
Advancing Wasserstein Convergence Analysis of Score-Based Models: Insights from Discretization and Second-Order Acceleration

Yifeng Yu
Tsinghua University
yyf22@mails.tsinghua.edu.cn

Lu Yu *
City University of Hong Kong
lu.yu@cityu.edu.hk

Abstract

Score-based diffusion models have emerged as powerful tools in generative modeling, yet their theoretical foundations remain underexplored. In this work, we focus on the Wasserstein convergence analysis of score-based diffusion models. Specifically, we investigate the impact of various discretization schemes, including Euler discretization, exponential integrators, and midpoint randomization methods. Our analysis provides the first quantitative comparison of these discrete approximations, emphasizing their influence on convergence behavior. Furthermore, we explore scenarios where Hessian information is available and propose an accelerated sampler based on the local linearization method. We establish the first Wasserstein convergence analysis for such a Hessian-based method, showing that it achieves an improved convergence rate of order $\tilde{O}(\sqrt{d}/\varepsilon)$, which significantly outperforms the standard rate $\tilde{O}(d/\varepsilon^2)$ of vanilla diffusion models. Numerical experiments on synthetic data and the MNIST dataset validate our theoretical insights.

1 Introduction

Diffusion models have become a pivotal framework in modern generative modeling, achieving notable success across fields such as image generation [11, 17, 31, 34], natural language processing [30], and computational biology [1, 42]. These models add noise to data via a forward process and learn to reverse it, reconstructing data from noise. This approach enables them to capture the underlying structure of complex, high-dimensional data distributions. For a detailed review of diffusion models, we refer the readers to [6, 39, 43].

A widely adopted formulation of diffusion models is the score-based generative model (SGM), implemented using stochastic differential equations (SDEs) [36]. Broadly speaking, SGMs rely on two key stochastic processes: a forward process that gradually transforms data samples into pure noise, and a backward process that reverses this transformation, recovering the target data distribution from noise.

Despite the remarkable empirical success of diffusion models across various applications, their theoretical understanding remains limited. In recent years, there has been a rapidly expanding body of research on the convergence theory of diffusion models. Generally, these contributions can be divided into two main approaches, each focusing on different metrics and divergences. The first category investigates convergence bounds based on α -divergence, including the Kullback–Leibler (KL) divergence and the total variation (TV) distance (see e.g., [5, 7, 8, 22, 26, 41]). Among these works, several explore acceleration techniques that leverage higher-order information about the log density (see e.g., [19, 24, 27]). The second category focuses on convergence bounds in Wasserstein

*Corresponding author

distance, which is often considered more practical and informative for estimation tasks. One line of work within this category assumes strong log-concavity of the data distribution and access to accurate estimates of the score function [3, 13, 37, 38]. Another line of work focuses on specific structural assumptions of the data distribution [10, 14, 29].

Much of the existing literature on the convergence theory of diffusion models relies on the Euler discretization method. Notably, [5] compare the behavior of Euler discretization and exponential integrators [18, 47] in terms of KL divergence. Additionally, [10] provide a comparative analysis of these two schemes, though without formal theoretical guarantees. A comprehensive and systematic understanding of how different discretization schemes influence convergence performance in diffusion models remains underexplored. Furthermore, while convergence analyses of accelerated diffusion models primarily focus on TV or KL distances, studies investigating Wasserstein convergence for these accelerations remain lacking².

In this work, we address these challenges by analyzing the Wasserstein convergence of score-based diffusion models when the data distribution has a smooth and strongly log-concave density. Specifically, we investigate the impact of different discretization schemes on convergence behavior. Beyond the widely used Euler method and exponential integrator, we explore the midpoint randomization method. This method was initially introduced in [32] for discretizing kinetic Langevin diffusion [9] and then has been extensively studied in log-concave sampling complexity theory [16, 21, 44–46]. It was later applied to diffusion models [15, 23], showing improved KL and TV convergence performance over vanilla models and offering easy parallelization.

We also consider scenarios where accurate estimates of the Hessian of the log density are accessible. Inspired by [33], we propose a novel sampler based on the *local linearization* method. Our analysis shows that this approach significantly accelerates convergence in Wasserstein distance.

Our contribution can be summarized as follows.

- We establish convergence guarantees for SGMs in the Wasserstein-2 distance under various discretization methods, including the Euler method, exponential integrators, the midpoint randomization method, and a hybrid approach combining the latter two.
- We introduce a novel Hessian-based accelerated sampler for the stochastic diffusion process, leveraging the local linearization method. We then establish its Wasserstein convergence analysis in Theorem 4, achieving state-of-the-art order of $\tilde{\mathcal{O}}(\sqrt{d}/\varepsilon)$.
- Section 5 compares the performance of SGMs under four discretization schemes and the proposed Hessian-based method on both synthetic data and the MNIST dataset. The results align with our theory and highlight the acceleration of the proposed second-order method.

In summary, our analysis provides a quantitative comparison of different discrete approximations, offering practical guidance for choosing discretization. Moreover, we present the first Wasserstein convergence analysis of an accelerated sampler that leverages the second-order information about log-densities. This accelerated sampler achieves a faster convergence rate $\tilde{\mathcal{O}}(\sqrt{d}/\varepsilon)$, compared to the standard rate $\tilde{\mathcal{O}}(d/\varepsilon^2)$ of vanilla diffusion models. These results contribute to the understanding of Wasserstein convergence in score-based models, shedding light on aspects that have not been extensively explored before.

Notation. Let $\mathbb{R}^d$ be the d -dimensional Euclidean space and I_d the identity matrix. The gradient and the Hessian of a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ are denoted by ∇f and $\nabla^2 f$. Given any pair of measures μ and ν , the Wasserstein-2 distance between μ and ν is defined as

$$W_2(\mu, \nu) = \left(\inf_{\varrho \in \Gamma(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 d\varrho(x, y) \right)^{1/2},$$

where the infimum is taken over all joint distributions ϱ that have μ and ν as marginals. For two symmetric $d \times d$ matrices A and B , we use $A \preceq B$ or $B \succeq A$ to denote the relation that $B - A$ is positive semi-definite. For any random vector X , let $\mathcal{L}(X)$ denote its law, and define $\|X\|_{\mathbb{L}_2} := \sqrt{\mathbb{E}[\|X\|^2]}$, where $\|\cdot\|$ denotes the Euclidean norm. For any random matrix A , define $\|A\|_{\mathbb{L}_2} := \sqrt{\mathbb{E}[\|A\|_2^2]}$, where $\|\cdot\|_2$ denotes the matrix 2-norm.

²Due to space constraints, we defer the discussion of related theoretical advancements in accelerating samplers for diffusion models to Appendix A.

2 Background and Our Setting

Framework. We consider the forward process

$$dX_t = f(X_t, t) dt + g(X_t, t) dB_t, \quad (1)$$

where the initial point $X_0 \sim p_0$ follows the data distribution, and B_t denotes the standard d -dimensional Brownian motion. Here, the drift $f : \mathbb{R}^d \times \mathbb{R}_+ \rightarrow \mathbb{R}^d$ and the function $g : \mathbb{R}^d \times \mathbb{R}_+ \rightarrow \mathbb{R}^{d \times d}$ are diffusion parameters. Some conditions are necessary to ensure that the SDE (1) is well-defined. In practice, various choices for the pair (f, g) are employed, depending on the specific needs of the model; for a detailed survey, we refer to [39]. For clarity, we adopt the simplest possible choice in this work by setting $f(X_t, t) = -X_t/2$ and $g(X_t, t) = 1$. This results in the Ornstein-Uhlenbeck process, which is described by the following SDE:

$$dX_t = -\frac{1}{2}X_t dt + dB_t. \quad (2)$$

The forward process (2) is run until a sufficiently large time $T > 0$, at which point the corrupted marginal distribution of X_T , denoted by p_T , is expected to approximate the standard Gaussian distribution. Then, diffusion models generate new data by reversing the SDE (2), which leads to the following backward SDE

$$dX_t^\leftarrow = \frac{1}{2}(X_t^\leftarrow + 2\nabla \log p_{T-t}(X_t^\leftarrow)) dt + dW_t, \quad (3)$$

where $X_0^\leftarrow \sim p_T$, and the term $\nabla \log p_t$, referred to as the *score function* for p_t , is represented by the gradient of the log density function of p_t . Additionally, W_t denotes another standard Brownian motion independent of B_t . Under mild conditions, when initialized at $X_0^\leftarrow \sim p_T$, the backward process $\{X_t^\leftarrow\}_{0 \leq t \leq T}$ has the same distribution as the forward process $\{X_{T-t}\}_{0 \leq t \leq T}$ [2, 4]. As a result, running the reverse diffusion $X_t^\leftarrow$ from $t = 0$ to T will generate a sample from the target data distribution p_0 . Note that the density p_T is unknown; we approximate it using the distribution

$$\hat{p}_T = \mathcal{N}(0, (1 - e^{-T})I_d)$$

as proposed in [13]. Therefore, we derive a reverse diffusion process defined by

$$dY_t = \frac{1}{2}(Y_t + 2\nabla \log p_{T-t}(Y_t)) dt + dW_t, \quad Y_0 \sim \hat{p}_T. \quad (4)$$

Score Matching. Another challenge in working with (3) is that the score function $\nabla \log p_t$ is unknown, as the distribution p_t is not explicitly available. In practice, rather than using the exact score function $\nabla \log p_{T-t}$, approximate estimates for it are learned from the data by training neural networks on a score-matching objective [20, 35, 40]. This objective is given by

$$\underset{\theta \in \Theta}{\text{minimize}} \quad \mathbb{E}[\|s_\theta(t, X_t) - \nabla \log p_t(X_t)\|^2],$$

where $\{s_\theta : \theta \in \Theta\}$ is a sufficiently rich function class, such as that of neural network. Substituting the learned score estimate s_* into the backward process (3), we obtain the following practical continuous-time backward SDE,

$$dX_t^\leftarrow = \frac{1}{2}(X_t^\leftarrow + 2s_*(T-t, X_t^\leftarrow)) dt + dW_t. \quad (5)$$

Since this continuous backward SDE cannot be simulated exactly, it is typically approximated using discretization methods.

Discretization Schemes. We outline the four discretization methods considered in this work for solving the practical reverse SDE (5). Let $h > 0$ be the step size. Without loss of generality, we assume $T = Nh$, where N is a positive integer. For simplicity, we denote $\frac{1}{2}X_t^\leftarrow + s_*(T-t, X_t^\leftarrow)$ by $\gamma(T-t, X_t^\leftarrow)$, and define

$$\Delta_h W_t := W_{t+h} - W_t, \quad \bar{\Delta}_h W_t := \int_t^{t+h} e^{\frac{t+h-s}{2}} dW_s.$$

• **EULER-MARUYAMA SCHEME:** Given the step size h , the following approximation holds

$$X_{t+h}^\leftarrow = X_t^\leftarrow + \int_0^h \gamma(T-(t+v), X_{t+v}^\leftarrow) dv + \Delta_h W_t \approx X_t^\leftarrow + h\gamma(T-t, X_t^\leftarrow) + \Delta_h W_t.$$

We derive the following discretized process for $n = 0, \dots, N - 1$:

$$\vartheta_{n+1}^{\text{EM}} = (1 + h/2)\vartheta_n^{\text{EM}} + hs_*(T - nh, \vartheta_n^{\text{EM}}) + \sqrt{h}\xi_n,$$

where $\vartheta_0^{\text{EM}} \sim \hat{p}_T$ and $\xi_n \sim \mathcal{N}(0, I_d)$.

• **EXPONENTIAL INTEGRATOR:** Inspired by the work [18], [47] propose a more refined discretization method which solves the backward SDE (3) explicitly, yielding the following approximation

$$\begin{aligned} X_{t+h}^{\leftarrow} &= e^{\frac{h}{2}} X_t^{\leftarrow} + \int_0^h e^{\frac{h-v}{2}} s_*(T - t - v, X_{t-v}^{\leftarrow}) dv + \bar{\Delta}_h W_t \\ &\approx e^{\frac{h}{2}} X_t^{\leftarrow} + 2(e^{\frac{h}{2}} - 1)s_*(T - t, X_t^{\leftarrow}) + \bar{\Delta}_h W_t. \end{aligned}$$

We derive the following discretized process for $n = 0, \dots, N - 1$:

$$\vartheta_{n+1}^{\text{EI}} = e^{\frac{h}{2}} \vartheta_n^{\text{EI}} + 2(e^{\frac{h}{2}} - 1)s_*(T - nh, \vartheta_n^{\text{EI}}) + \sqrt{e^h - 1}\xi_n$$

with the initial point $\vartheta_0^{\text{EI}} \sim \hat{p}_T$ and $\xi_n \sim \mathcal{N}(0, I_d)$.

• **VANILLA MIDPOINT RANDOMIZATION:** Unlike the Euler method, the midpoint randomization method evaluates the function $\gamma(T - t, X_t^{\leftarrow})$ at a random point within the time interval $[0, h]$ rather than at the start. Let U be a random variable uniformly distributed in $[0, 1]$ and independent of the Brownian motion W_t . The randomized midpoint method exploits the approximation

$$\begin{aligned} X_{t+h}^{\leftarrow} &= X_t^{\leftarrow} + \int_0^h \gamma(T - t - v, X_{t+v}^{\leftarrow}) dv + \Delta_h W_t \\ &\approx X_t^{\leftarrow} + h\gamma(T - t - hU, X_{t+hU}^{\leftarrow}) + \Delta_h W_t. \end{aligned} \quad (6)$$

The idea behind the randomized midpoint method is to introduce an U in $[0, 1]$, making $h\gamma(T - t - hU, X_{t+hU}^{\leftarrow})$ an estimator for integral $\int_0^h \gamma(T - t - v, X_{t+v}^{\leftarrow}) dv$.

Furthermore, the intermediate term $X_{t+hU}^{\leftarrow}$ is generated by employing the Euler method. We then derive the following discretized process for $n = 0, \dots, N - 1$:

Step 1 Generate $\xi'_n, \xi''_n \sim \mathcal{N}(\mathbf{0}, I_d)$ and $U_n \sim \text{Unif}[0, 1]$. Set $\xi_n = \sqrt{U_n}\xi'_n + \sqrt{1 - U_n}\xi''_n$.

Step 2 With the initialization $\vartheta_0^{\text{REM}} \sim \hat{p}_T$, define

$$\begin{aligned} \vartheta_{n+U}^{\text{REM}} &= \vartheta_n^{\text{REM}} + hU_n\gamma(T - nh, \vartheta_n^{\text{REM}}) + \sqrt{hU_n}\xi'_n, \\ \vartheta_{n+1}^{\text{REM}} &= \vartheta_n^{\text{REM}} + h\gamma(T - (n + U_n)h, \vartheta_{n+U}^{\text{REM}}) + \sqrt{h}\xi_n. \end{aligned}$$

• **EXPONENTIAL INTEGRATOR WITH MIDPOINT RANDOMIZATION:** Combining midpoint randomization with the exponential integrator approach, we propose the following new discretization process for $n = 0, \dots, N - 1$:

Step 1 Generate $\xi'_n, \xi''_n \sim \mathcal{N}(\mathbf{0}, I_d)$ and $U_n \sim \text{Unif}[0, 1]$. Set $\xi_n = \rho_n\xi'_n + \sqrt{1 - \rho_n^2}\xi''_n$ with

$$\rho_n = e^{\frac{h(1+U_n)}{2}} (1 - e^{-hU_n}) \left[(e^{hU_n} - 1)(e^h - 1) \right]^{-1/2}.$$

Step 2 With the initialization $\vartheta_0^{\text{REI}} \sim \hat{p}_T$, define

$$\begin{aligned} \vartheta_{n+U}^{\text{REI}} &= e^{hU_n/2} \vartheta_n^{\text{REI}} + 2(e^{hU_n/2} - 1)s_*(T - nh, \vartheta_n^{\text{REI}}) + \sqrt{e^{hU_n} - 1}\xi'_n, \\ \vartheta_{n+1}^{\text{REI}} &= e^{h/2} \vartheta_n^{\text{REI}} + he^{(1-U_n)h/2} s_*(T - (n + U_n)h, \vartheta_{n+U}^{\text{REI}}) + \sqrt{e^h - 1}\xi_n. \end{aligned}$$

The resulting discrete process is then solved to generate new samples that approximately follow the data distribution p_0 .

3 Wasserstein Convergence Analysis under Various Discretization Schemes

In this section, we study the convergence of diffusion models under EM, EI, REM and REI discretizations of the continuous backward SDE (3). Specifically, we establish the upper bounds on

the Wasserstein-2 distance between the distribution of the N -th output of the SGMs under these discretization schemes and the target distribution

$$W_2(\mathcal{L}(\vartheta_N^\alpha), p_0), \quad \alpha \in \{\text{EM}, \text{EI}, \text{REM}, \text{REI}\}.$$

Additionally, we analyze the number of iterations N required for the Wasserstein distance to achieve a pre-specified error level ε under each discretization scheme. For clarity of presentation, we omit constants in the main text, retaining only the key components that affect convergence rates. Full bounds with constants are provided in the proofs.

To establish the convergence analysis, we require the following assumption on target density p_0 .

Assumption 1. *The target density p_0 is m_0 -strongly log-concave, and the score function $\nabla \log p_0$ is L_0 -Lipschitz.*

Under Assumption 1, p_t is $m(t)$ -strongly log-concave, $\nabla \log p_t$ is $L(t)$ -Lipschitz. Moreover, $m(t)$ is lower bounded by $m_{\min} = \min(1, m_0)$, and $L(t)$ is upper bounded by $L_{\max} = 1 + L_0$, as summarized in Lemma 6 and 7 (see Appendix B). We also assume that the score function $\nabla \log p_t(x)$ exhibits linear growth in $\|x\|$, as stated below.

Assumption 2. *There exists a constant $M_1 > 0$ such that for $n = 0, 1, \dots, N-1$, it holds that*

$$\sup_{nh \leq t, s \leq (n+1)h} \|\nabla \log p_{T-t}(x) - \nabla \log p_{T-s}(x)\| \leq M_1 h(1 + \|x\|), \quad \forall x.$$

The above condition is a relaxation of the standard Lipschitz condition on the score function. Moreover, we require the following assumption on the score-matching approximation at each point ϑ_n .

Assumption 3. *Given a small $\varepsilon_{sc} > 0$, the score estimator satisfies*

$$\sup_{0 \leq n \leq N} \|\nabla \log p_{T-nh}(\vartheta_n) - s_*(T - nh, \vartheta_n)\|_{\mathbb{L}_2} \leq \varepsilon_{sc}.$$

Assumption 1, 2 and 3 are standard in the Wasserstein convergence analysis of the score-based diffusion model. These assumptions were previously adopted in [12, 13] and can be easily verified in the Gaussian case.

3.1 Euler-Maruyama Method and Exponential Integrator

In the following theorem, we quantify the Wasserstein distance between the distribution of $\vartheta_N^\alpha, \alpha \in \{\text{EM}, \text{EI}\}$ and the target distribution p_0 .

Theorem 1. *Suppose that Assumptions 1, 2 and 3 hold, it holds that*

$$W_2(\mathcal{L}(\vartheta_N^\alpha), p_0) \lesssim e^{-m_{\min} T} \|X_0\|_{\mathbb{L}_2} + \mathcal{C}_1^\alpha \sqrt{dh} + \mathcal{C}_2^\alpha \varepsilon_{sc}, \quad \alpha \in \{\text{EM}, \text{EI}\}, \quad (7)$$

$$\text{where} \quad \mathcal{C}_1^{\text{EM}} = \frac{L_{\max} + 1/2}{m_{\min} - 1/2} \quad \text{and} \quad \mathcal{C}_2^{\text{EM}} = \frac{1}{m_{\min} - 1/2},$$

$$\mathcal{C}_1^{\text{EI}} = \frac{L_{\max}}{m_{\min} - 1/2} \quad \text{and} \quad \mathcal{C}_2^{\text{EI}} = \frac{1}{m_{\min} - 1/2}$$

with $m_{\min} = \min(1, m_0)$ and $L_{\max} = 1 + L_0$.

Before comparing the above bound with existing ones, we state a direct consequence.

Corollary 2. *Given a small $\varepsilon > 0$ and $\varepsilon_{sc} = \mathcal{O}(\varepsilon)$, the Wasserstein distance satisfies $W_2(\mathcal{L}(\vartheta_N^\alpha), p_0) < \varepsilon, \alpha \in \{\text{EM}, \text{EI}\}$ after $N = \mathcal{O}(\frac{d}{\varepsilon^2} \log(\frac{\sqrt{d}}{\varepsilon}))$ iterations, provided that $T = \mathcal{O}(\log(\frac{\sqrt{d}}{\varepsilon}))$ and $h = \mathcal{O}(\frac{\varepsilon^2}{d})$.*

We now explain the upper bound in Theorem 1, which decomposes the total error into three parts: initialization, discretization, and score-matching errors. The **first term** on the right-hand side of display (7) bounds the error arising from initializing the reverse idealized continuous-time SDE (4) at $\hat{p}_T$ instead of p_T . The **second term** in (7) captures the discretization error from the discretization scheme, while the **third term** reflects the score matching error.

The term $-1/2$ in $m_{\min} - 1/2$ arises from the drift term of the forward SDE (2), as demonstrated in Lemma 8 in the appendix. We refer interested readers to the appendix for further details. More generally, if the forward SDE takes the form $dX_t = -\beta X_t dt + dB_t$, then the bound becomes $m(t) - \beta$, reflecting a dependence on the coefficient β . Although the current theory still assumes that the data distribution p_0 is strongly log-concave, the condition $m_0 > 1/2$ naturally generalizes to $m_0 > \beta$ for any $\beta > 0$.

The convergence rates of EM method obtained in Theorem 1 and Corollary 2 align with Theorem 2 and Proposition 5 in [13]. Moreover, we note that the convergence rate of EM and EI schemes are comparable, which is consistent with the error bounds for these two schemes in KL divergence established in Theorem 1 of [5], where $N = \Omega(T^2)$ in their setting.

3.2 Randomized Midpoint Method

Since the randomized midpoint method involves the i.i.d. uniformly distributed random variable U_n , the resulting score matching function $s_*(T - t, x)$ can be evaluated at any $t \in [0, T]$. To proceed, we impose a regularity condition on the deviation of the estimated score from the true score at these points. For this, we introduce the following auxiliary stochastic processes. Given $U_n = u$, define the conditional realization of the random vector $\vartheta_{n+U}^{\text{REM}}$ via

$$\vartheta_{n+u}^{\text{REM}} := \left(1 + \frac{uh}{2}\right) \vartheta_n^{\text{REM}} + uh s_*(T - nh, \vartheta_n^{\text{REM}}) + \sqrt{uh} \xi_n.$$

Similarly, we define the following conditional realization of $\vartheta_{n+U}^{\text{REI}}$

$$\vartheta_{n+u}^{\text{REI}} := e^{uh/2} \vartheta_n^{\text{REI}} + 2(e^{uh/2} - 1) s_*(T - nh, \vartheta_n^{\text{REI}}) + \sqrt{e^{uh} - 1} \xi'_n.$$

We impose the following assumption on score estimates, which extends Assumption 3.

Assumption 4. *There exists a constant $\varepsilon_{sc} > 0$ such that for any $u \in [0, 1]$ and $n = 0, \dots, N$,*

$$\|\nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^\alpha) - s_*(T - (n+u)h, \vartheta_{n+u}^\alpha)\|_{\mathbb{L}_2} \leq \varepsilon_{sc}, \quad \alpha \in \{\text{REM}, \text{REI}\}.$$

In what follows, we provide the upper bound for the Wasserstein-2 distance between the law of $\vartheta_N^\alpha, \alpha \in \{\text{REM}, \text{REI}\}$ and the data distribution p_0 .

Theorem 3. *Suppose that Assumptions 1, 2 and 4 hold, then for $\alpha \in \{\text{REM}, \text{REI}\}$,*

$$W_2(\mathcal{L}(\vartheta_N^\alpha), p_0) \lesssim e^{-m_{\min} T} \|X_0\|_{\mathbb{L}_2} + \mathcal{C}_1^\alpha(d) \sqrt{h} + \mathcal{C}_2^\alpha \varepsilon_{sc},$$

$$\text{where} \quad \mathcal{C}_1^{\text{REM}}(d) = \frac{\sqrt{d/3} L_{\max} + 1/2\sqrt{3}}{m_{\min} - 1/2} \quad \text{and} \quad \mathcal{C}_2^{\text{REM}} = \frac{3}{m_{\min} - 1/2},$$

$$\mathcal{C}_1^{\text{REI}}(d) = \frac{\sqrt{d/3} L_{\max}}{(m_{\min} - 1/2)} \quad \text{and} \quad \mathcal{C}_2^{\text{REI}} = \frac{3}{m_{\min} - 1/2}$$

with $L_{\max}$ and $m_{\min}$ as defined in Theorem 1.

The convergence rate of these two schemes is generally consistent with EM, EI methods, differing only in the coefficients. As shown in display (6), the key idea behind the randomized midpoint method is to introduce a uniformly distributed random variable U_n to evaluate the term $\gamma(T - t, X_t^\leftarrow)$ at a random point within the time interval $[0, h]$. In the proofs provided in Appendix B.3 and B.4 (corresponding to $\alpha = \text{REM}$ and $\alpha = \text{REI}$, respectively), we demonstrate that $\mathbb{E}_{U_n}[\vartheta_{n+1}^\alpha]$ yields an accurate approximation to the true distribution, with an error of order $\mathcal{O}(h^{5/2}) + \mathcal{O}(h)\varepsilon_{sc}$. However, this randomization also introduces a variance term $\|\vartheta_{n+1}^\alpha - \mathbb{E}_{U_n}[\vartheta_{n+1}^\alpha]\|_{\mathbb{L}_2}$, of order $\mathcal{O}(h^{3/2}) + \mathcal{O}(h)\varepsilon_{sc}$, which obscures the benefits of the improved estimation. As a result, the midpoint randomization offers no improvement in convergence over EM and EI methods.

Although midpoint randomization itself does not improve convergence in our setting, it enables parallel computation [15, 23], significantly reducing computational complexity and enhancing efficiency.

