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# DYNAMICS AND VARIATIONAL INTEGRATORS OF STOCHASTIC HAMILTONIAN SYSTEMS

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**Abstract.** Stochastic action integral and Lagrange formalism of stochastic Hamiltonian systems are written through construing the stochastic Hamiltonian systems as nonconservative systems with white noise as the nonconservative 'force'. Stochastic Hamilton's principle and its discrete version are derived. Based on these, a systematic approach of producing symplectic numerical methods for stochastic Hamiltonian systems, i.e., the stochastic variational integrators are established. Numerical tests show validity of this approach.

**Key Words.** Hamilton's principle, stochastic Hamiltonian systems, symplectic methods, variational integrators.

## 1. Introduction

The Hamiltonian formalism of a deterministic mechanical system is

$$dp = -\frac{\partial H}{\partial q}dt, \quad p(0) = p_0, \tag{1}$$

$$dq = \frac{\partial H}{\partial p}dt, \quad q(0) = q_0, \tag{2}$$

where $H(p, q)$ is Hamiltonian function. A stochastic Hamiltonian system is a Hamiltonian system under certain random disturbances, represented as (Milstein et al., [18])

$$dp = -\frac{\partial H}{\partial q}dt - \sum_{k=1}^{m}\frac{\partial H_k}{\partial q}\circ dW_k(t), \quad p(0) = p_0, \tag{3}$$

$$dq = \frac{\partial H}{\partial p}dt + \sum_{k=1}^{m}\frac{\partial H_k}{\partial p}\circ dW_k(t), \quad q(0) = q_0, \tag{4}$$

where $W_k(t)$ $(k = 1, \cdots, m)$ are $m$ independent standard Wiener processes, called noises. The small circle '$\circ$' before $dW_k(t)$ denotes stochastic differential equations of Stratonovich sense.

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Both the deterministic and stochastic Hamiltonian systems have an intrinsic property-the symplecticity, i.e., the preservation of the symplectic structure (Hairer et al., [7], Milstein et al., [18], [19], Poincaré, [21])

$$dp(t) \wedge dq(t) = dp_0 \wedge dq_0, \quad \forall t \geq 0. \tag{5}$$

Geometrically, it means the preservation of area along phase flow of the system (Hairer, [7]).

In numerical simulation, property (5) of the theoretical solution $(p(t), q(t))$ is expected to be preserved by the numerical solution $(p_n, q_n)$, that is

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n, \quad \forall n \geq 1. \tag{6}$$

Such numerical methods are called symplectic methods. Since the qualitative behavior (5) is preserved, symplectic methods show significant superiority than non-symplectic methods, especially in long-time simulation. Pioneering work on deterministic symplectic methods goes back to de Vogelaere ([28] 1956), Ruth ([23] 1983) and Feng Kang et al. ([4] 1985, [5] 1986, [6] 1989). Since then, there has been an accelerating interest and effort on the study of such methods, which is now an important subject of computational mathematics and scientific computing. On the contrary, although there has been much effort on numerical methods for SDEs, e.g. [1], [2], [10], [11], [12], [13] etc., systematic research on stochastic symplectic methods, marked by the work of Milstein et al. ([18], [19], 2002), is still rare. In these works, they gave some symplectic Runge-Kutta type methods. Systematic construction of stochastic symplectic methods is still an open problem.

Variational integrators ([7], [14], [17], [25], [29]) have been an important approach of creating symplectic methods. They are tightly connected with the Hamilton's principle and its discrete version ([15], [16], [27]). For stochastic Hamiltonian systems, however, the main difficulty in constructing the variational integrators is the formulation of the stochastic Hamilton's principle.

In this article, we start from the point of view of construing the stochastic Hamiltonian systems as nonconservative systems, for which the white noise is a nonconservative 'force'. We then propose the formulation of the stochastic action integral, Euler-Lagrange equations of motion, as well as the stochastic Hamilton's principle. Based on these, the theory of stochastic variational integrators is constructed.

The second section derives the stochastic Hamilton's principle. Stochastic variational integrators are constructed in section 3. Section 4 are examples and numerical experiments.

## 2. Stochastic Hamilton's Principle

The Hamiltonian system (1)-(2) is a conservative mechanical system. Its Lagrangian formalism is ([7])

$$\frac{\partial L}{\partial q} = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}, \tag{7}$$

where $p = \frac{\partial L}{\partial \dot{q}}$, called the Legendre transform, and $L(q(t), \dot{q}(t))$ is the Lagrangian function.

**Theorem 2.1 (Deterministic Hamilton's Principle)** ([7]). *The $q(t)$ satisfying the Lagrange equation of motion (7) minimizes the action integral*

$$\mathcal{S}(q) = \int_{t_0}^{t_1} L(q(t), \dot{q}(t))dt \tag{8}$$

*among all curves $q(t)$ that connect $q(t_0) = q_0$ and $q(t_1) = q_1$ with $\delta q(t_0) = \delta q(t_1) = 0$.*

Proof of the theorem can be found in [7].

Now the question is, is there a stochastic version of the Hamilton's principe, and what is the formulation of the stochastic action integral and the stochastic Lagrange equation of motion? For answer of these questions, we consider nonconservative mechanical systems.

Suppose the nonconservative force is $\mathbf{F}$. Under the influence of $\mathbf{F}$, the action integral is generalized to the form ([20], [22])

$$\tilde{\mathcal{S}} = \int_{t_0}^{t_1} (L - A)dt, \tag{9}$$

where $A$ is the work done by the nonconservative force $\mathbf{F}$, and

$$A = -\mathbf{F} \cdot \mathbf{r} \tag{10}$$

with $\mathbf{r} = \mathbf{r}(q, t)$ being the position vector. Let $\delta$ be a variation. Since a nonconservative force is independent of position $q$, it holds ([20], [22])

$$\delta A = -\mathbf{F} \cdot \delta\mathbf{r} = -\mathbf{F} \cdot \frac{\partial \mathbf{r}}{\partial q}\delta q. \tag{11}$$

Thus, the variation of $\tilde{\mathcal{S}}$ is

$$\begin{aligned} \delta\tilde{\mathcal{S}} &= \int_{t_0}^{t_1} (\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta\dot{q} - \delta A)dt \\ &= [\frac{\partial L}{\partial \dot{q}}\delta q]_{t_0}^{t_1} + \int_{t_0}^{t_1} [-\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) + \frac{\partial L}{\partial q} + \mathbf{F}^T\frac{\partial \mathbf{r}}{\partial q}]\delta q dt. \end{aligned} \tag{12}$$

From $\delta q(t_0) = \delta q(t_1) = 0$, it follows that

$$\begin{aligned} \delta\tilde{\mathcal{S}} &= 0 \\ \Leftrightarrow \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) &= \frac{\partial L}{\partial q} + \mathbf{F}^T\frac{\partial \mathbf{r}}{\partial q}. \end{aligned} \tag{13}$$

The equation (13) is the Lagrange equation of motion of a nonconservative system.

