

On the long-time integration of stochastic gradient systems

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Abstract

This article addresses the weak convergence of numerical methods for Brownian dynamics. Typical analyses of numerical methods for stochastic differential equations focus on properties such as the weak order which estimates the asymptotic (stepsize $h \rightarrow 0$) convergence behavior of the error of finite time averages. Recently it has been demonstrated, by study of Fokker-Planck operators, that a non-Markovian numerical method [Leimkuhler and Matthews, 2013] generates approximations in the long time limit with higher accuracy order (2nd order) than would be expected from its weak convergence analysis (finite-time averages are 1st order accurate). In this article we describe the transition from the transient to the steady-state regime of this numerical method by estimating the time-dependency of the coefficients in an asymptotic expansion for the weak error, demonstrating that the convergence to 2nd order is exponentially rapid in time. Moreover, we provide numerical tests of the theory, including comparisons of the efficiencies of the Euler-Maruyama method, the popular 2nd order Heun method, and the non-Markovian method.

1 Introduction

Stochastic gradient systems are stochastic differential equations in d dimensions having the form

$$dX = a(X)dt + \sigma dw, \quad X(0) = X_0, \quad (1.1)$$

where

$$a(x) := -\nabla V(x), \quad (1.2)$$

$V(x)$, $x \in \mathbf{R}^d$, is a potential energy function and $\sigma > 0$ is a constant which characterizes the strength of the additive noise, here described by a standard d -dimensional Wiener process $w(t)$. These systems originate in the work of Einstein [5, 6] to describe the motion of Brownian particles. They arise in mathematical models for chemistry, physics, biology and other areas, when the cumulative effect of unresolved degrees of freedom must be incorporated into a model to ensure its physical relevance. Under mild conditions on V , the system (1.1) is ergodic [8, 13] and has the unique invariant distribution $\rho_\beta \propto \exp(-\beta V)$, where $\beta = 2\sigma^{-2}$. Numerical methods for solving the equation (1.1) compute a discrete sequence of states X_1, X_2, \dots by iteratively approximating the short time evolution. The error in the numerical solution is typically quantified in either a *strong* sense (accuracy with respect to a particular stochastic path associated to (1.1)) or by reference to an evolving distribution (*weak* error, or error in averages); the latter is the focus of this article. Ideally, the discrete states are ultimately distributed in a way that is consistent with the invariant distribution, but for complex applications the introduction of error in the numerical process is inevitable. In this article we examine the asymptotic ($t \rightarrow \infty$) behavior of the weak error.

Undoubtedly, the most common numerical method for solving (1.1) is the Euler-Maruyama method which approximates $X(t_k)$, $t_k = hk$, by the iteration

$$X_{k+1} = X_k + ha(X_k) + \sigma\sqrt{h}\xi_{k+1}, \quad (1.3)$$

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where $\xi_k = (\xi_k^1, \dots, \xi_k^d)^\top$ and $\xi_k^i, i = 1, \dots, d, k = 1, \dots$, are i.i.d. random variables with the law $\mathcal{N}(0, 1)$. For analysis of the weak error, one considers a finite time interval $[0, \tau]$, with $\tau = hN$. The probability measure associated to (1.1) is described by a probability density $\rho(t, x)$ that evolves according to the Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = \mathcal{L}^\dagger \rho,$$

where \mathcal{L}^\dagger is the adjoint (in the L_2 sense) of the generator for (1.1), defined by

$$\mathcal{L} := \sum_{i=1}^d a^i(x) \frac{\partial}{\partial x^i} + \frac{\sigma^2}{2} \sum_{i=1}^d \frac{\partial^2}{(\partial x^i)^2}. \quad (1.4)$$

The solution $\rho(t, x)$ evolves from an initial probability distribution $\rho(0, x)$ to the steady state $\rho(\infty, x) = \rho_\beta$. Let φ be a test function (such as an element of the Schwartz space of C^∞ functions rapidly decaying at infinity). Then the average of φ at time τ may be taken to be

$$\bar{\varphi}(\tau) = \mathbf{E}_{\rho(\tau, \cdot)} \varphi \equiv \int_{\mathbb{R}^d} \varphi(x) \rho(\tau, x) dx. \quad (1.5)$$

The discretization scheme (1.3) may also be viewed as giving rise to an evolving probability distribution, and thus one may think of the iterates in (1.3), X_1, X_2, \dots , as being characterized by densities ρ_1, ρ_2, \dots . If stepsize h is used, then the average at time $\tau = Nh$ is given by

$$\hat{\varphi}(\tau, h) = \mathbf{E}_{\rho_N(\cdot)} \varphi \equiv \int_{\mathbb{R}^d} \varphi(x) \rho_N(x) dx. \quad (1.6)$$

It is natural to compare (1.5) and (1.6) as a means of quantifying the error as a function of h . We refer to this as the *weak error*. For the Euler-Maruyama method it is known (see, e.g. [7, 9, 15]) that

$$|\bar{\varphi}(\tau) - \hat{\varphi}(\tau, h)| = \mathcal{O}(h).$$

The Landau notation means that the given quantity is bounded for $h \rightarrow 0$ by Ch where C is a constant that is independent of the stepsize. A better way to write this is

$$|\bar{\varphi}(\tau) - \hat{\varphi}(\tau, h)| \leq C(\tau)h,$$

since C depends inherently on the time interval. This formula can be seen as a consequence of an asymptotic expansion of the weak error, as proposed by Talay and Tubaro [18] (see also [7, 9, 15]). We note that C also depends on the distribution of the initial state of the system, i.e. $\rho(0, x)$, as well as the particular observable, but we suppress these aspects in our notation. The asymptotic ($\tau \rightarrow \infty$) behavior of C describes the performance of the numerical method for computing averages with respect to the invariant distribution. For the Euler-Maruyama method, one finds that C is bounded as $\tau \rightarrow \infty$, thus one obtains first order approximation of averages both at finite time and in the long time limit.

In order to calculate averages in systems with complicated potentials and/or a large number of variables, one often must perform numerical calculations with a very long time interval. It is then desirable to use as large a timestep as is reasonable in the interest of reducing the computational effort, which is typically quantified in terms of the number of force evaluations. Weak first-order methods like Euler-Maruyama can be inefficient in practice. Schemes such as the second order stochastic Heun method [9, 15] can have greater efficiency: the stochastic Heun method uses two evaluations of the force $-\nabla V$ at each timestep, thus, in comparison to Euler-Maruyama, it must introduce less than about half the error at a given stepsize to be deemed superior. The alternative method discussed in this paper has been proposed in [11]:

$$X_{k+1} = X_k + ha(X_k) + \sigma \frac{\sqrt{h}}{2} (\xi_k + \xi_{k+1}), \quad (1.7)$$

where $\xi_k = (\xi_k^1, \dots, \xi_k^d)^\top$ and $\xi_k^i, i = 1, \dots, d, k = 1, \dots$, are i.i.d. random variables with the law $\mathcal{N}(0, 1)$. This method is very similar in form to the Euler-Maruyama method (1.3), and is as easy to implement, but the sums of successive random increments are not statistically independent, so the method

is fundamentally non-Markovian in nature. The scheme was motivated in [11] by an analysis of Langevin dynamics algorithms. In [12], the same method, along with some alternatives, was further analyzed from the perspective of the invariant measure, providing a rigorous foundation for the statement that the error in long-time averaging computed using (1.7) is of order two, i.e.

$$\lim_{\tau \rightarrow \infty} |\bar{\varphi}(\tau) - \hat{\varphi}(\tau, h)| \leq Kh^2.$$

The remarkable feature of this estimate is that the second order accuracy is achieved with only a single evaluation of the force at each timestep. The result of [12] relies on study of the invariant distribution and a Baker-Campbell-Hausdorff expansion of the generator of the process. Such an operator-based approach does not clarify the progression from finite time averaging to infinite time averaging and, in particular, nothing is demonstrated in [11, 12] about the weak accuracy of the method. In this article, we address this issue directly, studying the way that the finite-time averages obtained using the numerical scheme (1.7) converge, as $\tau \rightarrow \infty$, to steady-states of the numerical method. To do this, we compute the Talay-Tubaro expansion at finite time and show that

$$|\bar{\varphi}(\tau) - \hat{\varphi}(\tau, h)| \leq C_0(\tau)h + C_1(\tau)h^2 + \dots,$$

Then we demonstrate that

$$\lim_{\tau \rightarrow \infty} C_0(\tau) = 0,$$

implying a *superconvergence* property in the long-time limit. Moreover, we show that this convergence is exponential in τ .

