

we have

$$
\mathbb{E}\left[L^2\left\|\hat{\mathbf{x}}_{k,t+r\eta} - \hat{\mathbf{x}}_{k,r\eta}\right\|^2\right] + \mathbb{E}\left[\left\|\nabla \log \frac{p_{k,S-r\eta}(\hat{\mathbf{x}}_{k,r\eta})}{p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,r\eta})}\right\|^2\right] \le 4\epsilon,
$$

and the proof is completed. ■

Appendix E. Lemmas for Bounding Score Estimation Error

Lemma 14 (Recursive Form of Score Functions) *Under the notation in Section A, for any $k \in \mathbb{N}_{0,K-1}$ and $t \in [0, S]$, the score function can be written as*

$$\nabla_{\boldsymbol{x}} \log p_{k,S-t}(\boldsymbol{x}) = \mathbb{E}_{\mathbf{x}' \sim q_{k,S-t}(\cdot|\boldsymbol{x})}\left[-\frac{\boldsymbol{x} - e^{-(S-t)}\mathbf{x}'}{\left(1-e^{-2(S-t)}\right)}\right]$$

where the conditional density function $q_{k,S-t}(\cdot|\boldsymbol{x})$ is defined as

$$q_{k,S-t}(\boldsymbol{x}'|\boldsymbol{x}) \propto \exp\left(\nabla \log p_{k,0}(\boldsymbol{x}') - \frac{\left\|\boldsymbol{x} - e^{-(S-t)}\boldsymbol{x}'\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right).$$

Proof When the OU process, i.e., SDE 1, is selected as the forward path, for any $k \in \mathbb{N}_{0,K}$ and $t \in [0, S]$, the transition kernel has a closed form, i.e.,

$$p_{k,t|0}(\boldsymbol{x}|\boldsymbol{x}_0) = \left(2\pi\left(1-e^{-2t}\right)\right)^{-d/2} \cdot \exp\left[\frac{-\left\|\boldsymbol{x} - e^{-t}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2t}\right)}\right], \quad \forall\, 0 \le t \le S.$$

In this condition, we have

$$\begin{aligned} p_{k,S-t}(\boldsymbol{x}) &= \int_{\mathbb{R}^d} p_{k,0}(\boldsymbol{x}_0) \cdot p_{k,S-t|0}(\boldsymbol{x}|\boldsymbol{x}_0) \mathrm{d}\boldsymbol{x}_0 \\ &= \int_{\mathbb{R}^d} p_{k,0}(\boldsymbol{x}_0) \cdot \left(2\pi\left(1-e^{-2(S-t)}\right)\right)^{-d/2} \cdot \exp\left[\frac{-\left\|\boldsymbol{x} - e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right] \mathrm{d}\boldsymbol{x}_0 \end{aligned}$$

Plugging this formulation into the following equation

$$\nabla_{\boldsymbol{x}} \log p_{k,S-t}(\boldsymbol{x}) = \frac{\nabla p_{k,S-t}(\boldsymbol{x})}{p_{k,S-t}(\boldsymbol{x})},$$

we have

$$\begin{aligned} \nabla_{\boldsymbol{x}} \log p_{k,S-t}(\boldsymbol{x}) =& \frac{\nabla \int_{\mathbb{R}^d} p_{k,0}(\boldsymbol{x}_0) \cdot \left(2\pi\left(1-e^{-2(S-t)}\right)\right)^{-d/2} \cdot \exp\left[\frac{-\left\|\boldsymbol{x}-e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right] \mathrm{d}\boldsymbol{x}_0}{\int_{\mathbb{R}^d} p_{k,0}(\boldsymbol{x}_0) \cdot \left(2\pi\left(1-e^{-2(S-t)}\right)\right)^{-d/2} \cdot \exp\left[\frac{-\left\|\boldsymbol{x}-e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right] \mathrm{d}\boldsymbol{x}_0} \\ =& \frac{\int_{\mathbb{R}^d} p_{k,0}(\boldsymbol{x}_0) \cdot \exp\left(\frac{-\left\|\boldsymbol{x}-e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right) \cdot \left(-\frac{\boldsymbol{x}-e^{-(S-t)}\boldsymbol{x}_0}{\left(1-e^{-2(T-t)}\right)}\right) \mathrm{d}\boldsymbol{x}_0}{\int_{\mathbb{R}^d} p_{k,0}(\boldsymbol{x}_0) \cdot \exp\left(\frac{-\left\|\boldsymbol{x}-e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right) \mathrm{d}\boldsymbol{x}_0} \\ =& \mathbb{E}_{\mathbf{x}_0 \sim q_{k,S-t}(\cdot|\boldsymbol{x})}\left[-\frac{\boldsymbol{x} - e^{-(S-t)}\mathbf{x}_0}{\left(1-e^{-2(S-t)}\right)}\right] \end{aligned} \tag{18}$$

where the density function $q_{T-t}(\cdot|\boldsymbol{x})$ is defined as

$$q_{k,S-t}(\boldsymbol{x}_0|\boldsymbol{x}) = \frac{p_{k,0}(\boldsymbol{x}_0)\cdot\exp\left(\frac{-\left\|\boldsymbol{x}-e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right)}{\int_{\mathbb{R}^d} p_{k,0}(\boldsymbol{x}_0)\cdot\exp\left(\frac{-\left\|\boldsymbol{x}-e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right)\mathrm{d}\boldsymbol{x}_0}$$

$$\propto \exp\left(-f_{k,0}(\boldsymbol{x}_0) - \frac{\left\|\boldsymbol{x}-e^{-(S-t)}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2(S-t)}\right)}\right),$$

where $p_{k,0} \propto \exp(-f_{k,0})$. Hence, the proof is completed. ■

Lemma 15 (Strong log-concavity and L-smoothness of the auxiliary targets) *Under the notation in Section A, for any $k \in \mathbb{N}_{0,K-1}$, $r \in \mathbb{N}_{0,R-1}$ and $\boldsymbol{x} \in \mathbb{R}^d$, we define the auxiliary target distribution as*

$$q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x}) \propto \exp\left(\nabla \log p_{k,0}(\boldsymbol{x}') - \frac{\left\|\boldsymbol{x}-e^{-(S-r\eta)}\boldsymbol{x}'\right\|^2}{2\left(1-e^{-2(S-r\eta)}\right)}\right).$$

We define

$$\mu_r \coloneqq \frac{1}{2}\cdot\frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}} \quad \text{and} \quad L_r \coloneqq \frac{3}{2}\cdot\frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}.$$

Then, we have

$$\mu_r \boldsymbol{I} \preceq -\nabla^2 \log q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x}) \preceq L_r \boldsymbol{I}$$

when the segment length S satisfies $S = \frac{1}{2}\log\left(\frac{2L+1}{2L}\right)$.

Proof We begin with the formulation of $\nabla^2 \log q_{k,S-t}$, i.e.,

$$-\nabla^2 \log q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x}) = -\nabla^2 \log p_{k,0}(\boldsymbol{x}') + \frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}\boldsymbol{I}. \tag{19}$$

By supposing $S = \frac{1}{2}\log\left(\frac{2L+1}{2L}\right)$, we have

$$\frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}} \geq \frac{e^{-2S}}{1-e^{-2S}} = 2L \geq 2\left\|\nabla^2 \log p_{k,0}\right\|.$$

Plugging this inequality into Eq 19, we have

$$-\nabla^2 p_{k,0}(\boldsymbol{x}') + \frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}\cdot\boldsymbol{I} \preceq \left(\left\|\nabla^2 \log p_{k,0}(\boldsymbol{x}')\right\| + \frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}\right)\cdot\boldsymbol{I}$$

$$\preceq \frac{3}{2}\cdot\frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}\cdot\boldsymbol{I} = L_r\boldsymbol{I}.$$

Besides, it has

$$-\nabla^2 p_{k,0}(\boldsymbol{x}') + \frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}\cdot\boldsymbol{I} \succeq \left(-\left\|\nabla^2 \log p_{k,0}(\boldsymbol{x}')\right\| + \frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}\right)\cdot\boldsymbol{I}$$

$$\succeq \frac{1}{2}\cdot\frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}\cdot\boldsymbol{I} = \mu_r\boldsymbol{I}.$$

Hence, the proof is completed. ■

E.1. Score Estimation Error from Empirical Mean

Lemma 16 *With a little abuse of notation, for each $i \in \mathbb{N}_{1,n_{k,r}}$ in Alg 1, we denote the underlying distribution of* ***output particles*** *as $\mathbf{x}'_i \sim q'_{k,S-r\eta}$ and suppose it satisfies LSI with the constant μ'_r. Then, for any $\boldsymbol{x} \in \mathbb{R}^d$, we have*

$$\mathbb{P}\left[\left\|-\frac{1}{n_{k,r}}\sum_{i=1}^{n_{k,r}}\mathbf{x}'_i + \mathbb{E}_{\mathbf{x}'\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\| \le 2\epsilon'\right] \ge 1-\delta$$

by requiring the sample number $n_{k,r}$ to satisfy

$$n_{k,r} \ge \frac{\max\left\{d, -2\log\delta\right\}}{\mu'_r \epsilon'^2}.$$

Proof For any $\boldsymbol{x} \in \mathbb{R}^d$, we set

$$\boldsymbol{b}' := \mathbb{E}_{q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right] \quad \text{and} \quad \sigma' := \mathbb{E}_{\left\{\mathbf{x}'_i\right\}_{i=1}^{n_{k,r}} \sim q'^{(n_{k,r})}_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\left\|\sum_{i=1}^{n_{k,r}}\mathbf{x}'_i - \mathbb{E}\left[\sum_{i=1}^{n_{k,r}}\mathbf{x}'_i\right]\right\|\right].$$

We begin with the following probability

$$\begin{aligned}
&\mathbb{P}_{\left\{\mathbf{x}'_i\right\}_{i=1}^{n_{k,r}} \sim q'^{(n_{k,r})}_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\left\|-\frac{1}{n_{k,r}}\sum_{i=1}^{n_{k,r}}\mathbf{x}'_i + \mathbb{E}_{\mathbf{x}'\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|^2 \ge \left(\frac{\sigma'}{n_{k,r}} + \epsilon'\right)^2\right] \\
=&\mathbb{P}_{\left\{\mathbf{x}'_i\right\}_{i=1}^{n_{k,r}} \sim q'^{(n_{k,r})}_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\left\|\sum_{i=1}^{n_{k,r}}\mathbf{x}'_i - n_{k,r}\boldsymbol{b}'\right\| \ge \sigma' + n_{k,r}\epsilon'\right]
\end{aligned} \tag{20}$$

To lower bound this probability, we expect to utilize Lemma 33 which requires the following two conditions:

- The distribution of $\sum_{i=1}^{n_{k,r}}\mathbf{x}'_i$ satisfies LSI, and its LSI constant can be obtained.
- The formulation $\left\|\sum_{i=1}^{n_{k,r}}\mathbf{x}'_i - n_{k,r}\boldsymbol{b}'\right\| \ge \sigma' + n_{k,r}\epsilon'$ can be presented as $F \ge \mathbb{E}[F] + \mathrm{bias}$ where F is a 1-Lipschitz function.

For the first condition, by employing Lemma 29, we have that the LSI constant of

$$\sum_{i=1}^{n_{k,r}}\mathbf{x}'_i \sim \underbrace{q'_{k,S-r\eta}(\cdot|\boldsymbol{x}) * q'_{k,S-r\eta}(\cdot|\boldsymbol{x}) \cdots * q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}_{n_{k,r}}$$

is $\mu'_r/n_{k,r}$. For the second condition, we set the function $F(\boldsymbol{x}) = \|\boldsymbol{x} - n_{k,r}\boldsymbol{b}'\| : \mathbb{R}^d \to \mathbb{R}$ is 1-Lipschitz because

$$\|F\|_{\mathrm{Lip}} = \sup_{\boldsymbol{x}\neq\boldsymbol{y}}\frac{|F(\boldsymbol{x}) - F(\boldsymbol{y})|}{\|\boldsymbol{x}-\boldsymbol{y}\|} = \sup_{\boldsymbol{x}\neq\boldsymbol{y}}\frac{|\|\boldsymbol{x}\| - \|\boldsymbol{y}\||}{\|(\boldsymbol{x}-\boldsymbol{y})\|} = 1.$$

Besides, we have

$$F\left(\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i\right) = \left\|\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i - n_{k,r}\boldsymbol{b}'\right\| \quad \text{and} \quad \mathbb{E}\left[F\left(\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i\right)\right] = \sigma'$$

where the second equation follows from the definition of σ'. Therefore, with Lemma 33, we have

$$\mathbb{P}_{\{\mathbf{x}'_i\}_{i=1}^{n_{k,r}} \sim q'^{(n_{k,r})}_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\left\|\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i - n_{k,r}\boldsymbol{b}'\right\| \geq \sigma' + n_{k,r}\epsilon'\right] \leq \exp\left(-\frac{\mu'_r \epsilon'^2 n_{k,r}}{2}\right). \tag{21}$$

Then, we consider the range of σ' and have

$$\begin{aligned}\sigma' =& n_{k,r} \cdot \mathbb{E}_{\{\mathbf{x}'_i\}_{i=1}^{n_{k,r}} \sim q'^{(n_{k,r})}_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left\|\frac{1}{n_{k,r}}\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i - \boldsymbol{b}'\right\| \\ \leq & n_{k,r} \cdot \sqrt{\mathrm{var}\left(\frac{1}{n_{k,r}}\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i\right)} = \sqrt{n_{k,r}\mathrm{var}\left(\mathbf{x}'_i\right)} \leq \sqrt{\frac{n_{k,r} d}{\mu'_r}},\end{aligned} \tag{22}$$

the first inequality follows from Holder's inequality and the last follows from Lemma 35. Combining Eq 21 and Eq 22, it has

$$\mathbb{P}_{\{\mathbf{x}'_i\}_{i=1}^{n_{k,r}} \sim q'^{(n_{k,r})}_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\left\|-\frac{1}{n_{k,r}}\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i + \mathbb{E}_{\mathbf{x}' \sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|^2 \geq \left(\sqrt{\frac{d}{\mu'_r n_{k,r}}} + \epsilon'\right)^2\right] \leq \exp\left(-\frac{\mu'_r \epsilon'^2 n_{k,r}}{2}\right).$$

By requiring

$$\frac{d}{\mu'_r n_{k,r}} \leq \epsilon'^2 \quad \text{and} \quad -\frac{\mu'_r \epsilon'^2 n_{k,r}}{2} \leq \log\delta, \tag{23}$$

we have

$$\begin{aligned}&\mathbb{P}\left[\left\|-\frac{1}{n_{k,r}}\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i + \mathbb{E}_{\mathbf{x}' \sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\| \leq 2\epsilon'\right] \\ &= 1 - \mathbb{P}\left[\left\|-\frac{1}{n_{k,r}}\sum_{i=1}^{n_{k,r}} \mathbf{x}'_i + \mathbb{E}_{\mathbf{x}' \sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\| \geq 2\epsilon'\right] \geq 1 - \delta.\end{aligned}$$

Noted that Eq. 23 implies the sample number $n_{k,r}$ should satisfy

$$n_{k,r} \geq \frac{d}{\mu'_r \epsilon'^2} \quad \text{and} \quad n_{k,r} \geq \frac{2\log\delta^{-1}}{\mu'_r \epsilon'^2}.$$

Hence, the proof is completed. ■

E.2. Score Estimation Error from Mean Gap

Lemma 17 *For any given $(k,r,\boldsymbol{x})$ in Alg 1, suppose the distribution $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$ satisfies*

$$\mu_r \boldsymbol{I} \preceq -\nabla^2 \log q_{k,S-r\eta}(\cdot|\boldsymbol{x}) \preceq L_r \boldsymbol{I},$$

and $\mathbf{x}'_j \sim q'_j(\cdot|\boldsymbol{x})$ corresponds to Line 9 of Alg 1. If $0 < \tau_r \le \mu_r/(8L_r^2)$, we have

$$\mathrm{KL}\left(q'_{j+1}(\cdot|\boldsymbol{x}) \| q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) \le e^{-\mu_r\tau_r}\mathrm{KL}\left(q'_j(\cdot|\boldsymbol{x}) \| q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) + 28L_r^2 d\tau_r^2$$

when the score estimation satisfies $\left\|\nabla \log p_{k,0} - \boldsymbol{v}'\right\|_\infty \le L_r\sqrt{2d\tau_r}$.

