

IMPROVED CONVERGENCE RATE FOR DIFFUSION PROBABILISTIC MODELS

Anonymous authors

Paper under double-blind review

ABSTRACT

Score-based diffusion models have achieved remarkable empirical performance in the field of machine learning and artificial intelligence for their ability to generate high-quality new data instances from complex distributions. Improving our understanding of diffusion models, including mainly convergence analysis for such models, has attracted a lot of interests. Despite a lot of theoretical attempts, there still exists significant gap between theory and practice. Towards to close this gap, we establish an iteration complexity at the order of $d^{1/3}\varepsilon^{-2/3}$, which is better than $d^{5/12}\varepsilon^{-1}$, the best known complexity achieved before our work. This convergence analysis is based on a randomized midpoint method, which is first proposed for log-concave sampling (Shen & Lee, 2019), and then extended to diffusion models by Gupta et al. (2024). Our theory accommodates ε -accurate score estimates, and does not require log-concavity on the target distribution. Moreover, the algorithm can also be parallelized to run in only $O(\log^2(d/\varepsilon))$ parallel rounds in a similar way to prior works.

1 INTRODUCTION

Score-based diffusion models are a class of generative models that have gained prominence in the field of machine learning and artificial intelligence for their ability to generate high-quality new data instances from complex distributions (Dhariwal & Nichol, 2021; Ho et al., 2020; Sohl-Dickstein et al., 2015; Song & Ermon, 2019; Song et al., 2021). These models operate by gradually transforming noise into samples from the target distribution through a denoising process guided by pretrained neural networks that approximate the score functions. In practice, score-based diffusion models have demonstrated remarkable performance in generating realistic and diverse content across various domains (Croitoru et al., 2023; Ramesh et al., 2022; Rombach et al., 2022; Saharia et al., 2022), achieving state-of-the-art performance in generative AI.

The development of score-based diffusion models is closely related to the theory of stochastic processes. At a high level, we consider a forward process:

$$X_0 \xrightarrow{\text{add noise}} X_1 \xrightarrow{\text{add noise}} \dots \xrightarrow{\text{add noise}} X_T,$$

which draws a sample from the target data distribution (i.e., $X_0 \sim p_{\text{data}}$), and then progressively diffuses it to Gaussian noise over time. The key step of the diffusion model is to construct a reverse process:

$$Y_T \xrightarrow{\text{denoise}} Y_{T-1} \xrightarrow{\text{denoise}} \dots \xrightarrow{\text{denoise}} Y_0,$$

satisfying $Y_t \stackrel{d}{\approx} X_t$ for all t , which starts with pure Gaussian noise (i.e., $Y_T \sim \mathcal{N}(0, I_d)$) and gradually converts it back to a new sample Y_0 sharing a similar distribution to X_0 . Evidently, the most crucial step of the diffusion model lies in effective design of the reverse process. To accomplish this goal, Y_{t-1} in each step is typically obtained from Y_t with the aid of score functions ($s_t^* = \nabla \log p_{X_t}$), which are pre-trained by means of score matching techniques (e.g., Hyvärinen & Dayan (2005); Ho et al. (2020); Hyvärinen (2007); Vincent (2011); Song & Ermon (2019); Pang et al. (2020)).

Due to the impressive empirical success, in the past few years, there have been a lot of works exploring the convergence of diffusion models (De Bortoli, 2022; Gao et al., 2023; Lee et al., 2022;

2023; Chen et al., 2022; Benton et al., 2023; Chen et al., 2023; Li et al., 2023; 2024b; Gupta et al., 2024; Chen et al., 2024b; Li et al., 2024a; Li & Yan, 2024). They typically treat the score matching stage as a blackbox and study how the sampling steps T and the score estimation error will affect the sampling accuracy. Given the observation that there still exists a huge gap between prior theories and practice, this paper is devoted to improving the convergence theory for diffusion models.

1.1 MOTIVATION

Following the most existing works, let’s focus on the total variation distance between distributions of the target data and generated samples. Let d be the dimension, and ε denote the accuracy which means the total variation is smaller than ε . For the general target distribution, Benton et al. (2023) provides first linear d -dependency rate with an iteration complexity d/ε^2 . Later on, Li et al. (2024b) achieves an improved complexity scaling as d/ε , while with a burn-in cost d^2 .

However, such kind of result is still far away from practical observations. For example, for two typical image datasets, CIFAR-10 with $d = 32 \times 32 \times 3 = 3072$ and ImageNet 256×256 with $d = 256 \times 256 \times 3 = 196608$, it is sufficient to use about 50 steps to generate good samples (Song et al., 2021; Nichol & Dhariwal, 2021), which is much smaller than the theoretical requirement. To close this gap, people try to derive faster convergence rate through exploiting extra data distribution properties, such as low-dimensional structure (Li & Yan, 2024) and smoothness of score functions (Gupta et al., 2024; Chen et al., 2024b). Following this line of work, the scope of this paper lies in establishing some convergence theory for diffusion models towards aligning more closely with practical requirements.

1.2 OUR CONTRIBUTIONS

Focusing on the diffusion models with L -smooth score functions, this paper develops an improved iteration complexity as following (up to some logarithmic factors):

$$Ld^{1/3}\varepsilon^{-2/3},$$

which is inspired by the randomized mid-point design (Shen & Lee, 2019; Gupta et al., 2024). In what follows, let us make a brief comparison between our results and the state-of-the-art results about the convergence rate of score-based generative models.

- *Comparison under smoothness condition.* Similarly, Chen et al. (2024b) also studied the convergence theory by assuming smooth score functions. Recently, the iteration complexity is improved by Gupta et al. (2024); Chen et al. (2024b) in this setting, which, to ensure ε -accuracy, scales as $\tilde{O}(L^{5/3}d^{5/12}\varepsilon^{-1})$. This means that our convergence rate improves prior works by a factor of $L^{2/3}d^{1/12}\varepsilon^{-1/3}$.
- *Comparison under general condition.* Without the smoothness condition on score functions, Benton et al. (2023) proved an iteration complexity at the order of $d\varepsilon^{-2}$, which first exhibits linear dependency in the data dimension d . This bound is improved to $\tilde{O}(d/\varepsilon)$ by Li et al. (2024b) when the number of steps is larger than $\tilde{O}(d^2)$. In comparison, to achieve ε -accuracy, our theory improves these works provided that the Lipschitz conditions of score functions satisfy

$$L < d^{2/3}\varepsilon^{-4/3}, \quad \text{for } \varepsilon > d^{-1/2} \quad \text{or} \quad L < d^{2/3}\varepsilon^{-1/3}, \quad \text{for } \varepsilon < d^{-1/2}.$$

Hopefully, such relations can be satisfied in most real cases, for example, considering ImageNet 256×256 , this requirement becomes $L < 3381$ for $\varepsilon \approx 1$ and $L < 72845$ for $\varepsilon \approx 0.1$.

2 PRELIMINARY

In this section, we introduce some basics and notations of score-based generative models. The diffusion generative model typically encompasses two processes: a forward process and a reverse process, as described below.

Forward process. Starting from X_0 drawn from some target distribution p_{data} , the forward process evolves as follows:

$$X_t = \sqrt{\alpha_t}X_{t-1} + \sqrt{1 - \alpha_t}W_t, \quad 1 \leq t \leq T, \quad (1)$$

where $0 < \alpha_t < 1$, and $\{W_t\}_{1 \leq t \leq T}$ is a sequence of independent noise vectors drawn from $W_t \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, I_d)$. In addition, let's define

$$\bar{\alpha}_t := \prod_{k=1}^t \alpha_k, \quad 1 \leq t \leq T, \quad (2)$$

which will be helpful in our following analysis. The diffusion models draw a lot of motivations from the stochastic differential equations. Hence, let's also introduce the continuous-time limit of the forward diffusion process, which can be modeled as

$$dX_\tau = -\frac{1}{2(1-\tau)}X_\tau d\tau + \frac{1}{\sqrt{1-\tau}}dB_\tau, \quad \text{for } 0 \leq \tau < 1, \quad (3)$$

where B_τ denotes some Brownian motion.

Reverse process. The core of diffusion models lies in constructing a reverse-time process with nearly identical marginals as the forward process, namely, $Y_\tau \stackrel{d}{\approx} X_\tau$. Fortunately, it is shown that there exists some probability flow ODE

$$dY_\tau = -\frac{1}{2(1-\tau)}(Y_\tau + \nabla \log p_{X_\tau}(Y))d\tau, \quad (4)$$

which can achieve our goal, such that if we start from $Y_{\tau_0} \sim p_{X_{\tau_0}}$ for any $0 \leq \tau_0 < 1$, it can be ensured that $Y_\tau \stackrel{d}{\approx} X_\tau$ for all $0 \leq \tau < 1$. Then the design of reverse process is equivalent to discretize the above ODE process (4), as well as estimate $\nabla \log p_{X_\tau}$, which is also called score function.

Score functions. The score functions are crucial for score-based generative modeling, and the definition of score function is as follows.

Definition 1. The score function, denoted by $s_t^* : \mathbb{R}^d \rightarrow \mathbb{R}^d (1 \leq t \leq T)$, is defined as

$$s_t^*(x) := \nabla \log p_{X_t}(x) = -\frac{1}{1-\bar{\alpha}_t} \int_{x_0} p_{X_0|X_t}(x_0|x)(x - \sqrt{1-\bar{\alpha}_t}x_0)dx_0, \quad 1 \leq t \leq T. \quad (5)$$

Following the same way as prior analysis, we assume access to faithful estimates of the score functions s_t^* across all intermediate steps t as following.

Assumption 1. We assume access to an estimate $s_t(\cdot)$ for each $s_t^*(\cdot)$ with the averaged ℓ_2 score estimation error as

$$\varepsilon_{\text{score}}^2 = \frac{1}{T} \sum_{t=1}^T \mathbb{E}_{x \sim q_t} [\|s_t(x) - s_t^*(x)\|_2^2] =: \frac{1}{T} \sum_{t=1}^T \varepsilon_t^2. \quad (6)$$

In addition, we mainly focus on the case with smooth score functions in this paper, which is stated below.

Assumption 2. Assume that $s_t^*(x)$ and $s_t(x)$ are Lipschitz for all t such that

$$\|s_t^*(x_1) - s_t^*(x_2)\|_2 \leq L\|x_1 - x_2\|_2; \quad (7a)$$

$$\|s_t(x_1) - s_t(x_2)\|_2 \leq L\|x_1 - x_2\|_2. \quad (7b)$$

Target data distribution. Following prior works, we also need the following assumption on the target data distribution p_{data} to establish our theory.

Assumption 3. We assume that the target distribution p_{data} has bounded second-order moment in the sense that

$$R := \mathbb{E}[\|X_0\|_2^2] < T^{c_R} \quad (8)$$

for arbitrarily large constant $c_R > 0$.

Here, this assumption requires the second-order moment of p_{data} to be exceedingly large (given that the exponent c_R can be arbitrarily large), which is a mild assumption.

3 MAIN RESULTS

In this section, we first introduce a new score-based sampler with randomized midpoints, which is modified from Gupta et al. (2024) for ease of analysis. Then, we prove a faster convergence rate for this sampler based on a new analysis framework, which might be useful for improving convergence guarantees for other variations of samplers. Finally, we also provide a parallel sampling strategy for our sampler following the similar idea from prior works (Gupta et al., 2024; Chen et al., 2024a).

3.1 ALGORITHM

This part is devoted to explaining the details of our score-based sampler with randomized midpoints. Before proceeding, let's first specify the choice of learning rates to be used in our sampler.

Randomized schedule. Similar to prior works, we adopt the following randomized learning rate schedule

$$\bar{\alpha}_t \sim \text{Unif}(\hat{\alpha}_t, \hat{\alpha}_{t-1}), \quad \text{for } t = 1, \dots, T+1, \quad (9a)$$

where Unif denotes the uniform distribution, and

$$\hat{\alpha}_{T+1} = \frac{1}{T^{c_0}}, \quad \text{and} \quad \hat{\alpha}_{t-1} = \hat{\alpha}_t + \frac{c_1 \hat{\alpha}_t (1 - \hat{\alpha}_t) \log T}{T} \quad (9b)$$

for some sufficiently large constants $c_0, c_1 > 0$ obeying c_1/c_0 sufficiently large.