We note that there are several recent papers (see [1, 2, 20] and references therein), where the idea of modified differential equations is exploited in order to construct higher-order schemes for computing ergodic limits. This approach provides the possibility of modifying schemes which are of weak order one on finite time intervals to provide second order approximations in ergodic limits. However, such modified schemes require either to evaluate derivative of forces or to perform two force evaluations [1], i.e., their computational cost is at least as high as for the Heun scheme and substantially higher than for (1.7). Furthermore, although the theoretical approaches in our paper and in [1] share some similarities, the results of [1] are not applicable to the non-Markovian approximation (1.7) and they do not also include an analysis demonstrating that the leading term in the error of their modified schemes goes to zero exponentially fast.

2 Preliminaries

Let (Ω, P, \mathcal{F}) be a sufficiently rich probability space on which the \mathcal{F}_t -measurable Wiener process $w(t)$ from (1.1) is defined as well as the sequence of random variables ξ_1, ξ_2, \dots from the method (1.7). We suppose that all components of random variables ξ_k arising in (1.7) and the Wiener process w are independent. This assumption will allow us to use Ito integrals of the form $\int_{t_k}^t b(s, X_{t_k, X_k}(s)) dw(s)$, $t \geq t_k$, where $b(s, x)$ is a deterministic ‘good’ function (also note that in this paper we are considering the weak-sense convergence only). In what follows $\mathbf{E}(\cdot)$ denotes expectation with respect to the measure P .

We use the following notation for the solution of (1.1): $X(t) = X_{t_0, x}(t)$ when $X(t_0) = x$, $t \geq t_0$, and also we will write $X_x(t)$ when $t_0 = 0$. Recall (see, e.g. [8]) that the process $X(t)$ is exponentially ergodic if for any $x \in \mathbf{R}^d$ and any function φ with a polynomial growth there are $C(x) > 0$ and $\lambda > 0$ such that

$$|\mathbf{E}\varphi(X_x(t)) - \varphi^{erg}| \leq C(x)e^{-\lambda t}, \quad t \geq 0, \quad (2.1)$$

where

$$\lim_{t \rightarrow \infty} \mathbf{E}\varphi(X_x(t)) = \int \varphi(x)\rho(x) dx := \varphi^{erg}. \quad (2.2)$$

The solution $X(t)$ of (1.1) is exponentially ergodic with the Gibbs invariant density

$$\rho(x) \propto \exp\left(-\frac{2}{\sigma^2}V(x)\right)$$

under the condition (see e.g. [8, 13]): there exist $c_0 \in \mathbf{R}$ and $c_1 > 0$ such that

$$(x, a(x)) \leq c_0 - c_1|x|^2. \quad (2.3)$$

Under this condition, for all $p \geq 1$

$$\mathbf{E}|X_x(t)|^{2p} \leq K(1 + |x|^{2p}e^{-\lambda t}), \quad (2.4)$$

where $K > 0$ and $0 < \lambda \leq c_1$ depend on p (see e.g. [8, 13]).

Introduce the operator L

$$L := \frac{\partial}{\partial t} + \mathcal{L},$$

where \mathcal{L} is the generator for (1.1) defined in (1.4). We recall that the function

$$u(t, x) = \mathbf{E}\varphi(X_{t,x}(\tau)) \quad (2.5)$$

satisfies the Cauchy problem for the backward Kolmogorov equation

$$\begin{aligned} Lu &= 0, \\ u(\tau, x) &= \varphi(x), \end{aligned} \quad (2.6)$$

i.e., $\partial u / \partial t = -Lu$ so

$$u(t, x) = e^{(t-\tau)\mathcal{L}}\varphi(x).$$

The transition density $p(t, x, y)$ for (1.1) satisfies the Fokker-Planck (forward Kolmogorov) equation

$$\begin{aligned} \frac{\partial p}{\partial t}(t, x, y) &= \mathcal{L}^\dagger p(t, x, y), \quad t > 0, \\ p(0, x, y) &= \delta(y - x), \end{aligned} \quad (2.7)$$

where \mathcal{L}^\dagger is adjoint of \mathcal{L} , and the invariant density $\rho(x)$ satisfies the stationary Fokker-Planck equation

$$\mathcal{L}^\dagger \rho(x) = 0. \quad (2.8)$$

3 Main result

We start with a simple illustrative example.

Example 3.1. Let $a(x) = -\alpha x$ with $\alpha > 0$, then $X(t)$ from (1.1) is the Ornstein-Uhlenbeck process, which is Gaussian with $\mathbf{E}X_x(t) = xe^{-\alpha t}$ and $Cov(X_x(s), X_x(t)) = \frac{\sigma^2}{2\alpha}(e^{-\alpha(t-s)} - e^{-\alpha(t+s)})$ for $s \leq t$. It is not difficult to calculate that for the Euler scheme (1.3):

$$\begin{aligned} \mathbf{E}X_N &= x_0(1 - \alpha h)^N = x_0e^{-\alpha\tau}(1 + \mathcal{O}(h)), \\ Var(X_N) &= \frac{\sigma^2}{2\alpha} \frac{1 - (1 - \alpha h)^{2N}}{1 + \alpha h} = \frac{\sigma^2}{2\alpha}(1 - e^{-2\alpha\tau}) - \frac{\sigma^2}{2}h + e^{-2\alpha\tau}\mathcal{O}(h) + \mathcal{O}(h^2), \quad \alpha h < 1, \end{aligned}$$

where $|\mathcal{O}(h^p)| \leq Kh$ with $K > 0$ independent of τ , and for the scheme (1.7):

$$\begin{aligned} \mathbf{E}X_N &= x_0(1 - \alpha h)^N = x_0e^{-\alpha\tau}(1 + \mathcal{O}(h)), \\ Var(X_N) &= \frac{\sigma^2}{2\alpha} \left[1 - \frac{(1 - \alpha h)^{2N}}{1 - \alpha h} \right] = \frac{\sigma^2}{2\alpha}(1 - e^{-2\alpha\tau}) + e^{-2\alpha\tau}\mathcal{O}(h). \end{aligned}$$

We see that although both schemes have first order accuracy on finite time intervals, the ergodic limit of the scheme (1.7) is exact while the ergodic limit of the Euler scheme approximates the ergodic limit of the Ornstein-Uhlenbeck process with order one which is usually the case for weak schemes of order one [19, 17, 14].

In what follows we will assume the following.

Assumption 3.1 *The potential $V(x) \in C^7(\mathbf{R}^d)$, its first-order derivatives grow not faster than a linear function at infinity and higher derivatives are bounded. The relations (1.2) and (2.3) hold. The function $\varphi(x)$ in (2.6) lies in $C^6(\mathbf{R}^d)$ and it and its derivatives grow not faster than a polynomial function at infinity.*

The most restrictive condition in Assumption 3.1 is the requirement for $a(x) = -\nabla V$ to be globally Lipschitz:

$$|a(x)|^2 \leq K(1 + |x|^2), \quad (3.1)$$

where $K > 0$ is independent of $x \in \mathbf{R}^d$. (Refer to Remark 3.1, below, and the example presented in Subsection 5.2.)