In (13), the Lagrangian function $L$ is considered as a function with independent variables $q, \dot{q}$ and $t$. It is pointed out in [26] that the Lagrange equation of motion can also be represented with generalized independent variables $p, q, \dot{p}, \dot{q}$ and $t$, where the position vector $\mathbf{r} = \mathbf{r}(p, q, t)$. This is called the redundancy of the Lagrange equation of motion. In this case, the Lagrange equations of motion are

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) = \frac{\partial L}{\partial q} + \mathbf{F}^T\frac{\partial \mathbf{r}}{\partial q}, \tag{14}$$

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{p}}) = \frac{\partial L}{\partial p} + \mathbf{F}^T\frac{\partial \mathbf{r}}{\partial p}, \tag{15}$$

which can contain linearly dependent equations due to the redundancy of the variable set $\{p, q, \dot{p}, \dot{q}, t\}$.

Based on (14)-(15) and a variational principle, it is derived in [26] that the generalized Hamiltonian equations of motion of a nonconservative system under the nonconservative force $\mathbf{F}$ are

$$\dot{p} = -\frac{\partial H}{\partial q}^T + \frac{\partial \mathbf{r}}{\partial q}^T \mathbf{F}, \tag{16}$$

$$\dot{q} = \frac{\partial H}{\partial p}^T - \frac{\partial \mathbf{r}}{\partial p}^T \mathbf{F}. \tag{17}$$

Formally, $dW(t)$ in a stochastic differential equation can be regarded as equal to $\dot{W}(t)dt$, although $W(t)$ is nowhere differentiable, and $\dot{W}(t) = \xi(t)$ is the white noise ([3],[10]). Under this consideration, a stochastic Hamiltonian system with one noise ($m = 1$ in (3)-(4)) can also be written as

$$\dot{p} = -\frac{\partial H}{\partial q}^T - \frac{\partial H_1}{\partial q}^T \circ \dot{W}, \tag{18}$$

$$\dot{q} = \frac{\partial H}{\partial p}^T + \frac{\partial H_1}{\partial p}^T \circ \dot{W}. \tag{19}$$

For the linear stochastic oscillator

$$\dot{p} = -q + \sigma \dot{W}(t), \quad p(0) = p_0, \tag{20}$$

$$\dot{q} = p, \quad q(0) = q_0, \tag{21}$$

where $\sigma > 0$ is a constant, let $H(p,q) = \frac{1}{2}(p^2 + q^2)$ and $H_1(p,q) = -\sigma q$, we have

$$\dot{p} = -\frac{\partial H}{\partial q} - \frac{\partial H_1}{\partial q} \circ \dot{W}(t), \quad p(0) = p_0, \tag{22}$$

$$\dot{q} = \frac{\partial H}{\partial p} + \frac{\partial H_1}{\partial p} \circ \dot{W}(t), \quad q(0) = q_0. \tag{23}$$

Thus the linear stochastic oscillator (20)-(21) is a stochastic Hamiltonian system ([8], [9]). It is studied in [24] that, with initial conditions $p_0 = 0$, $q_0 = 1$, the second moment of the solution of (20)-(21) satisfies

$$\mathbf{E}(p(t)^2 + q(t)^2) = 1 + \sigma^2 t, \tag{24}$$

i.e., the Hamiltonian function $H(p,q)$ grows linearly with respect to time $t$. This is different from the deterministic Hamiltonian systems, for which the Hamiltonian function is preserved for all $t$, if $t$ is not explicitly contained in $H$. This indicates that the stochastic Hamiltonian systems are Hamiltonian systems in certain generalized sense, or to say, that they are disturbed by certain nonconservative force. This force, different from usual nonconservative forces which dissipate energy of the system, may also 'add' energy to the system, as shown by the linear stochastic oscillator. We call it the random force. A natural association with the random force is the white noise $\xi(t)$, since it is the source of the disturbance, and independent of the position $q$.

On the other hand, compare (18)-(19) with (16)-(17), we find that, formally, the associations between $\dot{W}$ and $\mathbf{F}$, as well as $-H_1$ and $\mathbf{r}$ are reasonable. Under this consideration, stochastic Hamiltonian systems are a special kind of nonconservative systems, whereby $\dot{W}(t)$ functions as a nonconservative force.

According to (10), formally, the 'work' done by $\dot{W}(t)$ is

$$\bar{A} = H_1 \circ \dot{W}(t). \tag{25}$$

Consider (9), the action integral of the stochastic Hamiltonian system (18)-(19) should be

$$\begin{aligned} \bar{\mathcal{S}} &= \int_{t_0}^{t_1} (L - \bar{A})dt \\ &= \int_{t_0}^{t_1} Ldt - \int_{t_0}^{t_1} H_1 \circ dW(t), \end{aligned} \tag{26}$$

where $L$ is the Lagrangian function with respect to the deterministic (drift) part of the stochastic system, and is connected with the deterministic Hamiltonian function $H$ through the equation

$$L = p^T \dot{q} - H. \tag{27}$$

The last equation of (26) applies the relation $\dot{W}(t)dt = dW(t)$ once more.