Moreover, for ease of presentation, we let $K = c_2 L \log T$ for some constant $c_2 > 0$ such that $\frac{c_2}{c_1}$ sufficiently large, and $N = \frac{2T}{K}$. Then define for $n = 0, \dots, N$, and $k = 0, \dots, K-1$,

$$\hat{\tau}_{k,n} := 1 - \hat{\alpha}_{T - \frac{kN}{2} - n} \quad \text{and} \quad \tau_{k,n} := 1 - \bar{\alpha}_{T - \frac{kN}{2} - n + 1}, \quad (9c)$$

which satisfy the following lemma. The proof is postponed to Appendix B.1.

Lemma 1. *Our choice of learning schedules (9) satisfies*

$$1 - \tau_{0,0} \leq \hat{\alpha}_T \leq \frac{2}{T^{c_0}}, \quad \tau_{K,0} \leq 1 - \hat{\alpha}_1 \leq \frac{1}{T^{c_0}}, \quad \text{and} \quad \frac{\hat{\tau}_{k,n-1} - \hat{\tau}_{k,n}}{\hat{\tau}_{k,n-1}(1 - \hat{\tau}_{k,n-1})} = \frac{c_1 \log T}{T}. \quad (10)$$

Sampling procedure. With the learning schedule in hand, we are now ready to introduce the sampling procedure. The algorithm is actually a discretization of the probability ODE flow incorporated with some stochastic noise, which proceeds as follows. We start from $Y_0 \sim \mathcal{N}(0, I_d)$, and then for $k = 0, \dots, K-1$, we keep updating Y_k through the formula:

$$Y_{k+1} = \sqrt{\frac{1 - \tau_{k+1,0}}{1 - \tau_{k,N}}} Y_{k,N} + \sqrt{\frac{\tau_{k+1,0} - \tau_{k,N}}{1 - \tau_{k,N}}} Z_k, \quad (11a)$$

where $Z_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, I)$ and for $n = 1, \dots, N$, we compute

$$\begin{aligned} \frac{Y_{k,n}}{\sqrt{1 - \tau_{k,n}}} &= \frac{Y_k}{\sqrt{1 - \tau_{k,0}}} + \frac{s_{T - \frac{kN}{2} + 1}(Y_k)}{2(1 - \tau_{k,0})^{3/2}} (\tau_{k,0} - \hat{\tau}_{k,0}) + \sum_{i=1}^{n-1} \frac{s_{T - \frac{kN}{2} - i + 1}(Y_{k,i})}{2(1 - \tau_{k,i})^{3/2}} (\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i}) \\ &\quad + \frac{s_{T - \frac{kN}{2} - n + 2}(Y_{k,n-1})}{2(1 - \tau_{k,n-1})^{3/2}} (\hat{\tau}_{k,n-1} - \tau_{k,n}). \end{aligned} \quad (11b)$$

Here, we let $Y_{k,0} = Y_k$. Notice that for each step to calculate $Y_{k,n}$, only one additional score evaluation for $s_{T - \frac{kN}{2} - n + 2}(Y_{k,n-1})$ is needed. This implies that the total iteration complexity is $KN = 2T$.

3.2 CONVERGENCE ANALYSIS

We are now positioned to present the convergence guarantees — measured by the total variation distance between the forward and the reverse processes — for the proposed sampler (11). The proof is postponed to Section 4.

Theorem 1. *Suppose that Assumptions 1, 2, and 3 hold true. Then the sampling process (11) with the learning rate schedule (9) satisfies*

$$\mathrm{TV}(p_{\text{data}}, p_{Y_K}) \leq \frac{CL^{3/2}d^{1/2}\log^2 T}{T^{3/2}} + C\varepsilon_{\text{score}}\log^{1/2} T \quad (12)$$

for some constant $C > 0$ large enough.

We now take a moment to discuss the main implications of Theorem 1.

Iteration complexity. Let’s focus on the first term in (12), which corresponds to discretization error, and ignore the score estimation error. To ensure $\mathrm{TV}(p_{\text{data}}, p_{Y_K}) \leq \varepsilon$, it is sufficient to choose

$$T \gtrsim \frac{Ld^{1/3}\log^{4/3} T}{\varepsilon^{2/3}}.$$

As far as we know, the existing iteration complexity guarantees (with sub-linear dependency on d) are $\tilde{O}(L^{5/3}d^{5/12}\varepsilon^{-1})$ achieved in Gupta et al. (2024) and $\tilde{O}(L^2d^{1/2}\varepsilon^{-1})$ derived in Chen et al. (2024b). Our theory improves the prior results with at least $\tilde{O}(L^{2/3}d^{1/12}\varepsilon^{-1/3})$.

Dependency of score estimation error. Turning attention to the second term, the sampling accuracy scales as $\varepsilon_{\text{score}}\log^{1/2} T$, suggesting that our sampler is stable to imperfect score estimation. In comparison, the existing results (with sub-linear dependency on d) scale as $L^{1/2}d^{1/12}\varepsilon_{\text{score}}\log T$ and $L^{1/2}\varepsilon_{\text{score}}\log T$ in Gupta et al. (2024) and Chen et al. (2024b), respectively. Our theory exhibits a better dependency on score estimation error, which is similar to the results in Chen et al. (2022) and Benton et al. (2023).

Lipschitz condition of score functions. It is noteworthy that our better iteration complexity holds under the condition of Lipschitz continuity for score functions. Without this condition, the best results are $\tilde{O}(d\varepsilon^{-2})$ and $\tilde{O}(d\varepsilon^{-1} + d^2)$, which are achieved in Benton et al. (2023) and Li et al. (2024b), respectively. Our theory is better than such result when the Lipschitz constant for the score functions satisfies $L < d^{2/3}\varepsilon^{-4/3}$ for $\varepsilon > d^{-1/2}$, or $L < d^{2/3}\varepsilon^{-1/3}$ for $\varepsilon < d^{-1/2}$, and it is still unknown how to achieve sub-linear dependency on d in the general case.

3.3 PARALLEL SAMPLING

In this section, we provide a way to do parallel sampling for our proposed sampler that needs the similar number of parallel rounds as prior works (Gupta et al., 2024), while the number of parallel processors here is significantly reduced. In the following, we first introduce the parallel sampling procedure, and then present the theoretical guarantee. The analysis is postponed to the appendix.

Details of parallel sampling procedure. In the parallel sampling, all procedures are the same as the above sampler (11), except that we will update $Y_{k,n}$ for $n = 1, \dots, N$ at the same time. Specifically, we first initialize

$$\frac{Y_{0,k,n}}{\sqrt{1 - \tau_{k,n}}} = \frac{Y_k}{\sqrt{1 - \tau_{k,0}}}, \quad n = 1, \dots, N. \quad (13a)$$

Then we update all $Y_{k,n}$ for M rounds simultaneously: at the m -th round, we update $Y_{m,k,n}$ for $n = 1, \dots, N$ in the following way:

$$\frac{Y_{m,k,n}}{\sqrt{1 - \tau_{k,n}}} = \frac{Y_k}{\sqrt{1 - \tau_{k,0}}} + \frac{s_{T - \frac{kN}{2} + 1}(Y_k)}{2(1 - \tau_{k,0})^{3/2}}(\tau_{k,0} - \hat{\tau}_{k,0}) + \sum_{i=1}^{n-1} \frac{s_{T - \frac{kN}{2} - i + 1}(Y_{m-1,k,i})}{2(1 - \tau_{k,i})^{3/2}}(\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i})$$

$$+ \frac{s_{T-\frac{kN}{2}-n+2}(Y_{m-1,k,n-1})}{2(1-\tau_{k,n-1})^{3/2}}(\widehat{\tau}_{k,n-1}-\tau_{k,n}). \quad (13b)$$

Finally, we compute

$$Y_{k+1} = \sqrt{\frac{1-\tau_{k+1,0}}{1-\tau_{k,N}}}Y_{M,k,N} + \sqrt{\frac{\tau_{k+1,0}-\tau_{k,N}}{1-\tau_{k,N}}}Z_k, \quad (13c)$$

and we complete the update from Y_k to Y_{k+1} in the parallel way. In this parallel setting, the total number of parallel rounds to yield sample Y_K is MK , and N parallel processors are needed.

Theoretical guarantee of parallel sampling. The convergence guarantees for the above parallel sampling is as follows, whose proof can be found in Section 5:

Theorem 2. *With the same setting as Theorem 1, it is sufficient to choose*

$$N \gtrsim \frac{d^{1/3} \log^{1/3} T}{\varepsilon^{2/3}}, \quad MK \gtrsim L \log^2 T, \quad \text{and} \quad \varepsilon_{\text{score}}^2 \lesssim \varepsilon^2 \log^{-1} T \quad (14)$$

to achieve $\text{TV}(p_{\text{data}}, p_{Y_K}) \lesssim \varepsilon$ for the sampler (13).

Finally, let us briefly compare our theory with the prior works. This theorem states that the parallel sampler achieves ε -accuracy with respect to total variation distance through using $O(\log^2(Ld/\varepsilon))$ parallel rounds, which is similar to Gupta et al. (2024); Chen et al. (2024a). In addition, we only need $\widetilde{O}(d^{1/3}\varepsilon^{-2/3})$ parallel processors, which improves their results significantly.

4 ANALYSIS

This section is devoted to establishing Theorem 1. Before proceeding, we find it helpful to introduce the following notations. Without abuse of notations, we use X_τ to denote the continuous process as follows:

$$X_\tau \stackrel{d}{=} \sqrt{1-\tau}X_0 + \sqrt{\tau}Z, \quad \text{with } Z \sim \mathcal{N}(0, I), \quad \text{for } 0 \leq \tau \leq 1, \quad (15)$$

and the corresponding score function is

$$s_\tau^*(x) := \nabla \log p_{X_\tau}(x) = -\frac{1}{\tau} \int_{x_0} p_{X_0|X_\tau}(x_0|x)(x - \sqrt{1-\tau}x_0)dx_0.$$

In addition, we rewrite the sampling process with the continuous index as following:

$$\begin{aligned} \frac{Y_{\tau_{k,n}}}{\sqrt{1-\tau_{k,n}}} &= \frac{Y_k}{\sqrt{1-\tau_{k,0}}} + \frac{s_{\tau_{k,0}}(Y_k)}{2(1-\tau_k)^{3/2}}(\tau_{k,0} - \widehat{\tau}_{k,0}) + \sum_{i=1}^{n-1} \frac{s_{\tau_{k,i}}(Y_{\tau_{k,i}})}{2(1-\tau_{k,i})^{3/2}}(\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \\ &\quad + \frac{s_{\tau_{k,n-1}}(Y_{\tau_{k,n-1}})}{2(1-\tau_{k,n-1})^{3/2}}(\widehat{\tau}_{k,n-1} - \tau_{k,n}), \end{aligned}$$

and

$$Y_{k+1} = \sqrt{\frac{1-\tau_{k+1,0}}{1-\tau_{k,N}}}Y_{\tau_{k,N}} + \sqrt{\frac{\tau_{k+1,0}-\tau_{k,N}}{1-\tau_{k,N}}}Z_k,$$

where $Y_0 \sim \mathcal{N}(0, I)$ and $Z_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, I)$. Here, Y_k corresponds to the Y_k in the discrete case. In the following, it is enough to consider $T > c_3 L \log T$ for some constant $c_3 > 0$ large enough; otherwise, the desired bound holds trivially. The proof can be divided into three steps.