4 Second-order Acceleration

In this section, we propose an accelerated sampler that leverages Hessian estimation. The core idea behind the acceleration is the *Local Linearization Method*, introduced in [33], which approximates the drift term of an SDE using its Itô expansion over small time intervals. To illustrate this, we begin with a general framework for the backward process.

$$dx_t = \gamma(T - t, x_t) dt + \sigma dW_t, \quad (8)$$

where $\sigma > 0$ and W_t is the d -dimensional Brownian motion. We assume that $\gamma(t, x) \in C^{1,3}(\mathbb{R}_+ \times \mathbb{R}^d)$ and approximate it by a linear function in both state and time within each discretization step. Applying Itô's formula to $\gamma(T - t, x)$, we derive the following approximation for $\gamma(T - t, x_t) - \gamma(T - s, x_s)$

$$\left(\frac{\sigma^2}{2} \frac{\partial^2 \gamma}{\partial x^2}(T - s, x_s) - \frac{\partial \gamma}{\partial t}(T - s, x_s) \right) (t - s) + \frac{\partial \gamma}{\partial x}(T - s, x_s) \cdot (x_t - x_s).$$

Here and henceforth, we abbreviate the partial derivative $\frac{\partial^\alpha g(z)}{\partial z^\alpha} \Big|_{z=z_0}$ as $\frac{\partial^\alpha g}{\partial z^\alpha}(z_0)$. This allows us to express $\gamma(T - t, x_t)$ in the following form

$$\gamma(T - t, x_t) \approx \gamma(T - s, x_s) + L_s(x_t - x_s) + M_s(t - s), \quad (9)$$

with

$$L_s = \frac{\partial \gamma}{\partial x}(T - s, x_s) \quad \text{and} \quad M_s = \frac{\sigma^2}{2} \frac{\partial^2 \gamma}{\partial x^2}(T - s, x_s) - \frac{\partial \gamma}{\partial t}(T - s, x_s).$$

Here, L_s is the first-order spatial derivative of γ , capturing its local variation with respect to position x . The term M_s represents the temporal evolution of γ , incorporating information about how its shape changes over both space and time. Substituting display (9) into the original SDE (8), we obtain

$$dx_t = [\gamma(T - s, x_s) + L_s(x_t - x_s) + M_s(t - s)] dt + \sigma dW_t.$$

This formulation ensures that the discretized process preserves the essential structure of the original dynamics while remaining computationally tractable. Unlike discretization schemes in Section 2, which rely on direct numerical integration, this transformed SDE allows for analytical solutions within each small time interval.

Setting $\gamma(T - t, x) = x/2 + \nabla \log p_{T-t}(x)$, $\sigma = 1$, let $\Delta t \in [0, h]$ and $s = nh$. By Itô's formula, we derive the analytical expression for x_t . In the resulting expression, we denote x_s by ϑ_n^{SO} . Then, we obtain that for any $t \in [nh, (n+1)h]$, it holds that

$$x_t = \vartheta_n^{\text{SO}} + \int_{nh}^t \left(\frac{1}{2} \vartheta_n^{\text{SO}} + \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) + L_n(x_u - \vartheta_n^{\text{SO}}) + M_n(u - nh) \right) du + \int_{nh}^t dW_u \quad (10)$$

where

$$L_n = \frac{1}{2} I_d + \nabla^2 \log p_{T-nh}(\vartheta_n^{\text{SO}}), \quad M_n = \frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) - \frac{\partial}{\partial t} \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}).$$

Thus, L_n contains the Hessian of the score function. The term M_n measures the difference between the spatial and temporal changes in the score function, reflecting the balance between curvature effects and temporal adaptation in the diffusion process. Notice that $x_{(n+1)h}$ is the point we aim to approximate. For this, we need to estimate the score function and its higher-order derivatives to obtain accurate estimates of L_n and M_n , denoted by $s_*^{(L)}$ and $s_*^{(M)}$, respectively.

By the work of [28], higher-order derivatives of $\log p_t(x)$ with respect to x can be accurately estimated. Moreover, we show in Appendix C that $\partial_t \nabla \log p_t(x)$ can be expressed as a combination of up to second-order partial derivatives of $\log p_t(x)$ with respect to x . Thus, estimating $\partial_t \nabla \log p_t(x)$ requires no additional assumptions beyond those for accurately estimating $\partial_x^2 \nabla \log p_t(x)$. We also require the following assumption.

Assumption 5. For some constants $\varepsilon_{sc}^{(L)}, \varepsilon_{sc}^{(M)} > 0$, the estimate for high-order derivatives of the score function satisfies that

$$\sup_{0 \leq n \leq N-1} \left\| s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}}) - L_n \right\|_{\mathbb{L}_2} \leq \varepsilon_{sc}^{(L)},$$

$$\sup_{0 \leq n \leq N-1} \left\| s_*^{(M)}(T - nh, \vartheta_n^{\text{SO}}) - M_n \right\|_{\mathbb{L}_2} \leq \varepsilon_{sc}^{(M)}.$$

This assumption has been adopted in prior works [24] and [27]. Substituting these estimates into display (10) then gives

$$x_t = \vartheta_n^{\text{SO}} + \int_{nh}^t \left[\gamma(T - nh, \vartheta_n^{\text{SO}}) + s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})(x_u - \vartheta_n^{\text{SO}}) + s_*^{(M)}(T - nh, \vartheta_n^{\text{SO}})(u - nh) \right] du + \int_{nh}^t dW_u.$$

Let $\vartheta_{n+1}^{\text{SO}}$ denote $x_{(n+1)h}$. The second-order discretization scheme is given by³

$$\begin{aligned} \vartheta_{n+1}^{\text{SO}} &= \vartheta_n^{\text{SO}} + s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})^{-1} \left(e^{s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})h} - I_d \right) \left(\frac{1}{2} \vartheta_n^{\text{SO}} + s_*(T - nh, \vartheta_n^{\text{SO}}) \right) \\ &\quad + s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})^{-2} \left(e^{s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})h} - s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})h - I_d \right) s_*^{(M)}(T - nh, \vartheta_n^{\text{SO}}) \\ &\quad + \int_{nh}^{(n+1)h} e^{s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})[(n+1)h - t]} dW_t. \end{aligned}$$

We assume additional smoothness on the score function.

Assumption 6. Let $\|\cdot\|_F$ denote the Frobenius norm. There exists a positive constant L_F such that

$$\|\nabla^2 \log p_t(x) - \nabla^2 \log p_t(y)\|_F \leq L_F \|x - y\|, \quad \forall x, y \in \mathbb{R}^d.$$

As shown in Theorems 4 and 5 of [27], this condition plays a crucial role in bounding the Wasserstein distance for Hessian estimates and can be easily verified in the Gaussian case.

Assumption 7. There exists a constant $M_2 > 0$ such that, for any $n = 0, \dots, N - 1$ and $t \in [nh, (n + 1)h]$, it holds that

$$\|\nabla^2 \log p_{T-t}(x) - \nabla^2 \log p_{T-nh}(x)\| \leq M_2 h(1 + \|x\|), \quad \forall x \in \mathbb{R}^d.$$

We now quantify the W_2 distance between the generated distribution $\mathcal{L}(\vartheta_N^{\text{SO}})$ and the target p_0 .

Theorem 4. Suppose that Assumptions 1, 3, 5, 6 and 7 hold, then

$$W_2(\mathcal{L}(\vartheta_N^{\text{SO}}), p_0) \lesssim e^{-m_{\min} T} \|X_0\|_{\mathbb{L}_2} + \mathcal{C}_1^{\text{SO}}(d)h + \mathcal{C}_2^{\text{SO}} \left(\varepsilon_{sc} + \frac{2}{3} \sqrt{hd} \varepsilon_{sc}^{(L)} + \frac{1}{2} h \varepsilon_{sc}^{(M)} \right) \quad (11)$$

where $\mathcal{C}_1^{\text{SO}}(d) = e^{(L_{\max} - 1/2)h} \cdot \frac{\sqrt{d}(L_{\max}^{3/2} + \sqrt{2}L_F/4)}{m_{\min} - 1/2}$ and $\mathcal{C}_2^{\text{SO}} = \frac{e^{(L_{\max} - 1/2)h}}{m_{\min} - 1/2}$ with $L_{\max}$ and $m_{\min}$ as defined in Theorem 1.

Before discussing the results of this theorem, let us state its direct consequence.

Corollary 5. For a given $\varepsilon > 0$, the Wasserstein distance satisfies $W_2(\mathcal{L}(\vartheta_N^{\text{SO}}), p_0) < \varepsilon$ after $N = \mathcal{O} \left(\frac{\sqrt{d}}{\varepsilon} \log \left(\frac{\sqrt{d}}{\varepsilon} \right) \right)$ iterations, provided that $T = \mathcal{O} \left(\log \left(\frac{\sqrt{d}}{\varepsilon} \right) \right)$ and $h = \mathcal{O} \left(\frac{\varepsilon}{\sqrt{d}} \right)$.

In the above, we present the first Wasserstein convergence analysis of an accelerated sampler that utilizes accurate score function estimation and second-order information about log-densities. The total error arises from the same resources as in Theorem 1. The **first term** on the right-hand side of display (11) captures the initialization error. The **second term** reflects the benefit of second-order acceleration, where improved discretization reduces the error in approximating the reverse SDE. The **third term** accounts for errors in estimating both the spatial and temporal components of the score function, as well as the higher order terms L_n and M_n .

The accelerated convergence of this method is driven by two key innovations: approximating the drift term through its Itô expansion rather than endpoint evaluations, and deriving a closed-form solution to the integral equation (10) using the Itô formula, akin to Exponential Integrator techniques. Compared to the four schemes described in Section 3, the proposed second-order algorithm offers a clear computational advantage: it requires only $\tilde{\mathcal{O}}(1/\varepsilon)$ iterations (v.s. $\tilde{\mathcal{O}}(1/\varepsilon^2)$), and permits a

³Due to space limitations, we refer readers to Appendix E for a complete derivation.

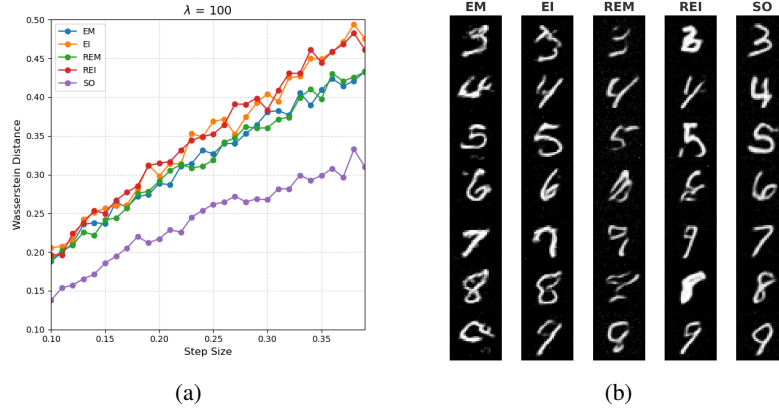


Figure 1: **(a)**: Errors of SGMs under EM, EI, REM, REI and SO with different choices of h . **(b)**: Samples generated by five different algorithms on the MNIST dataset.

larger step size $h = \mathcal{O}(\varepsilon)$, enabling faster progression in each iteration instead of $h = \mathcal{O}(\varepsilon^2)$. As a result, the second-order method achieves the same accuracy with fewer iterations and a larger step size, making it a more efficient method for approximating the target distribution.

We note that the convergence rate $\tilde{\mathcal{O}}(1/\varepsilon)$ matches that of the accelerated Denoising Diffusion Probabilistic Models (DDPM) sampler [17] proposed in [27], which achieves this rate in KL divergence and relies on Hessian estimation. Additionally, this rate aligns with the iteration complexity results in TV distance presented in [19] when setting $p = 1$ in their framework.

5 Numerical Studies

In this section, we compare the performance of the SGMs under EM, EI, REM, REI discretization schemes described in Section 2, as well as the second-order acceleration method (SO) proposed in Section 4, evaluated on both synthetic data and the MNIST dataset.

5.1 Experiments on Synthetic Data

We apply the five algorithms to the posterior of penalized logistic regression, defined by $p_0(\theta) \propto \exp(-f(\theta))$, with the potential function f defined via

$$f(\theta) = \frac{\lambda}{2} \|\theta\|^2 + \frac{1}{n_{\text{data}}} \sum_{i=1}^{n_{\text{data}}} \log(1 + \exp(-y_i x_i^\top \theta)),$$

where $\lambda > 0$ denotes the tuning parameter. The data $\{x_i, y_i\}_{i=1}^{n_{\text{data}}}$, composed of binary labels $y_i \in \{-1, 1\}$ and features $x_i = (x_{i,1}, \dots, x_{i,d})^\top \in \mathbb{R}^d$ generated from $x_{i,j} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 100)$. Set $\lambda = 100$ with $d = 20$ and $n_{\text{data}} = 100$. Appendix F provides additional results and implementation details. Figure 1a presents the W_2 distance measured along the first dimension between the empirical distributions of the samples from the five algorithms and the target distribution under different choices of h . These results support our theoretical findings: all discretization schemes from Section 2 exhibit similar convergence behavior, while the proposed Hessian-based sampler consistently achieves superior performance.

5.2 Real Data Analysis

We apply the four SGM discretization schemes and the second-order algorithm to the MNIST dataset. To accelerate the SO algorithm, we use Hessian-vector products (HVPs) instead of explicitly computing the Hessian. The results in Figure 1b demonstrate that SO outperforms the others. Additional results and implementation details are provided in Appendix G.

6 Discussion

The Wasserstein-2 distance, used in this paper, serves as a natural and practical metric for measuring errors in diffusion models. However, recent work on the convergence theory of diffusion models has also explored alternative metrics such as total variation distance and KL divergence. A promising direction for future research is to establish convergence guarantees with respect to these alternative distances.

Moreover, while this work makes progress in provably accelerating SDE-based diffusion sampling in Wasserstein distance, it would also be valuable to explore deterministic samplers based on probability flow ODEs.

Finally, for clarity and simplicity, we focus on a specific choice of drift functions f and g in the forward process, corresponding to the Ornstein–Uhlenbeck process. Extending this analysis to a more general framework with broader choices of (f, g) is an interesting avenue for future research.

Acknowledgments and Disclosure of Funding

Lu Yu is supported by the City University of Hong Kong Startup Fund and Hong Kong RGC Grant 21306325.

References

- [1] Namrata Anand and Tudor Achim. Protein structure and sequence generation with equivariant denoising diffusion probabilistic models. *arXiv preprint arXiv:2205.15019*, 2022.
- [2] Brian DO Anderson. Reverse-time diffusion equation models. *Stochastic Processes and their Applications*, 12(3):313–326, 1982.
- [3] Stefano Bruno, Ying Zhang, Dong-Young Lim, Ömer Deniz Akyildiz, and Sotirios Sabanis. On diffusion-based generative models and their error bounds: The log-concave case with full convergence estimates. *arXiv preprint arXiv:2311.13584*, 2023.
- [4] Patrick Cattiaux, Giovanni Conforti, Ivan Gentil, and Christian Léonard. Time reversal of diffusion processes under a finite entropy condition. In *Annales de l’Institut Henri Poincaré (B) Probabilités et Statistiques*, volume 59, pages 1844–1881. Institut Henri Poincaré, 2023.
- [5] 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*, pages 4735–4763. PMLR, 2023.
- [6] Minshuo Chen, Song Mei, Jianqing Fan, and Mengdi Wang. An overview of diffusion models: Applications, guided generation, statistical rates and optimization. *arXiv preprint arXiv:2404.07771*, 2024.
- [7] 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.
- [8] 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, 2024.
- [9] Xiang Cheng, Niladri S Chatterji, Peter L Bartlett, and Michael I Jordan. Underdamped langevin mcmc: A non-asymptotic analysis. In *Conference on learning theory*, pages 300–323. PMLR, 2018.
- [10] Valentin De Bortoli. Convergence of denoising diffusion models under the manifold hypothesis. *arXiv preprint arXiv:2208.05314*, 2022.
- [11] Prafulla Dhariwal and Alexander Nichol. Diffusion models beat gans on image synthesis. *Advances in neural information processing systems*, 34:8780–8794, 2021.

- [12] Xuefeng Gao and Lingjiong Zhu. Convergence analysis for general probability flow odes of diffusion models in wasserstein distances. *arXiv preprint arXiv:2401.17958*, 2024.
- [13] 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.
- [14] Marta Gentiloni-Silveri and Antonio Ocello. Beyond log-concavity and score regularity: Improved convergence bounds for score-based generative models in w_2 -distance. *arXiv preprint arXiv:2501.02298*, 2025.
- [15] Shivam Gupta, Linda Cai, and Sitan Chen. Faster diffusion-based sampling with randomized midpoints: Sequential and parallel. *arXiv preprint arXiv:2406.00924*, 2024.
- [16] Ye He, Krishnakumar Balasubramanian, and Murat A Erdogdu. On the ergodicity, bias and asymptotic normality of randomized midpoint sampling method. *Advances in Neural Information Processing Systems*, 33:7366–7376, 2020.
- [17] Jonathan Ho, Ajay Jain, and Pieter Abbeel. Denoising diffusion probabilistic models. *Advances in neural information processing systems*, 33:6840–6851, 2020.
- [18] Marlis Hochbruck and Alexander Ostermann. Exponential integrators. *Acta Numerica*, 19: 209–286, 2010.
- [19] Daniel Zhengyu Huang, Jiaoyang Huang, and Zhengjiang Lin. Convergence analysis of probability flow ode for score-based generative models. *arXiv preprint arXiv:2404.09730*, 2024.
- [20] Aapo Hyvärinen and Peter Dayan. Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning Research*, 6(4), 2005.
- [21] Saravanan Kandasamy and Dheeraj Nagaraj. The poisson midpoint method for langevin dynamics: Provably efficient discretization for diffusion models. *arXiv preprint arXiv:2405.17068*, 2024.
- [22] Gen Li and Changxiao Cai. Provable acceleration for diffusion models under minimal assumptions. *arXiv preprint arXiv:2410.23285*, 2024.
- [23] Gen Li and Yuchen Jiao. Improved convergence rate for diffusion probabilistic models. *arXiv preprint arXiv:2410.13738*, 2024.
- [24] Gen Li, Yu Huang, Timofey Efimov, Yuting Wei, Yuejie Chi, and Yuxin Chen. Accelerating convergence of score-based diffusion models, provably. *arXiv preprint arXiv:2403.03852*, 2024.
- [25] Gen Li, Yuting Wei, Yuejie Chi, and Yuxin Chen. A sharp convergence theory for the probability flow odes of diffusion models. *arXiv preprint arXiv:2408.02320*, 2024.
- [26] Jiadong Liang, Zhihan Huang, and Yuxin Chen. Low-dimensional adaptation of diffusion models: Convergence in total variation. *arXiv preprint arXiv:2501.12982*, 2025.
- [27] Y Liang, P Ju, Y Liang, and N Shroff. Broadening target distributions for accelerated diffusion models via a novel analysis approach. *arXiv preprint arXiv:2402.13901*, 2024.
- [28] Chenlin Meng, Yang Song, Wenzhe Li, and Stefano Ermon. Estimating high order gradients of the data distribution by denoising. *Advances in Neural Information Processing Systems*, 34: 25359–25369, 2021.
- [29] Nikiforos Mimikos-Stamatopoulos, Benjamin J Zhang, and Markos A Katsoulakis. Score-based generative models are provably robust: an uncertainty quantification perspective. *arXiv preprint arXiv:2405.15754*, 2024.
- [30] Vadim Popov, Ivan Vovk, Vladimir Gogoryan, Tasnima Sadekova, and Mikhail Kudinov. Gradients: A diffusion probabilistic model for text-to-speech. In *International Conference on Machine Learning*, pages 8599–8608. PMLR, 2021.

- [31] Aditya Ramesh, Prafulla Dhariwal, Alex Nichol, Casey Chu, and Mark Chen. Hierarchical text-conditional image generation with clip latents. *arXiv preprint arXiv:2204.06125*, 1(2):3, 2022.
- [32] Ruoqi Shen and Yin Tat Lee. The randomized midpoint method for log-concave sampling. *Advances in Neural Information Processing Systems*, 32, 2019.
- [33] Isao Shoji. Approximation of continuous time stochastic processes by a local linearization method. *Math. Comput.*, 67:287–298, 1998. URL <https://api.semanticscholar.org/CorpusID:13430357>.
- [34] Jiaming Song, Chenlin Meng, and Stefano Ermon. Denoising diffusion implicit models. *arXiv preprint arXiv:2010.02502*, 2020.
- [35] Yang Song, Sahaj Garg, Jiaxin Shi, and Stefano Ermon. Sliced score matching: A scalable approach to density and score estimation. In *Uncertainty in Artificial Intelligence*, pages 574–584. PMLR, 2020.
- [36] Yang Song, Jascha Sohl-Dickstein, Diederik P Kingma, Abhishek Kumar, Stefano Ermon, and Ben Poole. Score-based generative modeling through stochastic differential equations. *arXiv preprint arXiv:2011.13456*, 2020.
- [37] Stanislas Strasman, Antonio Ocello, Claire Boyer, Sylvain Le Corff, and Vincent Lemaire. An analysis of the noise schedule for score-based generative models. *arXiv preprint arXiv:2402.04650*, 2024.
- [38] Wenpin Tang and Hanyang Zhao. Contractive diffusion probabilistic models. *arXiv preprint arXiv:2401.13115*, 2024.
- [39] Wenpin Tang and Hanyang Zhao. Score-based diffusion models via stochastic differential equations—a technical tutorial. *arXiv preprint arXiv:2402.07487*, 2024.
- [40] Pascal Vincent. A connection between score matching and denoising autoencoders. *Neural computation*, 23(7):1661–1674, 2011.
- [41] Yuchen Wu, Yuxin Chen, and Yuting Wei. Stochastic runge-kutta methods: Provable acceleration of diffusion models. *arXiv preprint arXiv:2410.04760*, 2024.
- [42] Minkai Xu, Lantao Yu, Yang Song, Chence Shi, Stefano Ermon, and Jian Tang. Geodiff: A geometric diffusion model for molecular conformation generation. *arXiv preprint arXiv:2203.02923*, 2022.
- [43] Ling Yang, Zhilong Zhang, Yang Song, Shenda Hong, Runsheng Xu, Yue Zhao, Wentao Zhang, Bin Cui, and Ming-Hsuan Yang. Diffusion models: A comprehensive survey of methods and applications. *ACM Computing Surveys*, 56(4):1–39, 2023.
- [44] Lu Yu and Arnak Dalalyan. Parallelized midpoint randomization for langevin monte carlo. *arXiv preprint arXiv:2402.14434*, 2024.
- [45] Lu Yu, Avetik Karagulyan, and Arnak Dalalyan. Langevin monte carlo for strongly log-concave distributions: Randomized midpoint revisited. *arXiv preprint arXiv:2306.08494*, 2023.
- [46] Yifeng Yu and Lu Yu. Randomized midpoint method for log-concave sampling under constraints. *arXiv preprint arXiv:2405.15379*, 2024.
- [47] Qinsheng Zhang and Yongxin Chen. Fast sampling of diffusion models with exponential integrator. *arXiv preprint arXiv:2204.13902*, 2022.

NeurIPS Paper Checklist

1. Claims

Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

Answer: [Yes]

Justification: The main claims in the abstract and introduction are substantiated by the detailed theoretical analyses are presented in the paper. These sections clearly outline our contributions and scope, which are consistently reflected throughout the findings.

Guidelines:

- The answer NA means that the abstract and introduction do not include the claims made in the paper.
- The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
- The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
- It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

2. Limitations

Question: Does the paper discuss the limitations of the work performed by the authors?

Answer: [Yes]

Justification: In the last section, some strong assumptions made in this work are highlighted, along with potential directions for relaxing these assumptions and generalizing the current findings.

Guidelines:

- The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
- The authors are encouraged to create a separate "Limitations" section in their paper.
- The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
- The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
- The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting. Or a speech-to-text system might not be used reliably to provide closed captions for online lectures because it fails to handle technical jargon.
- The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
- If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
- While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. The authors should use their best judgment and recognize that individual actions in favor of transparency play an important role in developing norms that preserve the integrity of the community. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

3. Theory assumptions and proofs

Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [Yes]

Justification: For all the theoretical results, we provide the full set of assumptions and complete proofs for them.

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.
- Inversely, any informal proof provided in the core of the paper should be complemented by formal proofs provided in appendix or supplemental material.
- Theorems and Lemmas that the proof relies upon should be properly referenced.

4. Experimental result reproducibility

Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

Answer: [Yes]

Justification: All information necessary to reproduce the main experimental results is provided in the main text and appendix.

Guidelines:

- The answer NA means that the paper does not include experiments.
- If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important, regardless of whether the code and data are provided or not.
- If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
- Depending on the contribution, reproducibility can be accomplished in various ways. For example, if the contribution is a novel architecture, describing the architecture fully might suffice, or if the contribution is a specific model and empirical evaluation, it may be necessary to either make it possible for others to replicate the model with the same dataset, or provide access to the model. In general, releasing code and data is often one good way to accomplish this, but reproducibility can also be provided via detailed instructions for how to replicate the results, access to a hosted model (e.g., in the case of a large language model), releasing of a model checkpoint, or other means that are appropriate to the research performed.
- While NeurIPS does not require releasing code, the conference does require all submissions to provide some reasonable avenue for reproducibility, which may depend on the nature of the contribution. For example
 - (a) If the contribution is primarily a new algorithm, the paper should make it clear how to reproduce that algorithm.
 - (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
 - (c) If the contribution is a new model (e.g., a large language model), then there should either be a way to access this model for reproducing the results or a way to reproduce the model (e.g., with an open-source dataset or instructions for how to construct the dataset).
 - (d) We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

5. Open access to data and code

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [\[Yes\]](#)

Justification: The datasets used in this work are either synthetic or publicly available, and the code for reproducing the results is provided in the supplementary materials.

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so “No” is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- The authors should provide instructions on data access and preparation, including how to access the raw data, preprocessed data, intermediate data, and generated data, etc.
- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

6. Experimental setting/details

Question: Does the paper specify all the training and test details (e.g., data splits, hyper-parameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer: [\[Yes\]](#)

Justification: Experimental settings and details are provided.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

7. Experiment statistical significance

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [\[No\]](#)

Justification: Statistical significance of the experiments is not applicable in this context.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.
- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).

- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).
- It should be clear whether the error bar is the standard deviation or the standard error of the mean.
- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

8. Experiments compute resources

Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

Answer: [Yes]

Justification: Sufficient information about the computational resources used is provided in appendix.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
- The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.
- The paper should disclose whether the full research project required more compute than the experiments reported in the paper (e.g., preliminary or failed experiments that didn't make it into the paper).

9. Code of ethics

Question: Does the research conducted in the paper conform, in every respect, with the NeurIPS Code of Ethics <https://neurips.cc/public/EthicsGuidelines>?

Answer: [Yes]

Justification: This work fully complies with the NeurIPS Code of Ethics.

Guidelines:

- The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
- If the authors answer No, they should explain the special circumstances that require a deviation from the Code of Ethics.
- The authors should make sure to preserve anonymity (e.g., if there is a special consideration due to laws or regulations in their jurisdiction).

10. Broader impacts

Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

Answer: [NA]

Justification: This is a theoretical work without addressing or having any societal impact.