For a stochastic Hamiltonian system with $m$ noises (3)-(4), (25) should be modified to

$$\bar{A} = \sum_{k=1}^{m} H_k \circ \dot{W}_k(t), \tag{28}$$

which is the sum of the 'work' done by each $\dot{W}_k(t)$. Consequently,

$$\begin{aligned} \bar{\mathcal{S}} &= \int_{t_0}^{t_1} (L - \bar{A})dt \\ &= \int_{t_0}^{t_1} Ldt - \sum_{k=1}^{m} \int_{t_0}^{t_1} H_k \circ dW_k(t). \end{aligned} \tag{29}$$

We call it the stochastic action integral. It follows from (14)-(15) that the Lagrange equations of motion of the stochastic Hamiltonian system (18)-(19) are

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) = \frac{\partial L}{\partial q} - \frac{\partial H_1}{\partial q} \circ \dot{W}(t), \tag{30}$$

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{p}}) = \frac{\partial L}{\partial p} - \frac{\partial H_1}{\partial p} \circ \dot{W}(t). \tag{31}$$

We call them the stochastic Lagrange equations of motion. When the number of noises is $m$, they have the form

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) = \frac{\partial L}{\partial q} - \sum_{k=1}^{m} \frac{\partial H_k}{\partial q} \circ \dot{W}_k(t), \tag{32}$$

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{p}}) = \frac{\partial L}{\partial p} - \sum_{k=1}^{m} \frac{\partial H_k}{\partial p} \circ \dot{W}_k(t). \tag{33}$$

**Lemma 2.2.** *If*

$$\int_a^b \sum_{i=1}^{n} F_i(t) g_i(t) dt = 0$$

*for any functions $g_i(t)$ $(1 \leq i \leq n)$, then $F_i(t) = 0$ almost everywhere for $t \in [a, b]$* and $1 \leq i \leq n$.

*Proof.* We make induction on $n$. If $n = 1$, $\int_a^b F_1(t)g_1(t)dt = 0$. Since $g_1(t)$ can be any function, take $g_1(t) = F_1(t)$. Thus

$$\int_a^b F_1(t)^2 dt = 0.$$

$F_1(t)^2 \geq 0$ implies that $F_1(t) = 0$ almost everywhere for $t \in [a, b]$.

Suppose $F_i(t) = 0$ almost everywhere for $t \in [a, b]$ and $1 \leq i \leq k$. When $i = k+1$,

$$\int_a^b \sum_{i=1}^{k+1} F_i(t)g_i(t)dt = \int_a^b (\sum_{i=1}^{k} F_i(t)g_i(t) + F_{k+1}(t)g_{k+1}(t))dt = 0.$$

Take $g_i(t) = F_i(t)$, $(i = 1, \cdots, k+1)$, we have

$$\int_a^b (\sum_{i=1}^{k} F_i^2 + F_{k+1}^2)dt = 0.$$

By the induction hypothesis, it holds

$$\int_a^b F_{k+1}^2(t)dt = 0 \quad \text{almost everywhere for } t \in [a, b],$$

which implies that $F_{k+1}(t) = 0$ almost everywhere for $t \in [a, b]$. □

**Theorem 2.3 (Stochastic Hamilton's Principle).** *The stochastic Lagrange equations of motion (32)-(33) minimize the stochastic action integral (29).*

*Proof.* The variation of $\bar{\mathcal{S}}$ in (29) is

$$\begin{aligned}
\delta\bar{\mathcal{S}} &= \int_{t_0}^{t_1} (\frac{\partial L}{\partial p}\delta p + \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{p}}\delta \dot{p} + \frac{\partial L}{\partial \dot{q}}\delta \dot{q})dt \\
&- \sum_{k=1}^{m} \int_{t_0}^{t_1} (\frac{\partial H_k}{\partial p}\delta p + \frac{\partial H_k}{\partial q}\delta q) \circ \dot{W}_k(t)dt \\
&= [\frac{\partial L}{\partial \dot{p}}\delta p]_{t_0}^{t_1} + [\frac{\partial L}{\partial \dot{q}}\delta q]_{t_0}^{t_1} + \int_{t_0}^{t_1} (\frac{\partial L}{\partial p} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{p}}) - \sum_{k=1}^{m} \frac{\partial H_k}{\partial p} \circ \dot{W}_k(t))\delta p dt \\
&+ \int_{t_0}^{t_1} (\frac{\partial L}{\partial q} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) - \sum_{k=1}^{m} \frac{\partial H_k}{\partial q} \circ \dot{W}_k(t))\delta q dt. \qquad (34)
\end{aligned}$$

The calculations in (34) can be put forward successfully because the stochastic integrals involved are of Stratonovich sense, which enables the application of the classical differential chain rule. Since $\delta q(t_0) = \delta q(t_1) = \delta p(t_0) = \delta p(t_1) = 0$, it follows from Lemma 2.2 that $\delta\bar{\mathcal{S}} = 0$ is equivalent to

$$\begin{aligned}
\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) &= \frac{\partial L}{\partial q} - \sum_{k=1}^{m} \frac{\partial H_k}{\partial q} \circ \dot{W}_k(t), \\
\frac{d}{dt}(\frac{\partial L}{\partial \dot{p}}) &= \frac{\partial L}{\partial p} - \sum_{k=1}^{m} \frac{\partial H_k}{\partial p} \circ \dot{W}_k(t).
\end{aligned}$$

□

**Example 2.1.** This example is aimed to show that the stochastic Lagrangian and Hamiltonian formalism are equivalent.

The Kubo oscillator

$$dp = -aqdt - \sigma q \circ dW(t), \quad p(0) = p_0, \tag{35}$$

$$dq = apdt + \sigma p \circ dW(t), \quad q(0) = q_0 \tag{36}$$

is a stochastic Hamiltonian system with

$$H(p,q) = \frac{a}{2}(p^2+q^2), \quad H_1(p,q) = \frac{\sigma}{2}(p^2+q^2), \tag{37}$$

where $a$ and $\sigma$ are constants, and $p$, $q$ are of one dimension. According to (27), we have

$$L(p,q,\dot{p},\dot{q}) = p\dot{q} - H(p,q) = p\dot{q} - \frac{a}{2}(p^2+q^2). \tag{38}$$

Thus the Lagrange equations of motion of the Kubo oscillator should, according to (30)-(31), have the form

$$\dot{p} = -aq - \sigma q \circ \dot{W}(t), \tag{39}$$

$$0 = \dot{q} - ap - \sigma p \circ \dot{W}(t), \tag{40}$$

which are, with initial conditions $p(0) = p_0$, $q(0) = q_0$, equivalent to the Hamiltonian equations of motion (35)-(36).

