Symplectic methods based on Padé approximation for linear stochastic Hamiltonian systems

Liying Sun

(In collaboration with Prof. Lijin Wang)

School of Mathematics sciences, University of Chinese Academy of Sciences

2015 Conference on Structure-preserving Algorithms
Dec. 27, Nanjing
Outline

1. Introduction

2. Symplectic schemes for LSHS I

3. Symplectic schemes for LSHS II

4. Numerical experiments
Outline

1. Introduction
2. Symplectic schemes for LSHS I
3. Symplectic schemes for LSHS II
4. Numerical experiments
Linear deterministic Hamiltonian system

2n-dim LDHS

\[ dp(t) = -\frac{\partial H(p(t), q(t))}{\partial q} dt, \quad p(t_0) = p_0, \]
\[ dq(t) = \frac{\partial H(p(t), q(t))}{\partial p} dt, \quad q(t_0) = q_0. \]

- Hamiltonian function: \( H(p, q) = \frac{1}{2} (p^\top, q^\top) C \begin{pmatrix} p \\ q \end{pmatrix}, \quad C^\top = C; \)
- Exact solution:
  \[ \begin{pmatrix} p(t) \\ q(t) \end{pmatrix} = e^{(t-t_0)J^{-1}C} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}. \]
Symplectic numerical schemes for LDHS

- Symplectic numerical schemes:

\[
\begin{bmatrix}
p_{n+1} \\
q_{n+1}
\end{bmatrix} = P_{(k,k)} \begin{bmatrix}
p_n \\
q_n
\end{bmatrix} = \frac{\sum_{i=0}^{k} \frac{(2k-i)!k!}{(2k)!i!(k-i)!} (hJ^{-1}C)^i}{\sum_{i=0}^{k} \frac{(2k-i)!k!}{(2k)!i!(k-i)!} (-hJ^{-1}C)^i} \begin{bmatrix}
p_n \\
q_n
\end{bmatrix},
\]

(1.2)

where \(P_{(k,k)}\) is a Padé approximation.

- Property 1: (1.2) is symplectic;

- Property 2: (1.2) is of 2k-th order accuracy.

**Question:** What about the numerical approximations for linear stochastic Hamiltonian systems?
Consider $2n$-dim LSHSs in Stratonovich sense,

\[
\begin{align*}
    dP &= -\frac{\partial H_0(P, Q)}{\partial Q} dt - \sum_{i=1}^{m} \frac{\partial H_i(P, Q)}{\partial Q} \circ dW^i(t), & P(t_0) = p, \\
    dQ &= \frac{\partial H_0(P, Q)}{\partial P} dt + \sum_{i=1}^{m} \frac{\partial H_i(P, Q)}{\partial P} \circ dW^i(t), & Q(t_0) = q.
\end{align*}
\] (2.1)

- $W^i(t), i = 1, \cdots, m$: independent standard Wiener processes;
- $H_i(P, Q), i = 0, \cdots, m$:

\[
H_i(P, Q) = \frac{1}{2} (P^\top, Q^\top) C_i \begin{pmatrix} P \\ Q \end{pmatrix}, \quad C_i = (C_i^\top)^	op.
\]
Let $C^i = JA^i$, $A^i \in sp(2n)$ satisfying $JA^i + (A^i)^T = O$, $i = 0, 1, \cdots, m$, LSHS (2.1) becomes

$$dX(t) = A^0 X dt + \sum_{i=1}^{m} A^i X \circ dW^i(t), \quad X(t_0) = (p^T, q^T)^T$$

whose solution is:

$$X(t) = \exp \left[ (t - t_0)A^0 + \sum_{i=1}^{m} (W^i(t) - W^i(t_0))A^i \right] X(t_0), \quad (2.2)$$

with $t_0 \leq t \leq t_0 + T$. 
the Taylor’s expansion: $\exp(M) = I + \sum_{i=1}^{+\infty} \frac{M^i}{i!}$, $M \in \mathbb{R}^{n\times n}$;

Padé approximation:

$$\exp(M) \sim P_{(r,s)}(M) = D_{(r,s)}^{-1}(M)N_{(r,s)}(M),$$

with

$$N_{(r,s)} = I + \sum_{i=1}^{r} \frac{(r + s - i)!r!}{(r + s)!i!(r - i)!}M^i := I + \sum_{i=1}^{r} a_i M^i,$$

$$D_{(r,s)} = I + \sum_{i=1}^{s} \frac{(r + s - i)!s!}{(r + s)!i!(s - i)!}(-M)^i := I + \sum_{i=1}^{s} b_i (-M)^i.$$ 

and

$$\exp(M) - P_{(r,s)}(M) = O(M^{r+s+1}). \quad (2.3)$$
Truncate the stochastic increments $\Delta W_n \approx \zeta_h \sqrt{h}$:

$$
\zeta_h = \begin{cases} 
\xi^i, & \text{if } |\xi^i| \leq M_l, \\
M_l, & \text{if } \xi^i > M_l, \\
-M_l, & \text{if } \xi^i < -M_l,
\end{cases}
$$

with $\xi^i \sim N(0, 1)$ and $M_l = \sqrt{2\ell|\ln h|}$, $\ell \geq 1$. Denote $B := hA^0 + \sum_{i=1}^{m} \Delta W_n A^i$ and $\bar{B} := hA^0 + \sqrt{h} \sum_{i=1}^{m} \zeta_h^i A^i$, we get the numerical schemes

$$
X^{(r,s)}_{n+1} = \left[I + \sum_{j=1}^{s} b_j (-\bar{B})^j \right]^{-1} \left[I + \sum_{j=1}^{r} a_j \bar{B}^j \right] X^{(r,s)}_n.
$$
The convergence of numerical schemes $X^{(r,s)}_n$