Guidelines:

- The answer NA means that there is no societal impact of the work performed.
- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.

- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.
- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.
- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

11. Safeguards

Question: Does the paper describe safeguards that have been put in place for responsible release of data or models that have a high risk for misuse (e.g., pretrained language models, image generators, or scraped datasets)?

Answer: [NA]

Justification: This work poses no such risks.

Guidelines:

- The answer NA means that the paper poses no such risks.
- Released models that have a high risk for misuse or dual-use should be released with necessary safeguards to allow for controlled use of the model, for example by requiring that users adhere to usage guidelines or restrictions to access the model or implementing safety filters.
- Datasets that have been scraped from the Internet could pose safety risks. The authors should describe how they avoided releasing unsafe images.
- We recognize that providing effective safeguards is challenging, and many papers do not require this, but we encourage authors to take this into account and make a best faith effort.

12. Licenses for existing assets

Question: Are the creators or original owners of assets (e.g., code, data, models), used in the paper, properly credited and are the license and terms of use explicitly mentioned and properly respected?

Answer: [NA]

Justification: This work does not use existing assets.

Guidelines:

- The answer NA means that the paper does not use existing assets.
- The authors should cite the original paper that produced the code package or dataset.
- The authors should state which version of the asset is used and, if possible, include a URL.
- The name of the license (e.g., CC-BY 4.0) should be included for each asset.
- For scraped data from a particular source (e.g., website), the copyright and terms of service of that source should be provided.
- If assets are released, the license, copyright information, and terms of use in the package should be provided. For popular datasets, paperswithcode.com/datasets has curated licenses for some datasets. Their licensing guide can help determine the license of a dataset.

- For existing datasets that are re-packaged, both the original license and the license of the derived asset (if it has changed) should be provided.
- If this information is not available online, the authors are encouraged to reach out to the asset's creators.

13. **New assets**

Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

Answer: [NA]

Justification: This work does not release new assets.

Guidelines:

- The answer NA means that the paper does not release new assets.
- Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.
- The paper should discuss whether and how consent was obtained from people whose asset is used.
- At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

14. **Crowdsourcing and research with human subjects**

Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

Answer: [NA]

Justification: This work does not involve crowdsourcing or research with human subjects.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Including this information in the supplemental material is fine, but if the main contribution of the paper involves human subjects, then as much detail as possible should be included in the main paper.
- According to the NeurIPS Code of Ethics, workers involved in data collection, curation, or other labor should be paid at least the minimum wage in the country of the data collector.

15. **Institutional review board (IRB) approvals or equivalent for research with human subjects**

Question: Does the paper describe potential risks incurred by study participants, whether such risks were disclosed to the subjects, and whether Institutional Review Board (IRB) approvals (or an equivalent approval/review based on the requirements of your country or institution) were obtained?

Answer: [NA]

Justification: This work does not involve crowdsourcing nor research with human subjects.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Depending on the country in which research is conducted, IRB approval (or equivalent) may be required for any human subjects research. If you obtained IRB approval, you should clearly state this in the paper.
- We recognize that the procedures for this may vary significantly between institutions and locations, and we expect authors to adhere to the NeurIPS Code of Ethics and the guidelines for their institution.
- For initial submissions, do not include any information that would break anonymity (if applicable), such as the institution conducting the review.

16. Declaration of LLM usage

Question: Does the paper describe the usage of LLMs if it is an important, original, or non-standard component of the core methods in this research? Note that if the LLM is used only for writing, editing, or formatting purposes and does not impact the core methodology, scientific rigorousness, or originality of the research, declaration is not required.

Answer: [NA]

Justification: This work does not involve LLMs as any important, original, or non-standard components.

Guidelines:

- The answer NA means that the core method development in this research does not involve LLMs as any important, original, or non-standard components.
- Please refer to our LLM policy (<https://neurips.cc/Conferences/2025/LLM>) for what should or should not be described.

A Discussion of Theoretical Advances in Accelerating Samplers for Diffusion Models

Score-based diffusion models can be formulated using either SDEs or their deterministic counterparts, known as probability flow ODEs [36]. While SDE-based samplers generate samples through stochastic simulation, ODE-based samplers provide a deterministic alternative. Theoretical advancements in accelerating these samplers have emerged only recently. A significant step toward designing provably accelerated, training-free methods was made by [24], who propose and analyze acceleration for both ODE- and SDE-based samplers. Their accelerated SDE sampler leverages higher-order expansions of the conditional density to enhance efficiency. This was followed by the work of [25], which provided convergence guarantees for probability flow ODEs. Furthermore, [19] studies the convergence properties of deterministic samplers based on probability flow ODEs, using the Runge-Kutta integrator; [41] propose and analyze a training-free acceleration algorithm for SDE-based samplers, based on the stochastic Runge-Kutta method. [27] proposes a novel accelerated SDE-based sampler when Hessian information is available. Another line of work involves the midpoint randomized method. In particular, [15] explore ODE acceleration by incorporating a randomized midpoint method, leveraging its advantages in parallel computation. A more recent work by [23] improved upon the ODE sampler proposed by [15], achieving the state-of-the-art convergence rate.

We note that all of these works provide convergence analysis in terms of either KL divergence or TV distance. Among these, [27] accelerates the stochastic DDPM sampler by leveraging precise score and Hessian estimations of the log density, even for possibly non-smooth target distributions. This is achieved through a novel Bayesian approach based on tilting factor representation and Tweedie's formula. [19] accelerates the ODE sampler by utilizing p -th ($p \geq 1$) order information of the score function, with the target distribution supported on a compact set and employing early stopping. These two works are the most similar to our proposed accelerated sampler in that they all rely on the Hessian information of the log density. However, their settings differ from ours, and their convergence analyses are neither directly applicable to our framework nor precisely expressed in terms of Wasserstein distance.⁴

B Proof of Section 3

We define several stochastic processes associated with the backward process $X_t^{\leftarrow}$ and the sample path ϑ_n . First, recall that $X_t^{\leftarrow}$ is described by the following SDE:

$$dX_t^{\leftarrow} = \left(\frac{1}{2} X_t^{\leftarrow} + \nabla \log p_t(X_t^{\leftarrow}) \right) dt + dW_t, \quad X_0^{\leftarrow} \sim p_T,$$

and $\{\vartheta_n^\alpha, 0 \leq n \leq N\}$ satisfies the iterative law:

$$\vartheta_{n+1}^\alpha = \mathcal{G}_h^\alpha(\vartheta_n^\alpha, \{W_t\}_{nh \leq t \leq (n+1)h}),$$

where $\alpha \in \{\text{EM}, \text{EI}, \text{REM}, \text{REI}, \text{SO}\}$.

Based on $X_t^{\leftarrow}$, we define the following two processes, $\{Y_t, 0 \leq t \leq T\}$ and $\{\tilde{Y}_t, 0 \leq t \leq h\}$. Y_t satisfies the SDE

$$dY_t = \left(\frac{1}{2} Y_t + \nabla \log p_{T-t}(Y_t) \right) dt + dW_t, \quad Y_0 \sim \hat{p}_T.$$

$\tilde{Y}_t$ actually relies on $X_t^{\leftarrow}$ on the time interval $[nh, (n+1)h]$ for each n . However, we only need this notation in the proof of one-step discretization error, then we allow for some slight abuse of notation by omitting n , since it will not lead to any confusion. Therefore, $\{\tilde{Y}_t, 0 \leq t \leq h\}$ satisfies

$$d\tilde{Y}_t = \left(\frac{1}{2} \tilde{Y}_t + \nabla \log p_{T-t}(\tilde{Y}_t) \right) dt + dW_t, \quad \tilde{Y}_0 = \vartheta_n. \quad (12)$$

⁴When the target distribution is compactly supported, Pinsker's inequality allows translating TV or KL divergence into Wasserstein distance. However, this often yields loose bounds, especially in high dimensions, where the actual Wasserstein distance may be much smaller.

Recall that we have defined two processes v_{n+u}^{REM} and v_{n+u}^{REI} in Section 3.2, that is, for any $u \in [0, 1]$ and $n = 0, \dots, N-1$,

$$\begin{aligned} v_{n+u}^{\text{REM}} &:= \left(1 + \frac{uh}{2}\right) v_n^{\text{REM}} + uh s_*(T - nh, v_n^{\text{REM}}) + \sqrt{uh} \xi_n, \\ v_{n+u}^{\text{REI}} &:= e^{uh/2} v_n^{\text{REI}} + 2(e^{uh/2} - 1) s_*(T - nh, v_n^{\text{REI}}) + \sqrt{e^{uh} - 1} \xi'_n. \end{aligned}$$

This section is devoted to proving the convergence rate of the diffusion model under various discretization schemes. To this end, we need the following auxiliary lemmas.

Lemma 6 (Lemma 9 in [13]). *Suppose that Assumption 1 holds. Then, $\nabla \log p_t(x)$ is $L(t)$ -Lipschitz, where $L(t)$ is given by*

$$L(t) = \min\{(1 - e^{-t})^{-1}, e^t L_0\} = \begin{cases} e^t L_0 & \text{if } t \leq \log(1 + \frac{1}{L_0}) \\ (1 - e^{-t})^{-1} & \text{if } t > \log(1 + \frac{1}{L_0}) \end{cases}.$$

Therefore,

$$L(t) \leq L_0 + 1.$$

Lemma 7 (Proof of Proposition 7 in [13]). *Suppose that Assumption 1 holds. Then, $\nabla \log p_t(x)$ is $m(t)$ -strongly log-concave, where $m(t)$ is given by*

$$m(t) = \frac{1}{e^{-t}/m_0 + (1 - e^{-t})}.$$

Therefore,

$$m(t) \geq \min\{1, m_0\}.$$

Combining these two lemmas, we conclude that the Hessian matrix of $\log p_t$ satisfies the following condition

$$-L(t)I_d \preceq \nabla^2 \log p_t(\cdot) \preceq -m(t)I_d.$$

We will frequently use Grönwall's inequality in the proof. Below, we present a specialized form tailored to the relevant processes.

Lemma 8. *Suppose the Assumption 1 holds, consider two stochastic processes H_t and G_t defined on the time interval $[t_1, t_2]$, if they satisfy the same SDE, especially motivated by the same Brownian motion, which means that*

$$\begin{aligned} dH_t &= \left(\frac{1}{2}H_t + \nabla \log p_{T-t}(H_t)\right) dt + dW_t, \\ dG_t &= \left(\frac{1}{2}G_t + \nabla \log p_{T-t}(G_t)\right) dt + dW_t. \end{aligned}$$

then for each $t \in [t_1, t_2]$,

$$\|H_t - G_t\|_{\mathbb{L}_2} \leq e^{-\int_{t_1}^t (m(T-s) - \frac{1}{2}) ds} \|H_{t_1} - G_{t_1}\|_{\mathbb{L}_2}.$$

Applying Lemma 8 to different processes and time intervals, we derive the following inequalities essential for our proof.

$$\left\|Y_{nh+t} - \tilde{Y}_t\right\|_{\mathbb{L}_2} \leq e^{-\int_{nh}^{nh+t} (m(T-s) - \frac{1}{2}) ds} \left\|Y_{nh} - \tilde{Y}_0\right\|_{\mathbb{L}_2}, \quad \forall t \in [0, h]. \quad (13)$$

$$\left\|Y_t - X_t^{\leftarrow}\right\|_{\mathbb{L}_2} \leq e^{-\int_0^t (m(T-s) - \frac{1}{2}) ds} \left\|Y_0 - X_0^{\leftarrow}\right\|_{\mathbb{L}_2}, \quad \forall t \in [0, T]. \quad (14)$$

which follow from the fact that $\{Y_t, 0 \leq t \leq T\}$, $\{\tilde{Y}_t, 0 \leq t \leq h\}$, $\{X_t^{\leftarrow}, 0 \leq t \leq T\}$ all satisfy the same SDE as in Lemma 8, by applying a time-shifting operator to $\tilde{Y}_t$.

B.1 Proof of Theorem 1: Part I

In this part, we provide the first part of the proof of Theorem 1, with respect to Euler-Maruyama method. To achieve this, we first prove the one-step discretization error in the following proposition.

Proposition 9. *Suppose that Assumption 1, 2 and 3 are satisfied. Then, the following two claims hold.*

(1) *Firstly, it holds that*

$$\begin{aligned} \left\| \tilde{Y}_h - \vartheta_{n+1}^{\text{EM}} \right\|_{\mathbb{L}_2} &\leq h^2 (C_1(n)^2 + M_1) \left\| Y_{nh} - \vartheta_n^{\text{EM}} \right\|_{\mathbb{L}_2} \\ &\quad + h^2 \left[C_1(n) \left(C_1(n) C_2(n) + \frac{1}{2} C_4 + C_3(n) \right) + M_1 (1 + C_2(n) + C_4) \right] \\ &\quad + h^{3/2} \sqrt{d} C_1(n) \\ &\quad + h \varepsilon_{sc}, \end{aligned}$$

where

$$\begin{aligned} C_1(n) &= \frac{1}{2} + \frac{1}{h} \int_{nh}^{(n+1)h} L(T-t) \, dt, \\ C_2(n) &= e^{-\int_0^{nh} (m(T-t) - \frac{1}{2}) \, dt} \|Y_0 - X_T\|_{\mathbb{L}_2}, \\ C_3(n) &= \frac{1}{h} \int_{nh}^{(n+1)h} (dL(T-t))^{1/2} \, dt, \\ C_4 &= \sup_{0 \leq t \leq T} \|X_t\|_{\mathbb{L}_2}. \end{aligned}$$

(2) *As a result,*

$$\left\| Y_{(n+1)h} - \vartheta_{n+1}^{\text{EM}} \right\|_{\mathbb{L}_2} \leq r_n^{\text{EM}} \left\| Y_{nh} - \vartheta_n^{\text{EM}} \right\|_{\mathbb{L}_2} + h^2 C_n^{\text{EM}} + h^{3/2} \sqrt{d} C_1(n) + h \varepsilon_{sc},$$

where

$$\begin{aligned} r_n^{\text{EM}} &= e^{-\int_{nh}^{(n+1)h} (m(T-t) - \frac{1}{2}) \, dt} + h^2 (C_1(n)^2 + M_1), \\ C_n^{\text{EM}} &= C_1(n) \left(C_1(n) C_2(n) + \frac{1}{2} C_4 + C_3(n) \right) + M_1 (1 + C_2(n) + C_4). \end{aligned}$$

Proof. We prove the two claims sequentially.

Proof of Claim (1). Rewrite display (12) in the integral form,

$$\tilde{Y}_h = \tilde{Y}_0 + \int_0^h \left(\frac{1}{2} \tilde{Y}_t + \nabla \log p_{T-nh-t}(\tilde{Y}_t) \right) dt + \int_{nh}^{(n+1)h} dW_t.$$

For Euler-Maruyama method, we can write $\vartheta_{n+1}^{\text{EM}}$ in integral form as follows

$$\vartheta_{n+1}^{\text{EM}} = \vartheta_n^{\text{EM}} + \int_{nh}^{(n+1)h} \left(\frac{1}{2} \vartheta_n^{\text{EM}} + s_*(T-nh, \vartheta_n^{\text{EM}}) \right) dt + \int_{nh}^{(n+1)h} dW_t.$$

Note that $\tilde{Y}_0 = \vartheta_n^{\text{EM}}$, then, it holds that

$$\begin{aligned} \|\tilde{Y}_h - \vartheta_{n+1}^{\text{EM}}\|_{\mathbb{L}_2} &= \left\| \frac{1}{2} \int_0^h (\tilde{Y}_t - \vartheta_n^{\text{EM}}) dt + \int_0^h (\nabla \log p_{T-nh-t}(\tilde{Y}_t) - s_*(T-nh, \vartheta_n^{\text{EM}})) dt \right\|_{\mathbb{L}_2} \\ &\leq \underbrace{\left\| \frac{1}{2} \int_0^h (\tilde{Y}_t - \tilde{Y}_0) dt + \int_0^h (\nabla \log p_{T-nh-t}(\tilde{Y}_t) - \nabla \log p_{T-nh-t}(\tilde{Y}_0)) dt \right\|_{\mathbb{L}_2}}_{\text{I}} \\ &\quad + \underbrace{\left\| \int_0^h (\nabla \log p_{T-nh-t}(\vartheta_n^{\text{EM}}) - \nabla \log p_{T-nh}(\vartheta_n^{\text{EM}})) dt \right\|_{\mathbb{L}_2}}_{\text{II}} \\ &\quad + \underbrace{\left\| \int_0^h (\nabla \log p_{T-nh}(\vartheta_n^{\text{EM}}) - s_*(T-nh, \vartheta_n^{\text{EM}})) dt \right\|_{\mathbb{L}_2}}_{\text{III}}. \end{aligned} \quad (15)$$

Here, we decompose the term $\|\tilde{Y}_h - \vartheta_{n+1}^{\text{EM}}\|_{\mathbb{L}_2}$ into a sum of three terms and then control each term individually.

For the term I of inequality (15), by Assumption 1 and Lipschitzness of $\nabla \log p_t$, we obtain

$$\begin{aligned} \text{I} &= \left\| \frac{1}{2} \int_0^h (\tilde{Y}_t - \tilde{Y}_0) dt + \int_0^h (\nabla \log p_{T-nh-t}(\tilde{Y}_t) - \nabla \log p_{T-nh-t}(\tilde{Y}_0)) dt \right\|_{\mathbb{L}_2} \\ &\leq \frac{1}{2} \int_0^h \|\tilde{Y}_t - \tilde{Y}_0\|_{\mathbb{L}_2} dt + \int_0^h L(T-nh-t) \|\tilde{Y}_t - \tilde{Y}_0\|_{\mathbb{L}_2} dt \\ &\leq \left(\frac{1}{2}h + \int_{nh}^{(n+1)h} L(T-t) dt \right) \sup_{0 \leq t \leq h} \|\tilde{Y}_t - \tilde{Y}_0\|_{\mathbb{L}_2}. \end{aligned}$$

We then proceed to derive the upper bound for the term $\sup_{0 \leq t \leq h} \|\tilde{Y}_t - \tilde{Y}_0\|_{\mathbb{L}_2}$.

Lemma 10. *When p_0 satisfies Assumption 1, it holds that*

$$\begin{aligned} \sup_{0 \leq t \leq h} \|\tilde{Y}_t - \tilde{Y}_0\|_{\mathbb{L}_2} &\leq \left(\frac{1}{2}h + \int_{nh}^{(n+1)h} L(T-t) dt \right) \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} \\ &\quad + \left(\frac{1}{2}h + \int_{nh}^{(n+1)h} L(T-t) dt \right) e^{-\int_0^{nh} (m(T-t) - \frac{1}{2}) dt} \|Y_0 - X_T\|_{\mathbb{L}_2} \\ &\quad + \frac{1}{2}h \sup_{0 \leq t \leq T} \|X_t\|_{\mathbb{L}_2} + \int_{nh}^{(n+1)h} (dL(T-t))^{1/2} dt + \sqrt{dh}. \end{aligned}$$

Notice that we have no initial limit on the $\tilde{Y}_t$ in Lemma 10, which means that we can use this lemma to any discretization scheme.

For the term II of (15), we first rely on Assumption 2 to derive

$$\begin{aligned} \text{II} &= \left\| \int_0^h (\nabla \log p_{T-nh-t}(\vartheta_n^{\text{EM}}) - \nabla \log p_{T-nh}(\vartheta_n^{\text{EM}})) dt \right\|_{\mathbb{L}_2} \\ &\leq \int_0^h \|\nabla \log p_{T-nh-t}(\vartheta_n^{\text{EM}}) - \nabla \log p_{T-nh}(\vartheta_n^{\text{EM}})\|_{\mathbb{L}_2} dt \\ &\leq h^2 M_1 (1 + \|\vartheta_n^{\text{EM}}\|_{\mathbb{L}_2}). \end{aligned}$$

Using the triangle inequality and (14), we obtain

$$\begin{aligned}\|\vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} &\leq \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} + \|Y_{nh} - X_{nh}^{\leftarrow}\|_{\mathbb{L}_2} + \|X_{nh}^{\leftarrow}\|_{\mathbb{L}_2} \\ &\leq \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} + e^{-\int_0^{nh} (m(T-t) - \frac{1}{2}) dt} \|Y_0 - X_T\|_{\mathbb{L}_2} + \sup_{0 \leq t \leq T} \|X_t\|_{\mathbb{L}_2}.\end{aligned}\quad (16)$$

For the term III of (15), it follows from Assumption 3 that

$$\begin{aligned}\text{III} &= \left\| \int_0^h (\nabla \log p_{T-nh}(\vartheta_n^{\text{EM}}) - s_*(T-nh, \vartheta_n^{\text{EM}})) dt \right\|_{\mathbb{L}_2} \\ &\leq \int_0^h \|\nabla \log p_{T-nh}(\vartheta_n^{\text{EM}}) - s_*(T-nh, \vartheta_n^{\text{EM}})\|_{\mathbb{L}_2} dt \\ &\leq h\varepsilon_{sc}.\end{aligned}$$

Combining these terms above, we obtain that

$$\begin{aligned}\|\tilde{Y}_h - \vartheta_{n+1}^{\text{EM}}\|_{\mathbb{L}_2} &\leq h^2(C_1(n)^2 + M_1) \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} \\ &\quad + h^2 \left[C_1(n) \left(C_1(n)C_2(n) + \frac{1}{2}C_4 + C_3(n) \right) + M_1(1 + C_2(n) + C_4) \right] \\ &\quad + h^{3/2}\sqrt{d}C_1(n) \\ &\quad + h\varepsilon_{sc},\end{aligned}\quad (17)$$

where

$$\begin{aligned}C_1(n) &= \frac{1}{2} + \frac{1}{h} \int_{nh}^{(n+1)h} L(T-t) dt, \\ C_2(n) &= e^{-\int_0^{nh} (m(T-t) - \frac{1}{2}) dt} \|Y_0 - X_T\|_{\mathbb{L}_2}, \\ C_3(n) &= \frac{1}{h} \int_{nh}^{(n+1)h} (dL(T-t))^{1/2} dt, \\ C_4 &= \sup_{0 \leq t \leq T} \|X_t\|_{\mathbb{L}_2}.\end{aligned}$$

This completes the proof of Claim (1).

Proof of Claim (2). By the triangle inequality, we have

$$\|Y_{(n+1)h} - \vartheta_{n+1}^{\text{EM}}\|_{\mathbb{L}_2} \leq \|Y_{(n+1)h} - \tilde{Y}_h\|_{\mathbb{L}_2} + \|\tilde{Y}_h - \vartheta_{n+1}^{\text{EM}}\|_{\mathbb{L}_2}. \quad (18)$$

Applying (13) to the first term of (18), we obtain that

$$\|Y_{(n+1)h} - \tilde{Y}_h\|_{\mathbb{L}_2}^2 \leq e^{-\int_{nh}^{(n+1)h} (2m(T-t) - 1) dt} \|Y_{nh} - \tilde{Y}_0\|_{\mathbb{L}_2}^2. \quad (19)$$

Notice that $\tilde{Y}_0 = \vartheta_n^{\text{EM}}$, it then follows that

$$\|Y_{(n+1)h} - \tilde{Y}_h\|_{\mathbb{L}_2} \leq e^{-\int_{nh}^{(n+1)h} (m(T-t) - \frac{1}{2}) dt} \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2}.$$

Claim (2) follows directly from our previous results and Claim (1). Since this step is independent of the discretization method, it applies to all the schemes discussed in this section. In the following analysis, we omit this step and proceed directly with the proof of the first claim. $\square$

We now proceed to derive the upper bound of the Wasserstein distance between the sample distribution generated after N iterations and the target distribution p_0 , based on the one-step discretization error bound given by Proposition 9.

First, note that

$$W_2(\mathcal{L}(\vartheta_N^{\text{EM}}, p_0) \leq \|\vartheta_N^{\text{EM}} - X_0\|_{\mathbb{L}_2} \leq \|Y_{Nh} - \vartheta_N^{\text{EM}}\|_{\mathbb{L}_2} + \|Y_{Nh} - X_0\|_{\mathbb{L}_2}.$$

Invoking Proposition 7 of [13], we have

$$\|Y_{Nh} - X_0\|_{\mathbb{L}_2} \leq e^{-\int_0^T m(t) dt} \|X_0\|_{\mathbb{L}_2}. \quad (20)$$

According to Proposition 9, by induction, we obtain that

$$\begin{aligned} \|Y_{Nh} - \vartheta_N^{\text{EM}}\|_{\mathbb{L}_2} &\leq r_{N-1}^{\text{EM}} \|Y_{(N-1)h} - \vartheta_{N-1}^{\text{EM}}\|_{\mathbb{L}_2} + \left(h^2 C_{N-1}^{\text{EM}} + h^{3/2} \sqrt{d} C_1(N-1) + h\varepsilon_{sc}\right) \\ &\leq \left(\prod_{j=0}^{N-1} r_j^{\text{EM}}\right) \|Y_0 - \vartheta_0^{\text{EM}}\|_{\mathbb{L}_2} + \sum_{k=0}^{N-1} \left(\prod_{j=k+1}^{N-1} r_j^{\text{EM}}\right) \left(h^2 C_k^{\text{EM}} + h^{3/2} \sqrt{d} C_1(k) + h\varepsilon_{sc}\right) \\ &= \sum_{k=0}^{N-1} \left(\prod_{j=k+1}^{N-1} r_j^{\text{EM}}\right) \left(h^2 C_k^{\text{EM}} + h^{3/2} \sqrt{d} C_1(k) + h\varepsilon_{sc}\right), \end{aligned} \quad (21)$$

where we define $\prod_{j=N}^{N-1} r_j^{\text{EM}} = 1$. Notice that

$$\begin{aligned} \prod_{j=k+1}^{N-1} r_j^{\text{EM}} &= \prod_{j=k+1}^{N-1} \left(e^{-\int_{jh}^{(j+1)h} (m(T-t) - \frac{1}{2}) dt} + h^2 (C_1(k)^2 + M_1)\right) \\ &\lesssim \prod_{j=k+1}^{N-1} e^{-h(m_{\min} - \frac{1}{2})} = e^{-h(m_{\min} - \frac{1}{2})(N-k-1)}. \end{aligned}$$

Therefore, we have

$$\begin{aligned} \|Y_{Nh} - \vartheta_N^{\text{EM}}\|_{\mathbb{L}_2} &\lesssim \sum_{k=0}^{N-1} e^{-h(m_{\min} - \frac{1}{2})(N-k-1)} \left(h^2 C_k^{\text{EM}} + h^{3/2} \sqrt{d} C_1(k) + h\varepsilon_{sc}\right) \\ &\leq \frac{1}{1 - e^{-h(m_{\min} - \frac{1}{2})}} \left(h^2 \max_{0 \leq k \leq N-1} C_k^{\text{EM}} + h^{3/2} \sqrt{d} \max_{0 \leq k \leq N-1} C_1(k) + h\varepsilon_{sc}\right) \\ &\lesssim \frac{1}{m_{\min} - 1/2} \left(\sqrt{dh} \max_{0 \leq k \leq N-1} C_1(k) + \varepsilon_{sc}\right). \end{aligned} \quad (22)$$

Recall the definition of $C_1(k)$ and the upper bound of $L(t)$, it follows that

$$\max_{0 \leq k \leq N-1} C_1(k) \leq \frac{1}{2} + L_{\max},$$

and thus we obtain that

$$\|Y_{Nh} - \vartheta_N^{\text{EM}}\|_{\mathbb{L}_2} \lesssim \sqrt{dh} \cdot \frac{L_{\max} + 1/2}{m_{\min} - 1/2} + \varepsilon_{sc} \cdot \frac{1}{m_{\min} - 1/2}.$$

Plugging this back into the previous display then we have

$$\mathcal{W}_2(\mathcal{L}(\vartheta_N^{\text{EM}}), p_0) \lesssim e^{-\int_0^T m(t) dt} \|X_0\|_{\mathbb{L}_2} + \sqrt{dh} \cdot \frac{L_{\max} + 1/2}{m_{\min} - 1/2} + \varepsilon_{sc} \cdot \frac{1}{m_{\min} - 1/2},$$

which completes the first part of the proof for Theorem 1.