Proof Suppose the loop in Line 6 of Alg 1 aims to draw a sample from the target distribution $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$ satisfying

$$q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x}) \propto \exp(-g_{k,r}(\boldsymbol{x}')) \coloneqq \exp\left(-f_{k,0}(\boldsymbol{x}') - \frac{\left\|\boldsymbol{x} - e^{-(S-r\eta)}\boldsymbol{x}'\right\|^2}{2(1-e^{-2(S-r\eta)})}\right).$$

The score function of the target, i.e., $\nabla g_{k,r}(\boldsymbol{x}')$, satisfies

$$\nabla g_{k,r}(\boldsymbol{x}') = \nabla f_{k,0}(\boldsymbol{x}') + \frac{-e^{-(S-r\eta)}\boldsymbol{x} + e^{-2(S-r\eta)}\boldsymbol{x}'}{1-e^{-2(S-r\eta)}}.$$

At the j-th iteration corresponding to Line 9 in Alg 1. The previous score is approximated by

$$\nabla g'(\boldsymbol{x}') = \boldsymbol{v}'(\boldsymbol{x}') + \frac{-e^{-(S-r\eta)}\boldsymbol{x} + e^{-2(S-r\eta)}\boldsymbol{x}'}{1-e^{-2(S-r\eta)}}.$$

where $\boldsymbol{v}'(\cdot)$ is used to approximate $\nabla \log p_{k,0}(\cdot)$ by calling Alg 1 recursively. Suppose $\mathbf{x}'_j = \boldsymbol{z}_0$, the j-th iteration is equivalent to the following SDE

$$\mathrm{d}\mathbf{z}_t = -\nabla g'(\boldsymbol{z}_0)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t,$$

we denote the underlying distribution of $\mathbf{z}_t$ as q_t. Similarly, we set q_{0t} as the joint distribution of $(\mathbf{z}_0, \mathbf{z}_t)$, and have

$$q_{0t}(\boldsymbol{z}_0, \boldsymbol{z}_t) = q_0(\boldsymbol{z}_0) \cdot q_{t|0}(\boldsymbol{z}_t|\boldsymbol{z}_0).$$

According to the Fokker-Planck equation, we have

$$\partial_t q_{t|0}(\boldsymbol{z}_t|\boldsymbol{z}_0) = \nabla \cdot \left(q_{t|0}(\boldsymbol{z}_t|\boldsymbol{z}_0) \cdot \nabla g'(\boldsymbol{z}_0)\right) + \Delta q_{t|0}(\boldsymbol{z}_t|\boldsymbol{z}_0)$$

In this condition, we have

$$\begin{aligned}
\partial_t q_t(\boldsymbol{z}_t) =& \int \frac{\partial q_{t|0}(\boldsymbol{z}_t|\boldsymbol{z}_0)}{\partial t} \cdot q_0(\boldsymbol{z}_0)\mathrm{d}\boldsymbol{z}_0 \\
=& \int \left[\nabla \cdot \left(q_{t|0}(\boldsymbol{z}_t|\boldsymbol{z}_0) \cdot \nabla g'(\boldsymbol{z}_0)\right) + \Delta q_{t|0}(\boldsymbol{z}_t|\boldsymbol{z}_0)\right] \cdot q_0(\boldsymbol{z}_0)\mathrm{d}\boldsymbol{z}_0 \\
=& \nabla \cdot \left(q_t(\boldsymbol{z}_t) \int q_{0|t}(\boldsymbol{z}_0|\boldsymbol{z}_t)\nabla g'(\boldsymbol{z}_0)\mathrm{d}\boldsymbol{z}_0\right) + \Delta q_t(\boldsymbol{z}_t).
\end{aligned}$$

For abbreviation, we suppose

$$q_*(\cdot) \coloneqq q_{k,S-r\eta}(\cdot|\boldsymbol{x}) \quad \text{and} \quad g_* \coloneqq g_{k,r}.$$

With these notations, the dynamic of the KL divergence between q_t and q_* is

$$\begin{aligned}
&\partial_t \mathrm{KL}\left(q_t \| q_*\right) = \int \partial_t q_t(\boldsymbol{z}_t) \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \mathrm{d}\boldsymbol{z}_t \\
&= \int \nabla \cdot \left[q_t(\boldsymbol{z}_t) \left(\int q_{0|t}(\boldsymbol{z}_0|\boldsymbol{z}_t) \nabla g'(\boldsymbol{z}_0) \mathrm{d}\boldsymbol{z}_0 + \nabla \log q_t(\boldsymbol{z}_t) \right) \right] \cdot \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \mathrm{d}\boldsymbol{z}_t \\
&= - \int q_t(\boldsymbol{z}_t) \left(\left\| \nabla \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \right\|^2 + \left\langle \int q_{0|t}(\boldsymbol{z}_0|\boldsymbol{z}_t) \nabla g'(\boldsymbol{z}_0) \mathrm{d}\boldsymbol{z}_0 + \nabla \log q_*(\boldsymbol{z}_t), \nabla \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \right\rangle \right) \mathrm{d}\boldsymbol{z}_t \\
&= - \int q_t(\boldsymbol{z}_t) \left\| \nabla \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \right\|^2 \mathrm{d}\boldsymbol{z}_t + \int q_{0t}(\boldsymbol{z}_0, \boldsymbol{z}_t) \left\langle \nabla g'(\boldsymbol{z}_0) - \nabla g_*(\boldsymbol{z}_t), \nabla \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \right\rangle \mathrm{d}(\boldsymbol{z}_0, \boldsymbol{z}_t) \\
&\le -\frac{3}{4} \int q_t(\boldsymbol{z}_t) \left\| \nabla \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \right\|^2 \mathrm{d}\boldsymbol{z}_t + \int q_{0t}(\boldsymbol{z}_0, \boldsymbol{z}_t) \left\| \nabla g'(\boldsymbol{z}_0) - \nabla g_*(\boldsymbol{z}_t) \right\|^2 \mathrm{d}(\boldsymbol{z}_0, \boldsymbol{z}_t) \\
&\le -\frac{3}{4} \int q_t(\boldsymbol{z}_t) \left\| \nabla \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \right\|^2 + 2 \int q_{0t}(\boldsymbol{z}_0, \boldsymbol{z}_t) \left\| \nabla g'(\boldsymbol{z}_0) - \nabla g_*(\boldsymbol{z}_0) \right\|^2 \mathrm{d}(\boldsymbol{z}_0, \boldsymbol{z}_t) \\
&\quad + 2 \int q_{0t}(\boldsymbol{z}_0, \boldsymbol{z}_t) \left\| \nabla g_*(\boldsymbol{z}_0) - \nabla g_*(\boldsymbol{z}_t) \right\|^2 \mathrm{d}(\boldsymbol{z}_0, \boldsymbol{z}_t).
\end{aligned} \tag{24}$$

Upper bound the first term in Eq 24. The target distribution q_* satisfies μ_r-strong convexity, i.e.,

$$\mu_r \boldsymbol{I} \preceq -\nabla^2 \log q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x}) = -\nabla^2 \log(q_*(\boldsymbol{x}')),$$

It means q_* satisfies LSI with the constant μ_r due to Lemma 28. Hence, we have

$$-\frac{3}{4} \int q_t(\boldsymbol{z}_t) \left\| \nabla \log \frac{q_t(\boldsymbol{z}_t)}{q_*(\boldsymbol{z}_t)} \right\|^2 \le -\frac{3\mu_r}{2} \mathrm{KL}\left(q_t \| q_*\right). \tag{25}$$

Upper bound the second term in Eq 24. We assume that there is a uniform upper bound ϵ_g satisfying

$$\left\| \nabla g'(\boldsymbol{z}) - \nabla g_*(\boldsymbol{z}) \right\| \le \epsilon_g \quad \Rightarrow \quad \int q_{0t}(\boldsymbol{z}_0, \boldsymbol{z}_t) \left\| \nabla g'(\boldsymbol{z}_0) - \nabla g_*(\boldsymbol{z}_0) \right\|^2 \mathrm{d}(\boldsymbol{z}_0, \boldsymbol{z}_t) \le \epsilon_g^2. \tag{26}$$

Upper bound the third term in Eq 24. Due to the monotonicity of $e^{-t}/(1-e^{-t})$, we have

$$2L \le \frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}} \le \frac{e^{-2\eta}}{1-e^{-2\eta}} \le \eta^{-1}$$

where we suppose $\eta \le 1/2$ without loss of the generality to establish the last inequality. Hence, the target distribution q_* satisfies

$$\begin{aligned}
& -\nabla^2 \log q_* = -\nabla^2 \log q_{k,S-r\eta}(\cdot|\boldsymbol{x}) = -\nabla^2 \log p_{k,0} + \frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}} \\
& \preceq \left\| \nabla^2 \log p_{k,0} \right\| \boldsymbol{I} + \frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}} \boldsymbol{I} \coloneqq L_r \boldsymbol{I} \preceq (L+\eta^{-1}) \boldsymbol{I},
\end{aligned}$$

where the last inequality follows from Assumption **[A1]**. This result implies the smoothness of q_*, and we have

$$
\begin{aligned}
&\int q_{0t}(\boldsymbol{z}_0,\boldsymbol{z}_t)\left\|\nabla g_*(\boldsymbol{z}_0)-\nabla g_*(\boldsymbol{z}_t)\right\|^2 \mathrm{d}(\boldsymbol{z}_0,\boldsymbol{z}_t)\\
\le& L_r^2\int q_{0t}(\boldsymbol{z}_0,\boldsymbol{z}_t)\left\|\boldsymbol{z}_t-\boldsymbol{z}_0\right\|^2 \mathrm{d}(\boldsymbol{z}_0,\boldsymbol{z}_t) = L_r^2\cdot \mathbb{E}_{q_{0t}}\left[\left\|-t\nabla g'(\boldsymbol{z}_0)+\sqrt{2t}\xi\right\|^2\right]\\
=& L_r^2\cdot\left(2td+t^2\mathbb{E}_{q_0}\left\|\nabla g'(\boldsymbol{z}_0)-\nabla g_*(\boldsymbol{z}_0)+\nabla g_*(\boldsymbol{z}_0)\right\|^2\right)\\
\le& 2L_r^2\cdot\left(td+t^2\epsilon_g^2+t^2\mathbb{E}_{q_0}\left\|\nabla g_*(\boldsymbol{z}_0)\right\|^2\right)\\
\le& 2L_r^2dt+2L_r^2\epsilon_g^2t^2+4L_r^3dt^2+\frac{8L_r^4t^2}{\mu_r}\mathrm{KL}\left(q_0\|q_*\right),
\end{aligned} \tag{27}
$$

where the last inequality follows from Lemma 36.

Hence, Combining Eq 24, Eq 25, Eq 26, Eq 27 with $t\le\tau_r\le 1/(2L_r)$ and $\epsilon_g^2\le 2L_r^2d\tau_r$, we have

$$
\begin{aligned}
\partial_t\mathrm{KL}\left(q_t\|q_*\right)\le& -\frac{3\mu_r}{2}\mathrm{KL}\left(q_t\|q_*\right)+2\epsilon_g^2+\frac{16L_r^4t^2}{\mu_r}\mathrm{KL}\left(q_0\|q_*\right)+4L_r^2dt+4L_r^2\epsilon_g^2t^2+8L_r^3dt^2\\
\le& -\frac{3\mu_r}{2}\mathrm{KL}\left(q_t\|q_*\right)+4L_r^2d\tau_r+\frac{16L_r^4\tau_r^2}{\mu_r}\mathrm{KL}\left(q_0\|q_*\right)+4L_r^2d\tau_r+8L_r^4d\tau_r^3+8L_r^3d\tau_r^2\\
\le& -\frac{3\mu_r}{2}\mathrm{KL}\left(q_t\|q_*\right)+\frac{16L_r^4t^2}{\mu_r}\mathrm{KL}\left(q_0\|q_*\right)+14L_r^2d\tau_r.
\end{aligned}
$$

Multiplying both sides by $\exp(\frac{3\mu_r t}{2})$, then the previous inequality can be written as

$$
\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{\frac{3\mu_r t}{2}}\mathrm{KL}\left(q_t\|q_*\right)\right)\le e^{\frac{3\mu_r t}{2}}\cdot\left(\frac{16L_r^4\tau_r^2}{\mu_r}\mathrm{KL}\left(q_0\|q_*\right)+14L_r^2d\tau_r\right).
$$

Integrating from $t=0$ to $t=\tau_r$, we have

$$
\begin{aligned}
e^{\frac{3\mu_r\tau_r}{2}}\mathrm{KL}\left(q_t\|q_*\right)-\mathrm{KL}\left(q_0\|q_*\right)\le& \frac{2}{3\mu_r}\cdot\left(e^{\frac{3\mu_r\tau_r}{2}}-1\right)\cdot\left(\frac{16L_r^4\tau_r^2}{\mu_r}\mathrm{KL}\left(q_0\|q_*\right)+14L_r^2d\tau_r\right)\\
\le& 2\tau_r\cdot\left(\frac{16L_r^4\tau_r^2}{\mu_r}\mathrm{KL}\left(q_0\|q_*\right)+14L_r^2d\tau_r\right)
\end{aligned}
$$

where the last inequality establishes due to the fact $e^c\le 1+2c$ when $0<c\le\frac{3}{2}\cdot\mu_r\tau_r\le 1$. It means we have

$$
\mathrm{KL}\left(q_t\|q_*\right)\le e^{-\frac{3\mu_r\tau_r}{2}}\cdot\left(1+\frac{32L_r^4\tau_r^3}{\mu_r}\right)\mathrm{KL}\left(q_0\|q_*\right)+e^{-\frac{3\mu_r\tau_r}{2}}\cdot 28L_r^2d\tau_r^2.
$$