4.1 STEP 1: INTRODUCE THE AUXILIARY SEQUENCE

Let $\Phi_{\tau_1 \rightarrow \tau_2}(x) := x_{\tau_2} |_{x_{\tau_1}=x}$ defined through the following ODE

$$d \frac{x_\tau}{\sqrt{1-\tau}} = -\frac{s_\tau^*(x_\tau)}{2(1-\tau)^{3/2}} d\tau. \quad (16)$$

Then, we have the following result, whose proof is postponed to Appendix B.2:

324 **Lemma 2.** *It can be shown that*

$$325 \Phi_{\tau_1 \rightarrow \tau_2}(X_{\tau_1}) \stackrel{d}{=} X_{\tau_2}. \quad (17)$$

326 *Moreover, assume that $\widehat{X}_0 \stackrel{d}{=} X_{\tau_{0,0}}$. Then we have for $0 \leq k < K$,*

$$327 \widehat{X}_{k+1} = \sqrt{\frac{1 - \tau_{k+1,0}}{1 - \tau_{k,N}}} \Phi_{\tau_{k,0} \rightarrow \tau_{k,N}}(\widehat{X}_k) + \sqrt{\frac{\tau_{k+1,0} - \tau_{k,N}}{1 - \tau_{k,N}}} Z_k \stackrel{d}{=} X_{\tau_{k+1,0}}, \quad (18)$$

328 *where $Z_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, I)$.*

329 Given the definition of \widehat{X}_k , we make the following decomposition:

$$330 \text{TV}(p_{\text{data}}, p_{Y_K}) \leq \text{TV}(p_{\text{data}}, p_{\widehat{X}_K}) + \text{TV}(p_{\widehat{X}_K}, p_{Y_K}), \quad (19a)$$

331 and

$$332 \begin{aligned} \text{TV}^2(p_{\widehat{X}_K}, p_{Y_K}) &\leq \frac{1}{2} \text{KL}(p_{\widehat{X}_K} \| p_{Y_K}) \leq \frac{1}{2} \text{KL}(p_{\widehat{X}_0, \dots, \widehat{X}_K} \| p_{Y_0, \dots, Y_K}) \\ &= \frac{1}{2} \text{KL}(p_{\widehat{X}_0} \| p_{Y_0}) + \frac{1}{2} \sum_{k=0}^{K-1} \mathbb{E}_{x_k \sim p_{\widehat{X}_k}} \left[\text{KL}(p_{\widehat{X}_{k+1} | \widehat{X}_k}(\cdot | x_k) \| p_{Y_{k+1} | Y_k}(\cdot | x_k)) \right], \end{aligned} \quad (19b)$$

333 where we make use of Pinsker's inequality and the data-processing inequality. In the next step, we will bound the divergence between $p_{\widehat{X}_{k+1} | \widehat{X}_k}$ and $p_{Y_{k+1} | Y_k}$, and the remaining terms can be controlled easily, which is left to the final step.

334 4.2 STEP 2: CONTROL THE DIVERGENCE BETWEEN $p_{\widehat{X}_{k+1} | \widehat{X}_k}$ AND $p_{Y_{k+1} | Y_k}$

335 Based on the update rule for $Y_{\tau_{k,n}}$, we let

$$336 \begin{aligned} \frac{y_{\tau_{k,n}}}{\sqrt{1 - \tau_{k,n}}} &= \frac{y_{\tau_{k,0}}}{\sqrt{1 - \tau_{k,0}}} + \frac{s_{\tau_{k,0}}(y_{\tau_{k,0}})}{2(1 - \tau_{k,0})^{3/2}} (\tau_{k,0} - \widehat{\tau}_{k,0}) + \sum_{i=1}^{n-1} \frac{s_{\tau_{k,i}}(y_{\tau_{k,i}})}{2(1 - \tau_{k,i})^{3/2}} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \\ &\quad + \frac{s_{\tau_{k,n-1}}(y_{\tau_{k,n-1}})}{2(1 - \tau_{k,n-1})^{3/2}} (\widehat{\tau}_{k,n-1} - \tau_{k,n}), \end{aligned}$$

337 for $n = 1, \dots, N$. Then notice that $\widehat{X}_{k+1} | \widehat{X}_k$ and $Y_{k+1} | Y_k$ are both normal distributions with the same variance $\frac{\tau_{k+1,0} - \tau_{k,N}}{1 - \tau_{k,N}}$ and different means $\sqrt{\frac{1 - \tau_{k+1,0}}{1 - \tau_{k,N}}} \Phi_{\tau_{k,0} \rightarrow \tau_{k,N}}(\widehat{X}_k)$ and $\sqrt{\frac{1 - \tau_{k+1,0}}{1 - \tau_{k,N}}} y_{\tau_{k,N}}$, respectively. This tells us that

$$338 \text{KL}(p_{\widehat{X}_{k+1} | \widehat{X}_k}(\cdot | x_k) \| p_{Y_{k+1} | Y_k}(\cdot | x_k)) = \frac{1 - \tau_{k+1,0}}{2(\tau_{k+1,0} - \tau_{k,N})} \|y_{\tau_{k,N}} - x_{\tau_{k,N}}\|_2^2, \quad (20)$$

339 when we set $x_{\tau_{k,0}}, y_{\tau_{k,0}} = x_k$, and $x_{\tau_{k,N}}$ is defined as $x_{\tau_{k,N}} = \Phi_{\tau_{k,0} \rightarrow \tau_{k,n}}(x_k)$.

340 Towards controlling the difference between $y_{\tau_{k,n}}$ and $x_{\tau_{k,N}}$, let's consider the ODE trajectory beginning from $x_{\tau_{k,0}} = x_k$, and define

$$341 \begin{aligned} \xi_{k,n}(x_k) &:= \frac{x_{\tau_{k,n}}}{\sqrt{1 - \tau_{k,n}}} - \frac{x_{\tau_{k,0}}}{\sqrt{1 - \tau_{k,0}}} - \frac{s_{\tau_{k,0}}(x_{\tau_{k,0}})}{2(1 - \tau_{k,0})^{3/2}} (\tau_{k,0} - \widehat{\tau}_{k,0}) \\ &\quad - \sum_{i=1}^{n-1} \frac{s_{\tau_{k,i}}(x_{\tau_{k,i}})}{2(1 - \tau_{k,i})^{3/2}} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) - \frac{s_{\tau_{k,n-1}}(x_{\tau_{k,n-1}})}{2(1 - \tau_{k,n-1})^{3/2}} (\widehat{\tau}_{k,n-1} - \tau_{k,n}), \end{aligned} \quad (21)$$

342 which denotes the discretization and estimation error of the ODE process (16), and is controlled in the following lemma. The proof is postponed to Appendix A.1.

Lemma 3. For any k and n , it can be seen that with probability at least $1 - T^{-100}$,

$$\mathbb{E}_{x_k \sim p_{\hat{X}_k}} [\|\xi_{k,n}(x_k)\|_2^2] \lesssim \sum_{i=1}^n \frac{L^3 d \log^4 T}{(1 - \hat{\tau}_{k,i-1})^2 T^3} (\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i}) + \frac{N \log^2 T}{T^2} \sum_{i=0}^{n-1} \hat{\tau}_{k,i} (1 - \hat{\tau}_{k,i})^{-1} \varepsilon_{T - \frac{kN}{2} - i + 1}^2, \quad (22)$$

where $\varepsilon_{T - \frac{kN}{2} - i + 1}^2$ is defined in (6).

With the above relation, we can bound the divergence as following. The proof is postponed to Appendix A.2.

Lemma 4. According to Lemma 3, it can be shown that

$$\mathbb{E}_{x_k \sim p_{\hat{X}_k}} \left[\text{KL} \left(p_{\hat{X}_{k+1} | \hat{X}_k}(\cdot | x_k) \parallel p_{Y_{k+1} | Y_k}(\cdot | x_k) \right) \right] \lesssim \frac{L^3 d \log^4 T}{T^3} + \frac{\log T}{T} \sum_{i=0}^{N-1} \varepsilon_{T - \frac{kN}{2} - i + 1}^2, \quad (23)$$

where $\varepsilon_{T - \frac{kN}{2} - i + 1}^2$ is defined in (6).

4.3 STEP 3: PUTTING EVERYTHING TOGETHER

The remaining terms in (19) can be bounded through the following lemma, whose proof can be found in Appendix B.3.

Lemma 5. Under our choice of learning schedule (9), we have

$$\text{TV}(p_{\text{data}}, p_{\hat{X}_K}) \leq \frac{1}{T^{10}} \quad \text{and} \quad \text{KL}(p_{\hat{X}_0} \parallel p_{Y_0}) \leq \frac{1}{T^{10}}. \quad (24)$$

Inserting (24) and (23) into (19) leads to

$$\text{TV}(p_{\text{data}}, p_{Y_K}) \lesssim \frac{1}{T^{10}} + \sqrt{\frac{1}{T^{10}} + \frac{L^3 d \log^4 T}{T^3} + \varepsilon_{\text{score}}^2 \log T} \lesssim \frac{L^{3/2} d^{1/2} \log^2 T}{T^{3/2}} + \varepsilon_{\text{score}} \log^{1/2} T,$$

and we conclude the proof here.

5 ANALYSIS FOR PARALLELIZATION (THEOREM 2)

By comparing the update rules for $Y_{k,n}$ and $Y_{m,k,n}$, it is natural to control the difference of the following two sequences:

$$\begin{aligned} \frac{y_{\tau_{k,n}}}{\sqrt{1 - \tau_{k,n}}} &= \frac{y_{\tau_{k,0}}}{\sqrt{1 - \tau_{k,0}}} + \frac{s_{\tau_{k,0}}(y_{\tau_{k,0}})}{2(1 - \tau_{k,0})^{3/2}} (\tau_{k,0} - \hat{\tau}_{k,0}) + \sum_{i=1}^{n-1} \frac{s_{\tau_{k,i}}(y_{\tau_{k,i}})}{2(1 - \tau_{k,i})^{3/2}} (\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i}) \\ &\quad + \frac{s_{\tau_{k,n-1}}(y_{\tau_{k,n-1}})}{2(1 - \tau_{k,n-1})^{3/2}} (\hat{\tau}_{k,n-1} - \tau_{k,n}), \end{aligned}$$

and

$$\begin{aligned} \frac{y_{m,\tau_{k,n}}}{\sqrt{1 - \tau_{k,n}}} &= \frac{y_{\tau_{k,0}}}{\sqrt{1 - \tau_{k,0}}} + \frac{s_{\tau_{k,0}}(y_{\tau_{k,0}})}{2(1 - \tau_{k,0})^{3/2}} (\tau_{k,0} - \hat{\tau}_{k,0}) + \sum_{i=1}^{n-1} \frac{s_{\tau_{k,i}}(y_{m-1,\tau_{k,i}})}{2(1 - \tau_{k,i})^{3/2}} (\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i}) \\ &\quad + \frac{s_{\tau_{k,n-1}}(y_{m-1,\tau_{k,n-1}})}{2(1 - \tau_{k,n-1})^{3/2}} (\hat{\tau}_{k,n-1} - \tau_{k,n}). \end{aligned}$$

The above update rules, together with the Lipschitz condition of score estimates, lead to

$$\frac{\|y_{m,\tau_{k,n}} - y_{\tau_{k,n}}\|_2}{\sqrt{1 - \tau_{k,n}}} \lesssim \frac{L \log T}{T} \sum_{i=1}^{n-1} \frac{\|y_{m-1,\tau_{k,i}} - y_{\tau_{k,i}}\|_2}{\sqrt{1 - \tau_{k,i}}}.$$

Applying the above relation recursively gives

$$\max_n \frac{\|y_{M, \tau_{k,n}} - y_{\tau_{k,n}}\|_2}{\sqrt{1 - \tau_{k,n}}} \leq \left(\frac{NL \log T}{T}\right)^M \max_n \frac{\|y_{0, \tau_{k,n}} - y_{\tau_{k,n}}\|_2}{\sqrt{1 - \tau_{k,n}}} \leq \frac{1}{\text{poly}(T)},$$

provided that $M \gtrsim \log T$ and $T \gtrsim NL \log T$. Thus as long as $N \gtrsim \frac{d^{1/3} \log^{1/3} T}{\varepsilon^{2/3}}$, which guarantees that $T \gtrsim \frac{Ld^{1/3} \log^{4/3} T}{\varepsilon^{2/3}}$, we can get the desired result immediately through just inserting the above error bound into Lemma 4. We omit the details here due to the similarity.