B.2 Proof of Theorem 1: Part II

This part aims to prove the Wasserstein convergence result for the Exponential Integrator (EI) scheme. We will prove this theorem using the same method as in Theorem 1. Following this approach, we first establish the one-step discretization error in the proposition below.

Proposition 11. *Suppose that Assumption 1, 3 and 2 hold, then one-step discretization error for Exponential Integrator scheme is obtained from the following two bounds.*

(1) It holds that

$$\begin{aligned} \|\tilde{Y}_h - \vartheta_{n+1}^{\text{El}}\|_{\mathbb{L}_2} &\leq h^2 \left(C_5(n)C_1(n) + M_1 \frac{2(e^{h/2} - 1)}{h} \right) \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} \\ &\quad + h^2 \left[C_5(n) \left(C_1(n)C_2(n) + \frac{1}{2}C_4 + C_3(n) \right) + \frac{2(e^{h/2} - 1)}{h} M_1(1 + C_2(n) + C_4) \right] \\ &\quad + h^{3/2} \sqrt{d} C_5(n) \\ &\quad + h \cdot \frac{2(e^{h/2} - 1)}{h} \varepsilon_{sc}, \end{aligned}$$

where

$$C_5(n) = \frac{1}{h} \int_{nh}^{(n+1)h} e^{\frac{1}{2}((n+1)h-t)} L(T-t) dt \approx C_1(n) - \frac{1}{2}.$$

(2) Therefore, we have the bound for one-step discretization error

$$\|Y_{(n+1)h} - \vartheta_{n+1}^{\text{El}}\|_{\mathbb{L}_2} \leq r_n^{\text{El}} \|Y_{nh} - \vartheta_n^{\text{El}}\|_{\mathbb{L}_2} + h^2 C_n^{\text{El}} + h^{3/2} \sqrt{d} C_5(n) + h \cdot \frac{2(e^{h/2} - 1)}{h} \varepsilon_{sc},$$

where

$$\begin{aligned} r_n^{\text{El}} &= e^{-\int_{nh}^{(n+1)h} (m(T-t) - \frac{1}{2}) dt} + h^2 \left(C_5(n)C_1(n) + M_1 \frac{2(e^{h/2} - 1)}{h} \right), \\ C_n^{\text{El}} &= C_5(n) \left(C_1(n)C_2(n) + \frac{1}{2}C_4 + C_3(n) \right) + \frac{2(e^{h/2} - 1)}{h} M_1(1 + C_2(n) + C_4). \end{aligned}$$

Here, the constants $C_i, i = 1, 2, 3, 4$ are as defined in Proposition 9.

Proof. We prove two claims in succession.

Proof of Claim (1). Consider the process defined in (12), which satisfies the SDE

$$d\tilde{Y}_t = \left[\frac{1}{2} \tilde{Y}_t + \nabla \log p_{T-nh-t}(\tilde{Y}_t) \right] dt + dW_t,$$

Instead of integrating both sides of the SDE, we use Itô's formula to $e^{-\frac{t}{2}} \tilde{Y}_t$, then we have

$$d(e^{-\frac{t}{2}} \tilde{Y}_t) = -\frac{1}{2} e^{-\frac{t}{2}} \tilde{Y}_t + e^{-\frac{t}{2}} d\tilde{Y}_t = e^{-\frac{t}{2}} \left(\nabla \log p_{T-nh-t}(\tilde{Y}_t) dt + dW_t \right),$$

and we notice that we can write it in an integral form.

$$\tilde{Y}_t = e^{t/2} \tilde{Y}_0 + \int_0^t e^{\frac{1}{2}(t-s)} \nabla \log p_{T-nh-s}(\tilde{Y}_s) ds + \int_{nh}^{nh+t} e^{\frac{1}{2}((n+1)h-s)} dW_s.$$

Then we obtain that

$$\tilde{Y}_h - \vartheta_{n+1}^{\text{El}} = \int_0^h e^{\frac{1}{2}(h-t)} (\nabla \log p_{T-nh-t}(\tilde{Y}_t) - s_*(T - nh, \vartheta_n^{\text{El}})) dt.$$

We make decomposition the same as the one in (15), that is

$$\begin{aligned} \nabla \log p_{T-nh-t}(\tilde{Y}_t) - s_*(T - nh, \vartheta_n^{\text{El}}) &= \nabla \log p_{T-nh-t}(\tilde{Y}_t) - \nabla \log p_{T-nh-t}(\tilde{Y}_0) \\ &\quad + \nabla \log p_{T-nh-t}(\vartheta_n^{\text{El}}) - \nabla \log p_{T-nh}(\vartheta_n^{\text{El}}) \\ &\quad + \nabla \log p_{T-nh}(\vartheta_n^{\text{El}}) - s_*(T - nh, \vartheta_n^{\text{El}}). \end{aligned}$$

It then follows that

$$\begin{aligned} \|\tilde{Y}_h - \vartheta_{n+1}^{\text{El}}\|_{\mathbb{L}_2} &\leq \int_0^h e^{\frac{1}{2}(h-t)} \left\| \nabla \log p_{T-nh-t}(\tilde{Y}_t) - s_*(T - nh, \vartheta_n^{\text{El}}) \right\|_{\mathbb{L}_2} dt \\ &\leq \int_0^h e^{\frac{1}{2}(h-t)} \left\| \nabla \log p_{T-nh-t}(\tilde{Y}_t) - \nabla \log p_{T-nh-t}(\tilde{Y}_0) \right\|_{\mathbb{L}_2} dt \\ &\quad + \int_0^h e^{\frac{1}{2}(h-t)} \left\| \nabla \log p_{T-nh-t}(\vartheta_n^{\text{El}}) - \nabla \log p_{T-nh}(\vartheta_n^{\text{El}}) \right\|_{\mathbb{L}_2} dt \\ &\quad + \int_0^h e^{\frac{1}{2}(h-t)} \left\| \nabla \log p_{T-nh}(\vartheta_n^{\text{El}}) - s_*(T - nh, \vartheta_n^{\text{El}}) \right\|_{\mathbb{L}_2} dt. \end{aligned}$$

Note that apart from the exponential term $e^{\frac{1}{2}(h-t)}$, the derivation of the remaining parts is completely consistent with that of (15), until we encounter the term involving ϑ_n^{EI} , at which point we obtain

$$\begin{aligned} \|\tilde{Y}_h - \vartheta_{n+1}^{\text{EI}}\|_{\mathbb{L}_2} &\leq \left(\int_0^h e^{\frac{1}{2}(h-t)} L(T - nh - t) dt \right) \sup_{0 \leq t \leq h} \|\tilde{Y}_t - \tilde{Y}_0\|_{\mathbb{L}_2} \\ &\quad + \left(\int_0^h e^{\frac{1}{2}(h-t)} dt \right) M_1 h (1 + \|\vartheta_n^{\text{EI}}\|_{\mathbb{L}_2}) \\ &\quad + \left(\int_0^h e^{\frac{1}{2}(h-t)} dt \right) \varepsilon_{sc}. \end{aligned}$$

By Lemma 10, we can bound the first term on the right-hand side of the previous display. Moreover, from (16), $\|\vartheta_n^{\text{EI}}\|_{\mathbb{L}_2}$ can be bounded similarly. Substituting all coefficients with $C_i(n)$ from Proposition 9, we obtain

$$\begin{aligned} \|\tilde{Y}_h - \vartheta_{n+1}^{\text{EI}}\|_{\mathbb{L}_2} &\leq h^2 \cdot C_5(n) \left[C_1(n) \|Y_{nh} - \vartheta_n^{\text{EI}}\|_{\mathbb{L}_2} + C_1(n)C_2(n) + \frac{1}{2}C_4 + C_3(n) \right] \\ &\quad + h^2 \cdot \frac{2(e^{h/2} - 1)}{h} M_1 \left[1 + \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} + C_2(n) + C_4 \right] \\ &\quad + h^{3/2} \sqrt{d} C_5(n) \\ &\quad + h \cdot \frac{2(e^{h/2} - 1)}{h} \varepsilon_{sc} \\ &= h^2 \left(C_5(n)C_1(n) + M_1 \frac{2(e^{h/2} - 1)}{h} \right) \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} \\ &\quad + h^2 \left[C_5(n) \left(C_1(n)C_2(n) + \frac{1}{2}C_4 + C_3(n) \right) + \frac{2(e^{h/2} - 1)}{h} M_1 (1 + C_2(n) + C_4) \right] \\ &\quad + h^{3/2} \sqrt{d} C_5(n) \\ &\quad + h \cdot \frac{2(e^{h/2} - 1)}{h} \varepsilon_{sc}, \end{aligned}$$

where

$$C_5(n) = \frac{1}{h} \int_{nh}^{(n+1)h} e^{\frac{1}{2}((n+1)h-t)} L(T-t) dt \approx C_1(n) - \frac{1}{2}.$$

Proof of Claim (2). The proof is omitted for brevity, as it merely requires incorporating $\|Y_{(n+1)h} - \tilde{Y}_h\|_{\mathbb{L}_2}$ into the conclusion of Claim (1), following a similar argument as in the proof of Claim (2) in Proposition 9. □

For the second part of the proof for Theorem 1, recall that in the first part, the three key steps (20), (21) and (22) lead to the desired result. We now revisit these steps within the framework of other discretization schemes.

Since (20) is independent of the discretization scheme, we can directly apply it throughout the proofs of Theorems 1, 3 and 4. For (21), we note that the h^2 term in r_j^α is neglected, which results in the same upper bound for $\prod_{j=k+1}^{N-1} r_j^\alpha$ across all discretization schemes.

Given the consistency of these two steps, for the remaining discretization schemes, we can directly derive an analogue of (22) from Claim (2). Therefore, in the subsequent proofs of these theorems, after establishing the corresponding proposition, we proceed directly from an expression similar to (22).

For this theorem, we begin the proof with the following inequality

$$\begin{aligned}\|Y_{Nh} - \vartheta_N^{\text{El}}\|_{\mathbb{L}_2} &\lesssim \frac{1}{m_{\min} - 1/2} \left(hC_n^{\text{El}} + h^{1/2}\sqrt{d} \max_{0 \leq k \leq N-1} C_5(k) + \varepsilon_{sc} \right) \\ &\lesssim \frac{1}{m_{\min} - 1/2} \left(\sqrt{dh} \max_{0 \leq k \leq N-1} C_5(k) + \varepsilon_{sc} \right) \\ &\leq \sqrt{dh} \cdot \frac{L_{\max}}{m_{\min} - 1/2} + \varepsilon_{sc} \cdot \frac{1}{m_{\min} - 1/2}.\end{aligned}$$

Combining this with the bound of $\|X_0 - Y_{Nh}\|_{\mathbb{L}_2}$, we obtain

$$\mathbb{W}_2(\mathcal{L}(\vartheta_N^{\text{El}}), p_0) \lesssim e^{-m_{\min}T} \|X_0\|_{\mathbb{L}_2} + \sqrt{dh} \cdot \frac{L_{\max}}{m_{\min} - 1/2} + \varepsilon_{sc} \cdot \frac{1}{m_{\min} - 1/2}$$

as desired.

B.3 Proof of Theorem 3: Part I

In this section, we prove the Wasserstein distance between the generated distribution $\mathcal{L}(\vartheta_N^{\text{REM}})$ and the target distribution. The following proposition is established for the one-step discretization error.

Proposition 12. *Suppose that Assumptions 1, 2 and 4 are satisfied, the following two claims hold.*

(1) *It holds that*

$$\begin{aligned}&\|\tilde{Y}_h - \vartheta_{n+1}^{\text{REM}}\|_{\mathbb{L}_2} \\ &\leq h^2 \left\{ \left[\int_0^1 \int_0^1 \left[|u-v|L(T-(n+u)h) \left(\frac{1}{2} + L(T-nh) \right) + M_1 \right]^2 du dv \right]^{1/2} \right. \\ &\quad \left. + \frac{1}{4\sqrt{3}}L(T-nh) + \frac{1}{8\sqrt{3}} \right\} \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\ &\quad + h^2 \left\{ \left\{ \int_0^1 \int_0^1 \left\{ (u-v) \left[\left(\frac{1}{2} + L(T-nh) \right) C_2(n) + \frac{1}{2}C_4 + (dL(T-nh))^{1/2} \right] L(T-(n+u)h) \right. \right. \right. \\ &\quad \left. \left. \left. + M_1(1+C_2(n)+C_4) \right\}^2 du dv \right\}^{1/2} \right. \\ &\quad \left. + \frac{1}{8\sqrt{3}}(C_2(n)+C_4) + \frac{1}{4\sqrt{3}} \left(L(T-nh)C_2(n) + (dL(T-nh))^{1/2} \right) \right\} \\ &\quad + h^{3/2} \left\{ \sqrt{d} \left[\int_0^1 \int_0^1 L(T-(n+u)h)^2 |u-v| du dv \right]^{1/2} + \frac{1}{2\sqrt{3}} \right\} \\ &\quad + 2h\varepsilon_{sc}.\end{aligned}$$

(2) *Moreover, it holds that*

$$\|Y_{(n+1)h} - \vartheta_{n+1}^{\text{REM}}\| \leq r_n^{\text{REM}} \|Y_{nh} - \vartheta_n\|_{\mathbb{L}_2} + h^2 C_{n,1}^{\text{REM}} + h^{3/2} C_{n,2}^{\text{REM}} + 3h\varepsilon_{sc},$$

where

$$\begin{aligned}r_n^{\text{REM}} &= e^{-\int_{nh}^{(n+1)h} (m(T-t) - \frac{1}{2}) dt} \\ &\quad + h^2 \left\{ \left[\int_0^1 \int_0^1 \left[|u-v|L(T-(n+u)h) \left(\frac{1}{2} + L(T-nh) \right) + M_1 \right]^2 du dv \right]^{1/2} \right. \\ &\quad \left. + \frac{1}{4\sqrt{3}}L(T-nh) + \frac{1}{8\sqrt{3}} \right\},\end{aligned}$$

$$\begin{aligned}
C_{n,1}^{\text{REM}} &= \left\{ \int_0^1 \int_0^1 \left\{ (u-v) \left[\left(\frac{1}{2} + L(T-nh) \right) C_2(n) + \frac{1}{2} C_4 + (dL(T-nh))^{1/2} \right] L(T-(n+u)h) \right. \right. \\
&\quad \left. \left. + M_1(1+C_2(n)+C_4) \right\}^2 du dv \right\}^{1/2} \\
&\quad + \frac{1}{8\sqrt{3}}(C_2(n)+C_4) + \frac{1}{4\sqrt{3}} \left(L(T-nh)C_2(n) + (dL(T-nh))^{1/2} \right), \\
C_{n,2}^{\text{REM}} &= \sqrt{d} \left[\int_0^1 \int_0^1 L(T-(n+u)h)^2 |u-v| du dv \right]^{1/2} + \frac{1}{2\sqrt{3}}.
\end{aligned}$$

Proof of Proposition 12. Proof of Claim (1). We make the following decomposition of one-step discretization error

$$\left\| \tilde{Y}_h - \vartheta_{n+1}^{\text{REM}} \right\|_{\mathbb{L}_2} \leq \left\| \tilde{Y}_h - \mathbb{E}_{U_n} [\vartheta_{n+1}^{\text{REM}}] \right\|_{\mathbb{L}_2} + \left\| \mathbb{E}_{U_n} [\vartheta_{n+1}^{\text{REM}}] - \vartheta_{n+1}^{\text{REM}} \right\|_{\mathbb{L}_2}. \quad (23)$$

We first derive the upper bound for the term $\left\| \tilde{Y}_h - \mathbb{E}_{U_n} [\vartheta_{n+1}^{\text{REM}}] \right\|_{\mathbb{L}_2}$. By the definitions of ϑ_n^{REM} and $\tilde{Y}_h$, we have

$$\begin{aligned}
&\left\| \tilde{Y}_h - \mathbb{E}_{U_n} [\vartheta_{n+1}^{\text{REM}}] \right\|_{\mathbb{L}_2} \\
&= \left\| \frac{1}{2} \int_0^h \tilde{Y}_t dt + \int_0^h \nabla \log p_{T-nh-t}(\tilde{Y}_t) dt - \frac{1}{2} h \mathbb{E}_{U_n}(\vartheta_{n+U}^{\text{REM}}) - h \mathbb{E}_{U_n}[s_*(T-(n+U_n)h, \vartheta_{n+U}^{\text{REM}})] \right\|_{\mathbb{L}_2}.
\end{aligned}$$

Notice that

$$\int_0^h \tilde{Y}_t dt = h \mathbb{E}_{U_n}[\tilde{Y}_{U_n h}], \quad \int_0^h \nabla \log p_{T-nh-t}(\tilde{Y}_t) dt = h \mathbb{E}_{U_n}[\nabla \log p_{T-(n+U_n)h}(\tilde{Y}_{U_n h})].$$

Plugging this back into the previous display then gives

$$\begin{aligned}
&\left\| \tilde{Y}_h - \mathbb{E}_{U_n} [\vartheta_{n+1}^{\text{REM}}] \right\|_{\mathbb{L}_2} \\
&= \left\| \frac{1}{2} h \mathbb{E}_{U_n}[\tilde{Y}_{U_n h}] + h \mathbb{E}_{U_n}[\nabla \log p_{T-(n+U_n)h}(\tilde{Y}_{U_n h})] - \frac{1}{2} h \mathbb{E}_{U_n}(\vartheta_{n+U}^{\text{REM}}) - h \mathbb{E}_{U_n}(s_*(T-(n+U_n)h, \vartheta_{n+U}^{\text{REM}})) \right\|_{\mathbb{L}_2} \\
&\leq \frac{1}{2} h \left\| \mathbb{E}_{U_n}[\tilde{Y}_{U_n h} - \vartheta_{n+U}^{\text{REM}}] \right\|_{\mathbb{L}_2} + h \left\| \mathbb{E}_{U_n}[\nabla \log p_{T-(n+U_n)h}(\tilde{Y}_{U_n h}) - s_*(T-(n+U_n)h, \vartheta_{n+U}^{\text{REM}})] \right\|_{\mathbb{L}_2}.
\end{aligned}$$

By the definition of $\tilde{Y}_{U_n h}$ and $\vartheta_{n+U_n}^{\text{REM}}$, we have

$$\begin{aligned}
&\left\| \mathbb{E}_{U_n}[\tilde{Y}_{U_n h} - \vartheta_{n+U_n}^{\text{REM}}] \right\|_{\mathbb{L}_2} \\
&= \left\| \mathbb{E}_{U_n} \left[\frac{1}{2} \int_0^{U_n h} (\tilde{Y}_t - \vartheta_n^{\text{REM}}) dt + \int_0^{U_n h} (\nabla \log p_{T-nh-t}(\tilde{Y}_t) - s_*(T-nh, \vartheta_n^{\text{REM}})) dt \right] \right\|_{\mathbb{L}_2} \\
&\leq \left\| \mathbb{E}_{U_n} \left[\frac{1}{2} \int_0^{U_n h} \left\| \tilde{Y}_t - \vartheta_n^{\text{REM}} \right\| dt + \int_0^{U_n h} \left\| \nabla \log p_{T-nh-t}(\tilde{Y}_t) - s_*(T-nh, \vartheta_n^{\text{REM}}) \right\| dt \right] \right\|_{\mathbb{L}_2} \\
&\leq \left\| \mathbb{E}_{U_n} \left[\frac{1}{2} \int_0^h \left\| \tilde{Y}_t - \vartheta_n^{\text{REM}} \right\| dt + \int_0^h \left\| \nabla \log p_{T-nh-t}(\tilde{Y}_t) - s_*(T-nh, \vartheta_n^{\text{REM}}) \right\| dt \right] \right\|_{\mathbb{L}_2} \\
&\leq \frac{1}{2} \int_0^h \left\| \tilde{Y}_t - \vartheta_n^{\text{REM}} \right\|_{\mathbb{L}_2} dt + \int_0^h \left\| \nabla \log p_{T-nh-t}(\tilde{Y}_t) - s_*(T-nh, \vartheta_n^{\text{REM}}) \right\|_{\mathbb{L}_2} dt.
\end{aligned}$$

The second inequality arises because the integrand is non-negative, the last inequality follows from the fact that the random variables inside the inner expectation $\mathbb{E}_{U_n}$ are independent of U_n , and thus the inner expectation can be ignored. Then using the same argument as in the proof of Proposition 9,

especially adopting the same procedure as the one following (15), we can apply the conclusion of Proposition 9 to the term above, then we obtain that

$$\begin{aligned}
\left\| \mathbb{E}_{U_n} [\tilde{Y}_{U_n h} - \vartheta_{n+U_n}^{\text{REM}}] \right\|_{\mathbb{L}_2} &\leq \left(\frac{1}{2} h + \int_{nh}^{(n+1)h} L(T-t) dt \right) \sup_{0 \leq t \leq h} \left\| \tilde{Y}_t - \tilde{Y}_0 \right\|_{\mathbb{L}_2} \\
&\quad + \int_{nh}^{(n+1)h} \left\| \nabla \log p_{T-nh-t}(\vartheta_n^{\text{REM}}) - s_*(T-nh, \vartheta_n^{\text{REM}}) \right\|_{\mathbb{L}_2} dt \\
&\leq h^2 (C_1(n)^2 + M_1) \left\| Y_{nh} - \vartheta_n^{\text{REM}} \right\|_{\mathbb{L}_2} \\
&\quad + h^2 \left[C_1(n) \left(C_1(n) C_2(n) + \frac{1}{2} C_4 + C_3(n) \right) + M_1 (1 + C_2(n) + C_4) \right] \\
&\quad + h^{3/2} \sqrt{d} C_1(n) \\
&\quad + h \varepsilon_{sc} \\
&\triangleq h^2 r_1 \left\| Y_{nh} - \vartheta_n^{\text{REM}} \right\|_{\mathbb{L}_2} + h^2 r_2 + h^{3/2} \sqrt{d} C_1(n) + h \varepsilon_{sc},
\end{aligned}$$

where

$$\begin{aligned}
r_1 &= C_1(n)^2 + M_1, \\
r_2 &= C_1(n) \left(C_1(n) C_2(n) + \frac{1}{2} C_4 + C_3(n) \right) + M_1 (1 + C_2(n) + C_4).
\end{aligned}$$

We now derive the upper bound of the second term in (23). Note that

$$\begin{aligned}
&\left\| \mathbb{E}_{U_n} [\nabla \log p_{T-(n+U_n)h}(\tilde{Y}_{(n+U_n)h}) - s_*(T-(n+U_n)h, \vartheta_{n+U_n}^{\text{REM}})] \right\|_{\mathbb{L}_2} \\
&= \left\| \int_0^1 \left(\nabla \log p_{T-(n+u)h}(\tilde{Y}_{(n+u)h}) - s_*(T-(n+u)h, \vartheta_{n+u}^{\text{REM}}) \right) du \right\|_{\mathbb{L}_2} \\
&\leq \int_0^1 \left\| \nabla \log p_{T-(n+u)h}(\tilde{Y}_{(n+u)h}) - s_*(T-(n+u)h, \vartheta_{n+u}^{\text{REM}}) \right\|_{\mathbb{L}_2} du \\
&\leq \int_0^1 \left(\left\| \nabla \log p_{T-(n+u)h}(\tilde{Y}_{(n+u)h}) - \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}}) \right\|_{\mathbb{L}_2} \right. \\
&\quad \left. + \left\| \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}}) - s_*(T-(n+u)h, \vartheta_{n+u}^{\text{REM}}) \right\|_{\mathbb{L}_2} \right) du \\
&\leq \int_0^1 L(T-(n+u)h) \left\| \tilde{Y}_{(n+u)h} - \vartheta_{n+u}^{\text{REM}} \right\|_{\mathbb{L}_2} du + \varepsilon_{sc},
\end{aligned} \tag{24}$$

the second inequality follows from the triangle inequality, and the last inequality depends on Assumption 1 and 4. By (17), changing the value of h to uh , we have

$$\begin{aligned}
&\left\| \tilde{Y}_{(n+u)h} - \vartheta_{n+u}^{\text{REM}} \right\|_{\mathbb{L}_2} \\
&\leq (uh)^2 (C_{1,n}(u)^2 + M_1) \left\| Y_{nh} - \vartheta_n^{\text{REM}} \right\|_{\mathbb{L}_2} \\
&\quad + (uh)^2 \left[C_{1,n}(u) \left(C_{1,n}(u) C_2(n) + \frac{1}{2} C_4 + C_{3,n}(u) \right) + M_1 (1 + C_2(n) + C_4) \right] \\
&\quad + (uh)^{3/2} \sqrt{d} C_{1,n}(u) \\
&\quad + uh \varepsilon_{sc},
\end{aligned} \tag{25}$$

where $C_{1,n}(u)$ and $C_{3,n}(u)$ is the uh -version of $C_1(n)$ and $C_3(n)$, respectively, that is

$$\begin{aligned}
C_{1,n}(u) &= \frac{1}{2} + \frac{1}{uh} \int_{nh}^{(n+u)h} L(T-t) dt, \\
C_{3,n}(u) &= \frac{1}{uh} \int_{nh}^{(n+u)h} (dL(T-t))^{1/2} dt,
\end{aligned}$$