By requiring $0<\tau_r\le\mu_r/(8L_r^2)$, we have

$$
1+\frac{32L_r^4\tau_r^3}{\mu_r}\le 1+\frac{\mu_r\tau_r}{2}\le e^{\frac{\mu_r\tau_r}{2}}\quad\text{and}\quad e^{-\frac{3\mu_r\tau_r}{2}}\le 1.
$$

Hence, there is

$$
\mathrm{KL}\left(q_t\|q_*\right)\le e^{-\mu_r\tau_r}\mathrm{KL}\left(q_0\|q_*\right)+28L_r^2d\tau_r^2, \tag{28}
$$

and the proof is completed. ■

Lemma 18 *In Alg 1, suppose the input is $(k, r, \boldsymbol{x}, \epsilon)$ and $k > 0$, if we choose the initial distribution of the inner loop to be*

$$q_0'(\boldsymbol{x}') \propto \exp\left(-\frac{\left\|\boldsymbol{x} - e^{-(S-r\eta)}\boldsymbol{x}'\right\|^2}{2(1-e^{-2(S-r\eta)})}\right),$$

then suppose $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$ satisfies LSI with the constant μ_r and L_r smoothness. Their KL divergence can be upper-bounded as

$$\log \mathrm{KL}\left(q_0'(\cdot)\|q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) \leq \log\|\boldsymbol{x}\|^2 + \log\left[\frac{L_r^2 M}{\mu_r^2}\cdot\frac{de^S}{1-e^{-2S}}\right] + \frac{Me^{-S}}{1-e^{-2S}}.$$

Proof According to Lemma 14, the density $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$ can be presented as

$$q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x}) \propto \exp\left(-f_{k,0}(\boldsymbol{x}') - \frac{\left\|\boldsymbol{x} - e^{-(S-r\eta)}\boldsymbol{x}'\right\|^2}{2(1-e^{-2(S-r\eta)})}\right)$$

where $f_{k,0}(\boldsymbol{x}') = \nabla \log p_{k,0}(\boldsymbol{x}')$. Since it satisfies LSI with the constant, .i.e, μ_r, due to Definition 3, we have

$$\begin{aligned} \mathrm{KL}\left(q_0'(\cdot)\|q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) &\leq \frac{1}{2\mu_r}\cdot\int q_0'(\boldsymbol{x}')\left\|\nabla f_{k,0}(\boldsymbol{x}')\right\|^2 \mathrm{d}\boldsymbol{x}' \\ &\leq \mu_r^{-1}\cdot\left(\int q_0'(\boldsymbol{x}')\left\|\nabla f_{k,0}(\boldsymbol{x}') - \nabla f_{k,0}(\boldsymbol{0})\right\|^2 \mathrm{d}\boldsymbol{x}' + \int q_0'(\boldsymbol{x}')\left\|\nabla f_{k,0}(\boldsymbol{0})\right\|^2 \mathrm{d}\boldsymbol{x}'\right). \end{aligned} \tag{29}$$

For the first term, we have

$$\begin{aligned} &\int q_0'(\boldsymbol{x}')\left\|\nabla f_{k,0}(\boldsymbol{x}') - \nabla f_{k,0}(\boldsymbol{0})\right\|^2 \mathrm{d}\boldsymbol{x}' \\ &\leq L_r^2\cdot\int q_0'(\boldsymbol{x}')\left\|\boldsymbol{x}'\right\|^2 \mathrm{d}\boldsymbol{x}' = L_r^2\cdot\mathbb{E}_{q_0'}\left[\|\mathbf{x}'\|^2\right] = L_r^2\cdot\left[\mathrm{Var}(\mathbf{x}') + \left\|\mathbb{E}\mathbf{x}'\right\|^2\right] \end{aligned}$$

where the first inequality follows from **[A1]**. The high-dimensional Gaussian distribution, i.e., q_0' satisfies

$$\left\|\mathbb{E}_{q_0'}\left[\mathbf{x}'\right]\right\| = e^{S-r\eta}\|\boldsymbol{x}\| \quad \text{and} \quad \mathrm{Var}(\mathbf{x}') \leq d\cdot\left(e^{2(S-r\eta)} - 1\right),$$

where the last inequality follows from Lemma 35, hence we have

$$\int q_0'(\boldsymbol{x}')\left\|\nabla f_{k,0}(\boldsymbol{x}') - \nabla f_{k,0}(\boldsymbol{0})\right\|^2 \mathrm{d}\boldsymbol{x}' \leq L_r^2\cdot e^{2(S-r\eta)}(d + \|\boldsymbol{x}\|^2). \tag{30}$$

Then we consider to bound the second term of Eq 29. According to the definition of $\nabla f_{k,0}$, with the transition kernel of the OU process, we have

$$\begin{aligned} -\nabla f_{k,0}(\boldsymbol{x}') &= \nabla \log p_{k,0}(\boldsymbol{x}') = \frac{\nabla p_{k,0}(\boldsymbol{x}')}{p_{k,0}(\boldsymbol{x}')} \\ &= \frac{\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\cdot\exp\left(\frac{-\left\|\boldsymbol{x} - e^{-kS}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2kS}\right)}\right)\cdot\left(-\frac{\boldsymbol{x} - e^{-kS}\boldsymbol{x}_0}{\left(1-e^{-2(T-t)}\right)}\right)\mathrm{d}\boldsymbol{x}_0}{\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\cdot\exp\left(\frac{-\left\|\boldsymbol{x} - e^{-kS}\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2kS}\right)}\right)\mathrm{d}\boldsymbol{x}_0}. \end{aligned}$$

Therefore, we have

$$
\begin{aligned}
\left\|\nabla f_{k,0}(\mathbf{0})\right\|^2 = & \left\| \frac{\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\cdot \exp\left(\frac{-e^{-2kS}\|\boldsymbol{x}_0\|^2}{2\left(1-e^{-2kS}\right)}\right)\cdot \frac{e^{-kS}\boldsymbol{x}_0}{\left(1-e^{-2kS}\right)}\mathrm{d}\boldsymbol{x}_0}{\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\cdot \exp\left(\frac{-e^{-2kS}\|\boldsymbol{x}_0\|^2}{2\left(1-e^{-2kS}\right)}\right)\mathrm{d}\boldsymbol{x}_0} \right\|^2 \\
\leq & \frac{e^{-kS}}{1-e^{-2kS}}\cdot \int p_*(\boldsymbol{x}_0)\cdot\|\boldsymbol{x}_0\|^2\,\mathrm{d}\boldsymbol{x}_0\cdot \frac{\int p_*(\boldsymbol{x}_0)\cdot\exp\left(\frac{-e^{-2kS}\|\boldsymbol{x}_0\|^2}{\left(1-e^{-2kS}\right)}\right)\mathrm{d}\boldsymbol{x}}{\left(\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\cdot \exp\left(\frac{-e^{-2kS}\|\boldsymbol{x}_0\|^2}{2\left(1-e^{-2kS}\right)}\right)\mathrm{d}\boldsymbol{x}_0\right)^2} \\
\leq & \frac{e^{-kS}}{1-e^{-2kS}}\cdot M\cdot\left(\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\cdot\exp\left(\frac{-e^{-2kS}\left\|\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2kS}\right)}\right)\mathrm{d}\boldsymbol{x}_0\right)^{-1}
\end{aligned}
\tag{31}
$$

where the first inequality follows from Holders' inequality, the second inequality follows from **[A2]**. With, the following range:

$$
\frac{e^{-2kS}}{1-e^{-2kS}} \leq \frac{e^{-kS}}{1-e^{-2kS}} \leq \frac{e^{-S}}{1-e^{-2S}}
$$

we plug Eq 30 and Eq 31 into Eq 29 and obtain

$$
\begin{aligned}
\log \mathrm{KL}\left(q_0'(\cdot)\|q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) \leq \log\Bigg[\mu_r^{-1}\cdot\Bigg(& L_r^2\cdot e^{2(S-r\eta)}(d+\|\boldsymbol{x}\|^2) \\
& + \frac{e^{-kS}}{1-e^{-2kS}}\cdot M\left(\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\cdot\exp\left(\frac{-e^{-2kS}\left\|\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2kS}\right)}\right)\mathrm{d}\boldsymbol{x}_0\right)^{-1}\Bigg)\Bigg]
\end{aligned}
$$

Without loss of generality, we suppose both RHS of Eq 30 and Eq 31 are larger than 1. Then, we have

$$
\begin{aligned}
& \log \mathrm{KL}\left(q_0'(\cdot)\|q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) \\
& \leq \log\left[\frac{L_r^2}{\mu_r^2}\cdot e^{2(S-r\eta)}M\cdot\frac{e^{-kS}}{1-e^{-2kS}}\cdot(d+\|\boldsymbol{x}\|^2)\right] - \log\left[\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\cdot\exp\left(\frac{-e^{-2kS}\left\|\boldsymbol{x}_0\right\|^2}{2\left(1-e^{-2kS}\right)}\right)\mathrm{d}\boldsymbol{x}_0\right] \\
& \leq \log\left[\frac{L_r^2 M}{\mu_r^2}\cdot\frac{e^S}{1-e^{-2S}}\cdot(d+\|\boldsymbol{x}\|^2)\right] + \frac{e^{-2kS}}{2(1-e^{-2kS})}\cdot\int_{\mathbb{R}^d} p_*(\boldsymbol{x}_0)\left\|\boldsymbol{x}_0\right\|^2\mathrm{d}\boldsymbol{x}_0 \\
& \leq \log\left[\frac{L_r^2 M}{\mu_r^2}\cdot\frac{e^S}{1-e^{-2S}}\cdot(d+\|\boldsymbol{x}\|^2)\right] + \frac{Me^{-S}}{1-e^{-2S}} \leq \log\|\boldsymbol{x}\|^2 + \log\left[\frac{L_r^2 M}{\mu_r^2}\cdot\frac{de^S}{1-e^{-2S}}\right] + \frac{Me^{-S}}{1-e^{-2S}}.
\end{aligned}
$$

Hence, the proof is completed. ■

Corollary 19 *For any given (k,r) in Alg 1 and $\boldsymbol{x}\in\mathbb{R}^d$, suppose the distribution $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$ satisfies*

$$
\mu_r\boldsymbol{I} \preceq -\nabla^2\log q_{k,S-r\eta}(\cdot|\boldsymbol{x}) \preceq L_r\boldsymbol{I},
$$

and $\mathbf{x}_j' \sim q_j'(\cdot|\boldsymbol{x})$. If $0<\tau_r\leq \mu_r/(8L_r^2)$, we have

$$
\mathrm{KL}\left(q_j'\|q_*\right) \leq \exp\left(-\mu_r\tau_r j\right)\cdot\mathrm{KL}\left(q_0'\|q_*\right) + \frac{32L_r^2 d\tau_r}{\mu_r}
$$

when the score estimation satisfies $\left\|\nabla\log p_{k,0}-\boldsymbol{v}'\right\|_\infty \leq L_r\sqrt{2d\tau_r}$.

Proof Due to the range $0 < \tau_r \le \mu_r/8L_r^2$, we have $\mu_r\tau_r \le 1/8$. In this condition, we have

$$1 - \exp\left(-\mu_r\tau_r\right) \ge \frac{7}{8}\cdot \mu_r\tau_r.$$

Plugging this into the following inequality obtained by the recursion of Eq. 28, we have

$$\begin{aligned}\mathrm{KL}\left(q_j'\|q_*\right) \le& \exp\left(-\mu_r\tau_r j\right)\cdot \mathrm{KL}\left(q_0'\|q_*\right) + \frac{28L_r^2 d\tau_r^2}{\left(1-\exp\left(-\mu_r\tau_r\right)\right)}\\ \le& \exp\left(-\mu_r\tau_r j\right)\cdot \mathrm{KL}\left(q_0'\|q_*\right) + \frac{32L_r^2 d\tau_r}{\mu_r}.\end{aligned}$$

In this condition, if we require the KL divergence to satisfy $\mathrm{KL}\left(q_j'\|q_*\right) \le \epsilon$, a sufficient condition is that

$$\exp\left(-\mu_r\tau_r j\right)\cdot \mathrm{KL}\left(q_0'\|q_*\right) \le \frac{\epsilon}{2} \quad \text{and} \quad \frac{32L_r^2 d\tau}{\mu_r} \le \frac{\epsilon}{2},$$

which is equivalent to

$$\tau_r \le \frac{\mu_r\epsilon}{64L_r^2 d} \quad \text{and} \quad j \ge \frac{1}{\mu_r\tau_r}\cdot \log\frac{2\mathrm{KL}\left(q_0'\|q_*\right)}{\epsilon}.$$

According to the upper bound of $\mathrm{KL}\left(q_0'\|q_*\right)$ shown in Lemma 18, we require

$$j \ge \frac{1}{\mu_r\tau_r}\cdot\left[\log\frac{\|\boldsymbol{x}\|^2}{\epsilon} + \log\left(\frac{2L_r^2 M}{\mu_r^2}\cdot\frac{de^S}{1-e^{-2S}}\right) + \frac{Me^{-S}}{1-e^{-2S}}\right].$$

■

E.3. Core Lemmas

Lemma 20 *In Alg 1, for any $k \in \mathbb{N}_{0,K-1}$, $r \in \mathbb{N}_{0,R-1}$ and $\boldsymbol{x} \in \mathbb{R}^d$, we have*

$$\mathbb{P}\left[\left\|\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}) - \nabla\log p_{k,S-r\eta}(\boldsymbol{x})\right\|^2 \le 10\epsilon\right] \ge 1-\delta$$

by requiring the segment length S, the sample number $n_{k,r}$ and the step size of inner loops τ_r and the iteration number of inner loops $m_{k,r}$ satisfy

$$\begin{aligned}&S = \frac{1}{2}\log\frac{2L+1}{2L}, \quad n_{k,r} \ge \frac{4}{\epsilon(1-e^{-2(S-r\eta)})}\cdot\max\left\{d, -2\log\delta\right\},\\ &\tau_r \le \frac{\mu_r}{64L_r^2 d}\cdot(1-e^{-2(S-r\eta)})\epsilon \quad \text{and} \quad m_{k,r} \ge \frac{64L_r^2 d}{\mu_r^2(1-e^{-2(S-r\eta)})\epsilon}\cdot\left[\log\frac{d\|\boldsymbol{x}\|^2}{(1-e^{-2(S-r\eta)})\epsilon} + C_{m,1}\right],\end{aligned}$$

where $C_{m,1} = \log\left(2M\cdot 3^2\cdot 5L\right) + M\cdot 3L$. In this condition that choosing the τ_r to its upper bound, we required the score estimation in the inner loop satisfies

$$\left\|\nabla\log p_{k,0}(\boldsymbol{x}') - \mathbf{v}'_{k,0}(\boldsymbol{x}')\right\| \le \frac{e^{-(S-r\eta)}\epsilon^{0.5}}{8}.$$

Proof With a little abuse of notation, for each loop $i\in\mathbb{N}_{1,n_{k,r}}$ in Line 4 of Alg 1, we denote the underlying distribution of **output particles** as $\mathbf{x}'_i\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})$ for any $k\in\mathbb{N}_{0,K-1}$, $r\in\mathbb{N}_{0,R-1}$ and $\boldsymbol{x}\in\mathbb{R}^d$ in this lemma. According to Line 11 in Alg 1, we have

$$
\begin{aligned}
&\left\|\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})-\nabla\log p_{k,S-r\eta}(\boldsymbol{x})\right\|^2\\
=&\left\|\frac{1}{n_{r,k}}\sum_{i=1}^{n_{r,k}}\left(-\frac{\boldsymbol{x}-e^{-(S-r\eta)}\mathbf{x}'_i}{1-e^{-2(S-r\eta)}}\right)-\mathbb{E}_{\mathbf{x}'\sim q_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[-\frac{\boldsymbol{x}-e^{-(S-r\eta)}\mathbf{x}'}{1-e^{-2(S-r\eta)}}\right]\right\|^2\\
=&\frac{e^{-2(S-r\eta)}}{\left(1-e^{-2(S-r\eta)}\right)^2}\cdot\left\|-\frac{1}{n_{r,k}}\sum_{i=1}^{n_{r,k}}\mathbf{x}'_i+\mathbb{E}_{\mathbf{x}'\sim q_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|^2\\
\le&\frac{2e^{-2(S-r\eta)}}{\left(1-e^{-2(S-r\eta)}\right)^2}\cdot\left\|-\frac{1}{n_{r,k}}\sum_{i=1}^{n_{r,k}}\mathbf{x}'_i+\mathbb{E}_{\mathbf{x}'\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|^2\\
&+\frac{2e^{-2(S-r\eta)}}{\left(1-e^{-2(S-r\eta)}\right)^2}\cdot\left\|-\mathbb{E}_{\mathbf{x}'\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]+\mathbb{E}_{\mathbf{x}'\sim q_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|^2
\end{aligned}
\tag{32}
$$

In the following, we respectively upper bound the concentration error and the mean gap between $q'_{k,S-r\eta}(\cdot|\boldsymbol{x})$ and $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$ corresponding to the former and the latter term in Eq 32.