6 DISCUSSION

In this paper, we establish a faster convergence rate for diffusion probabilistic models, which scales as $Ld^{1/3}\varepsilon^{-2/3}$, assuming smooth score functions. Our theory achieves at least $L^{2/3}d^{1/12}\varepsilon^{-1/3}$ improvement over prior works (Gupta et al., 2024; Chen et al., 2024b), and thereby aligns more closely with practical requirements. Recent researches (Benton et al., 2023; Li et al., 2024b) have shown an $O(d\varepsilon^{-1})$ dependence for diffusion models without the assumption of smoothness. However, it remains unclear whether any algorithm can achieve a sub-linear dependence on d in the absence of smoothness. We leave this as an open question for future research. Furthermore, estimating the Lipschitz constant in real-world cases would be highly beneficial, potentially broadening the applicability of our results.

REFERENCES

- Joe Benton, Valentin De Bortoli, Arnaud Doucet, and George Deligiannidis. Nearly d -linear convergence bounds for diffusion models via stochastic localization. In *The Twelfth International Conference on Learning Representations*, 2023.
- Haoxuan Chen, Yinuo Ren, Lexing Ying, and Grant M Rotskoff. Accelerating diffusion models with parallel sampling: Inference at sub-linear time complexity. *arXiv preprint arXiv:2405.15986*, 2024a.
- Hongrui Chen, Holden Lee, and Jianfeng Lu. Improved analysis of score-based generative modeling: User-friendly bounds under minimal smoothness assumptions. In *International Conference on Machine Learning*, pp. 4735–4763. PMLR, 2023.
- Sitan Chen, Sinho Chewi, Jerry Li, Yuanzhi Li, Adil Salim, and Anru R Zhang. Sampling is as easy as learning the score: theory for diffusion models with minimal data assumptions. *arXiv preprint arXiv:2209.11215*, 2022.
- Sitan Chen, Sinho Chewi, Holden Lee, Yuanzhi Li, Jianfeng Lu, and Adil Salim. The probability flow ode is provably fast. *Advances in Neural Information Processing Systems*, 36, 2024b.
- Florinel-Alin Croitoru, Vlad Hondru, Radu Tudor Ionescu, and Mubarak Shah. Diffusion models in vision: A survey. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 45(9): 10850–10869, 2023.
- Valentin De Bortoli. Convergence of denoising diffusion models under the manifold hypothesis. *Transactions on Machine Learning Research*, 2022.
- Prafulla Dhariwal and Alexander Nichol. Diffusion models beat gans on image synthesis. *Advances in neural information processing systems*, 34:8780–8794, 2021.
- Xuefeng Gao, Hoang M Nguyen, and Lingjiong Zhu. Wasserstein convergence guarantees for a general class of score-based generative models. *arXiv preprint arXiv:2311.11003*, 2023.
- Shivam Gupta, Linda Cai, and Sitan Chen. Faster diffusion-based sampling with randomized mid-points: Sequential and parallel. *arXiv preprint arXiv:2406.00924*, 2024.
- Jonathan Ho, Ajay Jain, and Pieter Abbeel. Denoising diffusion probabilistic models. *Advances in neural information processing systems*, 33:6840–6851, 2020.

- 486 Aapo Hyvärinen. Some extensions of score matching. *Computational statistics & data analysis*, 51
487 (5):2499–2512, 2007.
488
- 489 Aapo Hyvärinen and Peter Dayan. Estimation of non-normalized statistical models by score match-
490 ing. *Journal of Machine Learning Research*, 6(4), 2005.
491
- 492 Holden Lee, Jianfeng Lu, and Yixin Tan. Convergence for score-based generative modeling with
493 polynomial complexity. *Advances in Neural Information Processing Systems*, 35:22870–22882,
494 2022.
- 495 Holden Lee, Jianfeng Lu, and Yixin Tan. Convergence of score-based generative modeling for
496 general data distributions. In *International Conference on Algorithmic Learning Theory*, pp.
497 946–985. PMLR, 2023.
498
- 499 Gen Li and Yuling Yan. Adapting to unknown low-dimensional structures in score-based diffusion
500 models. *arXiv preprint arXiv:2405.14861*, 2024.
- 501 Gen Li, Yuting Wei, Yuxin Chen, and Yuejie Chi. Towards faster non-asymptotic convergence for
502 diffusion-based generative models. *arXiv preprint arXiv:2306.09251*, 2023.
503
- 504 Gen Li, Yu Huang, Timofey Efimov, Yuting Wei, Yuejie Chi, and Yuxin Chen. Accelerating con-
505 vergence of score-based diffusion models, provably. In *Forty-first International Conference on*
506 *Machine Learning*, 2024a.
- 507 Gen Li, Yuting Wei, Yuejie Chi, and Yuxin Chen. A sharp convergence theory for the probability
508 flow odes of diffusion models. *arXiv preprint arXiv:2408.02320*, 2024b.
509
- 510 Alexander Quinn Nichol and Prafulla Dhariwal. Improved denoising diffusion probabilistic models.
511 In *International conference on machine learning*, pp. 8162–8171. PMLR, 2021.
512
- 513 Tianyu Pang, Kun Xu, Chongxuan Li, Yang Song, Stefano Ermon, and Jun Zhu. Efficient learn-
514 ing of generative models via finite-difference score matching. *Advances in Neural Information*
515 *Processing Systems*, 33:19175–19188, 2020.
- 516 Aditya Ramesh, Prafulla Dhariwal, Alex Nichol, Casey Chu, and Mark Chen. Hierarchical text-
517 conditional image generation with clip latents. *arXiv preprint arXiv:2204.06125*, 1(2):3, 2022.
518
- 519 Robin Rombach, Andreas Blattmann, Dominik Lorenz, Patrick Esser, and Björn Ommer. High-
520 resolution image synthesis with latent diffusion models. In *Proceedings of the IEEE/CVF confer-*
521 *ence on computer vision and pattern recognition*, pp. 10684–10695, 2022.
- 522 Chitwan Saharia, William Chan, Saurabh Saxena, Lala Li, Jay Whang, Emily L Denton, Kamyar
523 Ghasemipour, Raphael Gontijo Lopes, Burcu Karagol Ayan, Tim Salimans, et al. Photorealistic
524 text-to-image diffusion models with deep language understanding. *Advances in neural informa-*
525 *tion processing systems*, 35:36479–36494, 2022.
526
- 527 Ruoqi Shen and Yin Tat Lee. The randomized midpoint method for log-concave sampling. *Advances*
528 *in Neural Information Processing Systems*, 32, 2019.
529
- 530 Jascha Sohl-Dickstein, Eric Weiss, Niru Maheswaranathan, and Surya Ganguli. Deep unsupervised
531 learning using nonequilibrium thermodynamics. In *International conference on machine learn-*
532 *ing*, pp. 2256–2265. PMLR, 2015.
- 533 Jiaming Song, Chenlin Meng, and Stefano Ermon. Denoising diffusion implicit models. In *Internat-*
534 *ional Conference on Learning Representations*, 2021.
535
- 536 Yang Song and Stefano Ermon. Generative modeling by estimating gradients of the data distribution.
537 *Advances in neural information processing systems*, 32, 2019.
- 538 Pascal Vincent. A connection between score matching and denoising autoencoders. *Neural compu-*
539 *tation*, 23(7):1661–1674, 2011.

A PROOF OF KEY LEMMAS IN THEOREM 1

A.1 PROOF OF LEMMA 3

We first make the following decomposition

$$\xi_{k,n} = \mathcal{E}_{1,1} + \mathcal{E}_{1,0} - \mathcal{E}_2 - \mathcal{E}_3,$$

where

$$\begin{aligned} \mathcal{E}_{1,1} &:= \frac{x_{\tau_{k,n}}}{\sqrt{1-\tau_{k,n}}} - \frac{x_{\widehat{\tau}_{k,n-1}}}{\sqrt{1-\widehat{\tau}_{k,n-1}}} - \frac{s_{\tau_{k,n-1}}^*(x_{\tau_{k,n-1}})}{2(1-\tau_{k,n-1})^{3/2}}(\widehat{\tau}_{k,n-1} - \tau_{k,n}); \\ \mathcal{E}_{1,0} &:= \frac{x_{\widehat{\tau}_{k,0}}}{\sqrt{1-\widehat{\tau}_{k,0}}} - \frac{x_{\tau_{k,0}}}{\sqrt{1-\tau_{k,0}}} - \frac{s_{\tau_{k,0}}^*(x_{\tau_{k,0}})}{2(1-\tau_{k,0})^{3/2}}(\tau_{k,0} - \widehat{\tau}_{k,0}); \\ \mathcal{E}_2 &:= \sum_{i=1}^{n-1} \left[\frac{s_{\tau_{k,i}}^*(x_{\tau_{k,i}})}{2(1-\tau_{k,i})^{3/2}}(\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) - \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau \right]; \\ \mathcal{E}_3 &:= \frac{s_{\tau_{k,0}}(x_{\tau_{k,0}}) - s_{\tau_{k,0}}^*(x_{\tau_{k,0}})}{2(1-\tau_{k,0})^{3/2}}(\tau_{k,0} - \widehat{\tau}_{k,0}) + \frac{s_{\tau_{k,n-1}}(x_{\tau_{k,n-1}}) - s_{\tau_{k,n-1}}^*(x_{\tau_{k,n-1}})}{2(1-\tau_{k,n-1})^{3/2}}(\widehat{\tau}_{k,n-1} - \tau_{k,n}) \\ &\quad + \sum_{i=1}^{n-1} \frac{1}{2(1-\tau_{k,i})^{3/2}}(s_{\tau_{k,i}}(x_{\tau_{k,i}}) - s_{\tau_{k,i}}^*(x_{\tau_{k,i}}))(\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}). \end{aligned}$$

In the following, we will control these three terms separately.

- For the first term, recalling the ODE in (16) and the conclusion (17) in Lemma 2, we have

$$\frac{x_{\tau_{k,n}}}{\sqrt{1-\tau_{k,n}}} - \frac{x_{\widehat{\tau}_{k,n-1}}}{\sqrt{1-\widehat{\tau}_{k,n-1}}} = \int_{\tau_{k,n}}^{\widehat{\tau}_{k,n-1}} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau.$$

Inserting into the definition of $\mathcal{E}_{1,1}$, we have

$$\begin{aligned} \mathcal{E}_{1,1} &= \int_{\tau_{k,n}}^{\widehat{\tau}_{k,n-1}} \left(\frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} - \frac{s_{\tau_{k,n-1}}^*(x_{\tau_{k,n-1}})}{2(1-\tau_{k,n-1})^{3/2}} \right) d\tau \\ &\stackrel{(a)}{=} - \int_{\tau_{k,n}}^{\widehat{\tau}_{k,n-1}} \left(\int_{\tau'}^{\tau_{k,n-1}} \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau \right) d\tau' \\ &\stackrel{(b)}{=} - \int_{\tau_{k,n}}^{\tau_{k,n-1}} \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} \left(\int_{\tau_{k,n}}^{\widehat{\tau}_{k,n-1}} \mathbf{1}(\tau' < \tau) d\tau' \right) d\tau \\ &= - \left(\int_{\tau_{k,n}}^{\widehat{\tau}_{k,n-1}} (\tau - \tau_{k,n}) \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau + \int_{\widehat{\tau}_{k,n-1}}^{\tau_{k,n-1}} (\widehat{\tau}_{k,n-1} - \tau_{k,n}) \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau \right), \end{aligned}$$

where (a) comes from the fact that

$$\frac{s_{\tau'}^*(x_{\tau'})}{2(1-\tau')^{3/2}} - \frac{s_{\tau_{k,n-1}}^*(x_{\tau_{k,n-1}})}{2(1-\tau_{k,n-1})^{3/2}} = \int_{\tau_{k,n-1}}^{\tau'} \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau$$

and the $\mathbf{1}(\tau' < \tau)$ in (b) denotes an indicator. Thus we have

$$\begin{aligned} \mathbb{E}_{x_k \sim p_{\widehat{X}_k}} [\|\mathcal{E}_{1,1}(x_k)\|_2^2 | \tau] &\lesssim \int_{\tau_{k,n}}^{\widehat{\tau}_{k,n-1}} (\tau - \tau_{k,n})^2 d\tau \mathbb{E}_{x_{\tau} \sim X_{\tau}} \left[\int_{\tau_{k,n}}^{\widehat{\tau}_{k,n-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} \right\|_2^2 d\tau \right] \\ &\quad + (\widehat{\tau}_{k,n-1} - \tau_{k,n})^2 (\tau_{k,n-1} - \widehat{\tau}_{k,n-1}) \mathbb{E}_{x_{\tau} \sim X_{\tau}} \left[\int_{\widehat{\tau}_{k,n-1}}^{\tau_{k,n-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} \right\|_2^2 d\tau \right] \\ &\leq (\widehat{\tau}_{k,n-1} - \tau_{k,n})^2 (\tau_{k,n-1} - \tau_{k,n}) \int_{\tau_{k,n}}^{\tau_{k,n-1}} \mathbb{E}_{x_{\tau} \sim X_{\tau}} \left[\left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} \right\|_2^2 \right] d\tau. \end{aligned}$$

594
595
596
597
598
599
600
601
602
603
604
605
606
607
608
609
610
611
612
613
614
615
616
617
618
619
620
621
622
623
624
625
626
627
628
629
630
631
632
633
634
635
636
637
638
639
640
641
642
643
644
645
646
647

We claim that

$$\mathbb{E}_{x_\tau \sim X_\tau} \left[\left\| \frac{\partial(1-\tau)^{-3/2} s_\tau^*(x_\tau)}{\partial \tau} \right\|_2^2 \right] \lesssim \left(L \vee \frac{1}{\tau} \right) \frac{L^2 d}{(1-\tau)^5}. \quad (25)$$

The proof is postponed to the end of this section.