## 3. Stochastic Variational Integrators

We first introduce the deterministic variational integrators ([7], [14], [17], [25], [29]). Regarding the action integral (8)

$$\mathcal{S}(q) = \int_{t_0}^{t_1} L(q(t), \dot{q}(t))dt$$

as a function of $(q_0, q_1)$, and finding partial derivatives of $\mathcal{S}$ with respect to $q_0$ and $q_1$, one gets

$$\begin{aligned}
\frac{\partial \mathcal{S}}{\partial q_0} &= \int_{t_0}^{t_1} (\frac{\partial L}{\partial q}\frac{\partial q}{\partial q_0} + \frac{\partial L}{\partial \dot{q}}\frac{\partial \dot{q}}{\partial q_0})dt \\
&= \frac{\partial L}{\partial \dot{q}}\frac{\partial q}{\partial q_0}|_{t_0}^{t_1} + \int_{t_0}^{t_1} (\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}})\frac{\partial q}{\partial q_0}dt \\
&= -\frac{\partial L}{\partial \dot{q}}(q_0, \dot{q}(t_0)) \\
&= -p_0^T,
\end{aligned} \tag{41}$$

where the last two equalities apply the Lagrange equation of motion (7) and the Legendre transform $p = \frac{\partial L}{\partial \dot{q}}^T$, respectively.

Similarly, it holds

$$\frac{\partial \mathcal{S}}{\partial q_1} = p_1^T. \tag{42}$$

Thus, one can write

$$d\mathcal{S} = \frac{\partial \mathcal{S}}{\partial q_0}dq_0 + \frac{\partial \mathcal{S}}{\partial q_1}dq_1 = -p_0^T dq_0 + p_1^T dq_1. \tag{43}$$

**Theorem 3.1** ([7]) *A mapping $g : (p,q) \mapsto (P,Q)$ is symplectic if and only if there exists locally a function $\mathcal{S}(p,q)$ such that*

$$P^T dQ - p^T dq = d\mathcal{S}.$$

According to (43) and Theorem 3.1, the mapping $(p_0, q_0) \mapsto (p_1, q_1)$ generated by $\mathcal{S}$ through the relations (41)-(42) is symplectic.

Think of the discrete Lagrangian ([7], [15], [16], [27]) as

$$L_h(q_n, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L(q(t), \dot{q}(t))dt, \tag{44}$$

where $q_n \doteq q(t_n)$, $q_{n+1} \doteq q(t_{n+1})$, and $h = t_{n+1} - t_n$. It approximates the local action integral on the small time interval $[t_n, t_{n+1}]$, and produces the symplectic mapping $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ through the relations ([7], [14], [15], [25], [27])

$$p_n = -\frac{\partial L_h}{\partial q_n}(q_n, q_{n+1}), \quad p_{n+1} = \frac{\partial L_h}{\partial q_{n+1}}(q_n, q_{n+1}). \tag{45}$$

The next problem is how to compute $L_h$. In fact, it can be approximated through applying different quadrature formulae, such as the trapezoidal or the midpoint rule ([14], [29]). The $\dot{q}(t)$ in the integrand of (44) can be approximated by $\frac{q_{n+1}-q_n}{t_{n+1}-t_n}$. Different quadrature formulae lead to different methods. For example, Gaussian quadrature gives the Gauss collocation method, and Lobatto quadrature gives the Lobatto IIIA-IIIB pair ([17]).

In stochastic case, we construct variational integrators based on the stochastic Hamilton's principle. Its discrete version includes finding $\{p_n, q_n\}_1^{N-1}$ that minimizing the sum

$$\bar{\mathcal{S}}_h(\{p_n, q_n\}_0^N) = \sum_{n=0}^{N-1} \bar{L}_h(p_n, q_n, p_{n+1}, q_{n+1}) \tag{46}$$

for given $(p_0, q_0)$ and $(p_N, q_N)$. Let $\frac{\partial \bar{\mathcal{S}}_h}{\partial q_n} = 0$ and $\frac{\partial \bar{\mathcal{S}}_h}{\partial p_n} = 0$, it follows the discrete stochastic Euler-Lagrange equations

$$\frac{\partial \bar{L}_h}{\partial q_n}(p_{n-1}, q_{n-1}, p_n, q_n) + \frac{\partial \bar{L}_h}{\partial q_n}(p_n, q_n, p_{n+1}, q_{n+1}) = 0, \tag{47}$$

$$\frac{\partial \bar{L}_h}{\partial p_n}(p_{n-1}, q_{n-1}, p_n, q_n) + \frac{\partial \bar{L}_h}{\partial p_n}(p_n, q_n, p_{n+1}, q_{n+1}) = 0 \tag{48}$$

for $n = 1, \cdots, N-1$. This gives a three-term recurrence formula for determining $q_1, \cdots, q_{N-1}$ and $p_1, \cdots, p_{N-1}$.

For a stochastic system with $m$ noises (3)-(4), think of the stochastic discrete Lagrangian $\bar{L}_h$ as

$$\bar{L}_h(p_n, q_n, p_{n+1}, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L dt - \sum_{k=1}^{m} \int_{t_n}^{t_{n+1}} H_k \circ dW_k(t). \tag{49}$$

When equality holds in (49), the solution $\{p_n, q_n\}_1^{N-1}$ of the discrete Euler-Lagrange equations (47)-(48) should equal $\{p(t_n), q(t_n)\}_1^{N-1}$, where $p(t)$ and $q(t)$ satisfy the continuous stochastic Lagrange equations (32)-(33). This is due to the stochastic Hamilton's principle stated in Theorem 2.3. Consequently, under the consideration in (49), solutions of (47)-(48) should approximately equal $\{p(t_n), q(t_n)\}_1^{N-1}$, and therefore become a numerical simulation of $p(t)$ and $q(t)$.