Introduce the multi-index $\mathbf{i} = (i_1, \dots, i_d)$ and $|\mathbf{i}| = \sum_{j=1}^d i_j$. Under Assumption 3.1, we have the following. The solution $u(t, x)$ of (2.6) belongs to $C^{\infty, 8}(\mathbf{R}_+ \times \mathbf{R}^d)$, the space of functions of t and x which have continuous partial derivatives through order 8 in the spatial variables. Moreover, for some constant $K > 0$, $\varkappa \in \mathbf{N}$, and $\lambda_u > 0$ (see, e.g. [19])

$$|u(t, x) - \varphi^{erg}| \leq K(1 + |x|^\varkappa)e^{-\lambda_u(\tau-t)}, \quad t \geq 0, \quad (3.2)$$

and

$$\left| \frac{\partial^{j+|\mathbf{i}|}}{\partial^j t \partial^{i_1} x^1 \dots \partial^{i_d} x^d} u(t, x) \right| \leq K(1 + |x|^\varkappa)e^{-\lambda_u(\tau-t)}, \quad (3.3)$$

for all $1 \leq |\mathbf{i}| \leq 8$ and $0 \leq j \leq 2$.

The proof of the following lemma (which is an analogue of the moments bound (2.4) for the scheme (1.7)) is rather standard and is omitted here.

Lemma 3.1 *Assume that (2.3) and (3.1) hold. Let X_k be defined by the scheme (1.7). Then for all sufficiently small $h > 0$ for all $p \geq 1$ there is $\gamma \in (0, 2c_1)$ and $K > 0$ such that*

$$\mathbf{E}|X_k|^{2p} \leq K(1 + |x|^{2p}e^{-\gamma t_k}). \quad (3.4)$$

We prove the following convergence and error expansion theorem for the scheme (1.7).

Theorem 3.1 *Let Assumption 3.1 hold. Then the scheme (1.7) is first order weakly convergent and for all sufficiently small $h > 0$ its error has the form*

$$\mathbf{E}\varphi(X_x(\tau)) - \mathbf{E}\varphi(X_N) = C_0(\tau, x)h + C(\tau, x)h^2, \quad (3.5)$$

where

$$C_0(\tau, x) = \mathbf{E} \int_0^\tau B_0(t, X_x(t)) dt, \quad (3.6)$$

$$B_0(t, x) = \frac{1}{2} \left[\sum_{i,j=1}^d a^j(x) \frac{\partial}{\partial x^j} a^i(x) \frac{\partial}{\partial x^i} u(t, x) + \frac{\sigma^2}{2} \sum_{i,j=1}^d \frac{\partial}{\partial x^j} a^i(x) \frac{\partial^2}{\partial x^i \partial x^j} u(t, x) + \frac{\sigma^2}{2} \sum_{i,j=1}^d \frac{\partial^2}{(\partial x^j)^2} a^i(x) \frac{\partial}{\partial x^i} u(t, x) \right],$$

and

$$|C(\tau, x)| \leq K(1 + |x|^\varkappa e^{-\lambda\tau}),$$

for some $K > 0$, $\varkappa \in \mathbf{N}$ and $\lambda > 0$ independent of h and τ .

Proof. Note that we shall use the letters K , \varkappa and λ to denote various constants which are independent of h , t , τ , x . We will exploit ideas from [15, Chapter 2] and, in particular, from the proof of Theorem 2.2.5 on the Talay-Tubaro expansion. It is convenient to introduce the additional notation for X_k from (1.7): $\bar{X}_{t_{k-1}, X_{k-1}}(t_k) = X_k$, which explicitly expresses the dependence on X_{k-1} .

Since $X_0 = x$, we have $X_{t_1, X_0, X_0}(t_1)(\tau) = X_x(\tau)$, and, using independence of X_k and $w(t) - w(t_k)$, $t \geq t_k$ for all k , we can write $X_{t_k, X_k}(\tau) = X_{t_{k+1}, X_{t_k, X_k}(t_{k+1})}(\tau)$, $k = 0, \dots, N-1$. Then (cf. [15, p. 101]):

$$\begin{aligned} \mathbf{E}\varphi(X_x(\tau)) &= \mathbf{E}\varphi(X_{t_1, X_0, X_0}(t_1)(\tau)) - \mathbf{E}\varphi(X_{t_1, X_1}(\tau)) + \mathbf{E}\varphi(X_{t_1, X_1}(\tau)) \\ &= \mathbf{E}\varphi(X_{t_1, X_0, X_0}(t_1)(\tau)) - \mathbf{E}\varphi(X_{t_1, X_1}(\tau)) + \mathbf{E}\varphi(X_{t_2, X_{t_1, X_1}(t_2)}(\tau)) \\ &\quad - \mathbf{E}\varphi(X_{t_2, X_2}(\tau)) + \mathbf{E}\varphi(X_{t_2, X_2}(\tau)) \\ &= \dots = \sum_{k=0}^{N-2} \left(\mathbf{E}\varphi(X_{t_{k+1}, X_{t_k, X_k}(t_{k+1})}(\tau)) - \mathbf{E}\varphi(X_{t_{k+1}, X_{k+1}}(\tau)) \right) + \mathbf{E}\varphi(X_{t_{N-1}, X_{N-1}}(\tau)). \end{aligned}$$

Using the definition (2.5) of $u(t, x)$ and independence of X_k and $w(t) - w(t_k)$, $t \geq t_k$, we get

$$\begin{aligned} \mathbf{E}\varphi(X_{t_{k+1}, X_{t_k, X_k}(t_{k+1})}(\tau)) &= \mathbf{E}\mathbf{E}(\varphi(X_{t_{k+1}, X_{t_k, X_k}(t_{k+1})}(\tau)) | X_{t_k, X_k}(t_{k+1})) = \mathbf{E}u(t_{k+1}, X_{t_k, X_k}(t_{k+1})), \\ \mathbf{E}\varphi(X_{t_{k+1}, X_{k+1}}(\tau)) &= \mathbf{E}\mathbf{E}(\varphi(X_{t_{k+1}, X_{k+1}}(\tau)) | \bar{X}_{t_k, X_k}(t_{k+1})) = \mathbf{E}u(t_{k+1}, \bar{X}_{t_k, X_k}(t_{k+1})). \end{aligned}$$

Also, since $u(\tau, x) = \varphi(x)$, we have $\mathbf{E}\varphi(X_{t_{N-1}, X_{N-1}}(\tau)) = \mathbf{E}u(t_N, X_{t_{N-1}, X_{N-1}}(t_N))$ and $\mathbf{E}\varphi(X_N) = \mathbf{E}u(t_N, \bar{X}_{t_{N-1}, X_{N-1}}(t_N))$. Combining the above expressions, we arrive at the following identity for the global error of the method (1.7):

$$\begin{aligned} R &:= \mathbf{E}\varphi(X_x(\tau)) - \mathbf{E}\varphi(X_N) \\ &= \sum_{k=0}^{N-1} \mathbf{E}(u(t_{k+1}, X_{t_k, X_k}(t_{k+1})) - u(t_{k+1}, \bar{X}_{t_k, X_k}(t_{k+1}))). \end{aligned} \tag{3.7}$$