Then we have

$$\begin{aligned} \mathbb{E}_{x_k \sim p_{\widehat{X}_k}} \left[\|\mathcal{E}_{1,1}(x_k)\|_2^2 \mid \tau \right] &\lesssim (\widehat{\tau}_{k,n-1} - \tau_{k,n})^2 (\tau_{k,n-1} - \tau_{k,n})^2 \left(L \vee \frac{1}{\tau_{k,n}} \right) \frac{L^2 d}{(1-\tau_{k,n-1})^5} \\ &\lesssim (\widehat{\tau}_{k,n-1} - \widehat{\tau}_{k,n})^2 (\widehat{\tau}_{k,n-2} - \widehat{\tau}_{k,n})^2 \left(L \vee \frac{1}{\widehat{\tau}_{k,n}} \right) \frac{L^2 d}{(1-\widehat{\tau}_{k,n-2})^5} \\ &\lesssim (\widehat{\tau}_{k,n-1} - \widehat{\tau}_{k,n}) \frac{L^3 d \log^3 T}{(1-\widehat{\tau}_{k,n-1})^2 T^3}. \end{aligned}$$

Here the last inequality comes from

$$\begin{aligned} &(\widehat{\tau}_{k,n-1} - \widehat{\tau}_{k,n}) (\widehat{\tau}_{k,n-2} - \widehat{\tau}_{k,n})^2 \left(L \vee \frac{1}{\widehat{\tau}_{k,n}} \right) \frac{L^2 d}{(1-\widehat{\tau}_{k,n-2})^5} \\ &\stackrel{(a)}{\lesssim} \frac{L^2 d (1-\widehat{\tau}_{k,n-1})^3 \log^3 T}{T^3 (1-\widehat{\tau}_{k,n-2})^5} \left(L \vee \frac{\widehat{\tau}_{k,n-1}}{\widehat{\tau}_{k,n}} \right) \\ &\stackrel{(b)}{\lesssim} \frac{L^3 d \log^3 T}{(1-\widehat{\tau}_{k,n-1})^2 T^3}, \end{aligned}$$

where (a) is due to the facts that $(\widehat{\tau}_{k,n-1} - \widehat{\tau}_{k,n}) \left(L \vee \frac{1}{\widehat{\tau}_{k,n}} \right) \lesssim \frac{(1-\widehat{\tau}_{k,n-1}) \log T}{T} \left(L \vee \frac{\widehat{\tau}_{k,n-1}}{\widehat{\tau}_{k,n}} \right)$ and $(\widehat{\tau}_{k,n-2} - \widehat{\tau}_{k,n})^2 \lesssim \frac{\log^2 T}{T^2} ((1-\widehat{\tau}_{k,n-2})^2 + (1-\widehat{\tau}_{k,n-1})^2) \lesssim \frac{\log^2 T}{T^2} (1-\widehat{\tau}_{k,n-1})^2$, (b) comes from $L \gtrsim \frac{\widehat{\tau}_{k,n-1}}{\widehat{\tau}_{k,n}}$ and

$$\left(\frac{1-\widehat{\tau}_{k,n-1}}{1-\widehat{\tau}_{k,n-2}} \right)^5 \leq \left(1 + \frac{c_1 \log T}{T} \right)^5 \lesssim 1.$$

We remark that if $n = 2$, then it suffices to replace $\widehat{\tau}_{k,n-2}$ in the proof with $\widehat{\tau}_{k-1, \frac{N}{2}}$.

In addition, we could bound $\mathcal{E}_{1,0}$ similarly as

$$\begin{aligned} \mathcal{E}_{1,0} &= \int_{\widehat{\tau}_{k,0}}^{\tau_{k,0}} \left(\frac{s_\tau^*(x_\tau)}{2(1-\tau)^{3/2}} - \frac{s_{\tau_{k,0}}^*(x_{\tau_{k,0}})}{2(1-\tau_{k,0})^{3/2}} \right) d\tau \\ &= - \int_{\widehat{\tau}_{k,0}}^{\tau_{k,0}} \left(\int_{\tau'}^{\tau_{k,0}} \frac{\partial}{\partial \tau} \frac{s_\tau^*(x_\tau)}{2(1-\tau)^{3/2}} d\tau \right) d\tau' \\ &= - \int_{\widehat{\tau}_{k,0}}^{\tau_{k,0}} \frac{\partial}{\partial \tau} \frac{s_\tau^*(x_\tau)}{2(1-\tau)^{3/2}} \left(\int_{\widehat{\tau}_{k,0}}^{\tau_{k,0}} \mathbb{1}(\tau' < \tau) d\tau' \right) d\tau \\ &= - \int_{\widehat{\tau}_{k,0}}^{\tau_{k,0}} (\tau - \widehat{\tau}_{k,0}) \frac{\partial}{\partial \tau} \frac{s_\tau^*(x_\tau)}{2(1-\tau)^{3/2}} d\tau. \end{aligned}$$

Moreover, for $k \geq 1$,

$$\begin{aligned} \mathbb{E}_{x_k \sim p_{\widehat{X}_k}} \left[\|\mathcal{E}_{1,0}(x_k)\|_2^2 \mid \tau \right] &\lesssim (\tau_{k,0} - \widehat{\tau}_{k,0})^3 \int_{\widehat{\tau}_{k,0}}^{\tau_{k,0}} \mathbb{E}_{x_\tau \sim X_\tau} \left[\left\| \frac{\partial}{\partial \tau} \frac{s_\tau^*(x_\tau)}{(1-\tau)^{3/2}} \right\|_2^2 \right] d\tau \\ &\lesssim \frac{\log^3 T \widehat{\tau}_{k-1, \frac{N}{2}-1}^3 (1-\widehat{\tau}_{k-1, \frac{N}{2}-1})^3}{T^3} \left(L \vee \frac{1}{\widehat{\tau}_{k,0}} \right) \frac{L^2 d (\widehat{\tau}_{k-1, \frac{N}{2}-1} - \widehat{\tau}_{k,0})}{(1-\widehat{\tau}_{k-1, \frac{N}{2}-1})^5} \\ &\lesssim \frac{L^3 d \log^3 T}{T^3} \frac{(\widehat{\tau}_{k,0} - \widehat{\tau}_{k,1})}{(1-\widehat{\tau}_{k,0})^2}, \end{aligned}$$

where the last inequality comes from

$$\frac{\widehat{\tau}_{k,0} - \widehat{\tau}_{k,1}}{(1-\widehat{\tau}_{k,0})^2} = \frac{c_1 \widehat{\tau}_{k,0} (1-\widehat{\tau}_{k,0}) \log T}{T(1-\widehat{\tau}_{k,0})^2} = \frac{c_1 \widehat{\tau}_{k,0} \log T}{T(1-\widehat{\tau}_{k,0})} \gtrsim \frac{c_1 \widehat{\tau}_{k-1, \frac{N}{2}-1} \log T}{T(1-\widehat{\tau}_{k-1, \frac{N}{2}-1})} \frac{1 - \frac{c_1 \log T}{T}}{1 + \frac{c_1 \log T}{T}}$$

648
649
650
651
652
653
654
655
656
657
658
659
660
661
662
663
664
665
666
667
668
669
670
671
672
673
674
675
676
677
678
679
680
681
682
683
684
685
686
687
688
689
690
691
692
693
694
695
696
697
698
699
700
701

$$\gtrsim \frac{c_1 \widehat{\tau}_{k-1, \frac{N}{2}-1} (1 - \widehat{\tau}_{k, \frac{N}{2}-1}) \log T}{T(1 - \widehat{\tau}_{k, \frac{N}{2}-1})^2} \gtrsim \frac{\widehat{\tau}_{k-1, \frac{N}{2}-1} - \widehat{\tau}_{k, 0}}{(1 - \widehat{\tau}_{k-1, \frac{N}{2}-1})^2}$$

by invoking Lemma 1. For $k = 0$, it suffices to define $\widehat{\tau}_{-1, \frac{N}{2}-1} = 1 - \widehat{\alpha}_{T+1}$.

- Next, we intend to bound \mathcal{E}_2 . For any integer $r > 0$, considering that $\mathbb{E}_{x_k \sim p_{\widehat{X}_k}} [\|\mathcal{E}_2(x_k)\|_2^2 | \tau]$ is a random variable independent on x_k , we use r random independent variables $x_k^{(j)} \sim p_{\widehat{X}_k}$, $j = 1, \dots, r$, and get

$$\begin{aligned} \mathbb{E} \left[\left(\mathbb{E}_{x_k \sim p_{\widehat{X}_k}} [\|\mathcal{E}_2(x_k)\|_2^2 | \tau] \right)^r \right] &= \mathbb{E} \left[\mathbb{E}_{x_k^{(j)} \sim p_{\widehat{X}_k}} \left[\prod_{1 \leq j \leq r} \|\mathcal{E}_2(x_k^{(j)})\|_2^2 | \tau \right] \right] \\ &= \mathbb{E}_{x_k^{(j)} \sim p_{\widehat{X}_k}} \left[\mathbb{E} \left[\prod_{1 \leq j \leq r} \|\mathcal{E}_2(x_k^{(j)})\|_2^2 | x_k^{(j)} \right] \right]. \end{aligned} \quad (26)$$

To control the above term, we first make the following observations about the expectation and bias of random variable $\frac{s_{\tau_{k,i}}^*(x_{\tau_{k,i}})}{2(1-\tau_{k,i})^{3/2}}$ conditioned on $x_k^{(j)}$:

$$\begin{aligned} \mathbb{E} \left[\frac{s_{\tau_{k,i}}^*(x_{\tau_{k,i}})}{2(1-\tau_{k,i})^{3/2}} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) | x_k^{(j)} \right] &\stackrel{(a)}{=} \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \frac{1}{\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}} d\tau \\ &= \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau, \end{aligned}$$

where (a) comes from the fact that $\tau_{k,i}$ is uniformly distributed within $[\widehat{\tau}_{k,i}, \widehat{\tau}_{k,i-1}]$, and

$$\begin{aligned} &\int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau - \frac{s_{\tau_{k,i}}^*(x_{\tau_{k,i}})}{2(1-\tau_{k,i})^{3/2}} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \\ &= \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \left[\frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} - \frac{s_{\tau_{k,i}}^*(x_{\tau_{k,i}})}{2(1-\tau_{k,i})^{3/2}} \right] d\tau \\ &= \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \int_{\tau_{k,i}}^{\tau'} \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau d\tau' \\ &= \left(\int_{\tau_{k,i}}^{\widehat{\tau}_{k,i-1}} \int_{\tau_{k,i}}^{\tau'} - \int_{\widehat{\tau}_{k,i}}^{\tau_{k,i}} \int_{\tau'}^{\tau_{k,i}} \right) \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau d\tau' \\ &= \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} (\tau - \tau_{k,i}) \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau. \end{aligned}$$

