Exponential Discrete Gradient Schemes for Simulating Stochastic Hamiltonian Systems Preserving Hamiltonian Functions

Jia-lin RUAN and Li-jin WANG*

University of Chinese Academy of Sciences, Yu Quan Lu 19 (Jia), Beijing 100049, China

*Corresponding author

Keywords: Stochastic Hamiltonian Systems, Numerical simulation, Structure-preserving methods.

Abstract. The paper investigates the exponential discrete gradient methods simulating stochastic Hamiltonian systems with invariant Hamiltonians. We show that the methods are nearly symplectic, and nearly preserve the invariant Hamiltonians. Numerical experiments illustrate effectiveness and efficiency of the simulation methods.

Introduction

Hamiltonian systems are very important dynamical systems. All physical processes where the dissipation can be neglected can be described as Hamiltonian systems ([1]). Stochastic Hamiltonian systems (SHSs) are Hamiltonian systems with certain random disturbances, and are described as ([2])

\[ dX(t) = J^{-1} \nabla H_0(X) dt + J^{-1} \sum_{r=1}^{m} \nabla H_r(X) \circ dW_r(t), \quad X(0) = x_0, \]  

(1)

where \( X \in \mathbb{R}^{2d} \), \( J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix} \), \( H_0 \) and \( H_r \) \( (r = 1, \cdots, m) \): \( \mathbb{R}^{2d} \rightarrow R \) are real functions ensuring existence and uniqueness of the solution of (1), called the Hamiltonians of the system (1). \((W_1(t), \cdots, W_m(t))\) is an \( m \)-dimensional standard Wiener process. As their deterministic counterpart, the stochastic Hamiltonian systems have an intrinsic structure, the symplectic structure, depicted as ([1,2,3])

\[ \partial \frac{X(t)}{\partial x_0} \int \frac{\partial X(t)}{\partial x_0} = J, \quad \forall \ t \geq 0. \]  

(2)

Geometrically, (2) means area preservation in the phase space along the phase flow of the Hamiltonian systems.

Exact solutions of Hamiltonian systems are in general difficult to be found, therefore numerical simulations become an import tool of investigating such systems. Numerous numerical methods were developed for deterministic and stochastic Hamiltonian systems, in particular, people pursue symplectic methods for such systems (see e.g. [1,2,3,4] and references therein), methods that can preserve the symplectic structure (2) of the system, characterized by

\[ \partial \frac{X_{n+1}}{\partial x_n} \int \frac{\partial X_{n+1}}{\partial x_n} = J, \quad \forall \ n \geq 0. \]  

(3)

More general, methods that can preserve structures of the original systems are called structure-preserving algorithms, such as the symplectic methods for Hamiltonian systems, energy-preserving methods for systems with invariant energy, and so on ([1,3]). Such methods turn out to be superior than other general-purpose methods, in qualitative behavior and long-time simulation.

In this paper, we investigate the stochastic exponential discrete gradient (SEDG) methods applied to the stochastic Hamiltonian systems with invariant Hamiltonians. We examine their properties in preserving the symplecticity and the Hamiltonians, and show that they can nearly preserve the symplecticity and the Hamiltonians within error of root mean-square order 1. We also illustrate
their root mean-square convergence order, and their performance in terms of structure preservation via numerical experiments.

Section 2 is devoted to theoretical analysis of the SEDG methods applied to the SHSs with invariant Hamiltonians. In Section 3 we perform numerical experiments.

**SEDG Scheme for SHSs with Invariant Hamiltonians**

Now we focus on the stochastic Hamiltonian system (1) for \( m=1 \) and when it has invariant Hamiltonian functions.

**Lemma 1** ([4]): For a 2d-dimensional stochastic Hamiltonian system

\[
dX(t) = J^{-1}\nabla H_0(X) dt + J^{-1}\nabla H_1(X) \circ dW_t, \quad X(0) = x_0,
\]

where \( X = (p^T q^T)^T, \ p, q \in \mathbb{R}^d \), the Hamiltonian functions \( H_i, (i = 0, 1) \) are invariant for the flow of the system (4), if and only if \( \{H_0, H_1\} = 0 \), where the Poisson bracket is defined as

\[
\{H_0, H_1\} = \sum_{k=0}^{d} \left( \frac{\partial H_1}{\partial p_k} \frac{\partial H_0}{\partial q_k} - \frac{\partial H_0}{\partial p_k} \frac{\partial H_1}{\partial q_k} \right).
\]

Consider the SHS (1) with \( m=1, H_0 = \frac{1}{2} X^T M X + U, H_1 = V \), and \( M \) symmetric,

\[
dX(t) = J^{-1}(MX(t) + \nabla U(X(t))) dt + J^{-1}\nabla V(X(t)) \circ dW(t), \quad X(t_0) = x_0
\]