Plugging the previous display (25) back into display (24), then rearranging and simplifying the expression, yields

$$\begin{aligned}
& \left\| \mathbb{E}_{U_n} [\nabla \log p_{T-(n+U_n)h}(\tilde{Y}_{(n+U_n)h}) - s_*(T - (n + U_n)h, \vartheta_{n+U_n}^{\text{REM}})] \right\|_{\mathbb{L}_2} \\
& \leq h^2 \left(\int_0^1 L(T - (n + u)h) u^2 (C_{1,n}(u)^2 + M_1) \, du \right) \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} \\
& \quad + h^2 \left\{ \int_0^1 L(T - (n + u)h) u^2 \left[C_{1,n}(u) \left(C_{1,n}(u) C_2(n) + \frac{1}{2} C_4 + C_{3,n}(u) \right) + M_1(1 + C_2(n) + C_4) \right] \, du \right\} \\
& \quad + h^{3/2} \left(\int_0^1 L(T - (n + u)h) u^{3/2} \, du \right) \sqrt{d} C_1(n) \\
& \quad + h \left(\int_0^1 L(T - (n + u)h) u \, du \right) \varepsilon_{sc} \\
& \quad + \varepsilon_{sc} \\
& \triangleq h^2 r_3 \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} + h^2 r_4 + h^{3/2} r_5 + h r_6 \varepsilon_{sc} + \varepsilon_{sc},
\end{aligned}$$

where

$$\begin{aligned}
r_3 &= \int_0^1 L(T - (n + u)h) u^2 (C_{1,n}(u)^2 + M_1) \, du, \\
r_4 &= \int_0^1 L(T - (n + u)h) u^2 \left[C_{1,n}(u) \left(C_{1,n}(u) C_2(n) + \frac{1}{2} C_4 + C_{3,n}(u) \right) \right] \, du + M_1(1 + C_2(n) + C_4), \\
r_5 &= \left(\int_0^1 L(T - (n + u)h) u^{3/2} \, du \right) \sqrt{d} C_1(n), \\
r_6 &= \int_0^1 L(T - (n + u)h) u \, du.
\end{aligned}$$

From the bounds we have obtained for two terms, it follows that

$$\begin{aligned}
& \left\| \tilde{Y}_h - \mathbb{E}_{U_n} [\vartheta_{n+1}^{\text{REM}}] \right\|_{\mathbb{L}_2} \\
& \leq h^3 \left(\frac{1}{2} r_1 + r_3 \right) \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} + h^3 \left(\frac{1}{2} r_2 + r_4 \right) + h^{5/2} \left(\frac{1}{2} \sqrt{d} C_1(n) + r_5 \right) + h^2 \left(\frac{1}{2} + r_6 \right) \varepsilon_{sc} + h \varepsilon_{sc}.
\end{aligned} \tag{26}$$

Considering the second term of one-step discretization error

$$\begin{aligned}
& \vartheta_{n+1}^{\text{REM}} - \mathbb{E}_{U_n} [\vartheta_{n+1}^{\text{REM}}] \\
&= \frac{1}{2} h \left[\vartheta_{n+U}^{\text{REM}} - \mathbb{E}_{U_n} [\vartheta_{n+U}^{\text{REM}}] \right] + h \left[s_*(T - (n + U_n)h, \vartheta_{n+U}^{\text{REM}}) - \mathbb{E}_{U_n} [s_*(T - (n + U_n)h, \vartheta_{n+U}^{\text{REM}})] \right] \\
&= \frac{1}{2} h \left[\frac{1}{2} h (U_n - \frac{1}{2}) \vartheta_n^{\text{REM}} + h (U_n - \frac{1}{2}) s_*(T - nh, \vartheta_n^{\text{REM}}) \right] \\
& \quad + \frac{1}{2} h \left[\int_{nh}^{(n+U_n)h} dW_t - \int_0^1 \left(\int_{nh}^{(n+u)h} dW_t \right) \, du \right] \\
& \quad + h \left[s_*(T - (n + U_n)h, \vartheta_{n+U}^{\text{REM}}) - \mathbb{E}_{U_n} [s_*(T - (n + U_n)h, \vartheta_{n+U}^{\text{REM}})] \right].
\end{aligned} \tag{27}$$

The second equality follows from the fact that

$$\begin{aligned}
\mathbb{E}_{U_n} [\vartheta_{n+U}^{\text{REM}}] &= \vartheta_n^{\text{REM}} + \frac{1}{2} h \mathbb{E}_{U_n} [U_n] \vartheta_n^{\text{REM}} + h \mathbb{E}_{U_n} [U_n] s_*(T - nh, \vartheta_n^{\text{REM}}) + \mathbb{E}_{U_n} \int_{nh}^{(n+U_n)h} dW_t \\
&= \vartheta_n^{\text{REM}} + \frac{1}{4} h \vartheta_n^{\text{REM}} + \frac{1}{2} h s_*(T - nh, \vartheta_n^{\text{REM}}) + \int_0^1 \left(\int_{nh}^{(n+u)h} dW_t \right) \, du,
\end{aligned}$$

since U_n is independent of ϑ_n^{REM} .

We proceed to bound each term in (27). For the first term, still notice that the independence between

U_n and ϑ_n^{REM} , then we find that

$$\begin{aligned} \left\| (U_n - \frac{1}{2}) \vartheta_n^{\text{REM}} \right\|_{\mathbb{L}_2} &= \left\{ \mathbb{E} \left[\mathbb{E}_{U_n} \left\| (U_n - \frac{1}{2}) \vartheta_n^{\text{REM}} \right\|^2 \right] \right\}^{1/2} \\ &= \left\{ \mathbb{E} \left[\mathbb{E}_{U_n} [(U_n - \frac{1}{2})^2] \cdot \|\vartheta_n^{\text{REM}}\|^2 \right] \right\}^{1/2} \\ &= \left\{ \mathbb{E} \left[\frac{1}{12} \|\vartheta_n^{\text{REM}}\|^2 \right] \right\}^{1/2} \\ &= \frac{1}{2\sqrt{3}} \|\vartheta_n^{\text{REM}}\|_{\mathbb{L}_2}. \end{aligned}$$

The bounding of another part of the first term follows in a similar manner, we obtain that

$$\left\| (U_n - \frac{1}{2}) s_*(T - nh, \vartheta_n^{\text{REM}}) \right\|_{\mathbb{L}_2} = \frac{1}{2\sqrt{3}} \|s_*(T - nh, \vartheta_n^{\text{REM}})\|_{\mathbb{L}_2}.$$

For the second term of (27), notice that due to Itô's isometry formula, for any well-defined stochastic process X_t and its Itô stochastic integral $I_t(X) = \int_0^t X_u dM_u$, we have

$$\mathbb{E}[I_t(X)^2] = \mathbb{E} \int_0^t X_u^2 d\langle M \rangle_u, \quad (28)$$

then we can establish a lemma.

Lemma 13. Suppose W_t is a d -dim standard Brownian motion, then

$$\left\| \int_{nh}^{(n+U_n)h} dW_t - \int_0^1 \left(\int_{nh}^{(n+u)h} dW_t \right) du \right\|_{\mathbb{L}_2}^2 \leq \frac{h}{3}.$$

For the third term of (27), we get

$$\begin{aligned} &\left\| s_*(T - (n + U_n)h, \vartheta_{n+U}^{\text{REM}}) - \mathbb{E}_{U_n} [s_*(T - (n + U_n)h, \vartheta_{n+U}^{\text{REM}})] \right\|_{\mathbb{L}_2} \\ &= \left\| \int_0^1 s_*(T - (n + U_n)h, \vartheta_{n+U}^{\text{REM}}) - s_*(T - (n + v)h, \vartheta_{n+v}^{\text{REM}}) dv \right\|_{\mathbb{L}_2} \\ &= \left\{ \mathbb{E} \int_0^1 \left[\int_0^1 s_*(T - (n + u)h, \vartheta_{n+u}^{\text{REM}}) - s_*(T - (n + v)h, \vartheta_{n+v}^{\text{REM}}) dv \right]^2 du \right\}^{1/2} \\ &\leq \left\{ \mathbb{E} \int_0^1 \int_0^1 [s_*(T - (n + u)h, \vartheta_{n+u}^{\text{REM}}) - s_*(T - (n + v)h, \vartheta_{n+v}^{\text{REM}})]^2 du dv \right\}^{1/2} \\ &= \left\{ \int_0^1 \int_0^1 \|s_*(T - (n + u)h, \vartheta_{n+u}^{\text{REM}}) - s_*(T - (n + v)h, \vartheta_{n+v}^{\text{REM}})\|_{\mathbb{L}_2}^2 du dv \right\}^{1/2}. \end{aligned}$$

Then by the triangle inequality and Assumption 4, we have

$$\begin{aligned} &\|s_*(T - (n + u)h, \vartheta_{n+u}^{\text{REM}}) - s_*(T - (n + v)h, \vartheta_{n+v}^{\text{REM}})\|_{\mathbb{L}_2} \\ &\leq \|s_*(T - (n + u)h, \vartheta_{n+u}^{\text{REM}}) - \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}})\|_{\mathbb{L}_2} \\ &\quad + \|s_*(T - (n + v)h, \vartheta_{n+v}^{\text{REM}}) - \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REM}})\|_{\mathbb{L}_2} \\ &\quad + \|\nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}}) - \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REM}})\|_{\mathbb{L}_2} \\ &\leq 2\varepsilon_{sc} + \|\nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}}) - \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REM}})\|_{\mathbb{L}_2}. \end{aligned} \quad (29)$$

Combining the three terms of (27) together, we have

$$\begin{aligned} \|\vartheta_{n+1}^{\text{REM}} - \mathbb{E}_{U_n} [\vartheta_{n+1}^{\text{REM}}]\|_{\mathbb{L}_2} &\leq \frac{1}{8\sqrt{3}} h^2 \|\vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} + \frac{1}{4\sqrt{3}} h^2 \|s_*(T - nh, \vartheta_n^{\text{REM}})\|_{\mathbb{L}_2} + \frac{1}{2\sqrt{3}} h^{3/2} \\ &\quad + h \left\{ \int_0^1 \int_0^1 \|\nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REM}}) - \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}})\|_{\mathbb{L}_2}^2 du dv \right\}^{1/2} \\ &\quad + 2h\varepsilon_{sc}. \end{aligned}$$

By applying the same technique used in the proofs of Proposition 9 and Proposition 11, the upper bounds for $\|\vartheta_n^{\text{REM}}\|_{\mathbb{L}_2}$ and $\|s_*(T - nh, \vartheta_n^{\text{REM}})\|_{\mathbb{L}_2}$ follows readily. Thus, the proposition follows immediately from the bound on the second last term. We now consider the case for $u > v$, due to Assumptions 1 and 2,

$$\begin{aligned} & \|\nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}}) - \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REM}})\|_{\mathbb{L}_2} \\ & \leq L(T - (n + u)h) \|\vartheta_{n+u}^{\text{REM}} - \vartheta_{n+v}^{\text{REM}}\|_{\mathbb{L}_2} + M_1 h \left(1 + \|\vartheta_{n+v}^{\text{REM}}\|_{\mathbb{L}_2}\right). \end{aligned}$$

Since

$$\begin{aligned} \|\vartheta_{n+u}^{\text{REM}} - \vartheta_{n+v}^{\text{REM}}\|_{\mathbb{L}_2} & \leq \frac{1}{2}(u - v)h \|\vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} + (u - v)h \|s_*(T - nh, \vartheta_n^{\text{REM}})\|_{\mathbb{L}_2} + \left\| \int_{(n+v)h}^{(n+u)h} dW_t \right\|_{\mathbb{L}_2} \\ & \leq \frac{1}{2}(u - v)h \left(\|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} + C_2(n) + C_4 \right) \\ & \quad + (u - v)h \left[\varepsilon_{sc} + L(T - nh) \left(\|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} + C_2(n) \right) + (dL(T - nh))^{1/2} \right] \\ & \quad + \sqrt{(u - v)h} \\ & \leq (u - v)h \left[\frac{1}{2} + L(T - nh) \right] \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\ & \quad + (u - v)h \left[\left(\frac{1}{2} + L(T - nh) \right) C_2(n) + \frac{1}{2} C_4 + (dL(T - nh))^{1/2} \right] \\ & \quad + \sqrt{(u - v)dh} + (u - v)h \varepsilon_{sc}. \end{aligned}$$

The second inequality follows from (16), Assumptions 1, 3 and Lemma 18. Similarly,

$$\begin{aligned} \|\vartheta_{n+v}^{\text{REM}}\|_{\mathbb{L}_2} & \leq \|\vartheta_{n+v}^{\text{REM}} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} + \|\vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\ & \leq vh \left[\frac{1}{2} + L(T - nh) \right] \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\ & \quad + vh \left[\left(\frac{1}{2} + L(T - nh) \right) C_2(n) + \frac{1}{2} C_4 + (dL(T - nh))^{1/2} \right] \\ & \quad + \sqrt{vdh} + v\varepsilon_{sc} \\ & \quad + \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} + C_2(n) + C_4. \end{aligned}$$

Therefore, we obtain that

$$\begin{aligned} & \|\nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}}) - \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REM}})\|_{\mathbb{L}_2} \\ & \leq h \left\{ (u - v) \left[\frac{1}{2} + L(T - nh) \right] L(T - (n + u)h) + M_1 \right\} \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\ & \quad + h^2 M_1 v \left[\frac{1}{2} + L(T - nh) \right] \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\ & \quad + h^2 v M_1 \left[\left(\frac{1}{2} + L(T - nh) \right) C_2(n) + \frac{1}{2} C_4 + (dL(T - nh))^{1/2} \right] \\ & \quad + h^{3/2} M_1 \sqrt{vd} \\ & \quad + h \left\{ (u - v) \left[\left(\frac{1}{2} + L(T - nh) \right) C_2(n) + \frac{1}{2} C_4 + (dL(T - nh))^{1/2} \right] L(T - (n + u)h) \right. \\ & \quad \left. + M_1 (1 + C_2(n) + C_4) \right\} \\ & \quad + h^{1/2} L(T - (n + u)h) \sqrt{(u - v)d} \\ & \quad + h(u - v) L(T - (n + u)h) \varepsilon_{sc} + h^2 M_1 v \varepsilon_{sc}. \end{aligned}$$

We claim that we only consider the lowest order of each part, which means the relative higher order term with the combination of d and h will be ignored. Then take the supremum with respect to v ,

$$\begin{aligned}
& \left\{ \int_0^1 \int_0^1 \left\| \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REM}}) - \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REM}}) \right\|_{\mathbb{L}_2}^2 du dv \right\}^{1/2} \\
& \leq h \left\{ \int_0^1 \int_0^1 \left[|u-v| L(T-(n+u)h) \left(\frac{1}{2} + L(T-nh) \right) + M_1 \right]^2 du dv \right\}^{1/2} \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\
& \quad + h^{1/2} \sqrt{d} \left[\int_0^1 \int_0^1 L(T-(n+u)h)^2 |u-v| du dv \right]^{1/2} \\
& \quad + h \left[\int_0^1 \int_0^1 (u-v)^2 L(T-(n+u)h)^2 du dv \right]^{1/2} \varepsilon_{sc}.
\end{aligned} \tag{30}$$

Combining the above,

$$\begin{aligned}
& \left\| \vartheta_{n+1}^{\text{REM}} - \mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REM}}] \right\|_{\mathbb{L}_2} \\
& \leq \frac{1}{8\sqrt{3}} h^2 \left(\|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} + C_2(n) + C_4 \right) \\
& \quad + \frac{1}{4\sqrt{3}} h^2 \left[\varepsilon_{sc} + L(T-nh) \left(\|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} + C_2(n) \right) + (dL(T-nh))^{1/2} \right] \\
& \quad + \frac{1}{2\sqrt{3}} h^{3/2} \\
& \quad + h^2 \left\{ \int_0^1 \int_0^1 \left[|u-v| L(T-(n+u)h) \left(\frac{1}{2} + L(T-nh) \right) + M_1 \right]^2 du dv \right\}^{1/2} \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\
& \quad + h^2 \left\{ \int_0^1 \int_0^1 \left\{ (u-v) \left[\left(\frac{1}{2} + L(T-nh) \right) C_2(n) + \frac{1}{2} C_4 + (dL(T-nh))^{1/2} \right] L(T-(n+u)h) \right. \right. \\
& \quad \left. \left. + M_1(1 + C_2(n) + C_4) \right\}^2 du dv \right\}^{1/2} \\
& \quad + h^{3/2} \sqrt{d} \left[\int_0^1 \int_0^1 L(T-(n+u)h)^2 |u-v| du dv \right]^{1/2} \\
& \quad + h^2 \left[\int_0^1 \int_0^1 (u-v)^2 L(T-(n+u)h)^2 du dv \right]^{1/2} \varepsilon_{sc} \\
& \quad + 2h\varepsilon_{sc} \\
& \lesssim h^2 \left\{ \left[\int_0^1 \int_0^1 \left[|u-v| L(T-(n+u)h) \left(\frac{1}{2} + L(T-nh) \right) + M_1 \right]^2 du dv \right]^{1/2} \right. \\
& \quad \left. + \frac{1}{4\sqrt{3}} L(T-nh) + \frac{1}{8\sqrt{3}} \right\} \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \\
& \quad + h^2 \left\{ \left\{ \int_0^1 \int_0^1 \left\{ (u-v) \left[\left(\frac{1}{2} + L(T-nh) \right) C_2(n) + \frac{1}{2} C_4 + (dL(T-nh))^{1/2} \right] L(T-(n+u)h) \right. \right. \right. \\
& \quad \left. \left. + M_1(1 + C_2(n) + C_4) \right\}^2 du dv \right\}^{1/2} \right. \\
& \quad \left. + \frac{1}{8\sqrt{3}} (C_2(n) + C_4) + \frac{1}{4\sqrt{3}} (L(T-nh)C_2(n) + (dL(T-nh))^{1/2}) \right\} \\
& \quad + h^{3/2} \left\{ \sqrt{d} \left[\int_0^1 \int_0^1 L(T-(n+u)h)^2 |u-v| du dv \right]^{1/2} + \frac{1}{2\sqrt{3}} \right\} \\
& \quad + 2h\varepsilon_{sc}.
\end{aligned} \tag{31}$$

Compared to the term $\tilde{Y}_h - \mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REM}}]$, we can focus on the lower-order terms, ignoring the score matching error. Therefore, we have

$$\begin{aligned}
& \left\| \tilde{Y}_{(n+1)h} - \vartheta_{n+1}^{\text{REM}} \right\|_{\mathbb{L}_2} \\
& \leq h^2 \left\{ \left[\int_0^1 \int_0^1 \left[|u-v| L(T - (n+u)h) \left(\frac{1}{2} + L(T-nh) \right) + M_1 \right]^2 du dv \right]^{1/2} \|Y_{nh} - \vartheta_n^{\text{REM}}\|_{\mathbb{L}_2} \right. \\
& \quad \left. + \frac{1}{4\sqrt{3}} L(T-nh) + \frac{1}{8\sqrt{3}} \right\} \\
& \quad + h^2 \left\{ \left\{ \int_0^1 \int_0^1 \left\{ (u-v) \left[\left(\frac{1}{2} + L(T-nh) \right) C_2(n) + \frac{1}{2} C_4 + (dL(T-nh))^{1/2} \right] L(T - (n+u)h) \right. \right. \right. \\
& \quad \left. \left. \left. + M_1(1 + C_2(n) + C_4) \right\}^2 du dv \right\}^{1/2} \right. \\
& \quad \left. + \frac{1}{8\sqrt{3}} (C_2(n) + C_4) + \frac{1}{4\sqrt{3}} \left(L(T-nh) C_2(n) + (dL(T-nh))^{1/2} \right) \right\} \\
& \quad + h^{3/2} \left\{ \sqrt{d} \left[\int_0^1 \int_0^1 L(T - (n+u)h)^2 |u-v| du dv \right]^{1/2} + \frac{1}{2\sqrt{3}} \right\} \\
& \quad + 3h\varepsilon_{sc}.
\end{aligned}$$

□

Returning to the proof of Theorem 3, by the conclusion of Proposition 12, we have

$$\begin{aligned}
\|Y_{Nh} - \vartheta_N^{\text{REM}}\|_{\mathbb{L}_2} & \lesssim \frac{1}{m_{\min} - 1/2} \left(h \max_{0 \leq k \leq N-1} C_{k,1}^{\text{REM}} + h^{1/2} \max_{0 \leq k \leq N-1} C_{k,2}^{\text{REM}} + 3\varepsilon_{sc} \right) \\
& \lesssim \sqrt{h} \cdot \frac{\sqrt{d/3} L_{\max} + \frac{1}{2\sqrt{3}}}{m_{\min} - 1/2} + \varepsilon_{sc} \cdot \frac{3}{m_{\min} - 1/2}.
\end{aligned}$$

This completes the first part of proof for Theorem 3.

B.4 Proof of Theorem 3: Part II

We begin with the following proposition.

Proposition 14. *Suppose that Assumptions 1, 2 and 4 are satisfied, the following two claims hold*

(I) *It holds that*

$$\begin{aligned}
& \left\| \tilde{Y}_h - \vartheta_{n+1}^{\text{REI}} \right\|_{\mathbb{L}_2} \\
& \leq h^2 \left\{ \int_0^1 \int_0^1 \left[|u-v| L(T - (n+u)h) \left(\frac{1}{2} + L(T-nh) \right) + M_1 \right. \right. \\
& \quad \left. \left. + \frac{1}{2} |u-v| L(T - (n+v)h) r_n^{\text{EI}}(v) \right]^2 du dv \right\}^{1/2} \|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} \\
& \quad + h^2 \left\{ \frac{e^{\frac{1}{2}(1-v)h} - e^{\frac{1}{2}(1-u)h}}{h} e^{\frac{1}{2}vh} L(T - (n+u)h) \left[C_2(n) + C_4 + 2L(T-nh)C_2(n) + (dL(T-nh))^{1/2} \right] \right. \\
& \quad \left. + e^{\frac{1}{2}(1-u)h} M_1 \left[1 + 2e^{\frac{1}{2}vh} \left(L(T-nh)C_2(n) + (dL(T-nh))^{1/2} \right) + C_2(n) + C_4 \right] \right. \\
& \quad \left. + \frac{|e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h}|}{h} \left(L(T - (n+v)h)C_2(n) + (dL(T - (n+v)h))^{1/2} \right) \right\}
\end{aligned}$$

$$+ h^{3/2} \sqrt{d} \left\{ \int_0^1 \int_0^1 L(T - (n+u)h)^2 |u-v| \, du \, dv \right\}^{1/2} \\ + 3h\varepsilon_{sc}.$$

(2) Furthermore, it holds that

$$\|Y_{(n+1)h} - \vartheta_{n+1}^{\text{REI}}\|_{\mathbb{L}_2} \leq r_n^{\text{REI}} \|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} + h^2 C_{n,1}^{\text{REI}} + h^{3/2} C_{n,2}^{\text{REI}} + 3h\varepsilon_{sc},$$

where

$$r_n^{\text{REI}} = e^{-\int_{nh}^{(n+1)h} (m(T-t) - \frac{1}{2}) \, dt} \\ + h^2 \left\{ \int_0^1 \int_0^1 \left[|u-v| L(T - (n+u)h) \left(\frac{1}{2} + L(T - nh) \right) \right. \right. \\ \left. \left. + M_1 + \frac{1}{2} |u-v| L(T - (n+v)h) r_n^{\text{EI}}(v) \right]^2 \, du \, dv \right\}^{1/2}, \\ C_{n,1}^{\text{REI}} = \frac{e^{\frac{1}{2}(1-v)h} - e^{\frac{1}{2}(1-u)h}}{h} e^{\frac{1}{2}vh} L(T - (n+u)h) \left[C_2(n) + C_4 + 2L(T - nh)C_2(n) + (dL(T - nh))^{1/2} \right] \\ + e^{\frac{1}{2}(1-u)h} M_1 \left[1 + 2e^{\frac{1}{2}vh} \left(L(T - nh)C_2(n) + (dL(T - nh))^{1/2} \right) + C_2(n) + C_4 \right] \\ + \frac{|e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h}|}{h} \left(L(T - (n+v)h)C_2(n) + (dL(T - (n+v)h))^{1/2} \right), \\ C_{n,2}^{\text{REI}} = \sqrt{d} \left\{ \int_0^1 \int_0^1 L(T - (n+u)h)^2 |u-v| \, du \, dv \right\}^{1/2}.$$

Proof of Proposition 14. This proposition can be proven following the same approach as in the proof of Proposition 12, with the only difference being the inclusion of the exponential coefficient term. However, this term does not significantly affect the overall proof.

Similarly, we make a decomposition as

$$\|\tilde{Y}_h - \vartheta_{n+1}^{\text{REI}}\|_{\mathbb{L}_2} \leq \|\tilde{Y}_h - \mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REI}}]\|_{\mathbb{L}_2} + \|\mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REI}}]\|_{\mathbb{L}_2}. \quad (32)$$

Note that

$$\tilde{Y}_h - \mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REI}}] = \int_0^h e^{\frac{1}{2}(h-t)} \nabla \log p_{T-nh-t}(\tilde{Y}_t) \, dt - h \mathbb{E}_{U_n} \left[e^{\frac{1}{2}(1-U_n)h} s_*(T - nh - U_n h, \vartheta_{n+U_n}^{\text{REI}}) \right] \\ = h \int_0^1 e^{\frac{1}{2}(1-u)h} \left(\nabla \log p_{T-nh-uh}(\tilde{Y}_{uh}) - s_*(T - nh - uh, \vartheta_{n+u}^{\text{REI}}) \right) \, du \\ = h \int_0^1 e^{\frac{1}{2}(1-u)h} \left(\nabla \log p_{T-nh-uh}(\tilde{Y}_{uh}) - \nabla \log p_{T-nh-uh}(\vartheta_{n+u}^{\text{REI}}) \right) \, du \\ + h \int_0^1 e^{\frac{1}{2}(1-u)h} \left(\nabla \log p_{T-nh-uh}(\vartheta_{n+u}^{\text{REI}}) - s_*(T - nh - uh, \vartheta_{n+u}^{\text{REI}}) \right) \, du.$$

Then, we obtain

$$\|\tilde{Y}_h - \mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REI}}]\|_{\mathbb{L}_2} \\ \leq h \int_0^1 \left\| e^{\frac{1}{2}(1-u)h} \left(\nabla \log p_{T-nh-uh}(\tilde{Y}_{uh}) - s_*(T - nh - uh, \vartheta_{n+u}^{\text{REI}}) \right) \right\|_{\mathbb{L}_2} \, du \\ \leq h \int_0^1 e^{\frac{1}{2}(1-u)h} L(T - nh - uh) \|\tilde{Y}_{uh} - \vartheta_{n+u}^{\text{REI}}\|_{\mathbb{L}_2} \, du + h \int_0^1 e^{\frac{1}{2}(1-u)h} \, du \varepsilon_{sc} \\ \leq h^3 \int_0^1 e^{\frac{1}{2}(1-u)h} L(T - nh - uh) u^2 \left(C_{5,n}(u) C_{1,n}(u) + M_1 \frac{2(e^{uh/2} - 1)}{uh} \right) \, du \|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} \\ + h^3 \int_0^1 e^{\frac{1}{2}(1-u)h} L(T - nh - uh) u^2 \left[C_{5,n}(u) \left(C_{1,n}(u) C_2(n) + \frac{1}{2} C_4 + C_{3,n}(u) \right) \right. \\ \left. + C_{2,n}(u) \left(C_{1,n}(u) C_2(n) + \frac{1}{2} C_4 + C_{3,n}(u) \right) \right] \, du \|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2}.$$

$$\begin{aligned}
& + \frac{2(e^{uh} - 1)}{uh} M_1(1 + C_2(n) + C_4) \Big] du \\
& + h^{5/2} \int_0^1 e^{\frac{1}{2}(1-u)h} L(T - nh - uh) u^{3/2} C_{5,n}(u) du \sqrt{d} \\
& + h^2 \int_0^1 e^{\frac{1}{2}(1-u)h} L(T - nh - uh) \frac{2(e^{uh/2} - 1)}{h} du \varepsilon_{sc} + h \frac{2(e^{h/2} - 1)}{h} \varepsilon_{sc}, \tag{33}
\end{aligned}$$

where

$$C_{5,n}(u) = \frac{1}{uh} \int_{nh}^{(n+u)h} e^{\frac{1}{2}((n+u)h-t)} L(T-t) dt.$$

In the third inequality, we can directly bound $\|\tilde{Y}_{uh} - \vartheta_{n+u}^{\text{REI}}\|_{\mathbb{L}_2}$, as it is a special case of Proposition 11,

where the step size is replaced by uh .