Furthermore, recalling that $\tau_{k,i} \geq \widehat{\tau}_{k,i}$, we have

$$\begin{aligned} &\left\| \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} d\tau - \frac{s_{\tau_{k,i}}^*(x_{\tau_{k,i}})}{2(1-\tau_{k,i})^{3/2}} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \right\|_2 \\ &\leq \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} \right\|_2 d\tau \\ &\leq (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} \right\|_2 d\tau. \end{aligned}$$

Then given $x_k^{(j)}$, according to Bernstein inequality, we have with probability at least $1 - \delta$,

$$\|\mathcal{E}_2(x_k^{(j)})\|_2^2 \lesssim \log \frac{r}{\delta} \sum_{i=1}^{n-1} \left[(\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} \right\|_2 d\tau \right]^2, \quad \forall 1 \leq j \leq r. \quad (27)$$

For convenience, we introduce a temporary variable as below.

$$A_{k,i} := \left[(\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{2(1-\tau)^{3/2}} \right\|_2 d\tau \right]^2.$$

We bound $A_{k,i}$ as

$$\begin{aligned}
A_{k,i} &= (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i})^2 \left[\int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{(1-\tau)^{3/2}} \right\|_2 d\tau \right]^2 \\
&\stackrel{(a)}{\leq} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i})^2 (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{(1-\tau)^{3/2}} \right\|_2^2 d\tau \\
&= (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i})^3 \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{(1-\tau)^{3/2}} \right\|_2^2 d\tau, \tag{28}
\end{aligned}$$

where (a) uses the cauchy-schwarz inequality. For another, notice the relation that for $\mathbb{P}(X > \log \frac{r}{\delta}) < \frac{\delta}{r}$ and $Y \sim \text{Exp}(1)$, the following inequality holds.

$$\mathbb{E}[X^r] \leq \mathbb{E}[Y^r] = r!.$$

Then the (27) implies that

$$\mathbb{E} \left[\prod_{1 \leq j \leq r} \|\mathcal{E}_2(x_k^{(j)})\|_2^2 | x_k^{(j)} \right] \lesssim r! \prod_{1 \leq j \leq r} \sum_{i=1}^{n-1} A_{k,i}. \tag{29}$$

Combining (28) and (29), we have that

$$\mathbb{E} \left[\prod_{1 \leq j \leq r} \|\mathcal{E}_2(x_k^{(j)})\|_2^2 | x_k^{(j)} \right] \lesssim r! \prod_{1 \leq j \leq r} \sum_{i=1}^{n-1} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i})^3 \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{(1-\tau)^{3/2}} \right\|_2^2 d\tau.$$

Inserting into (26), we have

$$\mathbb{E} \left[\left(\mathbb{E}_{x_k \sim p_{\widehat{X}_k}} [\|\mathcal{E}_2(x_k)\|_2^2 | \tau] \right)^r \right] \lesssim r! \prod_{1 \leq j \leq r} \sum_{i=1}^{n-1} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i})^3 \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \mathbb{E}_{x_{\tau} \sim X_{\tau}} \left[\left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{(1-\tau)^{3/2}} \right\|_2^2 \right] d\tau,$$

which tells us that with probability at least $1 - T^{-100}$,

$$\mathbb{E}_{x_k \sim p_{\widehat{X}_k}} [\|\mathcal{E}_2(x_k)\|_2^2 | \tau] \lesssim \log T \sum_{i=1}^{n-1} (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i})^3 \int_{\widehat{\tau}_{k,i}}^{\widehat{\tau}_{k,i-1}} \mathbb{E}_{x_{\tau} \sim X_{\tau}} \left[\left\| \frac{\partial}{\partial \tau} \frac{s_{\tau}^*(x_{\tau})}{(1-\tau)^{3/2}} \right\|_2^2 \right] d\tau.$$

- Finally we intend to bound the term \mathcal{E}_3 . Recalling that $\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i} = \frac{c_1 \log T}{T} \widehat{\tau}_{k,i-1} (1 - \widehat{\tau}_{k,i-1})$, $\tau_{k,0} - \widehat{\tau}_{k,0} \leq \frac{c_1 \log T}{T} \widehat{\tau}_{k-1, \frac{N}{2}-1} (1 - \widehat{\tau}_{k-1, \frac{N}{2}-1}) \lesssim \frac{c_1 \log T}{T} \left(1 + \frac{c_1 \log T}{T}\right) \widehat{\tau}_{k,0} (1 - \widehat{\tau}_{k,0}) \lesssim \frac{c_1 \log T}{T} \widehat{\tau}_{k,0} (1 - \widehat{\tau}_{k,0})$, and $\widehat{\tau}_{k,n-1} - \tau_{k,n} \leq \widehat{\tau}_{k,n-1} - \widehat{\tau}_{k,n} \leq \frac{c_1 \log T}{T} \widehat{\tau}_{k,n-1} (1 - \widehat{\tau}_{k,n-1})$ in Lemma 1, we have that

$$\begin{aligned}
&\left\| \frac{s_{\tau_{k,0}}(x_{\tau_{k,0}}) - s_{\tau_{k,0}}^*(x_{\tau_{k,0}})}{(1 - \tau_{k,0})^{3/2}} (\tau_{k,0} - \widehat{\tau}_{k,0}) \right\|_2 \\
&\lesssim \frac{\log T}{T} \widehat{\tau}_{k,0} (1 - \widehat{\tau}_{k,0})^{-1/2} \left\| s_{\tau_{k,0}}(x_{\tau_{k,0}}) - s_{\tau_{k,0}}^*(x_{\tau_{k,0}}) \right\|_2, \\
&\left\| \frac{s_{\tau_{k,n-1}}(x_{\tau_{k,n-1}}) - s_{\tau_{k,n-1}}^*(x_{\tau_{k,n-1}})}{2(1 - \tau_{k,n-1})^{3/2}} (\widehat{\tau}_{k,n-1} - \tau_{k,n}) \right\|_2 \\
&\lesssim \frac{\log T}{T} \widehat{\tau}_{k,n-1} (1 - \widehat{\tau}_{k,n-1})^{-1/2} \left\| s_{\tau_{k,n-1}}(x_{\tau_{k,n-1}}) - s_{\tau_{k,n-1}}^*(x_{\tau_{k,n-1}}) \right\|_2 \\
&\left\| \frac{1}{2(1 - \tau_{k,i})^{3/2}} (s_{\tau_{k,i}}(x_{\tau_{k,i}}) - s_{\tau_{k,i}}^*(x_{\tau_{k,i}})) (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \right\|_2 \\
&\lesssim \frac{\log T}{T} \widehat{\tau}_{k,i-1} (1 - \widehat{\tau}_{k,i-1})^{-1/2} \left\| s_{\tau_{k,i}}(x_{\tau_{k,i}}) - s_{\tau_{k,i}}^*(x_{\tau_{k,i}}) \right\|_2 \\
&\lesssim \frac{\log T}{T} \widehat{\tau}_{k,i} (1 - \widehat{\tau}_{k,i})^{-1/2} \left\| s_{\tau_{k,i}}(x_{\tau_{k,i}}) - s_{\tau_{k,i}}^*(x_{\tau_{k,i}}) \right\|_2,
\end{aligned}$$

which comes from the fact that $(1 - \tau_{k,i})^{-3/2} \leq (1 - \hat{\tau}_{k,i-1})^{-3/2} \leq (1 - \frac{c_1 \log T}{T})^{-3/2} (1 - \hat{\tau}_{k,i})^{-3/2} \lesssim (1 - \hat{\tau}_{k,i})^{-3/2}$ for $0 \leq i \leq n-1$, and $\hat{\tau}_{k,i-1} (1 - \hat{\tau}_{k,i-1})^{-1/2} \lesssim (1 + \frac{c_1 \log T}{T})^1 (1 - \frac{c_1 \log T}{T})^{-1/2} \hat{\tau}_{k,i} (1 - \hat{\tau}_{k,i})^{-1/2} \lesssim \hat{\tau}_{k,i} (1 - \hat{\tau}_{k,i})^{-1/2}$ due to Lemma 1. Thus we have that

$$\|\mathcal{E}_3\|_2 \lesssim \frac{\log T}{T} \sum_{i=0}^{n-1} \hat{\tau}_{k,i} (1 - \hat{\tau}_{k,i})^{-1/2} \|s_{\tau_{k,i}}(x_{\tau_{k,i}}) - s_{\tau_{k,i}}^*(x_{\tau_{k,i}})\|_2.$$

Putting everything together, we have

$$\begin{aligned} \mathbb{E}_{x_k \sim p_{\hat{\tau}_k}} [\|\xi_{k,n}(x_k)\|_2^2] &\lesssim \frac{L^3 d (\hat{\tau}_{k,n-1} - \hat{\tau}_{k,n}) \log^3 T}{T^3 (1 - \hat{\tau}_{k,n-1})^2} + \frac{L^3 d (\hat{\tau}_{k,0} - \hat{\tau}_{k,1}) \log^3 T}{T^3 (1 - \hat{\tau}_{k,0})^2} \\ &\quad + \log T \sum_{i=1}^n (\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i})^3 \int_{\hat{\tau}_{k,i}}^{\hat{\tau}_{k,i-1}} \mathbb{E}_{x_\tau \sim X_\tau} \left[\left\| \frac{\partial}{\partial \tau} \frac{s_\tau^*(x_\tau)}{(1-\tau)^{3/2}} \right\|_2^2 \right] d\tau \\ &\quad + \frac{N \log^2 T}{T^2} \sum_{i=0}^{n-1} \hat{\tau}_{k,i}^2 (1 - \hat{\tau}_{k,i})^{-1} \|s_{\tau_{k,i}}(x_{\tau_{k,i}}) - s_{\tau_{k,i}}^*(x_{\tau_{k,i}})\|_2^2. \end{aligned}$$

According to (25), we have that

$$\begin{aligned} &(\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i})^3 \int_{\hat{\tau}_{k,i}}^{\hat{\tau}_{k,i-1}} \mathbb{E}_{x_\tau \sim X_\tau} \left[\left\| \frac{\partial}{\partial \tau} \frac{s_\tau^*(x_\tau)}{(1-\tau)^{3/2}} \right\|_2^2 \right] d\tau \\ &\stackrel{(a)}{\lesssim} \frac{\log^3 T \hat{\tau}_{k,i-1}^3 (1 - \hat{\tau}_{k,i-1})^3}{T^3} \left(L \vee \frac{1}{\hat{\tau}_{k,i}} \right) \frac{L^2 d (\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i})}{(1 - \hat{\tau}_{k,i-1})^5} \\ &\lesssim \frac{L^3 d \log^3 T (\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i})}{T^3 (1 - \hat{\tau}_{k,i-1})^2}, \quad 1 \leq i \leq n, \end{aligned}$$

where (a) comes from Lemma 1, and the fact that $\hat{\tau}_{k,i-1}/\hat{\tau}_{k,i} \lesssim (1 + c_1 \log T/T) \lesssim 1$. In addition, the definition $\mathbb{E}[\|s_{\tau_{k,i}}(x_{\tau_{k,i}}) - s_{\tau_{k,i}}^*(x_{\tau_{k,i}})\|_2^2] = \varepsilon_{T - \frac{kN}{2} - i + 1}^2$ leads to our desired result.