Upper bound the concentration error. The choice of S, i.e., $S=\frac{1}{2}\log\left(\frac{2L+1}{2L}\right)$, Lemma 15 demonstrate that suppose

$$
\mu_r=\frac{1}{2}\cdot\frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}\quad\text{and}\quad L_r=\frac{3}{2}\cdot\frac{e^{-2(S-r\eta)}}{1-e^{-2(S-r\eta)}}.
$$

Then, we have

$$
\mu_r\boldsymbol{I}\preceq-\nabla^2\log q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x})\preceq L_r\boldsymbol{I}.
$$

According to Alg 1, we utilize ULA as the inner loop (Line 4 – Line 9) to sample from $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$. By requiring the step size, i.e., τ_r to satisfy $\tau_r\le 1/L_r$, with Lemma 32, we know that the underlying distribution of output particles of the inner loops satisfies, i.e., $q'_{k,S-r\eta}(\cdot|\boldsymbol{x})$ satisfies LSI with a constant μ'_r satisfying

$$
\mu'_r\ge\frac{\mu_r}{2}\ge\frac{e^{-2(S-r\eta)}}{4(1-e^{-2(S-r\eta)})}.
$$

In this condition, we employ Lemma 16, by requiring

$$
\begin{aligned}
n_{k,r}\ge&\frac{4}{\epsilon(1-e^{-2(S-r\eta)})}\cdot\max\left\{d,-2\log\delta\right\}\\
\ge&\frac{1}{\mu'_r}\cdot\left(\frac{e^{-(S-r\eta)}}{(1-e^{-2(S-r\eta)})\epsilon^{0.5}}\right)^2\cdot\max\left\{d,-2\log\delta\right\}.
\end{aligned}
$$

and obtain

$$
\begin{aligned}
&\mathbb{P}\left[\frac{2e^{-2(S-r\eta)}}{\left(1-e^{-2(S-r\eta)}\right)^2}\cdot\left\|-\frac{1}{n_{r,k}}\sum_{i=1}^{n_{r,k}}\mathbf{x}'_i+\mathbb{E}_{\mathbf{x}'\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|^2\le 2\epsilon\right]\\
=&\mathbb{P}\left[\left\|-\frac{1}{n_{r,k}}\sum_{i=1}^{n_{r,k}}\mathbf{x}'_i+\mathbb{E}_{\mathbf{x}'\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|\le\frac{(1-e^{-2(S-r\eta)})\epsilon^{0.5}}{e^{-(S-r\eta)}}\right]\ge 1-\delta.
\end{aligned}
$$

Upper bound the mean gap. According to Lemma 15 and Lemma 28, we know $q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x})$ satisfies LSI with constant

$$\mu_r \geq \frac{e^{-2(S-r\eta)}}{2(1-e^{-2(S-r\eta)})}.$$

By introducing the optimal coupling between $q_{k,S-r\eta}(\cdot|\boldsymbol{x})$ and $q'_{k,S-r\eta}(\cdot|\boldsymbol{x})$, we have

$$\begin{aligned}
&\left\|-\mathbb{E}_{\mathbf{x}'\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]+\mathbb{E}_{\mathbf{x}'\sim q_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|^2 \\
\leq & W_2^2\left(q'_{k,S-r\eta}(\cdot|\boldsymbol{x}), q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) \leq \frac{2}{\mu_r}\mathrm{KL}\left(q'_{k,S-r\eta}(\cdot|\boldsymbol{x})\| q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right),
\end{aligned} \tag{33}$$

where the last inequality follows from Talagrand inequality Vempala and Wibisono (2019). Hence, the mean gap can be upper-bounded as

$$\begin{aligned}
&\frac{2e^{-2(S-r\eta)}}{\left(1-e^{-2(S-r\eta)}\right)^2}\cdot\left\|-\mathbb{E}_{\mathbf{x}'\sim q'_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]+\mathbb{E}_{\mathbf{x}'\sim q_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[\mathbf{x}'\right]\right\|^2 \\
\leq & \frac{2e^{-2(S-r\eta)}}{\left(1-e^{-2(S-r\eta)}\right)^2}\cdot\frac{2}{\mu_r}\mathrm{KL}\left(q'_{k,S-r\eta}(\cdot|\boldsymbol{x})\| q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) \\
\leq & \frac{8}{\left(1-e^{-2(S-r\eta)}\right)}\mathrm{KL}\left(q'_{k,S-r\eta}(\cdot|\boldsymbol{x})\| q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right).
\end{aligned}$$

To provide ϵ-level upper bound, we expect the required accuracy of KL convergence of inner loops to satisfy

$$\mathrm{KL}\left(q'_{k,S-r\eta}(\cdot|\boldsymbol{x})\| q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) \leq (1-e^{-2(S-r\eta)})\epsilon.$$

According to Corollary 19, to achieve such accuracy, we require the step size and the iteration number of inner loops to satisfy

$$\begin{aligned}
&\tau_r \leq \frac{\mu_r}{64L_r^2 d}\cdot(1-e^{-2(S-r\eta)})\epsilon \quad \text{and} \\
&m_{k,r} \geq \frac{1}{\mu_r}\cdot\frac{64L_r^2 d}{\mu_r(1-e^{-2(S-r\eta)})\epsilon}\cdot\left[\log\frac{\|\boldsymbol{x}\|^2}{(1-e^{-2(S-r\eta)})\epsilon}+\log\left(\frac{2L_r^2 M}{\mu_r^2}\cdot\frac{de^S}{1-e^{-2S}}\right)+\frac{Me^{-S}}{1-e^{-2S}}\right].
\end{aligned}$$

To simplify notation, we suppose $L\geq 1$ without loss of generality, and we the following equations:

$$\begin{aligned}
&\frac{L_r}{\mu_r}=3, \quad e^S=\exp\left(\frac{1}{2}\log\frac{2L+1}{2L}\right)=\sqrt{\frac{2L+1}{2L}}, \\
&\left(1-e^{-2S}\right)^{-1}=(2L+1),
\end{aligned}$$

which implies

$$\begin{aligned}
&\log\frac{d\|\boldsymbol{x}\|^2}{(1-e^{-2(S-r\eta)})\epsilon}+\log\left(2M\cdot 3^2\cdot 5L\right)+M\cdot 3L \\
\geq & \log\frac{d\|\boldsymbol{x}\|^2}{(1-e^{-2(S-r\eta)})\epsilon}+\log\left(2M\cdot\frac{L_r^2}{\mu_r^2}\cdot\sqrt{\frac{2L+1}{2L}}\cdot(2L+1)\right)+M\cdot(2L+1)\cdot\sqrt{\frac{2L}{2L+1}} \\
= & \log\frac{d\|\boldsymbol{x}\|^2}{(1-e^{-2(S-r\eta)})\epsilon}+\log\left(\frac{2L_r^2 M}{\mu_r^2}\cdot\frac{e^S}{1-e^{-2S}}\right)+\frac{Me^{-S}}{1-e^{-2S}}.
\end{aligned}$$

Therefore, we only require $m_{k,r}$ satisfies

$$m_{k,r} \geq \frac{1}{\mu_r} \cdot \frac{64L_r^2 d}{\mu_r(1-e^{-2(S-r\eta)})\epsilon} \cdot \left[\log \frac{d\|\boldsymbol{x}\|^2}{(1-e^{-2(S-r\eta)})\epsilon} + C_{m,1}\right]$$

where $C_{m,1} = \log\left(2M \cdot 3^2 \cdot 5L\right) + M \cdot 3L$. For simplicity, we choose τ_r as its upper bound and lower bound, respectively. In this condition, we still require

$$\left\|\nabla \log p_{k,0} - \boldsymbol{v}'\right\| \leq \frac{e^{-(S-r\eta)}\epsilon^{0.5}}{8} \leq \frac{1}{4}\cdot\sqrt{\frac{\mu_r(1-e^{-2(S-r\eta)})}{2}\cdot\epsilon} \leq L_r\sqrt{2d\tau_r}$$

where the first inequality follows from the range of μ_r, and the last inequality is satisfied when we choose τ_r to its upper bound. Hence, the proof is completed. ∎

Lemma 21 (Errors from fine-grained score estimation) *Under the notation in Section A, suppose the step size satisfy $\eta = C_\eta(d+M)^{-1}\epsilon$, we have*

$$\begin{aligned}
&\mathbb{P}\left[\left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})\right\|^2 \leq 10\epsilon, \forall \boldsymbol{x}\in\mathbb{R}^d\right]\\
\geq&(1-\delta)\cdot\left(\min_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},\epsilon)} \mathbb{P}\left[\left\|\nabla \log p_{k,0}(\boldsymbol{x}') - \mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2 \leq \frac{\epsilon}{96}\right]\right)^{n_{k,r}(10\epsilon)\cdot m_{k,r}(10\epsilon,\boldsymbol{x})},
\end{aligned}$$

where $\mathbb{S}_{k,r}(\boldsymbol{x}, 10\epsilon)$ denotes the set of particles appear in Alg 1 when the input is $(k, r, \boldsymbol{x}, 10\epsilon)$. For any $(k, r) \in \mathbb{N}_{0,K-1} \times \mathbb{N}_{0,R-1}$ by requiring

$$\begin{aligned}
&n_{k,r}(10\epsilon) = C_n \cdot \frac{(d+M)\cdot\max\{d, -2\log\delta\}}{(10\epsilon)^2} \quad \text{where} \quad C_n = 2^6\cdot 5^2\cdot C_\eta^{-1},\\
&m_{k,r}(10\epsilon,\boldsymbol{x}) = C_m \cdot \frac{(d+M)^3\cdot\max\{\log\|\boldsymbol{x}\|^2, 1\}}{(10\epsilon)^3} \quad \text{where} \quad C_m = 2^9\cdot 3^2\cdot 5^3\cdot C_{m,1}C_\eta^{-1.5}.
\end{aligned}$$

Proof According to Line 9 of Alg 1, for any $\boldsymbol{x}\in\mathbb{R}^d$, the score estimation $\mathbf{v}^{\leftarrow}_{k,r\eta}$ is constructed by estimating the mean in RHS of the following expectation using $n_{k,r}$ samples (i.e., calculating the empirical mean):

$$\nabla_{\boldsymbol{x}} \log p_{k,S-r\eta}(\boldsymbol{x}) = \mathbb{E}_{\mathbf{x}'\sim q_{k,S-r\eta}(\cdot|\boldsymbol{x})}\left[-\frac{\boldsymbol{x} - e^{-(S-r\eta)}\mathbf{x}'}{\left(1-e^{-2(S-r\eta)}\right)}\right] \tag{34}$$

$$\text{where} \quad q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x}) \propto \exp\left(\log\ p_{k,0}(\boldsymbol{x}') - \frac{\left\|\boldsymbol{x} - e^{-(S-r\eta)}\boldsymbol{x}'\right\|^2}{2\left(1-e^{-2(S-r\eta)}\right)}\right). \tag{35}$$

Then in order to guarantee an accurate estimation for $\nabla_{\boldsymbol{x}} \log p_{k,S-r\eta}(\boldsymbol{x})$, i.e., denoted by $\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})$, with Lemma 20, we require

1. Get a precise estimation for $\nabla \log p_{k,0}(\boldsymbol{x}')$, in order to guarantee that the estimation for $\nabla \log q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x})$ is accurate. In particular, we require

$$\left\|\nabla \log p_{k,0}(\boldsymbol{x}'_{i,j}) - \mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}'_{i,j})\right\| \leq \frac{e^{-(S-r\eta)}\epsilon^{0.5}}{8}.$$

2. Based on the $\nabla \log q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x})$, we run ULA with appropriate step size τ_r and iteration number $m_{k,r}$ satisfying

$$\begin{aligned} &\tau_r \le \frac{\mu_r}{64L_r^2 d}\cdot (1-e^{-2(S-r\eta)})\epsilon \quad \text{and} \\ &m_{k,r} \ge \frac{64L_r^2 d}{\mu_r^2(1-e^{-2(S-r\eta)})\epsilon}\cdot \log \frac{2\mathrm{KL}\left(q_0'(\cdot)\|q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right)}{(1-e^{-2(S-r\eta)})\epsilon} \end{aligned} \tag{36}$$

to generate samples $\boldsymbol{x}'$ whose underlying distribution $q'_{k,S-r\eta}(\cdot|\boldsymbol{x})$ is sufficiently close to $q_{k,S-r\eta}(\boldsymbol{x}'|\boldsymbol{x})$, i.e.,

$$\mathrm{KL}\left(q'_{k,S-r\eta}(\cdot|\boldsymbol{x})\|q_{k,S-r\eta}(\cdot|\boldsymbol{x})\right) \le (1-e^{-2(S-r\eta)})\epsilon.$$

3. Generate a sufficient number of samples satisfying

$$n_{k,r} \ge \frac{4}{\epsilon(1-e^{-2(S-r\eta)})}\cdot \max\left\{d, -2\log\delta\right\}. \tag{37}$$

such that the empirical estimation of the expectation in (34) is accurate, i.e.,

$$\begin{aligned} &\mathbb{P}\left[\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}) - \tilde{\mathbf{v}}_{k,r\eta}(\boldsymbol{x})\|^2 \le 10\epsilon\right] \\ &= \mathbb{P}\left[\left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}) - \frac{1}{n_{k,r}}\sum_{i=1}^{n_{k,r}}\left[-\frac{\boldsymbol{x}-e^{-(S-r\eta)}\boldsymbol{x}'_{i,m_{k,r}}}{\left(1-e^{-2(S-r\eta)}\right)}\right]\right\| \le 10\epsilon\right] \ge 1-\delta. \end{aligned}$$

Due to the fact $r\eta \ge 0$, the first condition can be achieved by requiring

$$\left\|\nabla \log p_{k,0}(\boldsymbol{x}'_{i,j}) - \mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}'_{i,j})\right\| \le \sqrt{\frac{2}{3}}\cdot\frac{\epsilon^{0.5}}{8} \le \sqrt{\frac{2L}{2L+1}}\cdot\frac{\epsilon^{0.5}}{8} = \frac{e^{-S}\epsilon^{0.5}}{8} \le \frac{e^{-(S-r\eta)}\epsilon^{0.5}}{8},$$

where the second inequality is established by supposing $L \ge 1$ without loss of generality, and the last equation follows from the choice of S.