If we assume

\[
\{\frac{1}{2} X^T M X, V\} = 0, \quad \{U, V\} = 0,
\]

then the SHS (6) possesses invariant Hamiltonian functions \( H_i, (i = 0, 1) \), according to Lemma 1. Given an equidistant time discretization \( 0 = t_0 < t_1 < \cdots < t_n < \cdots < t_N = T \) with \( h = t_{n+1} - t_n \) for \( n = 0, \ldots, N - 1 \), we apply the following SEDG numerical scheme ([5]) to (6)

\[
X_{n+1} = \exp(Ah)X_n + h\phi(Ah) J^{-1}\nabla U(X_n, X_{n+1})
+ \exp(\frac{Ah}{2}) J^{-1}\nabla V(X_n, X_{n+1}) \Delta W_n,
\]

where \( A = J^{-1}M, \ \phi(z) := \frac{\exp(z) - 1}{z} \), \( \Delta W_n = W(t_{n+1}) - W(t_n) \), and the discrete gradient \( \nabla Y (Y = U, V) \) is defined as

\[
\nabla Y (y, \tilde{y}) := \frac{1}{2} (\nabla Y_0 (y, \tilde{y} + \nabla Y_0 (\tilde{y}, y), \quad \text{where}
\]

\[
\nabla Y_0 (y, \tilde{y}) := \begin{pmatrix}
\frac{Y(\tilde{y}^1, y^2, \ldots, y^{2d}) - Y(y^1, y^2, \ldots, y^{2d})}{\tilde{y}^1 - y^1} \\
\frac{Y(\tilde{y}^1, \tilde{y}^2, y^3, \ldots, y^{2d}) - Y(y^1, y^2, \ldots, y^{2d})}{\tilde{y}^2 - y^2} \\
\vdots \\
\frac{Y(\tilde{y}^1, \tilde{y}^2, \ldots, \tilde{y}^{2d}) - Y(y^1, y^2, \ldots, y^{2d})}{\tilde{y}^{2d} - y^{2d}}
\end{pmatrix}.
\]

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Moreover we simulate $\Delta W_n$ by $\zeta_n \sqrt{h}$, where $\zeta_n = \begin{cases} \xi, & |\xi| \leq C_h, \\ C_h, & \xi > C_h, \\ -C_h, & \xi < -C_h, \end{cases}$

$C_h = \sqrt{2k |\ln h|}, \ k \geq 2I$ for a method supposed to be of root mean-square convergence order $I$ ([2]). We have the following theorems regarding the convergence order and structure preserving properties of the scheme (8).

**Theorem 2** ([5]): Suppose the SHS (6) satisfies the conditions for existence and uniqueness of the solution, and in addition assume that $U, V \in C^1(R^d)$ with uniformly bounded derivatives, and $\nabla U, \nabla V, J^{-1} \text{Hess}(V) J^{-1} \nabla V$ have bounded second moments along the solution of (6). Then the numerical scheme (8) is of root mean-square convergence order 1, i.e.,

$$(E|X(t_n) - X_n|^2)^{1/2} = O(h), \ n = 1, \ldots, N.$$ 

For the proof of Theorem 2, the readers can refer to [5].

**Theorem 3**: Assume that $\partial_i U, \partial_i V \ (i = 1, 2)$ are bounded and symmetric. The SEDG scheme (8) for the SHS (6) nearly preserves the symplecticity of (6) within error of root mean-square order 1.

**Proof.** According to (8) we have

$$\frac{\partial X_{n+1}}{\partial X_n} = B_{n+1} B_2, \quad \text{where}$$

$$B_1 = I - h \phi(Ah) J^{-1} \partial_1 \nabla U - \Delta W_n \exp(Ah/2) J^{-1} \partial_2 \nabla V,$$

$$B_2 = \exp(Ah) + h \phi(Ah) J^{-1} \partial_1 \nabla U + \Delta W_n \exp(Ah/2) J^{-1} \partial_2 \nabla V.$$ 

(10)

Note that $\phi(Ah) = I + O(h)$, the invertibility of $B_n$ can be guaranteed by choosing sufficiently small step size $h$. Straightforward calculations yield

$$\frac{\partial X_{n+1}}{\partial X_n} \ T \frac{\partial X_{n+1}}{\partial X_n} = J + h(A^T J + JA) + \Delta W_n^2 (\partial_1 \nabla V J \partial_1 \nabla V - \partial_2 \nabla V J \partial_2 \nabla V) + O(h \Delta W_n),$$

where we have used the series expansion of the matrix exponential $\exp(Ah)$ and the Taylor expansion of $B_n^{-1}$ according to the rule of expanding $(1 - x)^{-1}$. Note that $A^T J + JA = 0$ due to symmetry of $M$. Then we have

$$\frac{\partial X_{n+1}}{\partial X_n} \ T \frac{\partial X_{n+1}}{\partial X_n} = J + R_n, \quad \text{with} \quad (E(R_n^2))^{1/2} = O(h).$$