Denote

$$S_h = \int_{t_n}^{t_{n+1}} L dt - \sum_{k=1}^{m} \int_{t_n}^{t_{n+1}} H_k \circ dW_k(t), \tag{50}$$

where $S_h$ is considered as a function of $p(t_n), q(t_n), p(t_{n+1})$ and $q(t_{n+1})$. We find

$$\begin{aligned}
\frac{\partial S_h}{\partial q(t_n)} &= \int_{t_n}^{t_{n+1}} (\frac{\partial L}{\partial q}\frac{\partial q}{\partial q(t_n)} + \frac{\partial L}{\partial p}\frac{\partial p}{\partial q(t_n)} + \frac{\partial L}{\partial \dot{q}}\frac{\partial \dot{q}}{\partial q(t_n)} + \frac{\partial L}{\partial \dot{p}}\frac{\partial \dot{p}}{\partial q(t_n)})dt \\
&- \sum_{k=1}^{m} \int_{t_n}^{t_{n+1}} (\frac{\partial H_k}{\partial q}\frac{\partial q}{\partial q(t_n)} + \frac{\partial H_k}{\partial p}\frac{\partial p}{\partial q(t_n)}) \circ dW_k(t) \\
&= [\frac{\partial L}{\partial \dot{q}}\frac{\partial q}{\partial q(t_n)}]_{t_n}^{t_{n+1}} + \int_{t_n}^{t_{n+1}} (\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \sum_{k=1}^{m}\frac{\partial H_k}{\partial q}\dot{W}_k(t))\frac{\partial q}{\partial q(t_n)}dt \\
&+ [\frac{\partial L}{\partial \dot{p}}\frac{\partial p}{\partial q(t_n)}]_{t_n}^{t_{n+1}} + \int_{t_n}^{t_{n+1}} (\frac{\partial L}{\partial p} - \frac{d}{dt}\frac{\partial L}{\partial \dot{p}} - \sum_{k=1}^{m}\frac{\partial H_k}{\partial p}\dot{W}_k(t))\frac{\partial p}{\partial q(t_n)}dt \\
&= -p(t_n)^T, \qquad (51)
\end{aligned}$$

where the last equality is due to (32)-(33) and the Legendre transform $p = \frac{\partial L}{\partial \dot{q}}$. Similarly,

$$\frac{\partial S_h}{\partial p(t_n)}(p(t_n), q(t_n), p(t_{n+1}), q(t_{n+1})) = -\frac{\partial L}{\partial \dot{p}}(p(t_n), q(t_n), p(t_{n+1}), q(t_{n+1})). \tag{52}$$

Motivated by (51)-(52) and (49), as well as the deterministic discrete Legendre transform ([7] and references therein), we introduce the stochastic discrete Legendre transform

$$p_n = -\frac{\partial \bar{L}_h}{\partial q_n}(p_n, q_n, p_{n+1}, q_{n+1}), \tag{53}$$

$$\frac{\partial L}{\partial \dot{p}}|_{t_n} = -\frac{\partial \bar{L}_h}{\partial p_n}(p_n, q_n, p_{n+1}, q_{n+1}). \tag{54}$$

Thus

$$p_{n+1} = -\frac{\partial \bar{L}_h}{\partial q_{n+1}}(p_{n+1}, q_{n+1}, p_{n+2}, q_{n+2}), \tag{55}$$

$$\frac{\partial L}{\partial \dot{p}}|_{t_{n+1}} = -\frac{\partial \bar{L}_h}{\partial p_{n+1}}(p_{n+1}, q_{n+1}, p_{n+2}, q_{n+2}). \tag{56}$$

Substituting (55)-(56) into (47)-(48) gives

$$p_{n+1} = \frac{\partial \bar{L}_h}{\partial q_{n+1}}(p_n, q_n, p_{n+1}, q_{n+1}), \tag{57}$$

$$\frac{\partial L}{\partial \dot{p}}|_{t_{n+1}} = \frac{\partial \bar{L}_h}{\partial p_{n+1}}(p_n, q_n, p_{n+1}, q_{n+1}). \tag{58}$$

Since $L = p^T\dot{q} - H(p,q)$, it follows that

$$\frac{\partial L}{\partial \dot{p}} = 0, \tag{59}$$

which, together with (53)-(54) and (57)-(58) implies

$$d\bar{L}_h = -p_n dq_n + p_{n+1} dq_{n+1}. \tag{60}$$

It is important to note that, in the derivation, the classical differential chain rule is applied because the stochastic integrals involved are of Stratonovich sense.

**Theorem 3.2.** *Suppose that $L$ and $H_k$ $(k = 1, \cdots, m)$ are sufficiently smooth with respect to $p$ and $q$, then the mapping $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ determined by (53)-(54) and (57)-(59) is symplectic.*

*Proof.* From (53)-(54) and (57)-(59) it follows

$$\begin{aligned} dp_{n+1} \wedge dq_{n+1} &= d(\frac{\partial \bar{L}_h}{\partial q_{n+1}}) \wedge dq_{n+1} = \frac{\partial^2 \bar{L}_h}{\partial q_{n+1} \partial q_n} dq_n \wedge dq_{n+1}, \\ dp_n \wedge dq_n &= d(-\frac{\partial \bar{L}_h}{\partial q_n}) \wedge dq_n = \frac{\partial^2 \bar{L}_h}{\partial q_n \partial q_{n+1}} dq_n \wedge dq_{n+1}, \end{aligned}$$

Smoothness of $L$ and $H_k$ with respect to $p$ and $q$ implies $\frac{\partial^2 \bar{L}_h}{\partial q_{n+1} \partial q_n} = \frac{\partial^2 \bar{L}_h}{\partial q_n \partial q_{n+1}}$. Consequently,

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n.$$

□

Quadrature formulae applied to the integrals in (49) will give approximations of $\bar{L}_h$. Next, stochastic symplectic mappings $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ can be generated through (53)-(54) and (57)-(59). We call this process the stochastic variational integrator.

## 4. Examples and Numerical Tests

We apply the stochastic variational integrator to construct symplectic schemes for different stochastic Hamiltonian systems. The resulted methods are either known methods, which show the validity of the stochastic variational integrator theory, or new methods, effectiveness of which are tested through numerical experiments.

**Example 4.1.** This example is aimed to show that a known symplectic scheme can be produced by the variational integrator.