For the second term of (32), we have

$$\begin{aligned}
& \vartheta_{n+1}^{\text{REI}} - \mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REI}}] \\
& = h e^{\frac{1}{2}(1-U_n)h} s_*(T - nh - U_n h, \vartheta_{n+U}^{\text{REI}}) - h \mathbb{E}_{U_n} \left[e^{\frac{1}{2}(1-U_n)h} s_*(T - nh - U_n h, \vartheta_{n+U}^{\text{REI}}) \right] \\
& = h \int_0^1 \left[e^{\frac{1}{2}(1-U_n)h} s_*(T - nh - U_n h, \vartheta_{n+U_n}^{\text{REI}}) - e^{\frac{1}{2}(1-v)h} s_*(T - nh - v h, \vartheta_{n+v}^{\text{REI}}) \right] dv.
\end{aligned}$$

Similar to display (29), we then obtain

$$\begin{aligned}
& \|\vartheta_{n+1}^{\text{REI}} - \mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REI}}]\|_{\mathbb{L}_2} \\
& \leq \left\{ \mathbb{E} \int_0^1 \left[h \int_0^1 e^{\frac{1}{2}(1-u)h} s_*(T - (n+u)h, \vartheta_{n+u}^{\text{REI}}) - e^{\frac{1}{2}(1-v)h} s_*(T - (n+v)h, \vartheta_{n+v}^{\text{REI}}) dv \right]^2 du \right\}^{1/2} \\
& \leq h \left\{ \int_0^1 \int_0^1 \left\| e^{\frac{1}{2}(1-u)h} s_*(T - (n+u)h, \vartheta_{n+u}^{\text{REI}}) - e^{\frac{1}{2}(1-v)h} s_*(T - (n+v)h, \vartheta_{n+v}^{\text{REI}}) \right\|_{\mathbb{L}_2}^2 du dv \right\}^{1/2} \\
& \leq h \left\{ \int_0^1 \int_0^1 \left\| e^{\frac{1}{2}(1-u)h} \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REI}}) - e^{\frac{1}{2}(1-v)h} \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REI}}) \right\|_{\mathbb{L}_2}^2 du dv \right\}^{1/2} \\
& \quad + 2h \left(\int_0^1 e^{(1-u)h} du \right)^{1/2} \varepsilon_{sc},
\end{aligned}$$

Using the same strategy as in display (30), we arrive at

$$\begin{aligned}
& \left\| e^{\frac{1}{2}(1-u)h} \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REI}}) - e^{\frac{1}{2}(1-v)h} \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REI}}) \right\|_{\mathbb{L}_2} \\
& \leq e^{\frac{1}{2}(1-u)h} \left\| \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REI}}) - \nabla \log p_{T-(n+u)h}(\vartheta_{n+v}^{\text{REI}}) \right\|_{\mathbb{L}_2} \\
& \quad + e^{\frac{1}{2}(1-u)h} \left\| \nabla \log p_{T-(n+u)h}(\vartheta_{n+v}^{\text{REI}}) - \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REI}}) \right\|_{\mathbb{L}_2} \\
& \quad + \left| e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h} \right| \left\| \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REI}}) \right\|_{\mathbb{L}_2} \\
& \leq e^{\frac{1}{2}(1-u)h} L(T - (n+u)h) \left\| \vartheta_{n+u}^{\text{REI}} - \vartheta_{n+v}^{\text{REI}} \right\|_{\mathbb{L}_2} \\
& \quad + e^{\frac{1}{2}(1-u)h} M_1 h (1 + \|\vartheta_{n+v}^{\text{REI}}\|_{\mathbb{L}_2}) \\
& \quad + \left| e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h} \right| \left[L(T - (n+v)h) \left(\|Y_{(n+v)h} - \vartheta_{n+v}^{\text{REI}}\|_{\mathbb{L}_2} + C_2(n) \right) + (dL(T - (n+v)h))^{1/2} \right].
\end{aligned}$$

The second inequality follows from Assumptions 1 and 2. We bound the term $\|\nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REI}})\|_{\mathbb{L}_2}$ by decomposing it as follows

$$\begin{aligned}
\|\nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REI}})\|_{\mathbb{L}_2} & \leq \left\| \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REI}}) - \nabla \log p_{T-(n+v)h}(Y_{(n+v)h}) \right\|_{\mathbb{L}_2} \\
& \quad + \left\| \nabla \log p_{T-(n+v)h}(Y_{(n+v)h}) - \nabla \log p_{T-(n+v)h}(X_{((n+v)h)}^{\leftarrow}) \right\|_{\mathbb{L}_2} \\
& \quad + \left\| \nabla \log p_{T-(n+v)h}(X_{T-(n+v)h}) \right\|_{\mathbb{L}_2}.
\end{aligned}$$

Without loss of generality, we consider the case where $u > v$; the other case follows similarly.

$$\begin{aligned}
& \|\vartheta_{n+u}^{\text{REI}} - \vartheta_{n+v}^{\text{REI}}\|_{\mathbb{L}_2} \\
&= (e^{\frac{1}{2}uh} - e^{\frac{1}{2}vh}) \|\vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} + \int_{vh}^{uh} e^{\frac{1}{2}t} dt \|s_*(T - nh, \vartheta_n^{\text{REI}})\|_{\mathbb{L}_2} \\
&\quad + \left\| \int_{nh}^{(n+u)h} e^{\frac{1}{2}((n+u)h-t)} dW_t - \int_{nh}^{(n+v)h} e^{\frac{1}{2}((n+v)h-t)} dW_t \right\|_{\mathbb{L}_2} \\
&\leq (e^{\frac{1}{2}(u-v)h} - 1) e^{\frac{1}{2}vh} \left(\|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} + C_2(n) + C_4 \right) \\
&\quad + 2(e^{\frac{1}{2}(u-v)h} - 1) e^{\frac{1}{2}vh} \left[\varepsilon_{sc} + L(T - nh) \left(\|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} + C_2(n) \right) + (dL(T - nh))^{1/2} \right] \\
&\quad + \left[(e^{uh} - 1) + (e^{vh} - 1) - 2(e^{\frac{u+v}{2}h} - e^{\frac{u-v}{2}h}) \right]^{1/2} \sqrt{d}.
\end{aligned} \tag{34}$$

Here, we apply the formula in (28) to bound the last term.

$$\begin{aligned}
& \left\| \int_{nh}^{(n+u)h} \mathbf{1}_{\{t \leq (n+v)h\}} (e^{\frac{1}{2}((n+u)h-t)} - e^{\frac{1}{2}((n+v)h-t)}) + \mathbf{1}_{\{t > (n+v)h\}} e^{\frac{1}{2}((n+u)h-t)} dW_t \right\|_{\mathbb{L}_2} \\
&= \sqrt{d} \left[\int_{nh}^{(n+v)h} (e^{\frac{1}{2}((n+u)h-t)} - e^{\frac{1}{2}((n+v)h-t)})^2 dt + \int_{(n+v)h}^{(n+u)h} e^{(n+u)h-t} dt \right]^{1/2} \\
&= \sqrt{d} \left[(e^{uh} - 1) + (e^{vh} - 1) - 2(e^{\frac{u+v}{2}h} - e^{\frac{u-v}{2}h}) \right]^{1/2},
\end{aligned}$$

We then bound the term $\|\vartheta_{n+v}^{\text{REI}}\|_{\mathbb{L}_2}$ following display (34) above. To this end, let $u = 0$, we then have

$$\begin{aligned}
\|\vartheta_{n+v}^{\text{REI}}\|_{\mathbb{L}_2} &\leq (e^{\frac{1}{2}vh} - 1) (\|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} + C_2(n) + C_4) \\
&\quad + 2(e^{\frac{1}{2}vh} - 1) \left[\varepsilon_{sc} + L(T - nh) \left(\|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} + C_2(n) \right) + (dL(T - nh))^{1/2} \right] \\
&\quad + \sqrt{d}(e^{vh} - 1)^{1/2} \\
&\quad + \|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} + C_2(n) + C_4.
\end{aligned}$$

Additionally, we can bound $\|Y_{(n+v)h} - \vartheta_{n+v}^{\text{REI}}\|_{\mathbb{L}_2}$, as it is a special case of the one-step discretization error under the Exponential Integrator scheme, where the step size is replaced by vh . Specifically, we have

$$\begin{aligned}
& \|Y_{(n+v)h} - \vartheta_{n+v}^{\text{REI}}\|_{\mathbb{L}_2} \\
&\leq r_n^{\text{EI}}(v) \|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} + h^2 C_n^{\text{EI}}(v) + h^{3/2} u^{3/2} \sqrt{d} C_{5,n}(v) + vh \frac{2(e^{\frac{1}{2}vh} - 1)}{vh} \varepsilon_{sc},
\end{aligned}$$

where

$$\begin{aligned}
r_n^{\text{EI}}(v) &= e^{-\int_{nh}^{(n+v)h} (m(T-t) - \frac{1}{2}) dt} + v^2 h^2 \left(C_{5,n}(v) C_{1,n}(v) + M_1 \frac{2(e^{\frac{1}{2}vh} - 1)}{vh} \right), \\
C_n^{\text{EI}}(v) &= C_{5,n}(v) \left(C_{1,n}(v) C_2(n) + \frac{1}{2} C_4 + C_{3,n}(v) \right) + \frac{2(e^{\frac{1}{2}vh} - 1)}{vh} M_1 (1 + C_2(n) + C_4).
\end{aligned}$$

Then, we obtain

$$\begin{aligned}
& \left\| e^{\frac{1}{2}(1-u)h} \nabla \log p_{T-(n+u)h}(\vartheta_{n+u}^{\text{REI}}) - e^{\frac{1}{2}(1-v)h} \nabla \log p_{T-(n+v)h}(\vartheta_{n+v}^{\text{REI}}) \right\|_{\mathbb{L}_2} \\
&\leq \left\{ 2(e^{\frac{1}{2}(1-v)h} - e^{\frac{1}{2}(1-u)h}) e^{\frac{1}{2}vh} L(T - (n+u)h) \left[\frac{1}{2} + L(T - nh) \right] \right. \\
&\quad \left. + e^{\frac{1}{2}(1-u)h} M_1 h \left[(e^{\frac{1}{2}vh} - 1) + 2(e^{\frac{1}{2}vh} - 1) L(T - nh) + 1 \right] \right\}
\end{aligned}$$

$$\begin{aligned}
& + \left| e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h} \right| L(T - (n+v)h) r_n^{\text{El}}(v) \Big\} \|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} \\
& + h^3 L(T - (n+v)h) \frac{|e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h}|}{h} C_n^{\text{El}}(v) \\
& + h^{5/2} L(T - (n+v)h) \frac{|e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h}|}{h} u^{3/2} \sqrt{d} C_{5,n}(v) \\
& + h^2 M_1 e^{\frac{1}{2}(1-u)h} \frac{e^{\frac{1}{2}vh} - 1}{h} (C_2(n) + C_4) \\
& + h^{3/2} M_1 e^{\frac{1}{2}(1-u)h} \sqrt{vd} \left(\frac{e^{vh} - 1}{vh} \right)^{1/2} \\
& + h \left\{ \frac{e^{\frac{1}{2}(1-v)h} - e^{\frac{1}{2}(1-u)h}}{h} e^{\frac{1}{2}vh} L(T - (n+u)h) \left[C_2(n) + C_4 + 2L(T - nh)C_2(n) + (dL(T - nh))^{1/2} \right] \right. \\
& \quad + e^{\frac{1}{2}(1-u)h} M_1 \left[1 + 2e^{\frac{1}{2}vh} \left(L(T - nh)C_2(n) + (dL(T - nh))^{1/2} \right) + C_2(n) + C_4 \right] \\
& \quad \left. + \frac{|e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h}|}{h} \left(L(T - (n+v)h)C_2(n) + (dL(T - (n+v)h))^{1/2} \right) \right\} \\
& + h^{1/2} L(T - (n+u)h) e^{\frac{1}{2}(1-u)h} \left[\frac{(e^{uh} - 1) + (e^{vh} - 1) - 2(e^{\frac{u+v}{2}h} - e^{\frac{u-v}{2}h})}{h} \right]^{1/2} \sqrt{d} \\
& + h^2 \varepsilon_{sc} L(T - (n+v)h) \frac{|e^{\frac{1}{2}(1-u)h} - e^{\frac{1}{2}(1-v)h}|}{h} \frac{2(e^{\frac{1}{2}vh} - 1)}{h} \\
& + h \varepsilon_{sc} \cdot 2e^{\frac{1}{2}(1-u)h} \left[L(T - (n+u)h) \frac{e^{\frac{1}{2}uh} - e^{\frac{1}{2}vh}}{h} + M_1 e^{\frac{1}{2}vh} \right].
\end{aligned}$$

Ignoring the higher-order terms, we take the supremum with respect to v and substitute it back into the original expression, yielding

$$\begin{aligned}
& \|\vartheta_{n+1}^{\text{REI}} - \mathbb{E}_{U_n}[\vartheta_{n+1}^{\text{REI}}]\|_{\mathbb{L}_2} \\
& \leq h \left\{ \int_0^1 \int_0^1 \left\| e^{\frac{1}{2}(1-u)h} s_*(T - (n+u)h, \vartheta_{n+u}^{\text{REI}}) - e^{\frac{1}{2}(1-v)h} s_*(T - (n+v)h, \vartheta_{n+v}^{\text{REI}}) \right\|_{\mathbb{L}_2}^2 du dv \right\}^{1/2} \\
& \leq h^2 \left\{ \int_0^1 \int_0^1 [|u - v| L(T - (n+u)h) \left(\frac{1}{2} + L(T - nh) \right) + M_1 \right. \right. \\
& \quad \left. \left. + \frac{1}{2} |u - v| L(T - (n+v)h) r_n^{\text{El}}(v) \right]^2 du dv \right\}^{1/2} \|Y_{nh} - \vartheta_n^{\text{REI}}\|_{\mathbb{L}_2} \\
& \quad + h^{3/2} \left\{ \int_0^1 \int_0^1 dL(T - (n+u)h)^2 |u - v| du dv \right\}^{1/2} + 2h \varepsilon_{sc}.
\end{aligned} \tag{35}$$

This completes the proof. □

Now, we have

$$\begin{aligned}
\|Y_{Nh} - \vartheta_N^{\text{REI}}\|_{\mathbb{L}_2} & \lesssim \frac{1}{m_{\min} - 1/2} \left(h \max_{0 \leq k \leq N-1} C_{n,1}^{\text{REI}} + \sqrt{h} \max_{0 \leq k \leq N-1} C_{n,2}^{\text{REI}} + 3\varepsilon_{sc} \right) \\
& \lesssim \frac{L_{\max}}{\sqrt{3}(m_{\min} - 1/2)} + \varepsilon_{sc} \frac{3}{m_{\min} - 1/2}.
\end{aligned}$$

The desired result follows readily.

C The proof of the upper bound of error of the second-order acceleration scheme

This section is dedicated to proving the Wasserstein convergence result for second-order acceleration. To this end, we first establish the following proposition.

Proposition 15. *Suppose that Assumptions 1, 3, 5, 6, 7 are satisfied, the following results hold.*

(1) *First, we have an upper bound for $\|\tilde{Y}_h - \vartheta_{n+1}^{\text{SO}}\|_{\mathbb{L}_2}$ as follows,*

$$\begin{aligned} \|\tilde{Y}_h - \vartheta_{n+1}^{\text{SO}}\|_{\mathbb{L}_2} &\leq A_{n,1} e^{(L(nh) - \frac{1}{2})h} h^2 \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + A_{n,2} e^{(L(nh) - \frac{1}{2})h} h^2 \\ &\quad + \left(h\varepsilon_{sc} + \frac{2}{3} \sqrt{d} h^{3/2} \varepsilon_{sc}^{(L)} + \frac{1}{2} h^2 \varepsilon_{sc}^{(M)} \right) e^{(L(T-nh) - \frac{1}{2})h}, \end{aligned}$$

where

$$\begin{aligned} A_{n,1} &= \sup_{nh \leq t \leq (n+1)h} \frac{1}{t^2} \int_0^t \left(\int_0^s [(1 + L(T - nh - u))L(T - nh - u) \right. \\ &\quad \left. + (1 + L(T - nh))L(T - nh)] du \right) ds, \\ A_{n,2} &= \sup_{nh \leq t \leq (n+1)h} \frac{1}{t^2} \left[\int_0^t \left(\int_0^s [(1 + L(T - nh - u))L(T - nh - u) \right. \right. \\ &\quad \left. \left. + (1 + L(T - nh))L(T - nh)] du \right) ds \cdot C_2(n) \right. \\ &\quad \left. + \sqrt{d} \int_0^t \left(\int_0^s \left[\left(\frac{1}{2} + L(T - nh - u) \right) L(T - nh - u)^{1/2} \right. \right. \right. \\ &\quad \left. \left. + \left(\frac{1}{2} + L(T - nh) \right) L(T - nh)^{1/2} \right] du \right) ds \right. \\ &\quad \left. + \int_0^t \left(\int_0^s \frac{1}{2} (L(T - nh - u) + L(T - nh)) du \right) ds \cdot C_4 \right] \\ &\quad + \frac{\sqrt{2}}{4} \sqrt{d} L_F. \end{aligned}$$

(2) *Furthermore, it holds that*

$$\begin{aligned} \|Y_{(n+1)h} - \vartheta_{n+1}^{\text{SO}}\|_{\mathbb{L}_2} &\leq r_n^{\text{SO}} \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + h^2 C_n^{\text{SO}} \\ &\quad + \left[h\varepsilon_{sc} + \frac{2}{3} \sqrt{d} h^{3/2} \varepsilon_{sc}^{(L)} + \frac{1}{2} h^2 \varepsilon_{sc}^{(M)} \right] e^{(L(T-nh) - \frac{1}{2})h}, \end{aligned}$$

where

$$\begin{aligned} r_n^{\text{SO}} &= e^{-\int_{nh}^{(n+1)h} (m(T-t) - \frac{1}{2}) dt} + h^2 A_{n,1} e^{(L(T-nh) - \frac{1}{2})h}, \\ C_n^{\text{SO}} &= A_{n,2} e^{(L(T-nh) - \frac{1}{2})h}. \end{aligned}$$

Proof. Recall the expression in display (44), which states that

$$x_t = \vartheta_n^{\text{SO}} + \int_{nh}^t \left(\frac{1}{2} \vartheta_n^{\text{SO}} + \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) + L_n(x_s - \vartheta_n^{\text{SO}}) + M_n(s - nh) \right) ds + \int_{nh}^t dW_s$$

with

$$\begin{aligned} L_n &= \frac{1}{2} I_d + \nabla^2 \log p_{T-nh}(\vartheta_n^{\text{SO}}) \in \mathbb{R}^{d \times d}, \\ M_n &= \frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) - \frac{\partial}{\partial t} \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) \in \mathbb{R}^d. \end{aligned}$$

Plugging the estimates of $\nabla \log p_{T-nh}(\vartheta_n^{\text{SO}})$, L_n and M_n into the previous display yields the following process for x_t^{SO}

$$\begin{aligned} x_t^{\text{SO}} &= \vartheta_n^{\text{SO}} + \int_{nh}^t \frac{1}{2} \vartheta_n^{\text{SO}} + s_*(T-nh, \vartheta_n^{\text{SO}}) \, ds \\ &\quad + \int_{nh}^t s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}})(x_s^{\text{SO}} - \vartheta_n^{\text{SO}}) + s_*^{(M)}(T-nh, \vartheta_n^{\text{SO}})(s-nh) \, ds + \int_{nh}^t dW_s. \end{aligned}$$

Then, we obtain

$$\begin{aligned} x_t^{\text{SO}} - x_t &= (t-nh)(s_*(T-nh, \vartheta_n^{\text{SO}}) - \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}})) \\ &\quad + (s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}}) - L_n) \int_{nh}^t (x_s^{\text{SO}} - \vartheta_n^{\text{SO}}) \, ds + L_n \int_{nh}^t (x_s^{\text{SO}} - x_s) \, ds \\ &\quad + (s_*^{(M)}(T-nh, \vartheta_n^{\text{SO}}) - M_n) \cdot \frac{1}{2}(t-nh)^2. \end{aligned}$$

Notice that

$$\|L_n\|_{\mathbb{L}_2} = \left\| \frac{1}{2} I_d + \nabla^2 \log p_{T-nh}(\vartheta_n^{\text{SO}}) \right\|_{\mathbb{L}_2} \leq L(T-nh) - \frac{1}{2}. \quad (36)$$

Combining this with Assumptions 3 and 5 then provides us with

$$\begin{aligned} &\|x_t^{\text{SO}} - x_t\|_{\mathbb{L}_2} \\ &\leq (t-nh)\varepsilon_{sc} + \varepsilon_{sc}^{(L)} \int_{nh}^t \|x_s^{\text{SO}} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} \, ds + \|L_n\|_{\mathbb{L}_2} \int_{nh}^t \|x_s^{\text{SO}} - x_s\| \, ds + \frac{1}{2}(t-nh)^2 \varepsilon_{sc}^{(M)} \\ &\lesssim \left(L(T-nh) - \frac{1}{2} \right) \int_{nh}^t \|x_s^{\text{SO}} - x_s\| \, ds + (t-nh)\varepsilon_{sc} + \frac{2}{3}\sqrt{d}(t-nh)^{3/2} \varepsilon_{sc}^{(L)} + \frac{1}{2}(t-nh)^2 \varepsilon_{sc}^{(M)}. \end{aligned}$$

We omit the constant of term $\frac{2}{3}\sqrt{d}(t-nh)^{3/2} \varepsilon_{sc}^{(L)}$ in the last inequality. To handle the resulting integral inequality, we invoke the following Grönwall-type inequality.

Lemma 16. *Let $z(t) \geq t_0$ satisfy the following inequality:*

$$z(t) \leq \alpha(t) + \int_{t_0}^t \beta(s)z(s) \, ds, \quad t \geq t_0,$$

where $\beta(s)$ is non-negative, and t_0 is the initial time. Then, the solution $z(t)$ satisfies the following bound:

$$z(t) \leq \alpha(t) + \int_{t_0}^t \alpha(s)\beta(s) \exp\left(\int_s^t \beta(r) \, dr\right) \, ds, \quad t \geq t_0.$$

Additionally, if $\alpha(t)$ is non-decreasing function, then

$$z(t) \leq \alpha(t) \exp\left(\int_{t_0}^t \beta(s) \, ds\right), \quad t \geq t_0.$$

Let

$$\begin{aligned} z(t) &= \|x_t^{\text{SO}} - x_t\|_{\mathbb{L}_2}, \\ \alpha(t) &= (t-nh)\varepsilon_{sc} + \frac{2}{3}\sqrt{d}(t-nh)^{3/2} \varepsilon_{sc}^{(L)} + \frac{1}{2}(t-nh)^2 \varepsilon_{sc}^{(M)}, \\ \beta(t) &= L(T-nh) - \frac{1}{2}, \end{aligned}$$

and set $t_0 = nh$. By Lemma 16, we have

$$\|\vartheta_{n+1}^{\text{SO}} - x_{(n+1)h}\|_{\mathbb{L}_2} \leq \left(h\varepsilon_{sc} + \frac{2}{3}\sqrt{d}h^{3/2} \varepsilon_{sc}^{(L)} + \frac{1}{2}h^2 \varepsilon_{sc}^{(M)} \right) e^{(L(T-nh)-\frac{1}{2})h}. \quad (37)$$

The original SDE can be rewritten as follows

$$\tilde{Y}_t = \tilde{Y}_0 + \int_0^t \left(\frac{1}{2} \tilde{Y}_s + \nabla \log p_{T-nh-s}(\tilde{Y}_s) \right) ds + \int_{nh}^{nh+t} dW_s.$$

Combining this with the definition of x_t in (44), we then have

$$\begin{aligned} \tilde{Y}_t - x_{nh+t} &= \int_0^t \left(\frac{1}{2} \tilde{Y}_s + \nabla \log p_{T-nh-s}(\tilde{Y}_s) - \frac{1}{2} \vartheta_n^{\text{SO}} - \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) - L_n(x_{nh+s} - \vartheta_n^{\text{SO}}) - M_n s \right) ds \\ &= \int_0^t L_n(\tilde{Y}_s - x_{nh+s}) ds + \int_0^t \left(\frac{1}{2} \tilde{Y}_s + \nabla \log p_{T-nh-s}(\tilde{Y}_s) - \frac{1}{2} \vartheta_n^{\text{SO}} - \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) \right) ds \\ &\quad - \int_0^t \left(\int_0^s L_n d\tilde{Y}_u \right) ds - \int_0^t \left(\int_0^s M_n du \right) ds \\ &= \int_0^t L_n(\tilde{Y}_s - x_{nh+s}) ds + \int_0^t \left(\int_0^s d \left(\frac{1}{2} \tilde{Y}_u + \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right) \right) ds \\ &\quad - \int_0^t \left(\int_0^s L_n d\tilde{Y}_u \right) ds - \int_0^t \left(\int_0^s M_n du \right) ds. \end{aligned}$$

We then apply the Itô formula to the term $d \left(\frac{1}{2} \tilde{Y}_u + \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right)$. Recall the definitions of L_n and M_n , and after rearranging the expression, we obtain

$$\begin{aligned} \tilde{Y}_t - x_{nh+t} &= \underbrace{\int_0^t L_n(\tilde{Y}_s - x_{nh+s}) ds}_{\text{I}} + \underbrace{\int_0^t \left(\int_0^s \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) d\tilde{Y}_u \right) ds}_{\text{II}} \\ &\quad + \underbrace{\int_0^t \left[\int_0^s \left(\frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh-u}(\tilde{Y}_u) - \partial_t \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right) \right.}_{\text{III}} \\ &\quad \left. - \left(\frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh}(\tilde{Y}_0) - \partial_t \nabla \log p_{T-nh}(\tilde{Y}_0) \right) du \right] ds}_{\text{III}}. \end{aligned}$$

In what follows, we derive the upper bounds for each term on the right-hand side of the previous display.