To investigate the setting of hyper-parameters, i.e., the number of samples for empirical mean estimation $n_{k,r}$ and the number of iterations for ULA $m_{k,r}$. We first reformulate them as two functions, i.e.,

$$\begin{aligned} &n_{k,r}(10\epsilon) = C_n\cdot\frac{(d+M)\cdot\max\{d,-2\log\delta\}}{(10\epsilon)^2} \quad \text{where} \quad C_n = 2^6\cdot 5^2\cdot C_\eta^{-1}, \\ &m_{k,r}(10\epsilon,\boldsymbol{x}) = C_m\cdot\frac{(d+M)^3\cdot\max\{\log\|\boldsymbol{x}\|^2,1\}}{(10\epsilon)^3} \quad \text{where} \quad C_m = 2^9\cdot 3^2\cdot 5^3\cdot C_{m,1}C_\eta^{-1.5}. \end{aligned}$$

since this presentation helps to explain the connection between them and the input of Alg 1. Different from the results shown in Lemma 20, $n_{k,r}(\cdot)$ and $m_{k,r}(\cdot,\cdot)$ is independent with k and r. However, these choices will still make Eq 36 and Eq 37 establish, because

$$\begin{aligned}
n_{k,r}(10\epsilon) =& \frac{16}{\epsilon}\cdot\frac{(d+M)}{C_\eta\epsilon}\cdot\max\left\{d,-2\log\delta\right\}\geq\frac{16}{\epsilon\eta}\cdot\max\left\{d,-2\log\delta\right\}\\
\geq& \frac{16}{\epsilon(1-e^{-2\eta})}\cdot\max\left\{d,-2\log\delta\right\}\geq\frac{16}{\epsilon(1-e^{-2(S-r\eta)})}\cdot\max\left\{d,-2\log\delta\right\}\\
m_{k,r}(10\epsilon,\boldsymbol{x}) =& 576\cdot\frac{(d+M)^3}{\epsilon^3}\cdot\frac{C_{m,1}}{C_\eta^{1.5}}\cdot\max\{\log\|\boldsymbol{x}\|^2,1\}\geq 64\cdot\frac{L_r^2}{\mu_r^2}\cdot\left(\frac{d}{\epsilon\eta}\right)^{1.5}\cdot C_{m,1}\cdot\max\{\log\|\boldsymbol{x}\|^2,1\}\\
\geq& 64\cdot\frac{L_r^2}{\mu_r^2}\cdot\frac{d}{\epsilon\eta}\log\frac{d}{\epsilon\eta}\cdot C_{m,1}\cdot\max\{\log\|\boldsymbol{x}\|^2,1\}\geq 64\cdot\frac{L_r^2}{\mu_r^2}\cdot\frac{d}{\epsilon\eta}\left(\log\frac{d\|\boldsymbol{x}\|^2}{\epsilon\eta}+C_{m,1}\right)\\
\geq& 64\cdot\frac{L_r^2}{\mu_r^2}\cdot\frac{d}{\epsilon(1-e^{-2\eta})}\left(\log\frac{d\|\boldsymbol{x}\|^2}{\epsilon(1-e^{-2\eta})}+C_{m,1}\right)\\
\geq& \frac{64L_r^2 d}{\mu_r^2(1-e^{-2(S-r\eta)})\epsilon}\cdot\left(\log\frac{d\|\boldsymbol{x}\|^2}{(1-e^{-2(S-r\eta)})\epsilon}+C_{m,1}\right)
\end{aligned}$$

with the proper choice of step size, i.e., $\eta = C_\eta(d+M)^{-1}\epsilon$. With these settings, Lemma 20 demonstrates that

$$\begin{aligned}
&\mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})\right\|^2\leq 10\epsilon,\forall\boldsymbol{x}\in\mathbb{R}^d\right|\\
&\left.\bigcap_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},10\epsilon)}\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\leq\frac{\epsilon}{96}\right]\geq 1-\delta.
\end{aligned}$$

where $\mathbb{S}_{k,r}(\boldsymbol{x},10\epsilon)$ denotes the set of particles appear in Alg 1 when the input is $(k,r,\boldsymbol{x},10\epsilon)$ except for the recursion. It satisfies $|\mathbb{S}_{k,r}(\boldsymbol{x},10\epsilon)| = n_{k,r}(10\epsilon)\cdot m_{k,r}(10\epsilon,\boldsymbol{x})$. Furthermore, we have

$$\begin{aligned}
&\mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})\right\|^2\leq 10\epsilon\right]\\
&\geq\mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})\right\|^2\leq 10\epsilon\,\middle|\bigcap_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},10\epsilon)}\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\leq\frac{\epsilon}{96}\right]\\
&\quad\cdot\mathbb{P}\left[\bigcap_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},10\epsilon)}\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\leq\frac{\epsilon}{96}\right]\\
&\geq(1-\delta)\cdot\mathbb{P}\left[\bigcap_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},10\epsilon)}\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\leq\frac{\epsilon}{96}\right].
\end{aligned}\tag{38}$$

Considering that for each $\boldsymbol{x}'_{i,j}$, the score estimation, i.e., $\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}'_{i,j})$ is independent, hence, we have

$$\begin{aligned}
&\mathbb{P}\left[\bigcap_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},10\epsilon)}\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\leq\frac{\epsilon}{96}\right]\\
&=\prod_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},10\epsilon)}\mathbb{P}\left[\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\leq\frac{\epsilon}{96}\right]\\
&\geq\left(\min_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},\epsilon)}\mathbb{P}\left[\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\leq\frac{\epsilon}{96}\right]\right)^{|\mathbb{S}_{k,r}(\boldsymbol{x},\epsilon)|}
\end{aligned}\tag{39}$$

Therefore, combining Eq 38 and Eq 39, we have

$$\begin{aligned}&\mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x})\right\|^2\le 10\epsilon\right]\\ \ge&(1-\delta)\cdot\left(\min_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x},\epsilon)}\mathbb{P}\left[\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\le\frac{\epsilon}{96}\right]\right)^{n_{k,r}(10\epsilon)\cdot m_{k,r}(10\epsilon,\boldsymbol{x})},\end{aligned}$$

and the proof is completed. ■

Corollary 22 (Errors from coarse-grained score estimation) *Under the notation in Section A, suppose the step size satisfy $\eta=C_1(d+M)^{-1}\epsilon$, we have*

$$\begin{aligned}&\mathbb{P}\left[\left\|\nabla\log p_{k+1,0}(\boldsymbol{x})-\mathbf{v}^{\leftarrow}_{k,0}(\boldsymbol{x})\right\|^2\le 10\epsilon,\forall\boldsymbol{x}\in\mathbb{R}^d\right]\\ \ge&(1-\delta)\cdot\left(\min_{\boldsymbol{x}'\in\mathbb{S}_{k,0}(\boldsymbol{x},\epsilon)}\mathbb{P}\left[\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\le\frac{\epsilon}{96}\right]\right)^{n_{k,0}(10\epsilon)\cdot m_{k,0}(10\epsilon,\boldsymbol{x})},\end{aligned}\tag{40}$$

where $\mathbb{S}_{k,0}(\boldsymbol{x},10\epsilon)$ denotes the set of particles appear in Alg 1 when the input is $(k,0,\boldsymbol{x},10\epsilon)$. For any $k\in\mathbb{N}_{1,K-1}$ by requiring

$$\begin{aligned}&n_{k,0}(10\epsilon)=C_n\cdot\frac{(d+M)\cdot\max\{d,-2\log\delta\}}{(10\epsilon)^2}\quad\text{where}\quad C_n=2^6\cdot5^2\cdot C_\eta^{-1},\\ &m_{k,0}(10\epsilon,\boldsymbol{x})=C_m\cdot\frac{(d+M)^3\cdot\max\{\log\|\boldsymbol{x}\|^2,1\}}{(10\epsilon)^3}\quad\text{where}\quad C_m=2^9\cdot3^2\cdot5^3\cdot C_{m,1}C_\eta^{-1.5}.\end{aligned}$$

Besides, for any $\boldsymbol{x}\in\mathbb{R}^d$, we have

$$\mathbb{P}\left[\left\|\nabla\log p_{0,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{-1,0}(\boldsymbol{x}')\right\|^2\le\frac{\epsilon}{96},\forall\boldsymbol{x}'\in\mathbb{R}^d\right]=1$$

by requiring $\tilde{\mathbf{v}}_{-1,0}(\boldsymbol{x}')=-\nabla f_*(\boldsymbol{x}')$, which corresponds to Line 2 in Alg 1.

Proof When $k>0$, plugging $r=0$ into Lemma 21, we can obtain the result except inequality Eq 40. Instead, we have

$$\begin{aligned}&\mathbb{P}\left[\left\|\nabla\log p_{k,S}(\boldsymbol{x})-\mathbf{v}^{\leftarrow}_{k,0}(\boldsymbol{x})\right\|^2\le 10\epsilon,\forall\boldsymbol{x}\in\mathbb{R}^d\right]\\ \ge&(1-\delta)\cdot\left(\min_{\boldsymbol{x}'\in\mathbb{S}_{k,0}(\boldsymbol{x},\epsilon)}\mathbb{P}\left[\left\|\nabla\log p_{k,0}(\boldsymbol{x}')-\mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\le\frac{\epsilon}{96}\right]\right)^{n_{k,0}(10\epsilon)\cdot m_{k,0}(10\epsilon,\boldsymbol{x})}.\end{aligned}\tag{41}$$

Since the forward process, i.e., SDE 1, satisfies $\mathbf{x}_{k,S}=\mathbf{x}_{k+1,0}$, we have

$$p_{k,S}(\boldsymbol{x})=p_{k+1,0}(\boldsymbol{x})=\int p_*(\boldsymbol{y})\cdot\left(2\pi\left(1-e^{-2(k+1)S}\right)\right)^{-d/2}\cdot\exp\left[\frac{-\left\|\boldsymbol{x}-e^{-(k+1)S}\boldsymbol{y}\right\|^2}{2\left(1-e^{-2(k+1)S}\right)}\right]\mathrm{d}\boldsymbol{y},$$

which means $\nabla\log p_{k,S}=\nabla\log p_{k+1,0}$. Therefore, Eq 40 is established.

When $k=0$, due to the definition of $\tilde{\mathbf{v}}_{-1,0}$ in Eq 7, we know Eq 41 is established. Hence, the proof is completed. ■

Lemma 23 (Errors from score estimation) *Under the notation in Section A, suppose the step size satisfy $\eta = C_\eta (d+M)^{-1}\epsilon$, we have*

$$\mathbb{P}\left[\bigcap_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}} \left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right] \ge 1-\epsilon$$

with Alg 1 by properly choosing the number for mean estimations and ULA iterations. The total gradient complexity will be at most

$$\exp\left[\mathcal{O}\left(L^3\cdot\left(\log\frac{Ld+M}{\epsilon}\right)^3\cdot\max\left\{\log\log Z^2, 1\right\}\right)\right],$$

where Z is the maximal norm of particles that appear in Alg 2.

Proof We begin with lower bounding the following probability with $(i,j)\in\mathbb{N}_{0,K-1}\times\mathbb{N}_{0,R-1}$ and $(i,j)\neq(0,0)$,

$$\mathbb{P}\left[\left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right].$$

In the following part of this Lemma, we set $\eta = C_\eta(d+M)^{-1}\epsilon$ and denote δ as a tiny positive constant waiting for determining. With Lemma 21, we have

$$\begin{aligned}
&\mathbb{P}\left[\left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right]\\
\ge&(1-\delta)\cdot\left(\min_{\boldsymbol{x}'\in\mathbb{S}_{k,r}(\boldsymbol{x}^{\leftarrow}_{k,r\eta},10\epsilon)}\mathbb{P}\left[\left\|\nabla\log p_{k,0}(\boldsymbol{x}') - \mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\le\frac{10\epsilon}{960}\right]\right)^{n_{k,r}(10\epsilon)\cdot m_{k,r}(10\epsilon,\boldsymbol{x}^{\leftarrow}_{k,r\eta})}.
\end{aligned} \tag{42}$$

Then, if $k\ge 1$, for each item of the latter term, supposing $10\epsilon' = \epsilon/96$, Lemma 22 shows

$$\begin{aligned}
&\mathbb{P}\left[\left\|\nabla\log p_{k,0}(\boldsymbol{x}') - \mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\le\frac{\epsilon}{96}\right] = \mathbb{P}\left[\left\|\nabla\log p_{k,0}(\boldsymbol{x}') - \mathbf{v}^{\leftarrow}_{k-1,0}(\boldsymbol{x}')\right\|^2\le 10\epsilon'\right]\\
\ge&(1-\delta)\cdot\left(\min_{\boldsymbol{x}''\in\mathbb{S}_{k-1,0}(\boldsymbol{x}',10\epsilon')}\mathbb{P}\left[\left\|\nabla\log p_{k-1,0}(\boldsymbol{x}'') - \mathbf{v}^{\leftarrow}_{k-2,0}(\boldsymbol{x}'')\right\|^2\le\frac{\epsilon'}{96}\right]\right)^{n_{k,0}(10\epsilon')\cdot m_{k,r}(10\epsilon',\boldsymbol{x}')}\\
=&(1-\delta)\cdot\left(\min_{\boldsymbol{x}''\in\mathbb{S}_{k-1,0}(\boldsymbol{x}',\epsilon/96)}\mathbb{P}\left[\left\|\nabla\log p_{k-1,0}(\boldsymbol{x}'') - \mathbf{v}^{\leftarrow}_{k-2,0}(\boldsymbol{x}'')\right\|^2\le\frac{\epsilon}{96\cdot 960}\right]\right)^{n_{k,0}(\epsilon/96)\cdot m_{k,0}(\epsilon/96,\boldsymbol{x}')}.
\end{aligned}$$

Only particles that appear in the iteration will appear in powers of Eq 42. To simplify the notation, we set Z as the upper bound of the norm of particles appear in Alg 2,

$$\begin{aligned}
&m_{k,r}(10\epsilon,\boldsymbol{x})\le m_{k,r}(10\epsilon)\coloneqq C_m\cdot\frac{(d+M)^3\cdot\max\{2\log Z,1\}}{(10\epsilon)^3}\\
&\text{and}\quad u_{k,r}(\epsilon)\coloneqq n_{k,r}(\epsilon)\cdot m_{k,r}(\epsilon).
\end{aligned}$$