For the Kubo oscillator (35)-(36), (37)-(38) implies that the discrete Lagrangian is

$$\begin{aligned} \bar{L}_h &\approx \int_{t_n}^{t_{n+1}} L dt - \int_{t_n}^{t_{n+1}} H_1 \circ dW(t) \\ &= \int_{t_n}^{t_{n+1}} [p\dot{q} - \frac{a}{2}(p^2 + q^2)] dt - \int_{t_n}^{t_{n+1}} \frac{\sigma}{2}(p^2 + q^2) \circ dW(t) \\ &\approx h[\frac{p_{n+1} + p_n}{2} \cdot \frac{q_{n+1} - q_n}{h} - \frac{a}{2}((\frac{p_{n+1} + p_n}{2})^2 + (\frac{q_{n+1} + q_n}{2})^2)] \quad (61) \\ &- \frac{\sigma}{2} \Delta W_n [(\frac{p_{n+1} + p_n}{2})^2 + (\frac{q_{n+1} + q_n}{2})^2], \quad (62) \end{aligned}$$

where, in (61)-(62) the midpoint quadrature formula is applied to approximate the integrals, $\dot{q} \approx \frac{q_{n+1} - q_n}{h}$, and $\Delta W_n = W(t_{n+1}) - W(t_n)$.

Substituting the expression of $\bar{L}_h$ (61)-(62) into the relations

$$\frac{\partial \bar{L}_h}{\partial p_n} = \frac{\partial \bar{L}_h}{\partial p_{n+1}} = 0, \tag{63}$$

$$\frac{\partial \bar{L}_h}{\partial q_n} = -p_n, \tag{64}$$

$$\frac{\partial \bar{L}_h}{\partial q_{n+1}} = p_{n+1}, \tag{65}$$

which is the equivalent and concise form of (53)-(54) and (57)-(59), we get

$$\frac{ah+\sigma\Delta W_n}{2}(p_{n+1}+p_n) = q_{n+1}-q_n, \tag{66}$$

$$\frac{p_{n+1}+p_n}{2} + \frac{ah+\sigma\Delta W_n}{4}(q_{n+1}+q_n) = p_n, \tag{67}$$

$$\frac{p_{n+1}+p_n}{2} - \frac{ah+\sigma\Delta W_n}{4}(q_{n+1}+q_n) = p_{n+1}, \tag{68}$$

respectively. According to (66), replacing the $\frac{p_{n+1}+p_n}{2}$ in (67) and (68) by $\frac{q_{n+1}-q_n}{ah+\sigma\Delta W_n}$, whereby $ah+\sigma\Delta W_n$ is assumed to be nonzero, which can be ensured by suitably controlling $\Delta W_n$ in numerical simulation ([19]), we obtain

$$q_{n+1}-q_n + \frac{(ah+\sigma\Delta W_n)^2}{4}(q_{n+1}+q_n) = p_n(ah+\sigma\Delta W_n), \tag{69}$$

$$q_{n+1}-q_n - \frac{(ah+\sigma\Delta W_n)^2}{4}(q_{n+1}+q_n) = p_{n+1}(ah+\sigma\Delta W_n). \tag{70}$$

Taking sum and difference of the two equations (69) and (70) gives

$$p_{n+1} = p_n - ah\frac{q_{n+1}+q_n}{2} - \sigma\Delta W_n\frac{q_{n+1}+q_n}{2}, \tag{71}$$

$$q_{n+1} = q_n + ah\frac{p_{n+1}+p_n}{2} + \sigma\Delta W_n\frac{p_{n+1}+p_n}{2}, \tag{72}$$

which is just the midpoint rule proposed by Milstein et al. in [19]. Here we reproduce it through variational integrator.

**Example 4.2.** Now we illustrate through another example the approach of variational integrators in constructing stochastic symplectic schemes. The resulted method is again the midpoint rule, while in fact there could arise many other methods by applying different quadrature formulae to the integration of $\bar{L}(h)$, as well as using different forms of stochastic integrals.

For the model of synchrotron oscillations of particles in storage rings ([19])

$$dp = -\omega^2\sin q dt - \sigma_1\cos q\circ dW_1(t) - \sigma_2\sin q\circ dW_2(t), \quad p(0)=0, \tag{73}$$

$$dq = pdt, \quad q(0)=0, \tag{74}$$

where $\omega$, $\sigma_1$ and $\sigma_2$ are constants, and $p$, $q$ are scalars. It is a stochastic Hamiltonian system with

$$H = \frac{1}{2}p^2 - \omega^2\cos q, \quad H_1 = \sigma_1\sin q, \quad H_2 = -\sigma_2\cos q, \tag{75}$$

$$L = p\dot{q} - H = p\dot{q} + \omega^2\cos q - \frac{p^2}{2}. \tag{76}$$

Thus

$$\begin{aligned}
\bar{L}_h &\approx \int_{t_n}^{t_{n+1}} L dt - \sum_{k=1}^{2} \int_{t_n}^{t_{n+1}} H_k \circ dW_k(t) \\
&= \int_{t_n}^{t_{n+1}} (p\dot{q} + \omega^2 \cos q - \frac{p^2}{2}) dt - \int_{t_n}^{t_{n+1}} \sigma_1 \sin q \circ dW_1(t) \\
&+ \int_{t_n}^{t_{n+1}} \sigma_2 \cos q \circ dW_2(t) \\
&\approx h[\frac{p_{n+1}+p_n}{2} \cdot \frac{q_{n+1}-q_n}{h} + \omega^2 \cos(\frac{q_{n+1}+q_n}{2}) - \frac{1}{2}(\frac{p_{n+1}+p_n}{2})^2] \qquad (77) \\
&- \sigma_1 \Delta_n W_1 \sin(\frac{q_{n+1}+q_n}{2}) + \sigma_2 \Delta_n W_2 \cos(\frac{q_{n+1}+q_n}{2}), \qquad (78)
\end{aligned}$$

where, in (77) and (78), midpoint quadrature formula is applied, $\dot{q} \approx \frac{q_{n+1}-q_n}{h}$, and $\Delta_n W_i = W_i(t_{n+1}) - W_i(t_n)$ for $i = 1, 2$.