Expanding $u(t_{k+1}, \bar{X}_{t_k, X_k}(t_{k+1}))$ in powers of h around X_k by the usual Taylor formula, we obtain

$$\begin{aligned} \mathbf{E}u(t_{k+1}, \bar{X}_{t_k, X_k}(t_{k+1})) &= \mathbf{E}u(t_{k+1}, X_k) + \sum_{i=1}^d \mathbf{E} \left[\Delta X_k^i \frac{\partial}{\partial x^i} u(t_{k+1}, X_k) \right] \\ &\quad + \frac{1}{2} \sum_{i,j=1}^d \mathbf{E} \left[\Delta X_k^i \Delta X_k^j \frac{\partial^2}{\partial x^i \partial x^j} u(t_{k+1}, X_k) \right] \\ &\quad + \frac{1}{6} \sum_{i,j,l=1}^d \mathbf{E} \left[\Delta X_k^i \Delta X_k^j \Delta X_k^l \frac{\partial^3}{\partial x^i \partial x^j \partial x^l} u(t_{k+1}, X_k) \right] \\ &\quad + \frac{1}{24} \sum_{i,j,l,m=1}^d \mathbf{E} \left[\Delta X_k^i \Delta X_k^j \Delta X_k^l \Delta X_k^m \frac{\partial^4}{\partial x^i \partial x^j \partial x^l \partial x^m} u(t_{k+1}, X_k) \right] \\ &\quad + h^3 r_1(t_k, x), \end{aligned} \tag{3.8}$$

where

$$\Delta X_k = ha(X_k) + \sigma \frac{\sqrt{h}}{2} (\xi_k + \xi_{k+1})$$

and

$$|r_1(t_k, x)| \leq K(e^{-\lambda(\tau-t_k)} + |x|^{\varkappa} e^{-\lambda\tau}) \tag{3.9}$$

for some $K > 0$, $\varkappa \in \mathbf{N}$ and $\lambda > 0$ independent of h , x , t and τ . To derive the estimate (3.9), we used (3.3), the assumptions on $a(x)$ and its derivatives from Assumption 3.1, and (3.4).

Introduce the auxiliary process

$$X'_{k+1} = X_k + ha(X_k) + \sigma \frac{\sqrt{h}}{2} \xi_k.$$

Note that

$$X_k = X'_k + \sigma \frac{\sqrt{h}}{2} \xi_k.$$

Using the Taylor expansions around X'_k , we get for the second term in (3.8):

$$\begin{aligned} \sum_{i=1}^d \mathbf{E} \left[\Delta X_k^i \frac{\partial}{\partial x^i} u(t_{k+1}, X_k) \right] &= h \sum_{i=1}^d \mathbf{E} a^i(X_k) \frac{\partial}{\partial x^i} u(t_{k+1}, X_k) + \frac{\sigma^2}{4} h \sum_{i=1}^d \mathbf{E} \frac{\partial^2}{(\partial x^i)^2} u(t_{k+1}, X'_k) \\ &+ \frac{\sigma^4}{16} h^2 \sum_{i=1}^d \sum_{j=i+1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^2 (\partial x^j)^2} u(t_{k+1}, X'_k) + \frac{\sigma^4}{32} h^2 \sum_{i=1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^4} u(t_{k+1}, X'_k) + h^3 r_2(t_k, x); \end{aligned} \quad (3.10)$$

for the third term in (3.8):

$$\begin{aligned} \frac{1}{2} \sum_{i,j=1}^d \mathbf{E} \left[\Delta X_k^i \Delta X_k^j \frac{\partial^2}{\partial x^i \partial x^j} u(t_{k+1}, X_k) \right] &= \frac{1}{2} h^2 \sum_{i,j=1}^d \mathbf{E} \left[a^i(X_k) a^j(X_k) \frac{\partial^2}{\partial x^i \partial x^j} u(t_{k+1}, X_k) \right] \\ &+ \frac{\sigma^2}{4} h^2 \sum_{i,j=1}^d \mathbf{E} \left[\frac{\partial}{\partial x^j} a^i(X'_k) \frac{\partial^2}{\partial x^i \partial x^j} u(t_{k+1}, X'_k) \right] + \frac{\sigma^2}{4} h^2 \sum_{i,j=1}^d \mathbf{E} \left[a^i(X'_k) \frac{\partial^3}{\partial x^i (\partial x^j)^2} u(t_{k+1}, X'_k) \right] \\ &+ \frac{\sigma^2}{4} h \sum_{i,j=1}^d \mathbf{E} \frac{\partial^2}{(\partial x^i)^2} u(t_{k+1}, X'_k) + \frac{\sigma^4}{8} h^2 \sum_{i=1}^d \sum_{j=i+1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^2 (\partial x^j)^2} u(t_{k+1}, X'_k) \\ &+ \frac{\sigma^4}{16} h^2 \sum_{i=1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^4} u(t_{k+1}, X'_k) + r_3(t_k, x) h^3; \end{aligned} \quad (3.11)$$

for the fourth term in (3.8):

$$\begin{aligned} \frac{1}{6} \sum_{i,j,l=1}^d \mathbf{E} \left[\Delta X_k^i \Delta X_k^j \Delta X_k^l \frac{\partial^3}{\partial x^i \partial x^j \partial x^l} u(t_{k+1}, X_k) \right] &= \frac{\sigma^2}{4} h^2 \sum_{i,j=1}^d \mathbf{E} \left[a^i(X'_k) \frac{\partial^3}{\partial x^i (\partial x^j)^2} u(t_{k+1}, X'_k) \right] \\ &+ \frac{\sigma^4}{8} h^2 \sum_{i=1}^d \sum_{j=i+1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^2 (\partial x^j)^2} u(t_{k+1}, X'_k) + \frac{\sigma^4}{16} h^2 \sum_{i=1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^4} u(t_{k+1}, X'_k) + r_4(t_k, x) h^3; \end{aligned} \quad (3.12)$$

for the fifth term in (3.8):

$$\begin{aligned} \frac{1}{24} \sum_{i,j,l,m=1}^d \mathbf{E} \left[\Delta X_k^i \Delta X_k^j \Delta X_k^l \Delta X_k^m \frac{\partial^4}{\partial x^i \partial x^j \partial x^l \partial x^m} u(t_{k+1}, X_k) \right] \\ = \frac{\sigma^4}{16} h^2 \sum_{i=1}^d \sum_{j=i+1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^2 (\partial x^j)^2} u(t_{k+1}, X'_k) + \frac{\sigma^4}{32} h^2 \sum_{i=1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^4} u(t_{k+1}, X'_k) + r_5(t_k, x) h^3. \end{aligned} \quad (3.13)$$

The functions $r_i(t_k, x)$, $i = 2, \dots, 5$, satisfy estimates of the form (3.9), which are derived using the same facts as in the case of $r_1(t_k, x)$.

By Lemma 2.1.9 from [15, p. 99] and again using independence of X_k and $w(t) - w(t_k)$, $t \geq t_k$, we get

$$\mathbf{E} u(t_{k+1}, X_{t_k, X_k}(t_{k+1})) = \mathbf{E} u(t_{k+1}, X_k) + h \mathbf{E} \mathcal{L} u(t_{k+1}, X_k) + \frac{h^2}{2} \mathbf{E} \mathcal{L}^2 u(t_{k+1}, X_k) + r_6(t_k, x) h^3. \quad (3.14)$$