Upper bound for term I: The upper bound of the term I follows directly from the fact that

$$\|L_n\|_{\mathbb{L}_2} \leq L(T - nh) - \frac{1}{2}.$$

Upper bound for term II: To derive the upper bound for the second term, we expand the term $d\tilde{Y}_u$, yielding

$$\begin{aligned} &\left\| \int_0^s \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) d\tilde{Y}_u \right\|_{\mathbb{L}_2} \\ &\leq \left\| \int_0^s (\nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0)) \left(\frac{1}{2} \tilde{Y}_u + \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right) du \right\|_{\mathbb{L}_2} \\ &\quad + \left\| \int_0^s (\nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0)) dW_u \right\|_{\mathbb{L}_2} \\ &\leq \int_0^s \left\| \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) \right\|_{\mathbb{L}_2} \cdot \left\| \frac{1}{2} \tilde{Y}_u + \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} du \\ &\quad + \left(\int_0^s \left\| \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) \right\|_{\mathbb{L}_2}^2 du \right)^{1/2}. \end{aligned}$$

The second inequality follows from display (28). We note that by Assumptions 6 and 7, it holds that

$$\begin{aligned}
& \left\| \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) \right\|_{\mathbb{L}_2} \\
& \leq \left\| \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} + \left\| \nabla^2 \log p_{T-nh}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) \right\|_{\mathbb{L}_2} \\
& \leq M_2 h (1 + \|\tilde{Y}_u\|_{\mathbb{L}_2}) + L_F \|\tilde{Y}_u - \tilde{Y}_0\|_{\mathbb{L}_2} \\
& \leq M_2 h + (L_F + M_2 h) \|\tilde{Y}_u - \tilde{Y}_0\|_{\mathbb{L}_2} + M_2 h \|\vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} \\
& \lesssim L_F \sqrt{du},
\end{aligned}$$

Combining this with the previous display provides us with

$$\begin{aligned}
& \left\| \int_0^s \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) d\tilde{Y}_u \right\|_{\mathbb{L}_2} \\
& \lesssim \int_0^s L_F \sqrt{du} \cdot \left\| \frac{1}{2} \tilde{Y}_u + \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} du + \left(\int_0^s L_F^2 du du \right)^{1/2}.
\end{aligned}$$

Hence, we obtain

$$\begin{aligned}
\|\text{II}\|_{\mathbb{L}_2} &= \left\| \int_0^t \left(\int_0^s \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) d\tilde{Y}_u \right) ds \right\|_{\mathbb{L}_2} \\
&\leq \int_0^t \left\| \int_0^s \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) - \nabla^2 \log p_{T-nh}(\tilde{Y}_0) d\tilde{Y}_u \right\|_{\mathbb{L}_2} ds \\
&\leq \int_0^t \left[\int_0^s L_F \sqrt{du} \cdot \left\| \frac{1}{2} \tilde{Y}_u + \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} du + \left(\int_0^s L_F^2 du du \right)^{1/2} \right] ds \\
&\lesssim \frac{\sqrt{2}}{4} L_F \sqrt{dt^2}.
\end{aligned} \tag{38}$$

Upper bound for term III:

In Section 4, it is claimed that the partial derivative of $\nabla \log p_t$ with respect to t can be estimated without requiring additional assumptions. This is achieved by transforming the t -derivative into x -derivative via the Fokker-Planck equation, as detailed below.

$$\partial_t p_t(x) = \frac{d}{2} p_t(x) + \frac{1}{2} x^\top \nabla p_t(x) + \frac{1}{2} \sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2}. \tag{39}$$

We need the following auxiliary lemma.

Lemma 17. *Let p_t be the probability density function of X_t , then*

$$\begin{aligned}
& \sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \cdot \frac{1}{p_t(x)} = \text{Tr}(\nabla^2 \log p_t(x)) + \|\nabla \log p_t(x)\|^2, \\
& \nabla \left(\sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \right) \cdot \frac{1}{p_t(x)} = \nabla(\text{Tr}(\nabla^2 \log p_t(x))) + \nabla(\|\nabla \log p_t(x)\|^2) \\
& \quad + [\text{Tr}(\nabla^2 \log p_t(x)) + \|\nabla \log p_t(x)\|^2] \cdot \nabla \log p_t(x).
\end{aligned}$$

We begin by taking the gradient of $\log p_t$, and then compute the partial derivative of $\nabla \log p_t$ with respect to t . This results in

$$\partial_t \nabla \log p_t(x) = \partial_t \left(\frac{\nabla p_t(x)}{p_t(x)} \right) = \frac{\partial_t \nabla p_t(x)}{p_t(x)} - \frac{\nabla p_t(x)}{p_t(x)} \cdot \frac{\partial_t p_t(x)}{p_t(x)}.$$

Under certain regularity conditions, we can interchange the operators ∂_t and ∇ in the term $\partial_t \nabla p_t(x)$, and substitute $\partial_t p_t(x)$ by (39), it follows that

$$\partial_t \nabla \log p_t(x) = \frac{\nabla \partial_t p_t(x)}{p_t(x)} - \nabla \log p_t(x) \cdot \left(\frac{d}{2} + \frac{1}{2} x^\top \nabla \log p_t(x) + \frac{1}{2} \sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \cdot \frac{1}{p_t(x)} \right).$$

and

$$\begin{aligned} \frac{\nabla \partial_t p_t(x)}{p_t(x)} &= \frac{1}{p_t(x)} \cdot \nabla \left(\frac{d}{2} p_t(x) + \frac{1}{2} x^\top \nabla p_t(x) + \frac{1}{2} \sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \right) \\ &= \frac{d}{2} \frac{\nabla p_t(x)}{p_t(x)} + \frac{1}{2} \frac{\nabla p_t(x)}{p_t(x)} + \frac{1}{2} \frac{\nabla^2 p_t(x) x}{p_t(x)} + \frac{1}{2} \nabla \left(\sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \right) \cdot \frac{1}{p_t(x)} \\ &= \frac{d+1}{2} \nabla \log p_t(x) + \frac{1}{2} \frac{\nabla^2 p_t(x) x}{p_t(x)} + \frac{1}{2} \nabla \left(\sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \right) \cdot \frac{1}{p_t(x)}. \end{aligned}$$

Therefore, we obtain that

$$\begin{aligned} \partial_t \nabla \log p_t(x) &= \frac{d+1}{2} \nabla \log p_t(x) + \frac{1}{2} \frac{\nabla^2 p_t(x) x}{p_t(x)} + \frac{1}{2} \nabla \left(\sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \right) \cdot \frac{1}{p_t(x)} \\ &\quad - \nabla \log p_t(x) \cdot \left(\frac{d}{2} + \frac{1}{2} x^\top \nabla \log p_t(x) + \frac{1}{2} \sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \cdot \frac{1}{p_t(x)} \right) \\ &= \frac{1}{2} \nabla \log p_t(x) + \frac{1}{2} \left(\frac{\nabla^2 p_t(x) x}{p_t(x)} - \nabla \log p_t(x) \nabla \log p_t(x)^\top x \right) \\ &\quad + \frac{1}{2} \nabla \left(\sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \right) \cdot \frac{1}{p_t(x)} - \frac{1}{2} \nabla \log p_t(x) \sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \cdot \frac{1}{p_t(x)}. \end{aligned}$$

By Lemma 17, the last two terms above can be calculated. Additionally, it holds that

$$\nabla^2 \log p_t(x) = \frac{\nabla^2 p_t(x)}{p_t(x)} - \frac{\nabla p_t(x) \nabla p_t(x)^\top}{p_t(x)^2}.$$

Thus, $\partial_t \nabla \log p_t(x)$ can be simplified to

$$\begin{aligned} \partial_t \nabla \log p_t(x) &= \frac{1}{2} \nabla \log p_t(x) + \frac{1}{2} \nabla^2 \log p_t(x) x \\ &\quad + \frac{1}{2} \left[\nabla (\text{Tr}(\nabla^2 \log p_t(x))) + \nabla (\|\nabla \log p_t(x)\|^2) \right] \\ &\quad + \frac{1}{2} \left(\text{Tr}(\nabla^2 \log p_t(x)) + \|\nabla \log p_t(x)\|^2 \right) \cdot \nabla \log p_t(x) \\ &\quad - \frac{1}{2} \nabla \log p_t(x) \left(\text{Tr}(\nabla^2 \log p_t(x)) + \|\nabla \log p_t(x)\|^2 \right) \\ &= \frac{1}{2} \nabla \log p_t(x) + \frac{1}{2} \nabla^2 \log p_t(x) x + \frac{1}{2} \nabla (\text{Tr}(\nabla^2 \log p_t(x))) + \frac{1}{2} \nabla (\|\nabla \log p_t(x)\|^2). \end{aligned}$$

Notice that

$$\sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_t(x) = \frac{1}{2} \nabla (\text{Tr}(\nabla^2 \log p_t(x))).$$

Then, it follows that

$$\begin{aligned} &\frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_t(x) - \partial_t \nabla \log p_t(x) \\ &= - \left(\frac{1}{2} \nabla \log p_t(x) + \frac{1}{2} \nabla^2 \log p_t(x) x + \frac{1}{2} \nabla (\|\nabla \log p_t(x)\|^2) \right) \\ &= - \frac{1}{2} (\nabla \log p_t(x) + \nabla^2 \log p_t(x) x) + \nabla^2 \log p_t(x) \cdot \nabla \log p_t(x). \end{aligned}$$

Therefore we have

$$\begin{aligned}
& \left\| \frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh-u}(\tilde{Y}_u) - \partial_t \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} \\
& \leq \frac{1}{2} \left\| \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} + \frac{1}{2} \left\| \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} \left\| \tilde{Y}_u \right\|_{\mathbb{L}_2} \\
& \quad + \left\| \nabla^2 \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} \left\| \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} \\
& \leq \frac{1}{2} \left\| \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} + \frac{1}{2} L(T-nh-u) \left\| \tilde{Y}_u \right\|_{\mathbb{L}_2} + L(T-nh-u) \left\| \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2}.
\end{aligned}$$

The second inequality follows from Assumption 1. The bounds for $\left\| \tilde{Y}_u \right\|_{\mathbb{L}_2}$ and $\left\| \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2}$ can be derived according to the proof of Lemma 10. We then find

$$\begin{aligned}
& \left\| \frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh-u}(\tilde{Y}_u) - \partial_t \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} \\
& \leq \frac{1}{2} \left\| \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} + \frac{1}{2} L(T-nh-u) \left\| \tilde{Y}_u \right\|_{\mathbb{L}_2} + L(T-nh-u) \left\| \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} \\
& \leq \left(\frac{1}{2} + L(T-nh-u) \right) \left[L(T-nh-u) (\|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + C_2(n)) + (dL(T-nh-u))^{1/2} \right] \\
& \quad + \frac{1}{2} L(T-nh-u) (\|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + C_2(n) + C_4).
\end{aligned}$$

Therefore, we obtain

$$\begin{aligned}
\|\text{III}\|_{\mathbb{L}_2} & \leq \int_0^t \int_0^s \left\| \frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh-u}(\tilde{Y}_u) - \partial_t \nabla \log p_{T-nh-u}(\tilde{Y}_u) \right\|_{\mathbb{L}_2} du ds \\
& \quad + \int_0^t \int_0^s \left\| \frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh}(\tilde{Y}_0) - \partial_t \nabla \log p_{T-nh}(\tilde{Y}_0) \right\|_{\mathbb{L}_2} du ds \\
& \leq \int_0^t \int_0^s [(1 + L(T-nh-u))L(T-nh-u) + (1 + L(T-nh))L(T-nh)] du ds \cdot \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} \\
& \quad + \int_0^t \int_0^s [(1 + L(T-nh-u))L(T-nh-u) + (1 + L(T-nh))L(T-nh)] du ds \cdot C_2(n) \\
& \quad + \sqrt{d} \int_0^t \int_0^s \left[\left(\frac{1}{2} + L(T-nh-u) \right) L(T-nh-u)^{1/2} + \left(\frac{1}{2} + L(T-nh) \right) L(T-nh)^{1/2} \right] du ds \\
& \quad + \int_0^t \int_0^s \frac{1}{2} (L(T-nh-u) + L(T-nh)) du ds \cdot C_4.
\end{aligned} \tag{40}$$

For simplicity, we focus on the lowest-order term. Recall equations (36), (38) and (40), which lead to the following expression

$$\left\| \tilde{Y}_t - x_{nh+t} \right\|_{\mathbb{L}_2} \leq \left(L(T-nh) - \frac{1}{2} \right) \int_0^t \left\| \tilde{Y}_s - x_{nh+s} \right\|_{\mathbb{L}_2} ds + \left(A_{n,1} \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + A_{n,2} \right) \cdot t^2,$$

where

$$A_{n,1} = \sup_{nh \leq t \leq (n+1)h} \frac{1}{t^2} \int_0^t \int_0^s [(1 + L(T-nh-u))L(T-nh-u) + (1 + L(T-nh))L(T-nh)] du ds,$$

and

$$\begin{aligned} A_{n,2} = & \sup_{nh \leq t \leq (n+1)h} \frac{1}{t^2} \left[C_2(n) \int_0^t \int_0^s [(1 + L(T - nh - u))L(T - nh - u) + (1 + L(T - nh))L(T - nh)] \, du \, ds \right. \\ & + \sqrt{d} \int_0^t \int_0^s [(\frac{1}{2} + L(T - nh - u))L(T - nh - u)^{1/2} + (\frac{1}{2} + L(T - nh))L(T - nh)^{1/2}] \, du \, ds \\ & + \int_0^t \int_0^s \frac{1}{2} (L(T - nh - u) + L(T - nh)) \, du \, ds \cdot C_4 \Big] \\ & + \frac{\sqrt{2}}{4} \sqrt{d} L_F. \end{aligned}$$

Using Lemma 16 with

$$\begin{aligned} z(t) &= \left\| \tilde{Y}_t - x_{nh+t} \right\|_{\mathbb{L}_2}, \\ \alpha(t) &= (A_{n,1} \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + A_{n,2}) \cdot t^2, \\ \beta(t) &= L(T - nh) - \frac{1}{2}, \end{aligned}$$

set $t_0 = nh$, we then obtain

$$\begin{aligned} \left\| \tilde{Y}_h - x_{(n+1)h} \right\|_{\mathbb{L}_2} &\leq (A_{n,1} \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + A_{n,2}) h^2 \exp \left((L(T - nh) - \frac{1}{2})h \right) \\ &= A_{n,1} e^{(L(T-nh)-\frac{1}{2})h} h^2 \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + A_{n,2} e^{(L(T-nh)-\frac{1}{2})h} h^2. \end{aligned}$$

Invoking display (37), we arrive at

$$\begin{aligned} \left\| \tilde{Y}_h - \vartheta_{n+1}^{\text{SO}} \right\|_{\mathbb{L}_2} &\leq \left\| \tilde{Y}_h - x_{(n+1)h} \right\|_{\mathbb{L}_2} + \left\| \vartheta_{n+1}^{\text{SO}} - x_{(n+1)h} \right\|_{\mathbb{L}_2} \\ &\leq A_{n,1} e^{(L(T-nh)-\frac{1}{2})h} h^2 \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + A_{n,2} e^{(L(T-nh)-\frac{1}{2})h} h^2 \\ &\quad + \left[h\varepsilon_{sc} + \frac{2}{3} h^{3/2} \sqrt{d} \varepsilon_{sc}^{(L)} + \frac{1}{2} h^2 \varepsilon_{sc}^{(M)} \right] e^{(L(T-nh)-\frac{1}{2})h}. \end{aligned}$$

Furthermore, we can bound the coefficients $A_{n,1}$ and $A_{n,2}$ as follows,

$$\begin{aligned} A_{n,1} &\leq \frac{1}{t^2} \int_0^t \left(\int_0^s 2(1 + L_{\max}) L_{\max} \, du \right) \, ds = (1 + L_{\max}) L_{\max}, \\ A_{n,2} &\leq (1 + L_{\max}) L_{\max} C_2(n) + \sqrt{d} \left(\frac{1}{2} + L_{\max} \right) L_{\max}^{1/2} + \frac{1}{2} L_{\max} C_4 + \frac{\sqrt{2}}{4} \sqrt{d} L_F \\ &\lesssim \sqrt{d} \left(\frac{1}{2} + L_{\max} \right) L_{\max}^{1/2} + \frac{\sqrt{2}}{4} \sqrt{d} L_F. \end{aligned}$$

Collecting all the pieces then gives

$$\|Y_{nh} - \vartheta_{n+1}^{\text{SO}}\|_{\mathbb{L}_2} \leq r_n^{\text{SO}} \|Y_{nh} - \vartheta_n^{\text{SO}}\|_{\mathbb{L}_2} + C_n^{\text{SO}} h^2 + \left[h\varepsilon_{sc} + \frac{2}{3} h^{3/2} \varepsilon_{sc}^{(L)} + \frac{1}{2} h^2 \varepsilon_{sc}^{(M)} \right] e^{(L(T-nh)-\frac{1}{2})h},$$

where

$$\begin{aligned} r_n^{\text{SO}} &= e^{-\int_{nh}^{(n+1)h} (m(T-t) - \frac{1}{2}) \, dt} + A_{n,1} e^{(L(T-nh)-\frac{1}{2})h} h^2, \\ C_n^{\text{SO}} &= A_{n,2} e^{(L(T-nh)-\frac{1}{2})h}. \end{aligned}$$

□

From the result above, we finally obtain

$$\begin{aligned} \|Y_{Nh} - \vartheta_N^{\text{SO}}\|_{\mathbb{L}_2} &\lesssim \frac{1}{m_{\min} - 1/2} \left[h \max_{0 \leq k \leq N-1} C_k^{\text{SO}} + \left(\varepsilon_{sc} + \frac{2}{3} h^{1/2} \varepsilon_{sc}^{(L)} + \frac{1}{2} h \varepsilon_{sc}^{(M)} \right) e^{(L_{\max} - \frac{1}{2})h} \right] \\ &\lesssim h \cdot \frac{\sqrt{d} (L_{\max}^{3/2} + \sqrt{2} L_F/4) e^{(L_{\max} - \frac{1}{2})h}}{m_{\min} - 1/2} + \left(\varepsilon_{sc} + \frac{2}{3} \sqrt{hd} \varepsilon_{sc}^{(L)} + \frac{1}{2} h \varepsilon_{sc}^{(M)} \right) e^{(L_{\max} - \frac{1}{2})h}. \end{aligned}$$

This completes the proof of Theorem 4.

D Proof of Auxiliary Lemma

D.1 Proof of Lemma 8

We have

$$\begin{aligned} \frac{d \|H_t - G_t\|^2}{dt} &= 2 \left\langle H_t - G_t, \frac{d(H_t - G_t)}{dt} \right\rangle \\ &= 2 \left\langle H_t - G_t, \frac{1}{2}(H_t - G_t) + (\nabla \log p_{T-t}(H_t) - \nabla \log p_{T-t}(G_t)) \right\rangle \quad (41) \\ &= \|H_t - G_t\|^2 + 2 \langle H_t - G_t, \nabla \log p_{T-t}(H_t) - \nabla \log p_{T-t}(G_t) \rangle \\ &\leq (1 - 2m(T-t)) \|H_t - G_t\|^2. \end{aligned}$$

The last inequality follows from Lemma 6. Then, we take the derivative of $e^{-\int_{t_1}^t (2m(T-s)-1) ds} \|H_t - G_t\|^2$

$$\begin{aligned} &\frac{d}{dt} \left(e^{\int_{t_1}^t (2m(T-s)-1) ds} \|H_t - G_t\|^2 \right) \\ &= (2m(T-t) - 1) e^{-\int_{t_1}^t (2m(T-s)-1) ds} \|H_t - G_t\|^2 + e^{-\int_{t_1}^t (2m(T-s)-1) ds} \frac{d \|H_t - G_t\|^2}{dt} \\ &\leq 0. \end{aligned}$$

Therefore, we obtain that

$$e^{\int_{t_1}^t (2m(T-s)-1) ds} \|H_t - G_t\|^2 \leq \|H_{t_1} - G_{t_1}\|^2.$$

taking the expectation of both sides and then applying the square root yields the desired result.

D.2 Proof of Lemma 10

By the definition of $\tilde{Y}_h$, we have

$$\begin{aligned} \|\tilde{Y}_t - \tilde{Y}_0\|_{\mathbb{L}_2} &= \left\| \int_0^t \left(\frac{1}{2} \tilde{Y}_s + \nabla \log p_{T-nh-s}(\tilde{Y}_s) \right) ds + \int_{nh}^{nh+t} dW_s \right\|_{\mathbb{L}_2} \\ &\leq \int_0^t \frac{1}{2} \|\tilde{Y}_s\|_{\mathbb{L}_2} dt + \int_0^t \|\nabla \log p_{T-nh-s}(\tilde{Y}_s)\|_{\mathbb{L}_2} ds + \left\| \int_{nh}^{nh+t} dW_s \right\|_{\mathbb{L}_2}. \end{aligned}$$

To bound the first term, we observe that for any $s \in [0, h]$, the following holds

$$\begin{aligned} \|\tilde{Y}_s\|_{\mathbb{L}_2} &\leq \|Y_{nh+s}\|_{\mathbb{L}_2} + \|\tilde{Y}_s - Y_{nh+s}\|_{\mathbb{L}_2} \\ &\leq \|Y_{nh+s} - X_{nh+s}^{\leftarrow}\|_{\mathbb{L}_2} + \|X_{nh+s}^{\leftarrow}\|_{\mathbb{L}_2} + \|\tilde{Y}_s - Y_{nh+s}\|_{\mathbb{L}_2} \\ &\leq e^{-\int_0^{nh+s} (m(T-t)-\frac{1}{2}) dt} \|Y_0 - X_0^{\leftarrow}\|_{\mathbb{L}_2} + \|X_{T-(nh+s)}^{\leftarrow}\|_{\mathbb{L}_2} + e^{-\int_{nh}^s (m(T-u)-\frac{1}{2}) du} \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2} \\ &\leq e^{-\int_0^{nh} (m(T-t)-\frac{1}{2}) dt} \|Y_0 - X_T\|_{\mathbb{L}_2} + \sup_{0 \leq t \leq T} \|X_t\|_{\mathbb{L}_2} + \|Y_{nh} - \vartheta_n^{\text{EM}}\|_{\mathbb{L}_2}. \end{aligned}$$

Here, the second inequality follows from the Grönwall inequality applied on $\|Y_{nh+s} - X_{nh+s}^{\leftarrow}\|_{\mathbb{L}_2}$ and $\|\tilde{Y}_s - Y_{nh+s}\|_{\mathbb{L}_2}$, and the fact that $\|X_t\|_{\mathbb{L}_2} = \|X_{T-t}^{\leftarrow}\|_{\mathbb{L}_2}$. To bound the second term, we need the following lemma.

Lemma 18. *If the target distribution p_0 satisfies Assumption 1, it holds that*

$$\|\nabla \log p_t(X_t)\|_{\mathbb{L}_2} \leq (dL(t))^{1/2}.$$

According to Lemma 18, it follows that

$$\begin{aligned}
& \left\| \nabla \log p_{T-nh-s}(\tilde{Y}_s) \right\|_{\mathbb{L}_2} \\
& \leq \left\| \nabla \log p_{T-nh-s}(\tilde{Y}_s) - \nabla \log p_{T-nh-s}(X_{nh+s}^{\leftarrow}) \right\|_{\mathbb{L}_2} + \left\| \nabla \log p_{T-nh-s}(X_{nh+s}^{\leftarrow}) \right\|_{\mathbb{L}_2} \\
& \leq L(T-nh-s) \left\| \tilde{Y}_s - X_{nh+s}^{\leftarrow} \right\|_{\mathbb{L}_2} + (dL(T-nh-s))^{1/2} \\
& \leq L(T-nh-s) \left\| \tilde{Y}_0 - X_{nh}^{\leftarrow} \right\|_{\mathbb{L}_2} + (dL(T-nh-s))^{1/2} \\
& \leq L(T-nh-s) \left(\left\| \tilde{Y}_0 - Y_{nh} \right\|_{\mathbb{L}_2} + \left\| Y_{nh} - X_{nh}^{\leftarrow} \right\|_{\mathbb{L}_2} \right) + (dL(T-nh-s))^{1/2} \\
& \leq L(T-nh-s) \left(\left\| Y_{nh} - \vartheta_n^{\text{EM}} \right\|_{\mathbb{L}_2} + e^{-\int_0^{nh} (m(T-t) - \frac{1}{2}) dt} \left\| Y_0 - X_T \right\|_{\mathbb{L}_2} \right) + (dL(T-nh-s))^{1/2}.
\end{aligned}$$

Here, we use the fact that $\tilde{Y}_0 = \vartheta_n^{\text{EM}}$, and Grönwall inequality are used in the third inequality and the last one. This completes the proof.