Substituting the expression of $\bar{L}_h$ (77)-(78) into the relations (63)-(65), we obtain

$$\begin{aligned}
\frac{p_{n+1}+p_n}{2} &= \frac{q_{n+1}-q_n}{h}, \qquad (79) \\
\frac{p_{n+1}+p_n}{2} &= p_n - \frac{h\omega^2 + \sigma_2 \Delta_n W_2}{2} \sin(\frac{q_{n+1}+q_n}{2}) \\
&- \frac{\sigma_1 \Delta_n W_1}{2} \cos(\frac{q_{n+1}+q_n}{2}), \qquad (80) \\
\frac{p_{n+1}+p_n}{2} &= p_{n+1} + \frac{h\omega^2 + \sigma_2 \Delta_n W_2}{2} \sin(\frac{q_{n+1}+q_n}{2}) \\
&+ \frac{\sigma_1 \Delta_n W_1}{2} \cos(\frac{q_{n+1}+q_n}{2}). \qquad (81)
\end{aligned}$$

Replacing $\frac{p_{n+1}+p_n}{2}$ in (80) and (81) by the right-hand side of (79), and then taking sum and difference of the two obtained equations, it follows

$$\begin{aligned}
p_{n+1} &= p_n - (h\omega^2 + \sigma_2 \Delta_n W_2) \sin(\frac{q_{n+1}+q_n}{2}) \\
&- \sigma_1 \Delta_n W_1 \cos(\frac{q_{n+1}+q_n}{2}), \qquad (82) \\
q_{n+1} &= q_n + h \frac{p_{n+1}+p_n}{2}, \qquad (83)
\end{aligned}$$

which is just the midpoint rule applied to (73)-(74). Figure 4.1 illustrates a sample trajectory produced by the scheme (82)-(83).

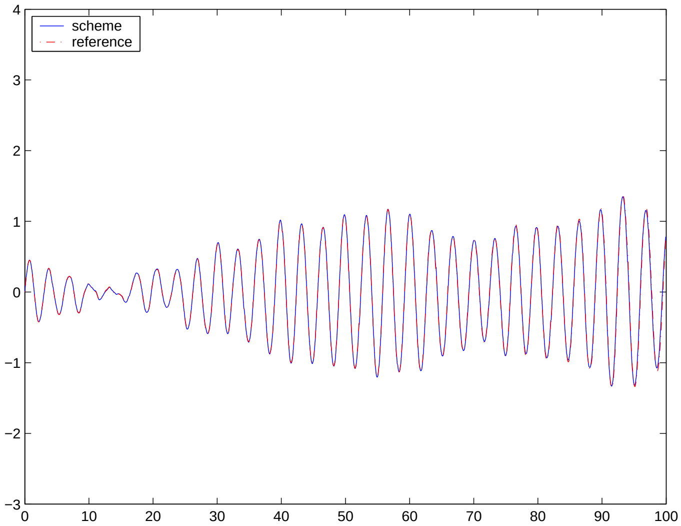


Figure 4.1: A sample trajectory of (82)-(83).

The solid line is produced by the scheme (82)-(83), and the dash-dotted reference line is a highly accurate simulation of the true solution $q(t)$ given in [19], i.e.

$$\begin{aligned} p_{n+1} &= p_n - h\omega^2 \sin(q_{n+1}) - (\sigma_1 \cos(q_{n+1})\Delta_n W_1 + \sigma_2 \sin(q_{n+1})\Delta_n W_2), \\ q_{n+1} &= q_n + hp_n. \end{aligned}$$

The two sample paths coincide visually. This shows the effectiveness of the numerical scheme (82)-(83). Data for the numerical test are $\sigma_1 = 0.2$, $\sigma_2 = 0.1$, $\omega = 2$, $t \in [0, 100]$, and the step-size is $h = 0.02$.

Since the scheme (82)-(83) is implicit, we applied fixed-point iteration to realize it. The number of iterations performed in each step is 100.

**Example 4.3.** The system with two additive noises ([18])

$$dp = -qdt + \gamma \circ dW_2(t), \quad p(0) = 0, \tag{84}$$

$$dq = pdt + \sigma \circ dW_1(t), \quad q(0) = 0, \tag{85}$$

is a stochastic Hamiltonian system with

$$\begin{aligned} H &= \frac{1}{2}(p^2 + q^2), \quad H_1 = \sigma p, \quad H_2 = -\gamma q, \\ L &= p\dot{q} - H = p\dot{q} - \frac{1}{2}(p^2 + q^2). \end{aligned} \tag{86}$$

Here $\sigma$ and $\gamma$ are constants, and $p$, $q$ are scalars. The discrete Lagrangian is

$$\begin{aligned} \bar{L}_h &\approx \int_{t_n}^{t_{n+1}} Ldt - \sum_{k=1}^{2} \int_{t_n}^{t_{n+1}} H_k \circ dW_k(t) \\ &= \int_{t_n}^{t_{n+1}} [p\dot{q} - \frac{1}{2}(p^2 + q^2)]dt - \int_{t_n}^{t_{n+1}} \sigma p \circ dW_1(t) + \int_{t_n}^{t_{n+1}} \gamma q \circ dW_2(t) \end{aligned} \tag{87}$$

The ($\lambda$)-integrals ([10]), denoted with $(\lambda)\int_0^T f(X(t),t)dW(t)$, $\quad(0\le\lambda\le 1)$, are defined as the mean-square limit of the sums (as $n\to\infty$)

$$S_n=\sum_{j=1}^{n} f((1-\lambda)X(t_j^{(n)})+\lambda X(t_{j+1}^{(n)}))(W(t_{j+1}^{(n)})-W(t_j^{(n)}))$$

for partitions $0=t_1^{(n)}<t_2^{(n)}<\cdots<t_{n+1}^{(n)}=T$, for which $\delta^{(n)}=\max_{1\le j\le n}(t_{j+1}^{(n)}-t_j^{(n)})\to 0$ as $n\to\infty$.