We have for the second term in (3.14):

$$\begin{aligned} h \mathbf{E} \mathcal{L} u(t_{k+1}, X_k) &= h \sum_{i=1}^d \mathbf{E} a^i(X_k) \frac{\partial}{\partial x^i} u(t_{k+1}, X_k) + \frac{\sigma^2}{2} h \sum_{i=1}^d \frac{\partial^2}{(\partial x^i)^2} u(t_{k+1}, X'_k) \\ &+ \frac{\sigma^4}{16} h^2 \sum_{i,j=1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^2 (\partial x^j)^2} u(t_{k+1}, X'_k) + r_7(t_k, x) h^3; \end{aligned} \quad (3.15)$$

for the third term in (3.14):

$$\begin{aligned}
\frac{h^2}{2} \mathbf{E} \mathcal{L}^2 u(t_{k+1}, X_k) &= \frac{h^2}{2} \sum_{i,j=1}^d \mathbf{E} a^i(X_k) a^j(X_k) \frac{\partial^2}{\partial x^i \partial x^j} u(t_{k+1}, X_k) \\
&+ \frac{h^2}{2} \sum_{i,j=1}^d \mathbf{E} a^j(X_k) \frac{\partial}{\partial x^j} a^i(X_k) \frac{\partial}{\partial x^i} u(t_{k+1}, X_k) + \frac{\sigma^2}{4} h^2 \sum_{i,j=1}^d \mathbf{E} a^i(X'_k) \frac{\partial^3}{\partial x^i (\partial x^j)^2} u(t_{k+1}, X'_k) \\
&+ \frac{\sigma^2}{4} h^2 \sum_{i,j=1}^d \mathbf{E} a^i(X'_k) \frac{\partial^3}{(\partial x^j)^2 \partial x^i} u(t_{k+1}, X'_k) + \frac{\sigma^2}{4} h^2 \sum_{i,j=1}^d \mathbf{E} \frac{\partial^2}{(\partial x^j)^2} a^i(X_k) \frac{\partial}{\partial x^i} u(t_{k+1}, X_k) \\
&+ \frac{\sigma^2}{2} h^2 \sum_{i,j=1}^d \mathbf{E} \frac{\partial}{\partial x^j} a^i(X'_k) \frac{\partial^2}{\partial x^i \partial x^j} u(t_{k+1}, X'_k) + \frac{\sigma^4}{8} h^2 \sum_{i,j=1}^d \mathbf{E} \frac{\partial^4}{(\partial x^i)^2 (\partial x^j)^2} u(t_{k+1}, X'_k) + r_8(t_k, x) h^3.
\end{aligned} \tag{3.16}$$

The functions $r_i(t_k, x)$, $i = 6, 7, 8$, satisfy estimates of the form (3.9), which are derived using the same facts as in the case of $r_1(t_k, x)$ except $r_6(t_k, x)$ where (2.4) was also used.

Let

$$r(t_k, x) = r_6(t_k, x) + r_7(t_k, x) + r_8(t_k, x) - r_5(t_k, x) - r_4(t_k, x) - r_3(t_k, x) - r_2(t_k, x) - r_1(t_k, x).$$

Substituting (3.8)-(3.16) in (3.7), we obtain

$$\begin{aligned}
R &= \frac{h^2}{2} \sum_{k=0}^{N-1} \left[\sum_{i,j=1}^d \mathbf{E} a^j(X_k) \frac{\partial}{\partial x^j} a^i(X_k) \frac{\partial}{\partial x^i} u(t_{k+1}, X_k) \right. \\
&\quad \left. + \frac{\sigma^2}{2} \sum_{i,j=1}^d \mathbf{E} \frac{\partial}{\partial x^j} a^i(X'_k) \frac{\partial^2}{\partial x^i \partial x^j} u(t_{k+1}, X'_k) + \frac{\sigma^2}{2} \sum_{i,j=1}^d \mathbf{E} \frac{\partial^2}{(\partial x^j)^2} a^i(X_k) \frac{\partial}{\partial x^i} u(t_{k+1}, X_k) \right] \\
&\quad + \sum_{k=0}^{N-1} \mathbf{E} r(t_k, X_k) h^3 \\
&= h^2 \mathbf{E} \sum_{k=0}^{N-1} \frac{1}{2} \left[\sum_{i,j=1}^d a^j(X_k) \frac{\partial}{\partial x^j} a^i(X_k) \frac{\partial}{\partial x^i} u(t_k, X_k) + \frac{\sigma^2}{2} \sum_{i,j=1}^d \frac{\partial}{\partial x^j} a^i(X_k) \frac{\partial^2}{\partial x^i \partial x^j} u(t_k, X_k) \right. \\
&\quad \left. + \frac{\sigma^2}{2} \sum_{i,j=1}^d \frac{\partial^2}{(\partial x^j)^2} a^i(X_k) \frac{\partial}{\partial x^i} u(t_k, X_k) \right] + \sum_{k=0}^{N-1} \mathbf{E} r(t_k, X_k) h^3 \\
&:= h^2 \mathbf{E} \sum_{k=0}^{N-1} B_0(t_k, X_k) + \sum_{k=0}^{N-1} \mathbf{E} r(t_k, X_k) h^3,
\end{aligned} \tag{3.17}$$

where (cf. (3.9))

$$|r(t_k, x)| \leq K(e^{-\lambda(\tau-t_k)} + |x|^\varkappa e^{-\lambda\tau}). \tag{3.18}$$

Due to the properties of $u(t, x)$ (see ((3.3)-(3.3)) and of $a(x)$ (see Assumption 3.1), we have

$$|B_0(t, x)| \leq K(1 + |x|^\varkappa) e^{-\lambda u(\tau-t)} \tag{3.19}$$

for some $K > 0$ and $\varkappa \in \mathbf{N}$ independent of h, x, t and τ . Using (3.19) and (3.4), we obtain from (3.17):

$$|R| \leq Kh(1 + |x|^\varkappa e^{-\lambda\tau}), \tag{3.20}$$

for some constants $K > 0$, $\varkappa \in \mathbf{N}$ and $\lambda > 0$ independent of h, x , and τ , i.e., the scheme (1.7) is of first weak order.

It remains to prove the expansion (3.5). Consider now the $(d + 1)$ -dimensional system

$$\begin{aligned} dX &= a(X)dt + \sigma dw(t), \quad X(0) = X_0, \\ dY &= B_0(t, X)dt, \quad Y(t_0) = 0. \end{aligned} \quad (3.21)$$

Solving (3.21) by the scheme (1.7), we get

$$\mathbf{E} \sum_{k=0}^{N-1} B_0(t_k, X_k)h = \mathbf{E}\bar{Y}(\tau) = \mathbf{E}Y(\tau) + r_B(\tau, x)h = C_0(\tau, x) + r_B(\tau, x)h, \quad (3.22)$$

where $C_0(\tau, x)$ is equal to

$$C_0(\tau, x) = \mathbf{E}Y(\tau) = \mathbf{E} \int_0^\tau B_0(s, X_x(s))ds \quad (3.23)$$

and

$$r_B(\tau, x)h = \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} [\mathbf{E}B_0(s, X_x(s)) - \mathbf{E}B_0(t_k, X_k)] ds. \quad (3.24)$$

Introduce

$$\tilde{B}_0(t, x) = B_0(t, x)e^{\lambda_u(\tau-t)}, \quad (3.25)$$

for which we have (cf. (3.19)):

$$|\tilde{B}_0(t, x)| \leq K(1 + |x|^\varkappa),$$

where $K > 0$ does not depend on x , t , and τ . Using the demonstrated first-order convergence of (1.7) (cf. (3.20)), it is not difficult to obtain that

$$\begin{aligned} |r_B(\tau, x)|h &\leq e^{-\lambda_u(\tau-t)} \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \left| \mathbf{E}\tilde{B}_0(s, X_x(s)) - \mathbf{E}\tilde{B}_0(t_k, X_k) \right| ds \\ &\leq e^{-\lambda_u(\tau-t)} h \sum_{k=0}^{N-1} \left| \mathbf{E}\tilde{B}_0(t_k, X_x(t_k)) - \mathbf{E}\tilde{B}_0(t_k, X_k) \right| + hK(1 + |x|^\varkappa e^{-\lambda\tau}) \\ &\leq hK(1 + |x|^\varkappa e^{-\lambda\tau}). \end{aligned} \quad (3.26)$$

The equality (3.17) together with (3.18) and (3.22)-(3.26) implies (3.5)-(3.6). \square

Now we prove that in the limit of $\tau \rightarrow \infty$ the scheme (1.7) has second order of accuracy in h .