Plugging this inequality into Eq 42, we have

$$\begin{aligned}
&\mathbb{P}\left[\left\|\nabla \log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right]\\
\ge&(1-\delta)^{1+u_{k,r}(10\epsilon)}\cdot\left(\mathbb{P}\left[\left\|\nabla\log p_{k-1,0}(\boldsymbol{x}'') - \mathbf{v}^{\leftarrow}_{k-2,0}(\boldsymbol{x}'')\right\|^2\le\frac{10\epsilon}{(960)^2}\right]\right)^{u_{k,r}(10\epsilon)\cdot u_{k,0}(\frac{\epsilon}{96})}.
\end{aligned}$$

Using Lemma 22 recursively, we will have

$$
\begin{aligned}
&\mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2\le 10\epsilon\right]\\
\ge&(1-\delta)^{1+u_{k,r}(10\epsilon)+u_{k,r}(10\epsilon)\cdot u_{k,0}\left(\frac{10\epsilon}{960}\right)+\ldots+u_{k,r}(10\epsilon)\cdot\prod_{i=k}^{2}u_{i,0}\left(\frac{10\epsilon}{960^{k-i+1}}\right)}\\
&\left(\mathbb{P}\left[\left\|\nabla\log p_{0,0}(\boldsymbol{x}')-\tilde{\mathbf{v}}_{-1,0}(\boldsymbol{x}')\right\|^2\le\frac{10\epsilon}{(960)^{k+1}},\forall \boldsymbol{x}'\in\mathbb{R}^d\right]\right)^{u_{k,r}(10\epsilon)\cdot\prod_{i=k}^{1}u_{i,0}\left(\frac{10\epsilon}{960^{k-i+1}}\right)}\\
=&(1-\delta)^{1+u_{k,r}(10\epsilon)+u_{k,r}(10\epsilon)\cdot u_{k,0}\left(\frac{10\epsilon}{960}\right)+\ldots+u_{k,r}(10\epsilon)\cdot\prod_{i=k}^{2}u_{i,0}\left(\frac{10\epsilon}{960^{k-i+1}}\right)}\\
\ge&1-\delta\cdot\left(1+u_{k,r}(10\epsilon)+u_{k,r}(10\epsilon)\cdot u_{k,0}\left(\frac{10\epsilon}{960}\right)+\ldots+u_{k,r}(10\epsilon)\cdot\prod_{i=k}^{2}u_{i,0}\left(\frac{10\epsilon}{960^{k-i+1}}\right)\right)
\end{aligned}
\tag{43}
$$

where the third inequality follows from the case $k=0$ in Lemma 22 and the last inequality follows from union bound.

Then, we start to upper bound the coefficient of δ. According to Lemma 21 and Lemma 22, it can be noted that the function $u_{k,r}(\cdot)$ is independent with k and r. It is actually because we provide a union bound for the sample number $n_{k,r}$ and the iteration number $m_{k,r}$ when $(k,r)\in\mathbb{N}_{0,K-1}\times\mathbb{N}_{0,R-1}$. Therefore, the explicit form of the uniformed u is defined as

$$
u(10\epsilon)=\underbrace{C_nC_m\cdot(d+m_2^2)^4\cdot\max\{d,\log(1/\delta^2)\}\cdot\max\{2\log Z,1\}}_{\text{independent with }\epsilon}\cdot(10\epsilon)^{-5}
$$

Then, we have

$$
u\left(\frac{10\epsilon}{960}\right)=u(10\epsilon)\cdot 960^5\quad\text{and}\quad u\left(\frac{10\epsilon}{960^i}\right)=u(10\epsilon)\cdot 960^{5i}.
$$

Combining this result with Eq 43, we obtain

$$
\begin{aligned}
&1+u_{k,r}(10\epsilon)+u_{k,r}(10\epsilon)\cdot u_{k,0}\left(\frac{10\epsilon}{960}\right)+\ldots+u_{k,r}(10\epsilon)\cdot\prod_{i=k}^{2}u_{i,0}\left(\frac{10\epsilon}{960^{k-i+1}}\right)\\
&\le(k+1)\cdot u(10\epsilon)\cdot\prod_{i=k}^{2}u\left(\frac{10\epsilon}{960^{5(k-i+1)}}\right)=(k+1)\cdot u(10\epsilon)\cdot\prod_{i=k}^{2}\left(u(10\epsilon)\cdot 960^{k-i+1}\right)\\
&=(k+1)\cdot 960^{2.5k(k-1)}\cdot u(10\epsilon)^k\le K\cdot 960^{2.5(K-1)(K-2)}\cdot u(10\epsilon)^{K-1}.
\end{aligned}
$$

Considering that $K=2/S\cdot\log[(Ld+M)/\epsilon]$, to bound RHS of the previous inequality, we have

$$
\begin{aligned}
&\log\left(960^{2.5(K-1)(K-2)}\cdot u(10\epsilon)^{K-1}\right)=2.5(K-1)(K-2)\log(960)+(K-1)\log(u(10\epsilon))\\
&\le 2.5\cdot\log(960)\cdot\left(\frac{2}{S}\log\frac{Ld+M}{\epsilon}\right)^2+\frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\left(\log C_nC_m+4\log(d+M)+\log d+\log\left(2\log\frac{1}{\delta}\right)\right.\\
&\quad\left.+\log\left(2\max\left\{\log Z,\frac{1}{2}\right\}\right)+\log(10^{-5})+5\log\frac{1}{\epsilon}\right).
\end{aligned}
$$

To make the result more clear, we set

$$
C_{u,1}\coloneqq\log(C_nC_m)+\log 2+\log\left(2\max\left\{\log Z,\frac{1}{2}\right\}\right)-5\log 10
$$

which is independent with d, ϵ and δ. Then, it has

$$\begin{aligned}
&\log\left(960^{2.5(K-1)(K-2)}\cdot u(10\epsilon)^{K-1}\right)\\
\le&\frac{70}{S^2}\left(\log\frac{Ld+M}{\epsilon}\right)^2+\frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\left[C_{u,1}+5\log(d+M)+\log\log\frac{1}{\delta}+5\log\frac{1}{\epsilon}\right].
\end{aligned}$$

which means

$$\begin{aligned}
&960^{2.5(K-1)(K-2)}\cdot u(10\epsilon)^{K-1}\\
&\le\exp\left[\frac{70}{S^2}\left(\log\frac{Ld+M}{\epsilon}\right)^2+\frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\left(C_{u,1}+5\log(d+M)+\log\log\frac{1}{\delta}+5\log\frac{1}{\epsilon}\right)\right]\\
&\le\mathrm{pow}\left(\frac{Ld+M}{\epsilon},\left(\left(\frac{70}{S^2}+\frac{10}{S}\right)\log\frac{Ld+M}{\epsilon}+\frac{2}{S}\log\log\frac{1}{\delta}+\frac{2C_{u,1}}{S}\right)\right)
\end{aligned}\tag{44}$$

where the last inequality suppose $L\ge 1$ as the previous settings. To simplify notation, we set

$$C_{u,2}\coloneqq\frac{70}{S^2}+\frac{10}{S}\quad\text{and}\quad C_{u,3}\coloneqq\frac{2C_{u,1}}{S}.$$

Plugging this result into Eq 43, we have

$$\begin{aligned}
&\mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2\le 10\epsilon\right]\\
&\ge 1-\delta\cdot K\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon},C_{u,2}\log\frac{Ld+M}{\epsilon}+\frac{2}{S}\log\log\frac{1}{\delta}+C_{u,3}\right).
\end{aligned}\tag{45}$$

With these conditions, we can lower bound score estimation errors along Alg 2. That is

$$\begin{aligned}
&\mathbb{P}\left[\bigcap_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}}\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2\le 10\epsilon\right]\\
=&\prod_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}}\mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2\le 10\epsilon\right]
\end{aligned}$$

where the first inequality establishes because the random variables, $\mathbf{v}^{\leftarrow}_{k,r\eta}$, are independent for each (k,r) pair. By introducing Eq 45, we have

$$\begin{aligned}
&\prod_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}}\mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})-\mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2\le 10\epsilon\right]\\
\ge&\left(1-\delta\cdot K\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon},C_{u,2}\log\frac{Ld+M}{\epsilon}+\frac{2}{S}\log\log\frac{1}{\delta}+C_{u,3}\right)\right)^{KR}\\
\ge&1-\delta\cdot K^2R\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon},C_{u,2}\log\frac{Ld+M}{\epsilon}+\frac{2}{S}\log\log\frac{1}{\delta}+C_{u,3}\right)\\
=&1-\delta\cdot\frac{4(d+M)}{SC_\eta\epsilon}\left(\log\frac{Ld+M}{\epsilon}\right)^2\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon},C_{u,2}\log\frac{Ld+M}{\epsilon}+\frac{2}{S}\log\log\frac{1}{\delta}+C_{u,3}\right)
\end{aligned}\tag{46}$$

where the first inequality follows from Eq 45 and the second inequality follows from the union bound, and the last inequality follows from the combination of the choice of the step size, i.e., $\eta = C_1(d+M)^{-1}\epsilon$ and the definition of K and R, i.e.,

$$K = \frac{T}{S} = \frac{2}{S}\log\frac{C_0}{\epsilon},\quad R = \frac{S}{\eta} = \frac{S(d+M)}{C_\eta \epsilon}.$$

It means when δ is small enough, we can control the recursive error with a high probability, i.e.,

$$\prod_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}} \mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right] \ge 1-\epsilon. \tag{47}$$

Compared with Eq 46, Eq 47 can be achieved by requiring

$$\underbrace{\frac{4(d+M)}{SC_\eta\epsilon}\left(\log\frac{Ld+M}{\epsilon}\right)^2 \cdot \mathrm{pow}\left(\frac{Ld+M}{\epsilon}, C_{u,2}\log\frac{Ld+M}{\epsilon}+C_{u,3}\right)}_{\text{defined as } C_B} \cdot \delta\mathrm{pow}\left(\frac{Ld+M}{\epsilon}, \frac{2}{S}\log\log\frac{1}{\delta}\right) \le \epsilon,$$

which can be obtained by requiring

$$\begin{aligned} & C_B\delta(-\log\delta)^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}} \le \epsilon \quad\Leftrightarrow\quad (-\log\delta)^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}} \le \frac{\epsilon}{C_B\delta} \\ \Leftrightarrow\quad & \frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log\log\frac{1}{\delta} \le \log\frac{\epsilon}{C_B\delta} \end{aligned} \tag{48}$$

We suppose $\delta = \epsilon/C_B \cdot a^{-2/S\cdot\log((Ld+M)/\epsilon)}$ and the last inequality of Eq 48 becomes

$$\mathrm{LHS} = \frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log\left[\log\frac{C_B}{\epsilon}+\frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log a\right] \le \frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log a = \mathrm{RHS},$$

which is hold if we require

$$a \ge \max\left\{\frac{2C_B}{\epsilon}, \left(\frac{Ld+M}{\epsilon}\right)^{2/S}, 1\right\}.$$

Because in this condition, we have

$$\log\frac{C_B}{\epsilon}+\frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log a \le \log\frac{a}{2} + (\log a)^2 \le \frac{2a}{5}+\frac{3a}{5} = a \quad \text{when} \quad a\ge 1,$$

where the first inequality follows from the monotonicity of function $\log(\cdot)$. Therefore, we have

$$\log\left[\log\frac{C_B}{\epsilon}+\frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log a\right] \le \log a$$

and Eq 48 establishes. Without loss of generality, we suppose $3C_B/\epsilon$ dominates the lower bound of a. Hence, the choice of δ can be determined.

After determining the choice of δ, the only problem left is the gradient complexity of Alg 2. The number of gradients calculated in Alg 2 is equal to the number of calls for $\tilde{\mathbf{v}}_{-1,0}$. According to Eq 43, we can easily note that the number of calls of $\tilde{\mathbf{v}}_{-1,0}$ is

$$u_{k,r}(10\epsilon)\cdot\prod_{i=k}^{1}u_{i,0}\left(\frac{10\epsilon}{960^{k-i+1}}\right)=u(10\epsilon)\prod_{i=k}^{1}u\left(\frac{10\epsilon}{960^{k-i+1}}\right)$$

for each (k,r) pair. We can upper bound RHS of the previous equation as

$$\begin{aligned}
&u(10\epsilon)\prod_{i=k}^{1}u\left(\frac{10\epsilon}{960^{k-i+1}}\right)=u(10\epsilon)\cdot\prod_{i=k}^{2}\left(u(10\epsilon)\cdot 960^{k-i+1}\right)\\
=&960^{2.5k(k-1)}\cdot u(10\epsilon)^{k}\le 960^{2.5(K-1)(K-2)}\cdot u(10\epsilon)^{K-1}.
\end{aligned}$$

Combining this result with the total number of (k,r) pair, i.e., T/η, the total gradient complexity can be relaxed as

$$\begin{aligned}
&\frac{T}{\eta}\cdot 960^{2.5k(k-1)}\cdot u(10\epsilon)^{k}\le K^2R\cdot 960^{2.5(K-1)(K-2)}\cdot u(10\epsilon)^{K-1}\\
&\le\frac{4(d+M)}{SC_\eta\epsilon}\left(\log\frac{Ld+M}{\epsilon}\right)^2\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon},C_{u,2}\log\frac{Ld+M}{\epsilon}+\frac{2}{S}\log\log\frac{1}{\delta}+C_{u,3}\right)\\
&=C_B\cdot(-\log\delta)^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}}\le\frac{\epsilon}{\delta}=C_B\cdot a^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}}
\end{aligned}\tag{49}$$

where the first inequality follows from the fact $T/\eta=KR$, the second inequality follows from the combination of the choice of the step size, i.e., $\eta=C_1(d+M)^{-1}\epsilon$ and the definition of K and R, i.e.,

$$K=\frac{T}{S}=\frac{2}{S}\log\frac{C_0}{\epsilon},\quad R=\frac{S}{\eta}=\frac{S(d+M)}{C_1\epsilon}$$

and the last inequality follows from 48. Choosing a as its lower bound, i.e., $2C_B/\epsilon$, RHS of Eq 49 satisfies

$$\begin{aligned}
&C_B\cdot a^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}}=C_B\cdot\left(\frac{2C_B}{\epsilon}\right)^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}}\le\left(\frac{2C_B}{\epsilon}\right)^{\frac{4}{S}\log\frac{Ld+M}{\epsilon}}\\
&\le\mathrm{pow}\left(\frac{8(d+M)}{SC_\eta\epsilon^2}\cdot\left(\log\frac{Ld+M}{\epsilon}\right)^2,\frac{4}{S}\log\frac{Ld+M}{\epsilon}\right)\\
&\quad\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon},\frac{4C_{u,2}}{S}\left(\log\frac{Ld+M}{\epsilon}\right)^2+\frac{4C_{u,3}}{S}\left(\log\frac{Ld+M}{\epsilon}\right)\right)\\
&=\exp\left[\mathcal{O}\left(\left(\log\frac{Ld+M}{\epsilon}\right)^3\right)\right].
\end{aligned}\tag{50}$$

If we consider the effect of the norm of particles and the dependency of smoothness L since we have

$$\begin{aligned}
&S=\frac{1}{2}\log\left(1+\frac{1}{2L}\right)=\Theta(L^{-1}),\quad\text{when}\quad L\ge 1,\\
&\frac{4C_{u,2}}{S}=\frac{70}{S^3}+\frac{10}{S^2}=\Theta(L^3),\quad\frac{4C_{u,3}}{S}=\frac{8C_{u,1}}{S^2}=\Theta\left(L^2\cdot\left(\max\left\{\log\log Z^2,1\right\}\right)\right),
\end{aligned}$$

Combining this result with Eq 50, the proof is completed. ■

Lemma 24 *Under the notation in Section A, suppose the step size satisfy $\eta = C_\eta(d+M)^{-1}\epsilon$, we have*

$$\mathbb{P}\left[\bigcap_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}} \left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right] \ge 1-\delta'$$

with Alg 1 by properly choosing the number for mean estimations and ULA iterations. The total gradient complexity will be at most

$$\exp\left(\mathcal{O}\left(\max\left\{\left(\log\frac{Ld+M}{\epsilon}\right)^3, \log\frac{Ld+M}{\epsilon}\cdot\log\frac{1}{\delta'}\right\}\cdot\max\left\{\log\log Z^2, 1\right\}\right)\right),$$

where Z is the maximal norm of particles appeared in Alg 2.