According to the definition of the Itô and Stratonovich integrals, they are special ($\lambda$) integrals with $\lambda=0$ and $\lambda=\frac{1}{2}$, respectively, and can transform to each other according to the formula

$$\int_0^T f(X,t)\circ dW(t)=\int_0^T f(X,t)dW(t)+\frac{1}{2}\int_0^T\frac{\partial f}{\partial X}(X,t)\cdot b(X,t)dt,$$

where $b(X,t)$ is the diffusion coefficient of the stochastic differential equation of $X$

$$dX=a(X,t)dt+b(X,t)dW(t).$$

Characterize the (1)-integral with a $*$ before $dW(t)$, it holds the following transform formula between the Stratonovich integrals and the (1)-integrals (see e.g. the discussion in [3]):

$$\int_0^T f(X,t)\circ dW(t)=\int_0^T f(X,t)*dW(t)-\frac{1}{2}\int_0^T\frac{\partial f}{\partial X}(X,t)\cdot b(X,t)dt.$$

Now we transform the first stochastic integral in (87) to the (1)-integral form

$$\int_{t_n}^{t_{n+1}}\sigma p\circ dW_1(t)=\int_{t_n}^{t_{n+1}}\sigma p*dW_1(t)-\frac{1}{2}\int_{t_n}^{t_{n+1}}\sigma\cdot 0dt,$$

and transform the second stochastic integral in (87) to its Itô form

$$\int_{t_n}^{t_{n+1}}\gamma q\circ dW_2(t)=\int_{t_n}^{t_{n+1}}\gamma q dW_2(t)+\frac{1}{2}\int_{t_n}^{t_{n+1}}\gamma\cdot 0dt,$$

where the "0"s in the above two formulae result from the fact that $dp$ does not contain $dW_1(t)$, whereas $dq$ does not contain $dW_2(t)$ in (84)-(85).

Thus the integral $\int_{t_n}^{t_{n+1}}\sigma p\circ dW_1(t)$ can be approximated by $\sigma p_{n+1}\Delta_n W_1$, and $\int_{t_n}^{t_{n+1}}\gamma q\circ dW_2(t)$ by $\gamma q_n\Delta_n W_2$. As a result, we obtain the following approximation of (87)

$$\bar{L}_h\approx h[p_{n+1}\cdot\frac{q_{n+1}-q_n}{h}-\frac{1}{2}(p_{n+1}^2+q_n^2)]-\sigma p_{n+1}\Delta_n W_1+\gamma q_n\Delta_n W_2, \tag{88}$$

where forward Euler quadrature is applied to $p$, and backward Euler quadrature to $q$ in the deterministic integral, and $\dot{q}$ is again approximated by $\frac{q_{n+1}-q_n}{h}$.

Substituting the expression of $\bar{L}_h$ (88) into (63)-(65), we get

$$p_{n+1} = p_n-hq_n+\gamma\Delta_n W_2, \tag{89}$$

$$q_{n+1} = q_n+hp_{n+1}+\sigma\Delta_n W_1, \tag{90}$$

which is the symplectic Euler-Maruyama method given by Milstein et al. in [18].

In the process above, if we transform the first stochastic integral in (87) to its Itô form while the second one to its (1)-integral form, and apply forward Euler quadrature to $q$ and backward Euler quadrature to $p$ in approximating the two integrals, we obtain

$$p_{n+1} = p_n - hq_{n+1} + \gamma\Delta_n W_2, \tag{91}$$
$$q_{n+1} = q_n + hp_n + \sigma\Delta_n W_1, \tag{92}$$

which is the adjoint method of (89)-(90). Its effect can be seen in Figure 4.2.

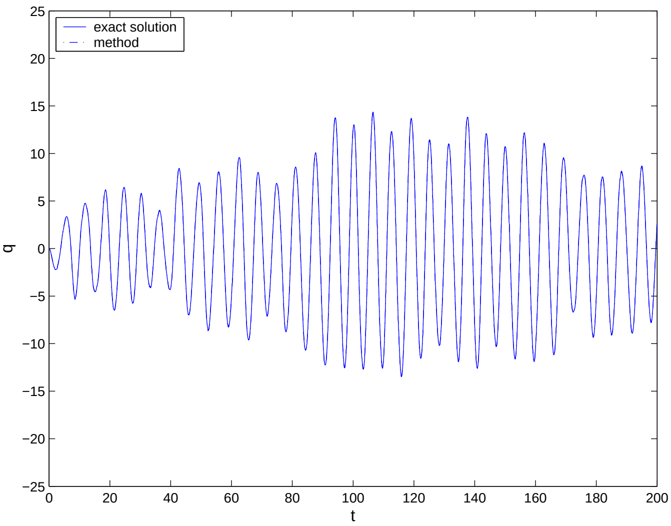


Figure 4.2: A sample trajectory of (89)-(90).

The solid line is a sample path of the exact solution $q(t)$, which satisfies the formula ([18])

$$Y(t_{k+1}) = FY(t_k) + u_k, \quad Y(0) = Y_0, \quad k = 0, 1, \cdots, N-1$$

for the discretization $0 = t_0 < t_1 < \cdots < t_N = T$, where $Y = \begin{pmatrix} q \\ p \end{pmatrix}$, $F = \begin{pmatrix} \cos h & \sin h \\ -\sin h & \cos h \end{pmatrix}$ with $h = t_{k+1} - t_k$, and

$$u_k = \begin{pmatrix} \sigma \int_{t_k}^{t_{k+1}} \cos(t_{k+1} - s) dW_1(s) + \gamma \int_{t_k}^{t_{k+1}} \sin(t_{k+1} - s) dW_2(s) \\ -\sigma \int_{t_k}^{t_{k+1}} \sin(t_{k+1} - s) dW_1(s) + \gamma \int_{t_k}^{t_{k+1}} \cos(t_{k+1} - s) dW_2(s) \end{pmatrix}.$$

The dash-dotted line is produced by the scheme (91)-(92). The two sample paths coincide visually. Data for creating the figure are $\gamma = 1$, $\sigma = 0$, $t \in [0, 200]$, and the step-size is $h = 0.02$.

**Conclusions.** The stochastic variational integrators are framed through investigating into the dynamics of stochastic Hamiltonian systems, and validated through performing several numerical tests. Construction of various concrete methods based on the stochastic variational integrator theory might be topics for further study.

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