**Theorem 4**: Under the assumptions of Theorem 2 and the conditions (7), the SEDG scheme (8) for the SHS (6) nearly preserves the Hamiltonian functions $H_i \ (i = 0, 1)$ within error of root mean-square order 1, i.e.,

$$(E|H_i(X_{n+1}) - H_i(X_n)|^2)^{1/2} = O(h), \quad i = 0, 1, \ n \geq 0.$$ 

**Proof.** According to (8), denoting $\Delta W_n$ by $\Delta W$ for simplicity, we have

$$\frac{1}{2} X_{n+1}^T M X_{n+1} = \frac{1}{2} X_n^T \exp(Ah)^T M \exp(Ah) X_n + h X_n^T \exp(Ah)^T M \phi(Ah) J^{-1} \nabla U$$

$$+ \frac{1}{2} h^2 J \phi(Ah)^T M \phi(Ah) J^{-1} \nabla U + \Delta W_n^2 \exp(Ah)^T M \exp(Ah/2) J^{-1} \nabla V$$

$$+ h \Delta W \nabla U J \phi(Ah)^T M \exp(Ah/2) J^{-1} \nabla V$$

$$+ \frac{1}{2} \Delta W^2 \nabla V J \exp(Ah/2) M \exp(Ah/2) J^{-1} \nabla V,$$

(13)
\[ U(X_{n+1}) - U(X_n) = X_n^T (\exp(Ah) - I)^T \nabla U + h \nabla U^T J \phi(Ah)^T \nabla U + \Delta W^T \nabla V^T J \exp(\frac{Ah}{2})^T \nabla U. \] (14)

Note that we have used the property of discrete gradients \( \nabla Y(y, \hat{y})^T (\hat{y} - y) = Y(\hat{y}) - Y(y) \) for (14). Then we have

\[ H_o(X_{n+1}) - H_o(X_n) = \frac{1}{2} \Delta W^T \nabla V(X_n)^T J M J^{-1} \nabla V(X_n) + R_{it}, \] (15)

under the assumption (7), and by performing series expansion of the discrete gradients, and the fact that \( \exp(Ah)^T M \exp(Ah) - M = 0 \) ([5]). (15) implies that \( E(H_o(X_{n+1}) - H_o(X_n))^2 = O(h^2) \). Similarly, we can derive that \( E(H_i(X_{n+1}) - H_i(X_n))^2 = O(h^2) \).

**Numerical Experiments**

We consider the Kubo oscillator (see e.g. [2])

\[
\text{d}X = \begin{pmatrix} 0 & -a \\ a & 0 \end{pmatrix} X \text{d}t + \begin{pmatrix} 0 & -\sigma \\ \sigma & 0 \end{pmatrix} X \circ \text{d}W(t), \quad X(0) = x_0,
\] (16)

where \( X = (x_1, x_2)^T, x_0 = (x_0^1, x_0^2)^T \). It is a stochastic Hamiltonian system with invariant Hamiltonian functions

\[
H_o(x_1, x_2) = \frac{a}{2}((x_1')^2 + (x_2')^2), \quad H_i(x_1, x_2) = \frac{\sigma}{2}((x_1')^2 + (x_2')^2).
\] (17)

In other words, the phase trajectory of the Kubo oscillator should be a circle with radius \( \sqrt{(x_0^1)^2 + (x_0^2)^2} \) and centered at the origin. The SEDG scheme (8) applied to the system (16) reads

\[
\begin{pmatrix} x_{n+1}^1 \\ x_{n+1}^2 \end{pmatrix} = \begin{pmatrix} \cos(\frac{ah}{2}) & -\sin(\frac{ah}{2}) \\ \sin(\frac{ah}{2}) & \cos(\frac{ah}{2}) \end{pmatrix} \begin{pmatrix} x_n^1 \\ x_n^2 \end{pmatrix} + \begin{pmatrix} \sin(\frac{ah}{2}) & \cos(\frac{ah}{2}) \\ 1 - \cos(\frac{ah}{2}) & \sin(\frac{ah}{2}) \end{pmatrix} \begin{pmatrix} -\frac{1}{2}(x_n^1 + x_n^2) \\ -\frac{1}{2}(x_n^1 + x_n^2) \end{pmatrix} + \begin{pmatrix} \cos(\frac{ah}{4}) & -\sin(\frac{ah}{4}) \\ \sin(\frac{ah}{4}) & \cos(\frac{ah}{4}) \end{pmatrix} \begin{pmatrix} \frac{1}{2}(x_n^1 + x_n^2) \\ \frac{1}{2}(x_n^1 + x_n^2) \end{pmatrix} \circ \Delta W_{n}.
\] (18)

Figure 1. A sample path \( x^2(t) \) (left) and the root mean-square convergence order (right) of the SEDG scheme (18) for the Kubo oscillator (16).
Figure 2. Preservation of \( H = (x^1)^2 + (x^2)^2 \) by the SEDG scheme (18) (left) and a strong 1.5 order Taylor scheme (right) for (16). Small circles, diamonds, and stars are numerical points by three different initial values, respectively.

As can be seen from Figure 1, the SEDG scheme (18) for (16) are of good accuracy, with root mean-square convergence order 1. Figure 2 shows the superiority of the SEDG scheme (18) compared with a strong 1.5 order Taylor scheme in preserving the invariant Hamiltonians.

Acknowledgement
This research was financially supported by the NNSFC No. 11471310, No. 11071251.

References