Proof In this lemma, we follow the same proof roadmap as that shown in Lemma 23. According to Eq 46, we have

$$\begin{aligned}&\prod_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}} \mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right]\\ \ge& 1-\delta\cdot\frac{4(d+M)}{SC_\eta\epsilon}\left(\log\frac{Ld+M}{\epsilon}\right)^2\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon}, C_{u,2}\log\frac{Ld+M}{\epsilon}+\frac{2}{S}\log\log\frac{1}{\delta}+C_{u,3}\right)\end{aligned}$$

where the parameter δ satisfies Lemma 21 under certain conditions. It means we can control the recursive error with a high probability, i.e.,

$$\prod_{\substack{k\in\mathbb{N}_{0,K-1}\\ r\in\mathbb{N}_{0,R-1}}} \mathbb{P}\left[\left\|\nabla\log p_{k,S-r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{x}^{\leftarrow}_{k,r\eta})\right\|^2 \le 10\epsilon\right] \ge 1-\delta'. \tag{51}$$

when δ satisfies

$$\underbrace{\frac{4(d+M)}{SC_\eta\epsilon}\left(\log\frac{Ld+M}{\epsilon}\right)^2\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon}, C_{u,2}\log\frac{Ld+M}{\epsilon}+C_{u,3}\right)}_{\text{defined as } C_B}\cdot\delta\mathrm{pow}\left(\frac{Ld+M}{\epsilon}, \frac{2}{S}\log\log\frac{1}{\delta}\right) \le \delta'.$$

We can reformulate the above inequality as follows.

$$\begin{aligned}&C_B\delta(-\log\delta)^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}} \le \delta' \quad\Leftrightarrow\quad (-\log\delta)^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}} \le \frac{\delta'}{C_B\delta}\\ \Leftrightarrow\quad& \frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log\log\frac{1}{\delta} \le \log\frac{\delta'}{C_B\delta}.\end{aligned} \tag{52}$$

By requiring $\delta = \delta'/C_B\cdot a^{-2/S\cdot\log((Ld+M)/\epsilon)}$, the last inequality of the above can be written as

$$\mathrm{LHS} = \frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log\left[\log\frac{C_B}{\delta'}+\frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log a\right] \le \frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log a = \mathrm{RHS},$$

when the choice of a satisfies

$$a \ge \max\left\{\frac{2C_B}{\delta'}, \left(\frac{Ld+M}{\epsilon}\right)^{2/S}, 1\right\}. \tag{53}$$

Since we have

$$\log\frac{C_B}{\delta'} + \frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log a \le \log\frac{a}{2} + (\log a)^2 \le \frac{2a}{5} + \frac{3a}{5} = a \quad \text{when} \quad a \ge 1,$$

where the first inequality follows from the monotonicity of function $\log(\cdot)$. Then, it has

$$\log\left[\log\frac{C_B}{\delta'} + \frac{2}{S}\log\frac{Ld+M}{\epsilon}\cdot\log a\right] \le \log a$$

and Eq 52 establishes.

To achieve the accurate score estimation with a high probability shown in Eq 51, the total gradient complexity will be

$$\frac{T}{\eta}\cdot 960^{2.5k(k-1)}\cdot u(10\epsilon)^k \le C_B\cdot a^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}}$$

shown in Eq 49. Plugging the choice of a (Eq 53) into the above inequality, we have

$$\begin{aligned}
C_B\cdot a^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}} &\le C_B\cdot\max\left\{\mathrm{pow}\left(\frac{2C_B}{\delta'}, \frac{2}{S}\log\frac{Ld+M}{\epsilon}\right), \mathrm{pow}\left(\frac{Ld+M}{\epsilon}, \frac{4}{S^2}\log\frac{Ld+M}{\epsilon}\right)\right\}\\
&\le \max\left\{\underbrace{\mathrm{pow}\left(\frac{2C_B}{\delta'}, \frac{4}{S}\log\frac{Ld+M}{\epsilon}\right)}_{\mathrm{Term\ Comp.1}}, \underbrace{C_B\cdot\mathrm{pow}\left(\frac{Ld+M}{\epsilon}, \frac{4}{S^2}\log\frac{Ld+M}{\epsilon}\right)}_{\mathrm{Term\ Comp.2}}\right\}
\end{aligned}$$

It can be easily noted that Term $\mathrm{Comp.2}$ will be dominated by Term $\mathrm{Comp.1}$. Then, we provide the upper bound of $\mathrm{Comp.1}$ as

$$\begin{aligned}
\log(\mathrm{Comp.1}) =& \frac{4}{S}\log\frac{Ld+M}{\epsilon}\cdot\left(\log 2C_B + \log(1/\delta')\right)\\
=& \frac{4}{S}\log\frac{Ld+M}{\epsilon}\cdot\left(\log\frac{8}{SC_\eta} + \log\frac{d+M}{\epsilon} + 2\log\log\frac{Ld+M}{\epsilon}\right.\\
&\left. + \log\frac{Ld+M}{\epsilon}\cdot\left(C_{u,2}\log\frac{Ld+M}{\epsilon} + C_{u,3}\right) + \log(1/\delta')\right)\\
=& \mathcal{O}\left(L^3\cdot\max\left\{\left(\log\frac{Ld+M}{\epsilon}\right)^3, \log\frac{Ld+M}{\epsilon}\cdot\log\frac{1}{\delta'}\right\}\right),
\end{aligned}$$

which utilizes similar techniques shown in Lemma 23 and means

$$C_B\cdot a^{\frac{2}{S}\log\frac{Ld+M}{\epsilon}} \le \exp\left(\mathcal{O}\left(L^3\cdot\max\left\{\left(\log\frac{Ld+M}{\epsilon}\right)^3, \log\frac{Ld+M}{\epsilon}\cdot\log\frac{1}{\delta'}\right\}\right)\right).$$

Hence, the proof is completed. ■

Appendix F. Auxiliary Lemmas

F.1. The chain rule of KL divergence

Lemma 25 (Lemma 6 in Chen et al. (2023a)) *Consider the following two Itô processes,*

$$\begin{aligned}\mathrm{d}\mathbf{x}_t =& \boldsymbol{f}_1(\mathbf{x}_t, t)\mathrm{d}t + g(t)\mathrm{d}B_t, \quad \mathbf{x}_0 = \boldsymbol{a},\\ \mathrm{d}\mathbf{y}_t =& \boldsymbol{f}_2(\mathbf{y}_t, t)\mathrm{d}t + g(t)\mathrm{d}B_t, \quad \mathbf{y}_0 = \boldsymbol{a},\end{aligned}$$

where $\boldsymbol{f}_1, \boldsymbol{f}_2 \colon \mathbb{R}^d \to \mathbb{R}$ and $g\colon \mathbb{R} \to \mathbb{R}$ are continuous functions and may depend on $\boldsymbol{a}$. We assume the uniqueness and regularity conditions:

- *The two SDEs have unique solutions.*
- *$\mathbf{x}_t, \mathbf{y}_t$ admit densities $p_t, q_t \in C^2(\mathbb{R}^d)$ for $t > 0$.*

Define the relative Fisher information between p_t and q_t by

$$\mathrm{FI}\left(p_t \| q_t\right) := \int p_t(\boldsymbol{x}) \left\| \nabla \log \frac{p_t(\boldsymbol{x})}{q_t(\boldsymbol{x})} \right\|^2 \mathrm{d}\boldsymbol{x}.$$

Then for any $t > 0$, the evolution of $\mathrm{KL}\left(p_t \| q_t\right)$ is given by

$$\frac{\partial}{\partial t}\mathrm{KL}\left(p_t \| q_t\right) = -\frac{g^2(t)}{2}\mathrm{FI}\left(p_t \| q_t\right) + \mathbb{E}\left[\left\langle \boldsymbol{f}_1(\mathbf{x}_t, t) - \boldsymbol{f}_2(\mathbf{x}_t, t), \nabla \log \frac{p(\mathbf{x}_t)}{q(\mathbf{x}_t)} \right\rangle\right].$$

Lemma 25 is applied to show the KL convergence between the underlying distribution of the SDEs that have the same diffusion term and a bounded difference between their drift terms.

Lemma 26 (Lemma 7 in Chen et al. (2023a)) *Under the notation in Section A, for $k \in \mathbb{N}_{0,K-1}$ and $r \in \mathbb{N}_{0,R-1}$, consider the reverse SDE starting from $\mathbf{x}^{\leftarrow}_{k,r\eta} = \boldsymbol{a}$*

$$\mathrm{d}\hat{\mathbf{x}}_{k,t} = \left[\hat{\mathbf{x}}_{k,t} + 2\nabla \log p_{k,S-t}(\hat{\mathbf{x}}_{k,t})\right] \mathrm{d}t + \sqrt{2}\mathrm{d}B_t, \quad \mathbf{x}^{\leftarrow}_{k,r\eta} = \boldsymbol{a} \tag{54}$$

and its discrete approximation

$$\mathrm{d}\mathbf{x}^{\leftarrow}_{k,t} = \left[\mathbf{x}^{\leftarrow}_{k,t} + 2\mathbf{v}^{\leftarrow}_{k,r\eta}\left(\mathbf{x}^{\leftarrow}_{k,r\eta}\right)\right] \mathrm{d}t + \sqrt{2}\mathrm{d}B_t, \quad \mathbf{x}^{\leftarrow}_{k,r\eta} = \boldsymbol{a} \tag{55}$$

for time $t \in [k\eta, (k+1)\eta]$. Let $\hat{p}_{k,t|r\eta}$ be the density of $\hat{\mathbf{x}}_{k,t}$ given $\hat{\mathbf{x}}_{k,r\eta}$ and $p^{\leftarrow}_{k,t|r\eta}$ be the density of $\mathbf{x}^{\leftarrow}_{k,t}$ given $\mathbf{x}^{\leftarrow}_{k,r\eta}$. Then, we have

- *For any $\boldsymbol{a} \in \mathbb{R}^d$, the two processes satisfy the uniqueness and regularity condition stated in Lemma 25, which means SDE 54 and SDE 55 have unique solutions and $\hat{p}_{k,t|r\eta}(\cdot|\boldsymbol{a}), p^{\leftarrow}_{k,t|r\eta}(\cdot|\boldsymbol{a}) \in C^2(\mathbb{R}^d)$ for $t \in (r\eta, (r+1)\eta]$.*
- *For a.e., $\boldsymbol{a} \in \mathbb{R}^d$, we have*

$$\lim_{t \to r\eta_+} \mathrm{KL}\left(\hat{p}_{k,t|r\eta}(\cdot|\boldsymbol{a}) \| \tilde{p}_{k,t|r\eta}(\cdot|\boldsymbol{a})\right) = 0.$$

Lemma 27 (Variant of Proposition 8 in Chen et al. (2023a)) *Under the notation in Section A and Algorithm 2, we have*

$$\begin{aligned}\mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right) \leq & \mathrm{KL}\left(\hat{p}_{K-1,0}\|p^{\leftarrow}_{K-1,0}\right)\\ & + \sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{(\hat{\mathbf{x}}_{k,t+r\eta},\hat{\mathbf{x}}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t.\end{aligned}$$

Proof Under the notation in Section A, for $k \in \mathbb{N}_{0,K-1}$ and $r \in \mathbb{N}_{0,R-1}$, let $\hat{p}_{k,t|r\eta}$ be the density of $\hat{\mathbf{x}}_{k,t}$ given $\hat{\mathbf{x}}_{k,r\eta}$ and $p^{\leftarrow}_{k,t|r\eta}$ be the density of $\mathbf{x}^{\leftarrow}_{k,t}$ given $\mathbf{x}^{\leftarrow}_{k,r\eta}$. According to Lemma 26 and Lemma 25, for any $\mathbf{x}^{\leftarrow}_{k,r\eta} = \boldsymbol{a}$, we have

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{KL}\left(\hat{p}_{k,t|r\eta}(\cdot|\boldsymbol{a})\|p^{\leftarrow}_{k,t|r\eta}(\cdot|\boldsymbol{a})\right)\\ &= -\mathrm{FI}\left(\hat{p}_{k,t|r\eta}(\cdot|\boldsymbol{a})\|p^{\leftarrow}_{k,t|r\eta}(\cdot|\boldsymbol{a})\right) + 2\mathbb{E}_{\mathbf{x}\sim\hat{p}_{k,t|r\eta}(\cdot|\boldsymbol{a})}\left[\left\langle \nabla\log p_{k,S-t}(\mathbf{x}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{a}), \nabla\log\frac{\hat{p}_{k,t|r\eta}(\mathbf{x}|\boldsymbol{a})}{p^{\leftarrow}_{k,t|r\eta}(\mathbf{x}|\boldsymbol{a})}\right\rangle\right]\\ &\leq \mathbb{E}_{\mathbf{x}\sim\hat{p}_{k,t|r\eta}(\cdot|\boldsymbol{a})}\left[\left\|\nabla\log p_{k,S-t}(\mathbf{x}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{a})\right\|^2\right].\end{aligned}$$

Due to Lemma 26, for any $\boldsymbol{a}\in\mathbb{R}^d$, we have

$$\lim_{t\to r\eta_+}\mathrm{KL}\left(\hat{p}_{k,t|r\eta}(\cdot|\boldsymbol{a})\|p^{\leftarrow}_{k,t|r\eta}(\cdot|\boldsymbol{a})\right) = 0,$$

which implies

$$\mathrm{KL}\left(\hat{p}_{k,t|r\eta}(\cdot|\boldsymbol{a})\|p^{\leftarrow}_{k,t|r\eta}(\cdot|\boldsymbol{a})\right) = \int_{r\eta}^t \mathbb{E}_{\mathbf{x}\sim\hat{p}_{\tau|r\eta}(\cdot|\boldsymbol{a})}\left[\left\|\nabla\log p_{k,S-\tau}(\mathbf{x}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\boldsymbol{a})\right\|^2\right]\mathrm{d}\tau.$$