Proof of Claim (25). We first make the following decomposition

$$\frac{\partial(1-\tau)^{-3/2} s_\tau^*(x_\tau)}{\partial \tau} = \frac{\partial(1-\tau)^{-3/2} s_\tau^*(\sqrt{1-\tau}x)}{\partial \tau} \Big|_{x=\frac{x_\tau}{\sqrt{1-\tau}}} + \frac{\partial(1-\tau)^{-3/2} s_\tau^*(\sqrt{1-\tau}x)}{\partial x} \Big|_{x=\frac{x_\tau}{\sqrt{1-\tau}}} \frac{\partial x_\tau / \sqrt{1-\tau}}{\partial \tau},$$

where

$$\left\| \frac{\partial(1-\tau)^{-3/2} s_\tau^*(\sqrt{1-\tau}x)}{\partial x} \right\| \leq (1-\tau)^{-1} L,$$

and

$$\mathbb{E}_{x_\tau \sim X_\tau} \left[\left\| \frac{\partial x_\tau / \sqrt{1-\tau}}{\partial \tau} \right\|_2^2 \right] \leq \mathbb{E}_{x_\tau \sim X_\tau} \left[\left\| \frac{s_\tau^*(x_\tau)}{2(1-\tau)^{3/2}} \right\|_2^2 \right] \lesssim \frac{d}{\tau(1-\tau)^3}.$$

Then it is sufficient to control the first term.

Denote

$$\bar{\tau} := \max \left\{ 0, \tau - \frac{1-\tau}{2L} \right\},$$

which satisfies that

$$\frac{1-\tau}{\tau-\bar{\tau}} = 2L \vee \frac{1-\tau}{\tau} \asymp L \vee \frac{1}{\tau} \quad \text{and} \quad 1-\bar{\tau} \asymp 1-\tau.$$

Then according to the relation

$$X_\tau = \sqrt{\frac{1-\tau}{1-\bar{\tau}}} X_{\bar{\tau}} + \sqrt{\frac{\tau-\bar{\tau}}{1-\bar{\tau}}} Z,$$

the score function can also be expressed as

$$\begin{aligned} s_\tau^*(\sqrt{1-\tau}x) &= -\frac{\sqrt{(1-\tau)(1-\bar{\tau})}}{\tau-\bar{\tau}} \int_y p_{X_\tau|X_\tau}(y|\sqrt{1-\tau}x)(\sqrt{1-\bar{\tau}}x-y)dy \\ &= \sqrt{\frac{1-\bar{\tau}}{1-\tau}} \int_y p_{X_\tau|X_\tau}(y|\sqrt{1-\tau}x) \nabla \log p_{X_\tau}(y) dy, \end{aligned}$$

where

$$p_{X_\tau|X_\tau}(y|\sqrt{1-\tau}x) \propto p_{X_\tau}(y) \exp\left(-\frac{(1-\tau)\|\sqrt{1-\bar{\tau}}x-y\|_2^2}{2(\tau-\bar{\tau})}\right),$$

This gives us

$$\begin{aligned} \frac{\partial(1-\tau)^{-3/2}s_\tau^*(\sqrt{1-\tau}x)}{\partial\tau} &= \frac{2\sqrt{1-\bar{\tau}}}{(1-\tau)^3} \int_y p_{X_\tau|X_\tau}(y|\sqrt{1-\tau}x)(\sqrt{1-\bar{\tau}}x-y)dy \\ &\quad + \frac{\sqrt{1-\bar{\tau}}}{(1-\tau)^2} \int_y \frac{\partial}{\partial\tau} p_{X_\tau|X_\tau}(y|\sqrt{1-\tau}x) \nabla \log p_{X_\tau}(y) dy \end{aligned}$$

In addition, with basic calculations, it can be shown that

$$\mathbb{E}_{\sqrt{1-\tau}x \sim X_\tau} \left[\left\| \sqrt{\frac{1-\bar{\tau}}{1-\tau}} \int_y p_{X_\tau|X_\tau}(y|\sqrt{1-\tau}x) \nabla \log p_{X_\tau}(y) dy \right\|_2^2 \right] \leq \frac{d}{\tau},$$

and

$$\mathbb{E}_{\sqrt{1-\tau}x \sim X_\tau} \left[\left\| \int_y \frac{\partial}{\partial\tau} p_{X_\tau|X_\tau}(y|\sqrt{1-\tau}x) \nabla \log p_{X_\tau}(y) dy \right\|_2^2 \right] \leq \frac{L^2(1-\bar{\tau})^2 d}{(1-\tau)^3(\tau-\bar{\tau})}.$$

where the latter relation can be derived in a similar way to Lemma 1 in [Chen et al. \(2024b\)](#), and it is omitted here for simplicity. Putting everything together leads to

$$\mathbb{E}_{\sqrt{1-\tau}x \sim X_\tau} \left[\left\| \frac{\partial(1-\tau)^{-3/2}s_\tau^*(\sqrt{1-\tau}x)}{\partial\tau} \right\|_2^2 \right] \lesssim \frac{d}{\tau(1-\tau)^5} + \frac{L^2(1-\bar{\tau})^3 d}{(1-\tau)^7(\tau-\bar{\tau})} \lesssim \left(L \vee \frac{1}{\tau}\right) \frac{L^2 d}{(1-\tau)^5}.$$

A.2 PROOF OF LEMMA 4

According to (20), we have that

$$\begin{aligned} \text{KL}(p_{\hat{X}_{k+1}|\hat{X}_k}(\cdot|x_k) \| p_{Y_{k+1}|Y_k}(\cdot|x_k)) &= \frac{1-\tau_{k+1,0}}{2(\tau_{k+1,0}-\tau_{k,N})} \|y_{\tau_{k,N}} - x_{\tau_{k,N}}\|_2^2 \\ &\stackrel{(i)}{\lesssim} \frac{T}{N\hat{\tau}_{k,N} \log T} \|y_{\tau_{k,N}} - x_{\tau_{k,N}}\|_2^2, \end{aligned} \quad (30)$$

where $y_{\tau_{k,N}}$ and $x_{\tau_{k,N}}$ are defined as

$$\begin{aligned} \frac{y_{\tau_{k,N}}}{\sqrt{1-\tau_{k,N}}} &= \frac{y_{\tau_{k,0}}}{\sqrt{1-\tau_{k,0}}} + \frac{s_{\tau_{k,0}}(y_{\tau_{k,0}})}{2(1-\tau_{k,0})^{3/2}} (\tau_{k,0} - \hat{\tau}_{k,0}) + \sum_{i=1}^{N-1} \frac{s_{\tau_{k,i}}(y_{\tau_{k,i}})}{2(1-\tau_{k,i})^{3/2}} (\hat{\tau}_{k,i-1} - \hat{\tau}_{k,i}) \\ &\quad + \frac{s_{\tau_{k,N-1}}(y_{\tau_{k,N-1}})}{2(1-\tau_{k,N-1})^{3/2}} (\hat{\tau}_{k,N-1} - \tau_{k,N}), \\ \frac{x_{\tau_{k,N}}}{\sqrt{1-\tau_{k,N}}} &= \frac{x_{\tau_{k,0}}}{\sqrt{1-\tau_{k,0}}} + \int_{\tau_{k,N}}^{\tau_{k,0}} \frac{s_\tau^*(x_\tau)}{2(1-\tau)^{3/2}} d\tau, \end{aligned}$$

according to (21) and (16), with $x_{\tau_{k,0}} = y_{\tau_{k,0}} = x_k$. Here the inequality (i) holds because

$$\begin{aligned} \tau_{k+1,0} - \tau_{k,N} &= \bar{\alpha}_{T-\frac{kN}{2}-N+1} - \bar{\alpha}_{T-\frac{kN}{2}-\frac{N}{2}+1} \geq \hat{\alpha}_{T-\frac{kN}{2}-N+1} - \hat{\alpha}_{T-\frac{kN}{2}-\frac{N}{2}} \\ &= \sum_{i=1}^{\frac{N}{2}+1} \left(\hat{\alpha}_{T-\frac{kN}{2}-N+i} - \hat{\alpha}_{T-\frac{kN}{2}-N+i+1} \right) \gtrsim \frac{N\hat{\alpha}_{T-\frac{kN}{2}-\frac{N}{2}}(1-\hat{\alpha}_{T-\frac{kN}{2}-N+1}) \log T}{T} \end{aligned}$$

$$= \frac{N(1 - \widehat{\tau}_{k+1,0})\widehat{\tau}_{k,N} \log T}{T} \gtrsim \frac{N(1 - \tau_{k+1,0})\widehat{\tau}_{k,N} \log T}{T}.$$

Combining the above definitions, we have

$$\begin{aligned} \frac{y_{\tau_{k,n}} - x_{\tau_{k,n}}}{\sqrt{1 - \tau_{k,n}}} &= -\xi_{k,n} + \sum_{i=1}^{n-1} \frac{1}{2(1 - \tau_{k,i})^{3/2}} (s_{\tau_{k,i}}(y_{\tau_{k,i}}) - s_{\tau_{k,i}}(x_{\tau_{k,i}})) (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \\ &\quad + \frac{s_{\tau_{k,0}}(y_{\tau_{k,0}}) - s_{\tau_{k,0}}(x_{\tau_{k,0}})}{2(1 - \tau_{k,0})^{3/2}} (\tau_{k,0} - \widehat{\tau}_{k,0}) + \frac{s_{\tau_{k,n-1}}(y_{\tau_{k,n-1}}) - s_{\tau_{k,n-1}}(x_{\tau_{k,n-1}})}{2(1 - \tau_{k,n-1})^{3/2}} (\widehat{\tau}_{k,n-1} - \tau_{k,n}). \end{aligned}$$

According to Lemma 3, we have

$$\begin{aligned} \left\| \sum_{i=1}^{n-1} \frac{1}{2(1 - \tau_{k,i})^{3/2}} (s_{\tau_{k,i}}(y_{\tau_{k,i}}) - s_{\tau_{k,i}}(x_{\tau_{k,i}})) (\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}) \right\|_2 &\lesssim \sum_{i=1}^{n-1} \frac{L \log T}{T \sqrt{1 - \tau_{k,i}}} \|y_{\tau_{k,i}} - x_{\tau_{k,i}}\|_2, \\ \frac{\|s_{\tau_{k,0}}(y_{\tau_{k,0}}) - s_{\tau_{k,0}}(x_{\tau_{k,0}})\|_2}{2(1 - \tau_{k,0})^{3/2}} (\tau_{k,0} - \widehat{\tau}_{k,0}) &= 0, \\ \frac{\|s_{\tau_{k,n-1}}(y_{\tau_{k,n-1}}) - s_{\tau_{k,n-1}}(x_{\tau_{k,n-1}})\|_2}{2(1 - \tau_{k,n-1})^{3/2}} (\widehat{\tau}_{k,n-1} - \tau_{k,n}) &\lesssim \frac{L \log T}{T \sqrt{1 - \tau_{k,n-1}}} \|y_{\tau_{k,n-1}} - x_{\tau_{k,n-1}}\|_2, \end{aligned}$$

due to the L -Lipschitz property of s and the relation

$$\begin{aligned} \frac{\widehat{\tau}_{k,i-1} - \widehat{\tau}_{k,i}}{1 - \tau_{k,i}} &\lesssim \frac{(1 - \widehat{\tau}_{k,i-1}) \log T}{T(1 - \tau_{k,i})} \lesssim \frac{\log T}{T}, \\ \frac{\widehat{\tau}_{k,n-1} - \tau_{k,n}}{1 - \tau_{k,n-1}} &\lesssim \frac{(1 - \widehat{\tau}_{k,n-1}) \log T}{T(1 - \widehat{\tau}_{k,n-2})} \lesssim \frac{\log T}{T}, \quad n \geq 2. \end{aligned}$$

If $n = 1$, then the above inequality holds by replacing $\widehat{\tau}_{k,n-2}$ with $\widehat{\tau}_{k-1, \frac{N}{2}-1}$ and $\widehat{\tau}_{-1, \frac{N}{2}-1}$ is defined as $1 - \widehat{\alpha}_{T+1}$. Combining the above inequalities gives us

$$\frac{\|y_{\tau_{k,n}} - x_{\tau_{k,n}}\|_2}{\sqrt{1 - \tau_{k,n}}} \lesssim \frac{L \log T}{T} \sum_{i=1}^{n-1} \frac{\|y_{\tau_{k,i}} - x_{\tau_{k,i}}\|_2}{\sqrt{1 - \tau_{k,i}}} + \|\xi_{k,n}\|_2.$$