Theorem 3.2 *Let Assumption 3.1 hold. Then the coefficient $C_0(\tau, x)$ from (3.6) goes to zero as $\tau \rightarrow \infty$:*

$$|C_0(\tau, x)| \leq K(1 + |x|^\varkappa)e^{-\lambda\tau} \quad (3.27)$$

for some constants $K > 0$, $\varkappa \in \mathbf{N}$ and $\lambda > 0$, i.e., over a long integration time the scheme (1.7) is of order two up to exponentially small correction.

Proof. We have

$$\begin{aligned} C_0(\tau, x) &= \int_0^\tau \mathbf{E}B_0(t, X_x(t))dt = \int_0^\tau \int_{\mathbf{R}^d} B_0(t, y)p(t, x, y)dydt \\ &= \int_0^\tau \int_{\mathbf{R}^d} B_0(t, y)\rho(y)dydt + \int_0^\tau \int_{\mathbf{R}^d} B_0(t, y)[p(t, x, y) - \rho(y)]dydt, \end{aligned} \quad (3.28)$$

where $p(t, x, y)$ is the transition density for (1.1) (see (2.7)) and $\rho(y)$ is the invariant density. Using integration by parts and (1.2), it is not difficult to verify that for any $0 \leq t \leq \tau$:

$$\int_{\mathbf{R}^d} B_0(t, y) \exp\left(-\frac{2}{\sigma^2}V(y)\right) dy = 0. \quad (3.29)$$

Further, using geometric ergodicity of $X(t)$ (cf. (2.1)), we have for $\tilde{B}_0(s, x)$ from (3.25)

$$|\mathbf{E}\tilde{B}_0(s, X_x(t)) - \int_{\mathbf{R}^d} \tilde{B}_0(s, y)\rho(y)dy| \leq K(1 + |x|^\varkappa)e^{-\lambda_B t}, \quad 0 \leq s \leq \tau, \quad t > 0, \quad (3.30)$$

for some constants $K > 0$, $\varkappa \in \mathbf{N}$ and $\lambda_B > 0$ independent of x, t , and τ .

Using (3.30), we obtain for some $\lambda > 0$ and all sufficiently large $\tau > 0$:

$$\begin{aligned} \left| \int_0^\tau \int_{\mathbf{R}^d} B_0(t, y)[p(t, x, y) - \rho(y)]dydt \right| &= \left| \int_0^\tau e^{-\lambda(\tau-t)} \int_{\mathbf{R}^d} \tilde{B}_0(t, y)[p(t, x, y) - \rho(y)]dydt \right| \\ &\leq K(1 + |x|^\beta)e^{-\lambda\tau}, \end{aligned}$$

which implies (3.27). \square

Remark 3.1 We note that the global Lipschitz condition in Assumption 3.1 is not restrictive as the concept of rejecting exploding trajectories from [16, 17] can be used in implementing (1.7) when the coefficients of (1.1) are not globally Lipschitz.

4 Discussion

1. We emphasize that the fact that the average of $B_0(t, x)$ with respect to the invariant measure is equal to zero (see (3.29)) is the reason why the scheme (1.7) is second order accurate in approximating ergodic limits (see Theorem 3.2).
2. In the case of the Euler scheme (1.3) we get the same error expansion as (3.5) for the scheme (1.7) but with a different $B_0(t, x) = B_0^E(t, x)$ (see [15, Section 2.2.3]):

$$\begin{aligned} B_0^E(t, x) &= \frac{1}{2} \left[\sum_{i,j=1}^d a^j \frac{\partial u}{\partial x^j} a^i \frac{\partial u}{\partial x^i} + \frac{\sigma^2}{2} \sum_{i,j} \frac{\partial^2 a^j}{(\partial x^i)^2} \frac{\partial u}{\partial x^j} + \frac{\sigma^2}{2} \sum_{i,j=1}^d a^i \frac{\partial^3 u}{\partial x^i (\partial x^j)^2} \right. \\ &\quad \left. + \sigma^2 \sum_{i,j=1}^d \frac{\partial a^j}{\partial x^i} \frac{\partial^2 u}{\partial x^j \partial x^i} + \frac{\sigma^4}{6} \sum_{i,j=1}^d \frac{\partial^4 u}{(\partial x^i)^2 (\partial x^j)^2} \right]. \end{aligned}$$

The average of $B_0^E(t, x)$ with respect to the invariant measure is not equal to zero and, consequently, the Euler scheme (1.3) approximates ergodic limits with order one – the same order as its weak convergence over a finite time interval (see also Example 3.1).

3. Let a one-step weak approximation $\bar{X}_{t,x}(t+h)$ of the solution $X_{t,x}(t+h)$ of (1.1) generate a method of order p . Then, according to the Talay-Tubaro expansion [18] (see also [15, Section 2.2.3]), the global error of the method has the form

$$R := \mathbf{E}\varphi(X_x(\tau)) - \mathbf{E}\varphi(\bar{X}_x(\tau)) = C_0(\tau, x)h^p + \dots + C_n(\tau, x)h^{p+n} + O(h^{p+n+1}), \quad (4.1)$$

where $n \in \mathbf{N}$ (n can be arbitrarily large if the potential $V(x)$ belongs to $\mathbf{C}^\infty(\mathbf{R}^d)$, its first-order derivatives grow not faster than a linear function at infinity and its higher derivatives of any order are bounded) and the functions $C_0(\tau, x), \dots, C_n(\tau, x)$ are independent of h . It follows from the proof of Theorem 2.2.5 in [15] that the coefficients C_i in (4.1) can be presented in the form

$$C_i(\tau, x) = \int_0^\tau \mathbf{E}B_i(s, X_x(s))ds.$$

The function $B_0(s, x)$ is the coefficient at the leading term in the one-step error expansion of the method analogous to $B(s, x)$ in Theorem 3.1. The other $B_i(s, x)$, $i \geq 1$, consists of the coefficient at h^{p+i+1} from the one-step error expansion of the method (analogously to as $B_0(s, x)$ does at h^{p+1}) and of the coefficients at h^{p+i+1} from one-step error expansions for approximations of C_j with $j < i$ (see details in [15, Section 2.2.3]). Furthermore, one can deduce from the proof of Theorem 3.2 that if the averages of $B_i(s, x)$ $0 \leq i \leq q \leq n$, with respect to the invariant measure are equal to zero then in the limit of

$\tau \rightarrow \infty$ the scheme has $p + q$ order of accuracy in h . Hence, such a detailed one-step error analysis is the basis for discovering long time integration properties of numerical schemes and can serve as a guide in the construction of highly efficient numerical methods for computing ergodic limits for diffusions.

We observe that higher order methods for sampling from the Gibbs distribution have recently been constructed based on the idea of modified differential equations e.g. in [1]) but they are Markovian in comparison with the scheme (1.7) considered here. To our knowledge (see also the recent paper [20]), a non-Markovian scheme with order higher than 2 in computing ergodic limits has not yet been proposed. We note in particular the remarkable simplicity of the scheme (1.7), which requires just a single evaluation of force per step but nevertheless has second order accuracy in the computation of ergodic limits.

5 Numerical experiments

We compare the sampled distributions for the Euler-Maruyama scheme (1.3) with the second-order (in the sense of approximating ergodic limits) scheme (1.7), with both methods equal in cost (measured in terms of evaluations of the force). We also compare the sampled distributions with Heun’s method, a second-order scheme requiring two evaluations of $a(x) = -\nabla V(x)$:

$$\begin{aligned}\hat{X}_{k+1} &= X_k + ha(X_k) + \sigma\sqrt{h}\xi_{k+1}, \\ X_{k+1} &= X_k + \frac{h}{2} \left[a(\hat{X}_{k+1}) + a(X_k) \right] + \sigma\sqrt{h}\xi_{k+1}.\end{aligned}\tag{5.1}$$

As the scheme (1.7) computes exact long-time averages for all quadratic potential energy functions V , it is necessary to consider anharmonic models in order to capture the representative behavior of the scheme.