Integrating both sides of the equation, we have

$$\mathbb{E}_{\hat{\mathbf{x}}_{k,r\eta}\sim\hat{p}_{k,r\eta}}\left[\mathrm{KL}\left(\hat{p}_{k,t|r\eta}(\cdot|\hat{\mathbf{x}}_{k,r\eta})\|p^{\leftarrow}_{k,t|r\eta}(\cdot|\hat{\mathbf{x}}_{k,r\eta})\right)\right] \leq \int_{r\eta}^t \mathbb{E}\left[\left\|\nabla\log p_{k,S-\tau}(\hat{\mathbf{x}}_{k,\tau}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}\tau.$$

According to the chain rule of KL divergence Chen et al. (2023a), we have

$$\begin{aligned}&\mathrm{KL}\left(\hat{p}_{k,(r+1)\eta}\|p^{\leftarrow}_{k,(r+1)\eta}\right)\\ &\leq \mathrm{KL}\left(\hat{p}_{k,r\eta}\|p^{\leftarrow}_{k,r\eta}\right) + \mathbb{E}_{\hat{\mathbf{x}}_{k,r\eta}\sim\hat{p}_{k,r\eta}}\left[\mathrm{KL}\left(\hat{p}_{k,(r+1)\eta|r\eta}(\cdot|\hat{\mathbf{x}}_{k,r\eta})\|p^{\leftarrow}_{k,(r+1)\eta|r\eta}(\cdot|\hat{\mathbf{x}}_{k,r\eta})\right)\right]\\ &\leq \mathrm{KL}\left(\hat{p}_{k,r\eta}\|p^{\leftarrow}_{k,r\eta}\right) + \int_0^\eta \mathbb{E}_{(\hat{\mathbf{x}}_{k,t+r\eta},\hat{\mathbf{x}}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t.\end{aligned}$$

Summing over $r\in\{0,1,\ldots,R-1\}$, it has

$$\mathrm{KL}\left(\hat{p}_{k,R\eta}\|p^{\leftarrow}_{k,R\eta}\right) \leq \mathrm{KL}\left(\hat{p}_{k,0}\|p^{\leftarrow}_{k,0}\right) + \sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{(\hat{\mathbf{x}}_{k,t+r\eta},\hat{\mathbf{x}}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t.$$

Similarly, by considering all segments, we have

$$\begin{aligned}\mathrm{KL}\left(\hat{p}_{0,S}\|p^{\leftarrow}_{0,S}\right) \leq & \mathrm{KL}\left(\hat{p}_{K-1,0}\|p^{\leftarrow}_{K-1,0}\right) \\ & + \sum_{k=0}^{K-1}\sum_{r=0}^{R-1}\int_0^\eta \mathbb{E}_{(\hat{\mathbf{x}}_{k,t+r\eta},\hat{\mathbf{x}}_{k,r\eta})}\left[\left\|\nabla\log p_{k,S-(t+r\eta)}(\hat{\mathbf{x}}_{k,t+r\eta}) - \mathbf{v}^{\leftarrow}_{k,r\eta}(\hat{\mathbf{x}}_{k,r\eta})\right\|^2\right]\mathrm{d}t.\end{aligned}$$

■

Lemma 28 (Variant of Lemma 10 in Cheng and Bartlett (2018)) *Suppose $-\log p_*$ is m-strongly convex function, for any distribution with density function p, we have*

$$\mathrm{KL}\left(p\|p_*\right) \leq \frac{1}{2m}\int p(\boldsymbol{x})\left\|\nabla\log\frac{p(\boldsymbol{x})}{p_*(\boldsymbol{x})}\right\|^2\mathrm{d}\boldsymbol{x}.$$

By choosing $p(\boldsymbol{x}) = g^2(\boldsymbol{x})p_*(\boldsymbol{x})/\mathbb{E}_{p_*}\left[g^2(\mathbf{x})\right]$ for the test function $g\colon \mathbb{R}^d \to \mathbb{R}$ and $\mathbb{E}_{p_*}\left[g^2(\mathbf{x})\right] < \infty$, we have

$$\mathbb{E}_{p_*}\left[g^2\log g^2\right] - \mathbb{E}_{p_*}\left[g^2\right]\log\mathbb{E}_{p_*}\left[g^2\right] \leq \frac{2}{m}\mathbb{E}_{p_*}\left[\|\nabla g\|^2\right],$$

which implies p_* satisfies m-log-Sobolev inequality.

Lemma 29 *(Corollary 3.1 in Chafaï (2004)) If $\nu, \tilde{\nu}$ satisfy LSI with constants $\alpha, \tilde{\alpha} > 0$, respectively, then $\nu * \tilde{\nu}$ satisfies LSI with constant $(\frac{1}{\alpha} + \frac{1}{\tilde{\alpha}})^{-1}$.*

Lemma 30 (Lemma 16 in Vempala and Wibisono (2019)) *Suppose a probability distribution p satisfies LSI with constant $\mu > 0$. Let a map $T\colon \mathbb{R}^d \to \mathbb{R}^d$, be a differentiable L-Lipschitz map. Then, $\tilde{p} = T_{\#}p$ satisfies LSI with constant μ/L^2*

Lemma 31 (Lemma 17 in Vempala and Wibisono (2019)) *Suppose a probability distribution p satisfies LSI with a constant μ. For any $t > 0$, the probability distribution $\tilde{p}_t = p * \mathcal{N}(\mathbf{0}, t\boldsymbol{I})$ satisfies LSI with the constant $(\mu^{-1} + t)^{-1}$.*

Lemma 32 (Theorem 8 in Vempala and Wibisono (2019)) *Suppose $p \propto \exp(-f)$ is μ strongly log concave and L-smooth. If we conduct ULA with the step size satisfying $\eta \leq 1/L$, then, for any iteration number, the underlying distribution of the output particle satisfies LSI with a constant larger than $\mu/2$.*

Proof Suppose we run ULA from $\mathbf{x}_0 \sim p_0$ to $\mathbf{x}_k \sim p_k$ where the LSI constant of p_k is denoted as μ_k. When the step size of ULA satisfies $0 < \eta \leq 1/L$, due to the strong convexity of p, the map $\boldsymbol{x} \mapsto \boldsymbol{x} - \eta\nabla f(\boldsymbol{x})$ is $(1-\eta\mu)$-Lipschitz. Combining the LSI property of p_k and Lemma 30, the distribution of $\mathbf{x}_k - \eta\nabla f(\mathbf{x}_k)$ satisfies LSI with a constant $\mu_k/(1-\eta\mu)^2$. Then, by Lemma 31, $\mathbf{x}_{k+1} = \mathbf{x}_k - \eta\nabla f(\mathbf{x}_k) + \sqrt{2\eta}\mathcal{N}(0, \boldsymbol{I}) \sim p_{k+1}$ satisfies μ_{k+1}-LSI with

$$\frac{1}{\mu_{k+1}} \leq \frac{(1-\eta\mu)^2}{\mu_k} + 2\eta.$$

For any k, if there is $\mu_k \geq \mu/2$, with the setting of η, i.e., $\eta \leq 1/L \leq 1/\mu$, then

$$\frac{1}{\mu_{k+1}} \leq \frac{(1-\eta\mu)^2}{\mu/2} + 2\eta = \frac{2}{\mu} - 2\eta(1-\eta\mu) \leq \frac{2}{\mu}.$$

It means for any $k' > k$, we have $\mu_{k'} \geq \mu/2$. By requiring the LSI constant of initial distribution, i.e., p_0 to satisfy $\mu_0 \geq \mu/2$, we have the underlying distribution of the output particle satisfies LSI with a constant larger than $\mu/2$. Hence, the proof is completed. ■

Lemma 33 *If ν satisfies a log-Sobolev inequality with log-Sobolev constant μ then every 1-Lipschitz function f is integrable with respect to ν and satisfies the concentration inequality*

$$\nu\left\{f \geq \mathbb{E}_\nu[f] + t\right\} \leq \exp\left(-\frac{\mu t^2}{2}\right).$$

Proof According to Lemma 34, it suffices to prove that for any 1-Lipschitz function f with expectation $\mathbb{E}_\nu[f] = 0$,

$$\mathbb{E}\left[e^{\lambda f}\right] \leq e^{\lambda^2/(2\mu)}.$$

To prove this, it suffices, by a routine truncation and smoothing argument, to prove it for bounded, smooth, compactly supported functions f such that $\|\nabla f\| \leq 1$. Assume that f is such a function. Then for every $\lambda \geq 0$ the log-Sobolev inequality implies

$$\mathrm{Ent}_\nu\left(e^{\lambda f}\right) \leq \frac{2}{\mu}\mathbb{E}_\nu\left[\left\|\nabla e^{\lambda f/2}\right\|^2\right],$$

which is written as

$$\mathbb{E}_\nu\left[\lambda f e^{\lambda f}\right] - \mathbb{E}_\nu\left[e^{\lambda f}\right]\log\mathbb{E}\left[e^{\lambda f}\right] \leq \frac{\lambda^2}{2\mu}\mathbb{E}_\nu\left[\|\nabla f\|^2 e^{\lambda f}\right].$$

With the notation $\varphi(\lambda) = \mathbb{E}\left[e^{\lambda f}\right]$ and $\psi(\lambda) = \log\varphi(\lambda)$, the above inequality can be reformulated as

$$\begin{aligned}\lambda\varphi'(\lambda) \leq & \varphi(\lambda)\log\varphi(\lambda) + \frac{\lambda^2}{2\mu}\mathbb{E}_\nu\left[\|\nabla f\|^2 e^{\lambda f}\right] \\ \leq & \varphi(\lambda)\log\varphi(\lambda) + \frac{\lambda^2}{2\mu}\varphi(\lambda),\end{aligned}$$

where the last step follows from the fact $\|\nabla f\| \leq 1$. Dividing both sides by $\lambda^2\varphi(\lambda)$ gives

$$\left(\frac{\log(\varphi(\lambda))}{\lambda}\right)' \leq \frac{1}{2\mu}.$$

Denoting that the limiting value $\frac{\log(\varphi(\lambda))}{\lambda}\mid_{\lambda=0} = \lim_{\lambda\to 0^+}\frac{\log(\varphi(\lambda))}{\lambda} = \mathbb{E}_\nu[f] = 0$, we have

$$\frac{\log(\varphi(\lambda))}{\lambda} = \int_0^\lambda \left(\frac{\log(\varphi(t))}{t}\right)' dt \leq \frac{\lambda}{2\mu},$$

which implies that

$$\psi(\lambda) \leq \frac{\lambda^2}{2\mu} \Longrightarrow \varphi(\lambda) \leq \exp\left(\frac{\lambda^2}{2\mu}\right)$$

Then the proof can be completed by a trivial argument of Lemma 34. ■

Lemma 34 *Let* $\mathbf{x}$ *be a real random variable. If there exist constants* $C, A < \infty$ *such that* $\mathbb{E}\left[e^{\lambda \mathbf{x}}\right] \leq Ce^{A\lambda^2}$ *for all* $\lambda > 0$ *then*

$$\mathbb{P}\left\{\mathbf{x} \geq t\right\} \leq C \exp\left(-\frac{t^2}{4A}\right)$$

Proof According to the non-decreasing property of exponential function $e^{\lambda \boldsymbol{x}}$, we have

$$\mathbb{P}\left\{\mathbf{x} \geq t\right\} = \mathbb{P}\left\{e^{\lambda \mathbf{x}} \geq e^{\lambda t}\right\} \leq \frac{\mathbb{E}\left[e^{\lambda \mathbf{x}}\right]}{e^{\lambda t}} \leq C \exp\left(A\lambda^2 - \lambda t\right),$$

The first inequality follows from Markov inequality, and the second follows from the given conditions. By minimizing the RHS, i.e., choosing $\lambda = t/(2A)$, the proof is completed. ■

Lemma 35 *Suppose* q *is a distribution which satisfies LSI with constant* μ*, then its variance satisfies*

$$\int q(\boldsymbol{x}) \left\|\boldsymbol{x} - \mathbb{E}_{\tilde{q}}\left[\mathbf{x}\right]\right\|^2 \mathrm{d}\boldsymbol{x} \leq \frac{d}{\mu}.$$

Proof It is known that LSI implies Poincaré inequality with the same constant, i.e., μ, which means if for all smooth function $g \colon \mathbb{R}^d \to \mathbb{R}$,

$$\mathrm{var}_q\left(g(\mathbf{x})\right) \leq \frac{1}{\mu}\mathbb{E}_q\left[\left\|\nabla g(\mathbf{x})\right\|^2\right].$$

In this condition, we suppose $\boldsymbol{b} = \mathbb{E}_q[\mathbf{x}]$, and have the following equation

$$\begin{aligned}
&\int q(\boldsymbol{x}) \left\|\boldsymbol{x} - \mathbb{E}_q\left[\mathbf{x}\right]\right\|^2 \mathrm{d}\boldsymbol{x} = \int q(\boldsymbol{x}) \left\|\boldsymbol{x} - \boldsymbol{b}\right\|^2 \mathrm{d}\boldsymbol{x} \\
= &\int \sum_{i=1}^d q(\boldsymbol{x}) \left(\boldsymbol{x}_i - \boldsymbol{b}_i\right)^2 \mathrm{d}\boldsymbol{x} = \sum_{i=1}^d \int q(\boldsymbol{x}) \left(\langle \boldsymbol{x}, \boldsymbol{e}_i\rangle - \langle \boldsymbol{b}, \boldsymbol{e}_i\rangle\right)^2 \mathrm{d}\boldsymbol{x} \\
= &\sum_{i=1}^d \int q(\boldsymbol{x}) \left(\langle \boldsymbol{x}, \boldsymbol{e}_i\rangle - \mathbb{E}_q\left[\langle \mathbf{x}, \boldsymbol{e}_i\rangle\right]\right)^2 \mathrm{d}\boldsymbol{x} = \sum_{i=1}^d \mathrm{var}_q\left(g_i(\mathbf{x})\right)
\end{aligned}$$

where $g_i(\boldsymbol{x})$ is defined as $g_i(\boldsymbol{x}) \coloneqq \langle \boldsymbol{x}, \boldsymbol{e}_i\rangle$ and $\boldsymbol{e}_i$ is a one-hot vector (the i-th element of $\boldsymbol{e}_i$ is 1 others are 0). Combining this equation and Poincaré inequality, for each i, we have

$$\mathrm{var}_q\left(g_i(\mathbf{x})\right) \leq \frac{1}{\mu}\mathbb{E}_q\left[\left\|\boldsymbol{e}_i\right\|^2\right] = \frac{1}{\mu}.$$

Hence, the proof is completed. ■

Lemma 36 *(Lemma 12 in Vempala and Wibisono (2019)) Suppose* $p \propto \exp(-f)$ *satisfies Talagrand's inequality with constant* μ *and is* L*-smooth. For any* p'*,*

$$\mathbb{E}_{p'}\left[\left\|\nabla f(\mathbf{x})\right\|^2\right] \leq \frac{4L^2}{\mu}\mathrm{KL}\left(p' \| p\right) + 2Ld.$$