Applying the above relation recursively leads to

$$\frac{\|y_{\tau_{k,n}} - x_{\tau_{k,n}}\|_2}{\sqrt{1 - \tau_{k,n}}} \lesssim \frac{L \log T}{T} \sum_{i=1}^{n-1} \|\xi_{k,i}\|_2 + \|\xi_{k,n}\|_2,$$

provided that $T \gtrsim NL \log T$. For convenience, denote the upper bound of $\mathbb{E}_{x_k \sim p_{\widehat{x}_k}} [\|\xi_{k,n}(x_k)\|_2^2]$ in Lemma 3 as $\widehat{\xi}_{k,n}^2(x_k)$. Recall that $\widehat{\xi}_{k,n}^2(x_k)$ increases with n , and $T \gtrsim NL \log T$. Then we have

$$\begin{aligned} \mathbb{E}_{x_k \sim p_{\widehat{x}_k}} \left[\frac{\|y_{\tau_{k,N}} - x_{\tau_{k,N}}\|_2^2}{1 - \tau_{k,N}} \right] &\lesssim \frac{NL^2 \log^2 T}{T^2} \sum_{i=1}^{N-1} \widehat{\xi}_{k,N}^2 + \widehat{\xi}_{k,N}^2 \\ &\lesssim \left(1 + \frac{N^2 L^2 \log^2 T}{T^2} \right) \widehat{\xi}_{k,N}^2 \lesssim \widehat{\xi}_{k,N}^2. \end{aligned}$$

Inserting into (30), we have

$$\begin{aligned} \text{KL}(p_{\widehat{x}_{k+1}|\widehat{x}_k}(\cdot | x_k) \| p_{Y_{k+1}|Y_k}(\cdot | x_k)) &\lesssim \frac{T(1 - \tau_{k,N})}{N\widehat{\tau}_{k,N} \log T} \widehat{\xi}_{k,N}^2 \\ &\stackrel{(a)}{\lesssim} \frac{T(1 - \tau_{k,N})}{N\widehat{\tau}_{k,N} \log T} \left(\sum_{i=1}^N \frac{L^3 d \log^4 T}{(1 - \widehat{\tau}_{k,i-1})^2 T^3} (\widehat{\tau}_{k,i} - \widehat{\tau}_{k,i-1}) + \frac{N \log^2 T}{T^2} \sum_{i=0}^{N-1} \widehat{\tau}_{k,i} (1 - \widehat{\tau}_{k,i})^{-1} \varepsilon_{T - \frac{kN}{2} - i+1}^2 \right), \end{aligned} \tag{31}$$

where (a) uses Lemma 3. The first term is bounded by

$$\begin{aligned} \frac{T(1 - \tau_{k,N})}{N\widehat{\tau}_{k,N} \log T} \sum_{i=1}^N \frac{L^3 d \log^4 T}{(1 - \widehat{\tau}_{k,i-1})^2 T^3} (\widehat{\tau}_{k,i} - \widehat{\tau}_{k,i-1}) &\lesssim \frac{L^3 d \log^3 T (1 - \tau_{k,N})}{NT^2 \widehat{\tau}_{k,N}} \sum_{i=1}^N \frac{(\widehat{\tau}_{k,i} - \widehat{\tau}_{k,i-1})}{(1 - \widehat{\tau}_{k,i-1})^2} \\ &\lesssim \frac{L^3 d \log^4 T (1 - \tau_{k,N})}{NT^3 \widehat{\tau}_{k,N}} \sum_{i=1}^N \frac{\widehat{\tau}_{k,i-1}}{(1 - \widehat{\tau}_{k,i-1})} \\ &\lesssim \frac{L^3 d \log^4 T}{T^3} \frac{\widehat{\tau}_{k,0}(1 - \tau_{k,N})}{(1 - \widehat{\tau}_{k,0})\widehat{\tau}_{k,N}}. \end{aligned}$$

To further bound the above terms, we claim that provided $T \gtrsim N \log T$,

$$\frac{\widehat{\tau}_{k,0}(1 - \widehat{\tau}_{k,N})}{(1 - \widehat{\tau}_{k,0})\widehat{\tau}_{k,N}} \lesssim 1, \quad (32)$$

the proof of which is postponed to the end of this section. Then recalling that $\widehat{\tau}_{k,N} \leq \tau_{k,N}$, we have

$$\frac{T(1 - \tau_{k,N})}{N\widehat{\tau}_{k,N} \log T} \sum_{i=1}^{N-1} \frac{L^3 d \log^4 T}{(1 - \widehat{\tau}_{k,i})^2 T^3} (\widehat{\tau}_{k,i} - \widehat{\tau}_{k,i-1}) \lesssim \frac{L^3 d \log^4 T}{T^3}.$$

Next, the second term in (31) is bounded by

$$\begin{aligned} \frac{T(1 - \tau_{k,N})}{N\widehat{\tau}_{k,N} \log T} \frac{N \log^2 T}{T^2} \sum_{i=0}^{N-1} \widehat{\tau}_{k,i} (1 - \widehat{\tau}_{k,i})^{-1} \varepsilon_{T - \frac{kN}{2} - i + 1}^2 &\leq \frac{\log T}{T} \frac{(1 - \tau_{k,N})\widehat{\tau}_{k,0}}{\widehat{\tau}_{k,N}(1 - \widehat{\tau}_{k,0})} \sum_{i=0}^{N-1} \varepsilon_{T - \frac{kN}{2} - i + 1}^2 \\ &\stackrel{(a)}{\lesssim} \frac{\log T}{T} \sum_{i=0}^{N-1} \varepsilon_{T - \frac{kN}{2} - i + 1}^2, \end{aligned}$$

where (a) uses (32).

Combining these relations gives

$$\mathbb{E}_{x_k \sim p_{\widehat{X}_k}} \left[\text{KL} \left(p_{\widehat{X}_{k+1} | \widehat{X}_k}(\cdot | x_k) \parallel p_{Y_{k+1} | Y_k}(\cdot | x_k) \right) \right] \lesssim \frac{L^3 d \log^4 T}{T^3} + \frac{\log T}{T} \sum_{i=0}^{N-1} \varepsilon_{T - \frac{kN}{2} - i + 1}^2.$$

Proof of Claim (32). According to the definition of $\tau_{k,i}$, we have that

$$\frac{1 - \widehat{\tau}_{k,N}}{1 - \widehat{\tau}_{k,0}} = \frac{\widehat{\alpha}_{T - \frac{kN}{2} - N}}{\widehat{\alpha}_{T - \frac{kN}{2}}} \leq \left(1 + \frac{c_1 \log T}{T} \right)^N,$$

and

$$\frac{\widehat{\tau}_{k,0}}{\widehat{\tau}_{k,N}} = \frac{1 - \widehat{\alpha}_{T - \frac{kN}{2}}}{1 - \widehat{\alpha}_{T - \frac{kN}{2} - N}} \leq \left(1 - \frac{c_1 \log T}{T} \right)^{-N}.$$

Thus we have

$$\frac{(1 - \widehat{\tau}_{k,N})\widehat{\tau}_{k,0}}{(1 - \widehat{\tau}_{k,0})\widehat{\tau}_{k,N}} \leq \left(\frac{1 + \frac{c_1 \log T}{T}}{1 - \frac{c_1 \log T}{T}} \right)^N \leq \exp \left(\frac{2Nc_1 \log T}{1 - \frac{c_1 \log T}{T}} \right) \lesssim 1.$$

B PROOF OF AUXILIARY LEMMAS IN THEOREM 1

B.1 PROOF OF LEMMA 1

The first relation is immediately obtained by noticing that

$$1 - \tau_{0,0} = \bar{\alpha}_{T+1} \leq \widehat{\alpha}_T \leq 2\widehat{\alpha}_{T+1},$$

provided that $\frac{c_1 \log T}{T} < 1$.

Regarding the second inequality, for $T_0 = (1 - \frac{3c_0}{c_1})T + 1$ and $c_1 > 3c_0$, we claim that $\hat{\alpha}_{T_0} \geq \frac{1}{2}$; otherwise, we have

$$\hat{\alpha}_{t-1} = \hat{\alpha}_t \left(1 + \frac{c_1 \hat{\alpha}_t \log T}{T}\right) > \hat{\alpha}_t \left(1 + \frac{c_1 \log T}{2T}\right),$$

and then

$$\hat{\alpha}_{T_0} > \hat{\alpha}_{T+1} \left(1 + \frac{c_1 \log T}{2T}\right)^{T-T_0+1} > \frac{1}{2}.$$

Then if $c_1 > 5c_0$, we have

$$\tau_{K,0} = 1 - \bar{\alpha}_1 \leq 1 - \hat{\alpha}_1 \leq (1 - \hat{\alpha}_{T_0}) \left(1 - \frac{c_1 \log T}{2T}\right)^{T_0-1} \leq \frac{1}{T^{c_0}},$$

where we make use of the observation that for $t \leq T_0$,

$$1 - \hat{\alpha}_{t-1} = (1 - \hat{\alpha}_t) \left(1 - \frac{c_1 \hat{\alpha}_t \log T}{T}\right) \leq (1 - \hat{\alpha}_t) \left(1 - \frac{c_1 \log T}{2T}\right).$$

The third equation follows immediately from the definition of $\hat{\tau}_{k,n}$ that

$$\frac{\hat{\tau}_{k,n-1} - \hat{\tau}_{k,n}}{\hat{\tau}_{k,n-1}(1 - \hat{\tau}_{k,n-1})} = \frac{\hat{\alpha}_{T - \frac{kN}{2} - n} - \hat{\alpha}_{T - \frac{kN}{2} - n + 1}}{(1 - \hat{\alpha}_{T - \frac{kN}{2} - n + 1})\hat{\alpha}_{T - \frac{kN}{2} - n + 1}} = \frac{c_1 \log T}{T}.$$

B.2 PROOF OF LEMMA 2

Notice that the map Φ in (17) is just the integral form of (16), which is equivalent to

$$dx_\tau = -\frac{1}{2(1-\tau)}(x_\tau + s_\tau^*(x_\tau))d\tau.$$

This is the well-known probability ODE flow, which comes from Song et al. (2021) and is also used in Li et al. (2023).

The proof of (18) can be completed by using mathematical induction. Recalling that $\hat{X}_0 \stackrel{d}{=} X_{\tau_{0,0}}$, the (18) holds for $k+1 = 0$. Assume that (18) holds for $k+1 = h$. We have $\Phi_{\tau_{h-1,0} \rightarrow \tau_{h-1,N}}(\hat{X}_{h-1}) \stackrel{d}{=} X_{\tau_{h-1,N}}$. According to (15), we could immediately get that (18) holds for $k = h$.

B.3 PROOF OF LEMMA 5

According to Lemma 2, we know that $\hat{X}_0 \stackrel{d}{=} X_{\tau_{0,0}} = \sqrt{1 - \tau_{0,0}}X_0 + \sqrt{\tau_{0,0}}Z$ for some standard Gaussian variable Z . Then we have

$$\begin{aligned} \text{KL}(p_{\hat{X}_0} \| p_{Y_0}) &\leq \text{KL}(p_{X_{\tau_{0,0}}, X_0} \| p_{Y_0} p_{X_0}) = \mathbb{E}_{X_0 \sim p_{\text{data}}} [\text{KL}(p_{\hat{X}_0 | X_0} \| p_{Y_0})] \\ &= \frac{1}{2} \left[(1 - \tau_{0,0}) \mathbb{E}_{X_0 \sim p_{\text{data}}} \|X_0\|^2 - d \log(\tau_{0,0}) + d\tau_{0,0} - d \right] \\ &\leq \frac{1}{2} T^{c_R - c_0} + d \frac{(1 - \tau_{0,0})^2}{2\tau_{0,0}} \leq \frac{1}{2} T^{c_R - c_0} + \frac{d}{T^{2c_0}} \leq \frac{1}{T^{10}}, \end{aligned}$$

as long as $c_0 \geq \max\{c_R + 10, 10\}$, and $T \gtrsim d^{1/10}$. In addition, the analysis of $\text{TV}(p_{\text{data}}, p_{\hat{X}_K})$ can be found in the proof of Theorem 2 in (Chen et al., 2024b).