5.1 Anharmonic scalar model

We consider solutions to (1.1) using the one-dimensional potential energy function

$$V(x) = \cos(x),$$

with periodic $x \in [0, 2\pi)$.

5.1.1 Error in infinite time

We sample the configurational distribution $\exp(-V(x))$ using trajectories generated using the Euler-Maruyama scheme (1.3), Heun’s method (5.1) and the method (1.7), where the trajectory runs over a fixed time interval of $[0, 2 \times 10^8]$.

We note that the weak-sense convergence results are proved in Section 3 under the assumption that test functions $\varphi(x)$ are sufficiently smooth and they and their derivatives grow not faster than polynomial functions at infinity (see Assumption 3.1). This is a usual assumption in stochastic numerics [7, 9, 15]. At the same time, this assumption is not sufficient to guarantee convergence in distribution of the scheme (1.7), which would require to consider $\varphi(x)$ being step functions. In [3] first-order weak-sense convergence of the Euler scheme and the corresponding Talay-Tubaro error expansion were proved in the case of $\varphi(x)$ being measurable bounded functions, which, in particular, implies convergence in distribution of the Euler scheme. Further, first-order convergence for density of the Euler scheme was proved in [4]. Ideas from [3, 4] can be exploited to extend the convergence results obtained in Section 3 for the scheme (1.7) to include the case of nonsmooth $\varphi(x)$. Here we show and compare convergence in distribution of the scheme (1.7) and the other two tested methods experimentally.

For each scheme, we divide $[0, 2\pi]$ into 100 equal histogram bins to approximate the sampled distribution, and compare the observed density of bin i (denoted $\hat{\rho}_i$) to the exact canonical density of bin i (denoted ρ_i) computed to high precision using a numerical solver. The error in the distribution is then reported as either the approximate L_2 difference in the sampled distributions, or as the relative entropy (or Kullback-Leibler divergence [10]) of the two distributions, defined by $I = \int \rho(x) \ln[\rho(x)/\hat{\rho}(x)]dx$. The

relative entropy gives a measure of the information lost between two probability distributions. The two error quantities are approximated as

$$\text{Relative entropy error: } \sum_i \rho_i \ln \left(\frac{\rho_i}{\hat{\rho}_i} \right), \quad L_2 \text{ error: } \sqrt{\sum_i (\hat{\rho}_i - \rho_i)^2}.$$

We compute the configurational distribution using each scheme at 16 different timesteps, where the smallest is $h = 0.2$ and subsequent timesteps are increased by 10%. The distributions are averaged over 32 independent realizations per timestep, and the overall errors are plotted in Figure 1.

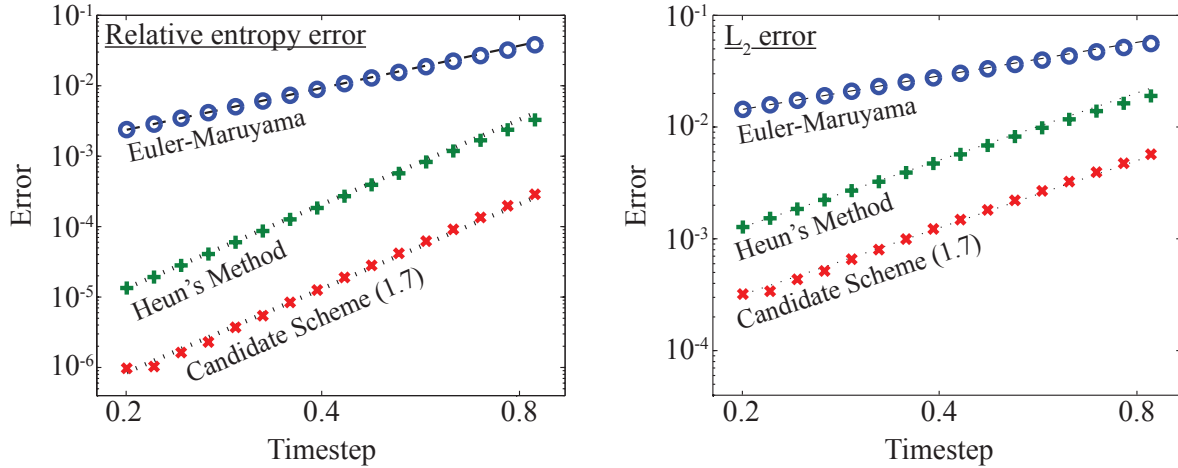


Figure 1: The error in computed distributions is plotted for each scheme at many stepsizes. We compare both the relative entropy (Kullback-Leibler divergence) and the L_2 error of the computed distributions of q . The plotted black guidelines give trends with respect to stepsize, with the dashed and dotted lines giving first and second order respectively in the right plot, and second and fourth order respectively in the left plot.

The results match the analysis given in Section 3 for the large-time regime. In the case of the L_2 error, the Euler-Maruyama scheme gives a first order error in the computed distribution, while the other schemes give second order errors. For the computation of relative entropy, we see a doubled rate of convergence (from first to second order, or from second to fourth order). Writing $\hat{\rho} = \rho(1 + \varepsilon\psi)$, where ε is a small parameter and $\int \psi \rho = 0$ (conservation of total probability), we have,

$$\int \rho \ln[1/(1 + \varepsilon\psi)] dx = - \int \rho \ln(1 + \varepsilon\psi) dx = - \int \rho(\varepsilon\psi - \varepsilon^2\psi^2 + \dots) dx = -\varepsilon^2 \int \psi^2 \rho dx + \dots$$

In the discrete context, if $\hat{\rho}_i = \rho_i + h^k \psi_i$ for an order k scheme, then we find that the relative entropy is proportional to h^{2k} . In practice, we observe that Heun's method and the method (1.7) give a fourth order relationship with the stepsize, whereas the Euler-Maruyama scheme has relative entropy proportional to ε^2 . The non-Markovian method gives approximately an order of magnitude improvement in this example.

5.1.2 Error in finite time

We consider the weak accuracy of the Euler-Maruyama scheme (1.3), Heun's method (5.1) and the method (1.7). In order to realize the evolving distribution computed for each scheme, we average over 2.56×10^9 independent trajectories with initial points drawn from a normal distribution with mean π and variance 1 (where the tails of the distribution outside the periodic region are cut off). We divide $[0, 2\pi]$ into 21 histogram bins, and run over $t \in [0, 9]$.