D.3 Proof of Lemma 13

For the stochastic integral of process X , we have

$$\mathbb{E}(I_t(X))^2 = \mathbb{E} \int_0^t X_u^2 d\langle M \rangle_u.$$

Then, we obtain

$$\begin{aligned}
& \left\| \int_{nh}^{(n+U_n)h} dW_t - \int_0^1 \left(\int_{nh}^{(n+u)h} dW_t \right) du \right\|_{\mathbb{L}_2}^2 \\
& = \mathbb{E} \left(\int_0^1 \int_{nh}^{(n+1)h} -\mathbf{1}_{\{U_n \leq u\}} \mathbf{1}_{\{(n+U_n)h \leq t \leq (n+u)h\}} + \mathbf{1}_{\{U_n > u\}} \mathbf{1}_{\{(n+u)h \leq t \leq (n+U_n)h\}} dW_t du \right)^2 \\
& \leq \int_0^1 \mathbb{E} \left(\int_{nh}^{(n+1)h} -\mathbf{1}_{\{U_n \leq u\}} \mathbf{1}_{\{(n+U_n)h \leq t \leq (n+u)h\}} + \mathbf{1}_{\{U_n > u\}} \mathbf{1}_{\{(n+u)h \leq t \leq (n+U_n)h\}} dW_t \right)^2 du \\
& = \int_0^1 \left(\mathbb{E} \int_{nh}^{(n+1)h} \mathbf{1}_{\{U_n \leq u\}} \mathbf{1}_{\{(n+U_n)h \leq t \leq (n+u)h\}} + \mathbf{1}_{\{U_n > u\}} \mathbf{1}_{\{(n+u)h \leq t \leq (n+U_n)h\}} dt \right) du \\
& = \int_0^1 (\mathbb{E} (\mathbf{1}_{\{U_n \leq u\}}(u - U_n)h + \mathbf{1}_{\{U_n > u\}}(U_n - u)h)) du \\
& = h \int_0^1 \left(u^2 - u + \frac{1}{2} \right) du \\
& = \frac{1}{3}h.
\end{aligned}$$

D.4 Proof of Lemma 16

Define the function $w(s)$ via

$$w(s) = \exp \left(- \int_{t_0}^s \beta(r) dr \right) \int_{t_0}^s \beta(r) z(r) dr, \quad \forall s \geq t_0.$$

Differentiating this function gives

$$w'(s) = \left(z(s) - \int_{t_0}^s \beta(r) z(r) dr \right) \beta(s) \exp \left(- \int_{t_0}^s \beta(r) dr \right) \leq \alpha(s) \beta(s) \exp \left(- \int_{t_0}^s \beta(r) dr \right).$$

Note that $w(t_0) = 0$. Integrating the function w from t_0 to t yields

$$w(t) \leq \int_{t_0}^t \alpha(s) \beta(s) \exp \left(- \int_{t_0}^s \beta(r) \, dr \right) \, ds.$$

By the definition of $w(s)$, we also have

$$\int_{t_0}^t \beta(s) z(s) \, ds = \exp \left(\int_{t_0}^t \beta(r) \, dr \right) w(t).$$

Combining the previous two displays provides us with

$$\int_{t_0}^t \beta(s) z(s) \, ds \leq \int_{t_0}^t \alpha(s) \beta(s) \exp \left(\int_s^t \beta(r) \, dr \right) \, ds.$$

By substituting this estimate into the inequality, we can obtain the first desired result. Furthermore, if α is non-decreasing, then for any $s \leq t$, it holds that $\alpha(s) \leq \alpha(t)$. This leads to

$$z(t) \leq \alpha(t) + \alpha(t) \int_{t_0}^t \beta(s) \exp \left(\int_s^t \beta(r) \, dr \right) \, ds.$$

which can be simplified to

$$z(t) \leq \alpha(t) \exp \left(\int_{t_0}^t \beta(r) \, dr \right), \quad t \geq t_0.$$

This completes the proof.

D.5 Proof of Lemma 17

Notice that

$$\begin{aligned} \nabla^2 \log p_t(x) &= - \frac{1}{p_t(x)^2} \nabla p_t(x) \nabla p_t(x)^\top + \frac{1}{p_t(x)} \nabla^2 p_t(x) \\ &= - \nabla \log p_t(x) \nabla \log p_t(x)^\top + \frac{1}{p_t(x)} \nabla^2 p_t(x), \end{aligned}$$

which indicates

$$\begin{aligned} \frac{1}{2} \sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \cdot \frac{1}{p_t(x)} &= \frac{1}{2} \operatorname{Tr} \left(\frac{1}{p_t(x)} \nabla^2 p_t(x) \right) \\ &= \frac{1}{2} \operatorname{Tr} \left(\nabla^2 \log p_t(x) + \nabla \log p_t(x) \nabla \log p_t(x)^\top \right) \\ &= \frac{1}{2} \operatorname{Tr} \left(\nabla^2 \log p_t(x) \right) + \frac{1}{2} \|\nabla \log p_t(x)\|^2, \end{aligned}$$

Additionally, we have

$$\begin{aligned} \nabla \left(\frac{\partial^2 \log p_t(x)}{\partial x_i^2} \right) &= \nabla \left(\frac{\partial^2 p_t(x)}{\partial x_i^2} \cdot \frac{1}{p_t(x)} - \left(\frac{\partial p_t(x)}{\partial x_i} \cdot \frac{1}{p_t(x)} \right)^2 \right) \\ &= \nabla \left(\frac{\partial^2 p_t(x)}{\partial x_i^2} \right) \cdot \frac{1}{p_t(x)} - \frac{\partial^2 p_t(x)}{\partial x_i^2} \cdot \frac{1}{p_t(x)} \cdot \nabla \log p_t(x) - \nabla \left(\left(\frac{\partial \log p_t(x)}{\partial x_i} \right)^2 \right). \end{aligned}$$

Then, we obtain

$$\begin{aligned} &\nabla \left(\sum_{i=1}^d \frac{\partial^2 p_t(x)}{\partial x_i^2} \right) \cdot \frac{1}{p_t(x)} \\ &= \nabla \left(\operatorname{Tr}(\nabla^2 \log p_t(x)) \right) + \left[\operatorname{Tr}(\nabla^2 \log p_t(x)) + \|\nabla \log p_t(x)\|^2 \right] \cdot \nabla \log p_t(x) + \nabla(\|\nabla \log p_t(x)\|^2). \end{aligned}$$

D.6 Proof of Lemma 18

Note that

$$\begin{aligned}\mathbb{E}(\|\nabla \log p_t(X_t)\|^2) &= \int_{\mathbb{R}^d} \|\nabla \log p_t(x)\|^2 p_t(x) dx \\ &= \lim_{R \rightarrow \infty} \int_{B(0,R)} \langle \nabla \log p_t(x), \nabla \log p_t(x) \rangle p_t(x) dx \\ &= \lim_{R \rightarrow \infty} \int_{B(0,R)} \langle \nabla \log p_t(x), \nabla p_t(x) \rangle dx,\end{aligned}$$

where $B(0, R)$ denotes the Euclidean ball with radius $R > 0$ centered at the origin. Using integration by parts, we then obtain

$$\begin{aligned}\mathbb{E}(\|\nabla \log p_t(X_t)\|^2) &= \lim_{R \rightarrow \infty} \int_{B(0,R)} -p_t(x) \Delta \log p_t(x) dx + \int_{\partial B(0,R)} p_t(x) \frac{\partial \log p_t(x)}{\partial \vec{n}} dS \\ &= \int_{\mathbb{R}^d} p_t(x) \cdot (-\Delta \log p_t(x)) dx \\ &\leq dL(t),\end{aligned}$$

where $\frac{\partial f}{\partial \vec{n}} = \nabla f \cdot \vec{n}$ represents the directional derivative along the normal vector $\vec{n}$ and dS denotes the surface integral over the spherical surface. Here we use the fact that $p_t(x)$ converges to 0 at an exponential rate as $\|x\|$ approaches infinity, and the fact that

$$-\Delta \log p_t(x) = -\text{Tr}(\nabla^2 \log p_t(x)) \in [0, dL(t)],$$

which follows from Lemma 6.

E Details for second-order acceleration

In this section, we present a complete derivation of the second-order acceleration scheme, detailing the implementation of Itô-Taylor expansions and Itô's formula. Building upon the general backward process framework

$$dx_t = \gamma(T - t, x_t) dt + \sigma dW_t, \quad (42)$$

where $\sigma > 0$ and W_t is the d -dimensional Brownian motion. We apply Itô's formula to $\gamma(T - t, x)$. This procedure generates an approximated structure of SDE (42),

$$dx_t = [\gamma(T - s, x_s) + L_s(x_t - x_s) + M_s(t - s)] dt + \sigma dW_t. \quad (43)$$

with

$$L_s = \frac{\partial \gamma}{\partial x}(T - s, x_s) \quad \text{and} \quad M_s = \frac{\sigma^2}{2} \frac{\partial^2 \gamma}{\partial x^2}(T - s, x_s) - \frac{\partial \gamma}{\partial t}(T - s, x_s)$$

which serves as the foundation for our subsequent second-order discretization. In Section 4, we demonstrate that this approximation preserves the core dynamical structure of the original SDE (42) while admitting a closed-form solution. This is achieved by replacing the intractable drift term $\gamma(T - t, x_s)$ with its Itô-expanded counterpart, which remains analytical tractable through explicit integration.

Applying Itô's formula to $e^{-L_s t} x_t$ yields

$$d(e^{-L_s t} x_t) = e^{-L_s t} (\gamma(T - s, x_s) - L_s x_s + M_s(t - s)) dt + e^{-L_s t} \sigma dW_t.$$

For fixed s , both sides of the equation permit closed-form integration. While the Brownian integral $\int_s^{s+\Delta t} e^{-L_s t} \sigma dW_t$ formally appears non-analytic, it equivalently manifests as a Gaussian random variable with explicitly computable variance. This enables full analytical representation for $x_{s+\Delta t}$

when integrating over $[s, s + \Delta t]$,

$$\begin{aligned} x_{s+\Delta t} &= e^{L_s \Delta t} x_s + \int_s^{s+\Delta t} e^{L_s(s+\Delta t-t)} dt (\gamma(T-s, x_s) - L_s x_s) \\ &\quad + \int_s^{s+\Delta t} e^{L_s(s+\Delta t-t)} (t-s) dt M_s + \sigma \int_s^{s+\Delta t} e^{L_s(s+\Delta t-t)} dW_t \\ &= x_s + L_s^{-1} (e^{L_s \Delta t} - 1) \gamma(T-s, x_s) + L_s^{-2} [(e^{L_s \Delta t} - 1) - L_s \Delta t] M_s \\ &\quad + \sigma \int_s^{s+\Delta t} e^{L_s(s+\Delta t-u)} dW_u. \end{aligned}$$

Having established the general framework, we now specialize to our core case through the parameterization: set $\gamma(T-t, x) = \frac{1}{2}x + \nabla \log p_{T-t}(x)$, $\sigma = 1$, let $\Delta t \in [0, h]$ and $s = nh$.

In the resulting expression, we denote x_s by ϑ_n^{SO} . Then for any $t \in [nh, (n+1)h]$, the solution admits the semi-analytic representation

$$\begin{aligned} x_t &= \vartheta_n^{\text{SO}} + \int_{nh}^t \left(\frac{1}{2} \vartheta_n^{\text{SO}} + \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) \right. \\ &\quad \left. + L_n(x_u - \vartheta_n^{\text{SO}}) + M_n(u - nh) \right) du + \int_{nh}^t dW_u \end{aligned} \quad (44)$$

where

$$\begin{aligned} L_n &= \frac{1}{2} I_d + \nabla^2 \log p_{T-nh}(\vartheta_n^{\text{SO}}) \\ M_n &= \frac{1}{2} \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2} \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}) - \frac{\partial}{\partial t} \nabla \log p_{T-nh}(\vartheta_n^{\text{SO}}). \end{aligned}$$

Though L_n and M_n are theoretically defined through exact derivatives in SDE (43), their practical evaluation requires approximations due to the score function's computational intractability. We implement these approximations via numerical methods or neural networks, with concrete techniques for L_n and M_n estimation provided separately in Appendix F and G. Substituting these approximations into the SDE (44) yields

$$\begin{aligned} x_t &= \vartheta_n^{\text{SO}} + \int_{nh}^t \left(\gamma(T-nh, \vartheta_n^{\text{SO}}) + s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}})(x_u - \vartheta_n^{\text{SO}}) \right. \\ &\quad \left. + s_*^{(M)}(T-nh, \vartheta_n^{\text{SO}})(u - nh) \right) du + \int_{nh}^t dW_u. \end{aligned}$$

Crucially, this substitution preserves the closed-form integrability of the original framework. Adopting the same exponential integration strategy as above, we derive a closed form of x_t . Let $\vartheta_{n+1}^{\text{SO}}$ denote $x_{(n+1)h}$, the second-order discretization scheme is given by

$$\begin{aligned} \vartheta_{n+1}^{\text{SO}} &= \vartheta_n^{\text{SO}} + s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}})^{-1} \left(e^{s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}})h} - I_d \right) \left(\frac{1}{2} \vartheta_n^{\text{SO}} + s_*(T-nh, \vartheta_n^{\text{SO}}) \right) \\ &\quad + s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}})^{-2} \left(e^{s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}})h} - s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}})h - I_d \right) s_*^{(M)}(T-nh, \vartheta_n^{\text{SO}}) \\ &\quad + \int_{nh}^{(n+1)h} e^{s_*^{(L)}(T-nh, \vartheta_n^{\text{SO}})[(n+1)h-t]} dW_t. \end{aligned}$$

Implementation specifics for handling the matrix exponentials and stochastic integral are addressed in Appendix G.

F Numerical Studies on Synthetic Data

We apply the five schemes to the posterior density of penalized logistic regression, defined by $p_0(\theta) \propto \exp(-f(\theta))$ with the potential function

$$f(\theta) = \frac{\lambda}{2} \|\theta\|^2 + \frac{1}{n_{\text{data}}} \sum_{i=1}^{n_{\text{data}}} \log(1 + \exp(-y_i x_i^\top \theta)),$$

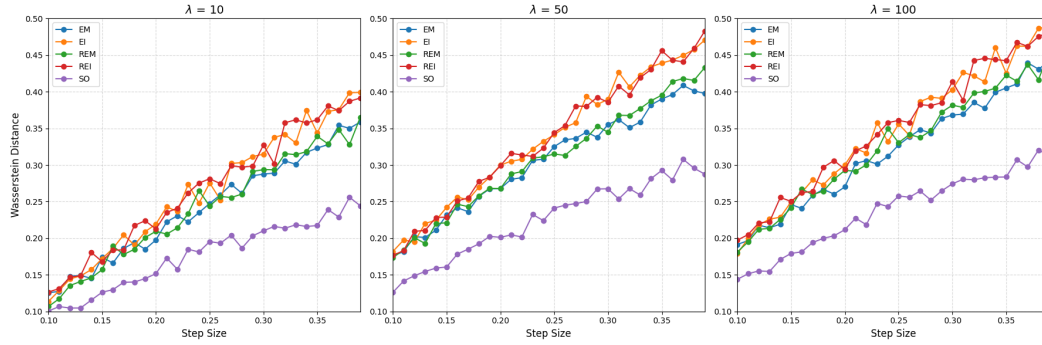


Figure 2: Error of various discretization schemes and second-order sampler with different choice of step size.

where $\lambda > 0$ denotes the tuning parameter. The data $\{x_i, y_i\}_{i=1}^{n_{\text{data}}}$, composed of binary labels $y_i \in \{-1, 1\}$ and features $x_i = (x_{i,1}, \dots, x_{i,d})^\top \in \mathbb{R}^d$ generated from $x_{i,j} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 100)$.

F.1 Implementation Details

In the numerical studies, we set $T = 10$, and the number of Monte Carlo iterations is chosen as the floor of T/h , where h varies according to the step size indicated in the figure. Figure 2 shows the Wasserstein distance measured along the first dimension between the empirical distributions of the N -th outputs from SGMs and the target distribution, with different choices of the step size h . In this simulation, we use the Monte-Carlo method to estimate the score function and the Hessian matrix.

F.2 Calculation

In this part, we derive explicit formulas for each coefficient term we need. First, the score function can be computed as

$$\begin{aligned} \nabla \log p_0(\theta) &= - \left(\lambda \theta + \frac{1}{n_{\text{data}}} \sum_{i=1}^{n_{\text{data}}} \frac{-y_i x_i \exp(-y_i x_i^\top \theta)}{1 + \exp(-y_i x_i^\top \theta)} \right) \\ &= - \left(\lambda \theta + \frac{1}{n_{\text{data}}} \sum_{i=1}^{n_{\text{data}}} \frac{-y_i x_i}{1 + \exp(y_i x_i^\top \theta)} \right). \end{aligned}$$

For simplicity, we denote the logistic sigmoid function $\sigma(u) = \frac{1}{1 + e^{-u}}$, then

$$\nabla \log p_0(\theta) = - \left(\lambda \theta + \frac{1}{n_{\text{data}}} \sum_{i=1}^{n_{\text{data}}} -y_i x_i \sigma(-y_i x_i^\top \theta) \right).$$

Since $\sigma'(u) = \sigma(u)[1 - \sigma(u)]$, we have

$$\begin{aligned} \nabla^2 \log p_0(\theta) &= - \left(\lambda I_d + \frac{1}{n_{\text{data}}} \sum_{i=1}^{n_{\text{data}}} y_i^2 \sigma(-y_i x_i^\top \theta) [1 - \sigma(-y_i x_i^\top \theta)] x_i x_i^\top \right) \\ &= - \lambda I_d - \frac{1}{n_{\text{data}}} \sum_{i=1}^{n_{\text{data}}} \sigma(-y_i x_i^\top \theta) [1 - \sigma(-y_i x_i^\top \theta)] x_i x_i^\top. \end{aligned}$$

As $x_i x_i^\top \succcurlyeq 0$, $\nabla^2 \log p_0(\theta) \preccurlyeq -\lambda I_d$. We also have that $\sigma(1 - y_i x_i^\top \theta) \in (0, 1)$, then

$$\begin{aligned} \nabla^2 \log p_0(\theta) &\succcurlyeq -\lambda I_d - \frac{1}{4n_{\text{data}}} \sum_{i=1}^{n_{\text{data}}} x_i x_i^\top \\ &\succcurlyeq - \left(\lambda + \frac{1}{n_{\text{data}}} \lambda_{\max} \left(\sum_{i=1}^{n_{\text{data}}} x_i x_i^\top \right) \right) I_d. \end{aligned}$$

Therefore,

$$m_0 = \lambda, \quad L_0 = \lambda + \frac{1}{n_{\text{data}}} \lambda_{\max} \left(\sum_i^{n_{\text{data}}} x_i x_i^\top \right).$$

Recall that the transition probability $p_{t|0}(\theta_t|\theta_0) = \phi(\theta_t; \mu_t, \Sigma_t)$, where $\mu_t = e^{-\frac{1}{2}t}\theta_0$, $\Sigma_t = (1 - e^{-t})I_d$, and $\phi(\theta, \mu, \Sigma)$ denotes the probability density function of $\mathcal{N}(\mu, \Sigma)$, then we have

$$\begin{aligned} p_t(\theta_t) &= \int_{\mathbb{R}^d} p_{t|0}(\theta_t|\theta_0) p_0(\theta_0) d\theta_0 \\ &= \int_{\mathbb{R}^d} \frac{1}{\sqrt{(2\pi)^d |\Sigma_t|}} \exp\left(-\frac{1}{2}(\theta_t - \mu_t)^\top \Sigma_t^{-1} (\theta_t - \mu_t)\right) p_0(\theta_0) d\theta_0 \\ &= \int_{\mathbb{R}^d} \frac{1}{[2\pi(1 - e^{-t})]^{d/2}} \exp\left(-\frac{1}{2(1 - e^{-t})} \|\theta_t - e^{-\frac{1}{2}t}\theta_0\|^2\right) p_0(\theta_0) d\theta_0 \\ &= \frac{1}{[2\pi(1 - e^{-t})]^{d/2}} \mathbb{E}_{\theta_0 \sim p_0} \left[\exp\left(-\frac{1}{2(1 - e^{-t})} \|\theta_t - e^{-\frac{1}{2}t}\theta_0\|^2\right) \right]. \end{aligned}$$

Hence,

$$\begin{aligned} \nabla p_t(\theta_t) &= \frac{1}{[2\pi(1 - e^{-t})]^{d/2}} \mathbb{E}_{\theta_0 \sim p_0} \left[\nabla \left(\exp\left(-\frac{1}{2(1 - e^{-t})} \|\theta_t - e^{-\frac{1}{2}t}\theta_0\|^2\right) \right) \right] \\ &= \frac{1}{[2\pi(1 - e^{-t})]^{d/2}} \mathbb{E}_{\theta_0 \sim p_0} \left[\exp\left(-\frac{1}{2(1 - e^{-t})} \|\theta_t - e^{-\frac{1}{2}t}\theta_0\|^2\right) \cdot \frac{-(\theta_t - e^{-\frac{1}{2}t}\theta_0)}{1 - e^{-t}} \right], \\ \nabla^2 p_t(\theta_t) &= \frac{1}{[2\pi(1 - e^{-t})]^{d/2}} \mathbb{E}_{\theta_0 \sim p_0} \left[\exp\left(-\frac{1}{2(1 - e^{-t})} \|\theta_t - e^{-\frac{1}{2}t}\theta_0\|^2\right) \right. \\ &\quad \left. \cdot \left(\frac{(\theta_t - e^{-\frac{1}{2}t}\theta_0)(\theta_t - e^{-\frac{1}{2}t}\theta_0)^\top}{(1 - e^{-t})^2} - \frac{1}{1 - e^{-t}} I_d \right) \right]. \end{aligned}$$

We can approximate $p_t(\theta_t)$, $\nabla p_t(\theta_t)$ and $\nabla^2 p_t(\theta_t)$ or even higher order derivative tensor of $p_t(\theta_t)$ by Monte Carlo method, therefore, we can compute score function and its high order derivative by

$$\nabla \log p_t(\theta_t) = \frac{\nabla p_t(\theta_t)}{p_t(\theta_t)}, \quad \nabla^2 \log p_t(\theta_t) = \frac{\nabla^2 p_t(\theta_t)}{p_t(\theta_t)} - \frac{\nabla p_t(\theta_t) \nabla p_t(\theta_t)^\top}{p_t(\theta_t)^2}.$$

G Real Data Analysis

G.1 Implementation Details

We set the step size $h = 0.2$ and $N = 2/h$. We conducted experiments on an NVIDIA RTX 4060 GPU (16GB VRAM). The training process required 2 GPU hours over 100 epochs with a batch size of 32, using CUDA 12.4, PyTorch 2.4, and torchvision 0.20.0. Figure 3 shows the digits generated by five algorithms, using the same score functions. The execution times for the algorithms are as follows: EM method 2 hour 12 min 49 s, EI method 2 hour 12 min 50 s, REM method 2 hour 13 min 30 s, REI method 2 hour 13 min 47 s, SO method 2 hour 14 min 05 s.

G.2 Score matching function for second order acceleration

For the MNIST dataset, we have demonstrated in the proof of Proposition 15 that computing third-order derivatives is unnecessary. Unlike existing high-order methods for estimating second-order scores [28], which require the joint training of score functions and Hessian matrices and consequently incur substantial computational overhead, our second-order algorithm avoids explicit computation of the Jacobian matrix. Furthermore, by employing Hessian-vector products (HVPs), we efficiently capture higher-order information, enabling our second-order acceleration method to achieve improved performance with reduced iteration complexity and manageable computational cost. More specifically, in the experiments of the MNIST dataset, we construct a U-Net architecture incorporating time and label embeddings to train the score function, where the time embedding operates



Figure 3: Comparative visualization of generated MNIST digits under various discretization schemes.

on the temporal variable t of the score function, while the label embedding leverages MNIST's categorical digit labels. This conditional formulation expresses the score function as $\nabla \log p(t, x | \text{label})$, enabling per-class score estimation through discriminative embedding propagation.

Recall iteration rule of the SO algorithm, we have

$$\begin{aligned} \vartheta_{n+1}^{\text{SO}} = & \vartheta_n^{\text{SO}} + s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})^{-1} \left(e^{s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})h} - I_d \right) \left(\frac{1}{2} \vartheta_n^{\text{SO}} + s_*(T - nh, \vartheta_n^{\text{SO}}) \right) \\ & + s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})^{-2} \left(e^{s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})h} - s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})h - I_d \right) s_*^{(M)}(T - nh, \vartheta_n^{\text{SO}}) \\ & + \int_{nh}^{(n+1)h} e^{s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})[(n+1)h-t]} dW_t. \end{aligned}$$

Note that

$$\int_{nh}^{(n+1)h} e^{s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})[(n+1)h-t]} dW_t \sim \mathcal{N} \left(0, \frac{1}{2} s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})^{-1} \left(e^{2s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}})h} - I_d \right) \right).$$

Let $g_n(\cdot) := s_*(T - nh, \cdot)$ denote the score matching function at time $T - nh$. Although the approximation of the Hessian matrix $\nabla^2 \log p_{T-nh}(\cdot)$ will not explicitly appear in the algorithmic implementation, we formally designate it as $H_n(\cdot)$ for notational clarity. Consequently, the estimators of L_n and M_n are chosen to be

$$\begin{aligned} s_*^{(L)}(T - nh, \vartheta_n^{\text{SO}}) &:= \frac{1}{2} I_d + H_n(\vartheta_n^{\text{SO}}) \\ s_*^{(M)}(T - nh, \vartheta_n^{\text{SO}}) &:= -\frac{1}{2} g_n(\vartheta_n^{\text{SO}}) - H_n(\vartheta_n^{\text{SO}}) \left(\frac{1}{2} \vartheta_n^{\text{SO}} + g_n(\vartheta_n^{\text{SO}}) \right). \end{aligned}$$

Employing the Taylor expansion, we have

$$\begin{aligned} (s_*^{(L)})^{-1} \left(e^{hs_*^{(L)}} - I_d \right) &= \sum_{k=1}^{\infty} \frac{h^k (s_*^{(L)})^{k-1}}{k!}, \\ (s_*^{(L)})^{-2} \left(e^{hs_*^{(L)}} - hs_*^{(L)} - I_d \right) &= \sum_{k=2}^{\infty} \frac{h^k (s_*^{(L)})^{k-2}}{k!}, \end{aligned}$$

$$\left[\frac{1}{2} (s_*^{(L)})^{-1} \left(e^{2hs_*^{(L)}} - I_d \right) \right]^{1/2} = \sqrt{h} \sum_{k=0}^{\infty} a_k (hs_*^{(L)})^k,$$

where $(a_0, a_1, a_2, a_3, a_4, a_5, a_6 \dots) = (1, \frac{1}{2}, \frac{5}{24}, \frac{1}{16}, \frac{79}{5760}, \frac{3}{1280}, \frac{71}{193536}, \dots)$. We thus reformulate all operators in the discretization scheme using matrix multiplications, which is a crucial step that avoids the explicit computation and storage of the full Hessian matrix H_t . This is achieved by leveraging Hessian-vector products (HVPs) via automatic differentiation, which reduces memory complexity to $\mathcal{O}(d)$ while retaining second-order curvature information. Specifically, given that g_n corresponds to the neural network's output and H_n represents its Jacobian matrix, we compute $H_n v$ for any vector v through PyTorch's reverse-mode differentiation (`torch.autograd.grad`). By iteratively applying this HVP procedure k times, we efficiently construct $H_n^k v$ for any $k \geq 0$. Through Taylor series expansion, these HVP-powered computations enable precise evaluation of each term in the discretization scheme.