As the exact solution is unknown, we compute a baseline solution using Heun's method with $h = 0.04$ over the time interval. This solution is compared to the evolving distributions for $h = 0.16, 0.24, 0.32$

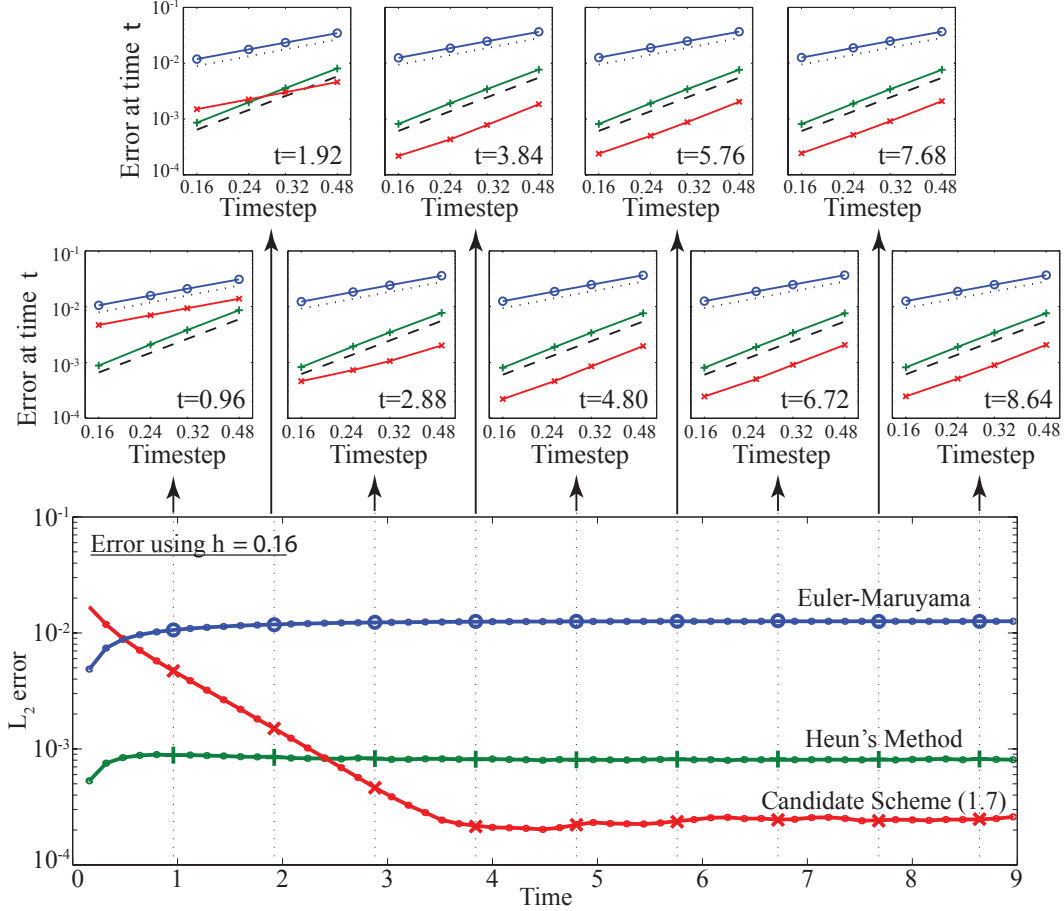


Figure 2: The lower plot shows the error in the distribution after time t , as computed using each scheme at $h = 0.16$. In the plots at the top, we compare the error growth with respect to stepsize h at multiples of $t = 0.96$. The Euler-Maruyama scheme (\circ), Heun's method ($+$) and the method (1.7) (\times) are compared to first order (dotted) and second order (dashed) guidelines.

and 0.48. The growth of the error at multiples of $t = 0.96$ is plotted at the top and bottom of Figure 2, along with guidelines to indicate the order of accuracy.

We plot the error after time t for each scheme, using $h = 0.16$, in the central plot of Figure 2. Initially the error in the scheme (1.7) reduces like $\exp(-\lambda t)$, but stabilizes after $t = 4$. This is due to the behavior described in Section 3, where only the first order component has an exponentially decreasing prefactor. The stabilization occurs when the h^2 part of the error begins to dominate the observed error.

5.2 Lennard-Jones box

As a more challenging problem, we compute the error in the radial distribution function for $r \in (0, 6)$ for a $6 \times 6 \times 6$ periodic box of 64 Lennard-Jones particles, with interaction potential

$$V(q) = \sum_{i=1}^{64} \sum_{j=i+1}^{64} r_{ij}^{-12} - r_{ij}^{-6}, \quad r_{ij} = \|q_i - q_j\|,$$

where q_i denotes the position of particle i , i.e., x in (1.1)-(1.2) is $3 \times 64 = 192$ -dimensional. We chose, arbitrarily, $\beta = 10$ and estimate the radial distribution function during simulation by dividing the interval $(0, 6)$ into 120 histogram bins of equal length, with the error computed as the L_2 difference between the exact and computed radial distributions.

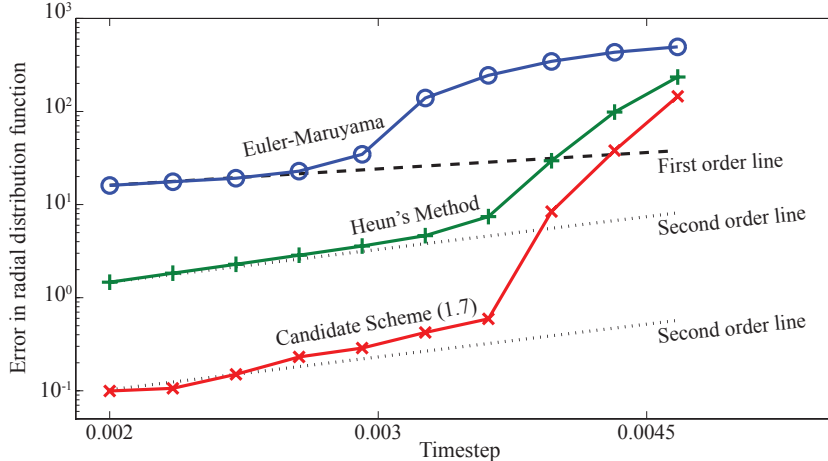


Figure 3: We plot the observed L_2 error in the computed radial distribution functions for a periodic box of 64 Lennard-Jones particles. The Euler-Maruyama (\circ) and the method (1.7) (\times) schemes require one force evaluation per step, while Heun’s method ($+$) requires two.

We observe that the Lipschitz condition (3.1) is not, formally, satisfied for many molecular dynamics potentials (including Lennard-Jones potentials) due to the presence of singularities. Nonetheless it is likely that, due to energetic considerations it would be possible to create a modified domain (a) in which typical solutions remain and (b) in which the Lipschitz condition (3.1) can be verified. The numerical example presented here strongly suggests that the global Lipschitz condition could be relaxed. More directly, the assumption (3.1) can be verified if the potential is replaced by one without singularities, e.g. by using instead Morse potentials, or by a smoothly truncated singular potential, or by a smooth Gaussian approximation of the singular potential [21].

Due to the size and complexity of the problem, we cannot use standard numerical solvers to compute the exact solution. Therefore we compute a baseline solution using the scheme (1.7) to compute 368 realizations of a 10^7 step trajectory (after a 10^6 step equilibration period), with a small stepsize of $h = 0.0016$.

We next compute the radial distribution functions computed using the three schemes in Section 5.1, at ten different timesteps beginning at $h = 0.002$ and with subsequent timesteps increasing by 10%. The trajectories were all taken over a constant time window of $[0, 20000]$, with sampling beginning after a 10^6 step equilibration.

We plot the error for all three schemes in Figure 3. For both the Euler-Maruyama scheme and Heun’s method we average over 32 realizations for each timestep that we consider. This was sufficient to resolve the error introduced by these discretization methods. However, the scheme (1.7) proved to be sufficiently accurate that further computation was required to discern the leading error term, with the error at each timestep computed using 256 realizations to reduce the sampling error.

The results show good agreement with the theory presented in Section 3. The method (1.7) demonstrates an order of magnitude improvement in the long-time error of averages compared to Heun’s method, while at the same time requiring half the cost (in terms of force evaluations).

6 Summary

In this article we have closed the gap in understanding between the typical weak error analysis of numerical discretization methods and the invariant measure accuracy of e.g. [11, 12, 1], demonstrating in particular that the non-Markovian numerical integration method (1.7) makes an exponentially rapid transition from first order weak accuracy to second order accuracy as $\tau \rightarrow \infty$. Our results are confirmed in several numerical experiments, with the ultimate conclusion being that the scheme (1.7) is typically superior to the Euler-Maruyama and Heun’s methods in terms of accuracy and efficiency for the purpose of averaging

in the long term (in the transient region, the other methods may of course be better, depending on the problem).

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