**Theorem (L. Sun and L. Wang, arXiv)**

The numerical method

$$X^{(r,s)}_{n+1} = \left[ I + \sum_{j=1}^{s} b_j(-\bar{B})^j \right]^{-1} \left[ I + \sum_{j=1}^{r} a_j\bar{B}^j \right] X^{(r,s)}_n$$

is of mean-square order $\frac{r+s}{2}$ with $M_l = \sqrt{2\ell|\ln h|}$, $\ell \geq r + s$. 
The symplecticity of numerical methods $X_{n}^{(k,k)}$

**Theorem (L. Sun and L. Wang, arXiv)**

The numerical method

$$
X_{n+1}^{(k,k)} = \left[ I + \sum_{j=1}^{k} b_j (-\bar{B})^j \right]^{-1} \left[ I + \sum_{j=1}^{k} a_j \bar{B}^j \right] X_{n}^{(r,s)}
$$

is symplectic.
Sketch of proof

**Goal:** 
\[ D_{(k,k)}^{-1}N_{(k,k)} := \left[ I + \sum_{j=1}^{k} b_j(-\bar{B})^j \right]^{-1} \left[ I + \sum_{j=1}^{k} a_j\bar{B}^j \right] \in Sp(2n) \]

Let \( N_{(k,k)}(\bar{B}) = F(\bar{B}) + G(\bar{B}) \), \( D_{(k,k)}(\bar{B}) = F(\bar{B}) - G(\bar{B}) \), where \( F(\bar{B}) = F(-\bar{B}) \) and \( G(\bar{B}) = -G(-\bar{B}) \). By the properties of \( \bar{B} \in sp(2n) \), we can obtain

\[
(N_{(k,k)}(\bar{B}))^\top JN_{(k,k)}(\bar{B}) = (D_{(k,k)}(\bar{B}))^\top JD_{(k,k)}(\bar{B}),
\]

(2.4)

which support that \( N_{(k,k)}^{-1}D_{(k,k)} \in Sp(2n) \) and \( X_n^{(k,k)} \) is symplectic. \( \square \)
Consider $2n$-dim LSHS II with additive noises,

$$
\begin{align*}
    d\tilde{P} &= -\frac{\partial \tilde{H}_0(\tilde{P}, \tilde{Q})}{\partial \tilde{Q}} dt + \sum_{i=1}^{m} \tilde{C}_1^i dW^i(t), \quad \tilde{P}(t_0) = \tilde{p}, \\
    d\tilde{Q} &= \frac{\partial \tilde{H}_0(\tilde{P}, \tilde{Q})}{\partial \tilde{P}} dt + \sum_{i=1}^{m} \tilde{C}_2^i dW^i(t), \quad \tilde{Q}(t_0) = \tilde{q},
\end{align*}
$$

- $\tilde{H}_0(\tilde{P}, \tilde{Q}) = \frac{1}{2}(\tilde{P}^\top, \tilde{Q}^\top)\tilde{C}^0 \begin{pmatrix} \tilde{P} \\ \tilde{Q} \end{pmatrix}$, $\tilde{C}^0 = (\tilde{C}^0)^\top$;

- $\tilde{C}_1^i, \tilde{C}_2^i$, $i = 1, \cdots, m$, are constant column vectors.
Denoting $R_i = (\tilde{C}_i^T, \tilde{C}_i^T)^T$, we have

$$dZ(t) = J^{-1}\tilde{C}^0 Z dt + \sum_{i=1}^{m} R_idW^i(t), \quad Z(t_0) = (\tilde{p}, \tilde{q})^T,$$

with exact solution:

$$Z(t) = e^{(t-t_0)J^{-1}\tilde{C}^0} Z(t_0) + \sum_{i=1}^{m} \int_{t_0}^{t} e^{(t-\theta)J^{-1}\tilde{C}^0} R_idW^i(\theta).$$
Denoting $B_1 = hJ^{-1}\tilde{C}^0$ and $B_2(\theta) = (t_{n+1} - \theta)J^{-1}\tilde{C}^0$, we get

$$Z(t_{n+1}) = e^{B_1}Z(t_n) + \sum_{i=1}^m \int_{t_n}^{t_{n+1}} e^{B_2(\theta)}R_i dW^i(\theta).$$

$$\int_{t_n}^{t_{n+1}} e^{B_2(\theta)}R_i dW^i(\theta)$$

$$P(\tilde{r}, 1) \rightarrow \int_{t_n}^{t_{n+1}} P(\tilde{r}, 1)(B_2(\theta))R_i dW^i(\theta)$$

$$h = N' h'$$

$$B_2^k = B_2(t_n + kh')$$

$$B_2^k = B_2(t_n + kh')$$

$$h = N' h'$$

$$h = N' h'$$

$$B_2^k = B_2(t_n + kh')$$

$$B_2^k = B_2(t_n + kh')$$

$$\sum_{k=0}^{N'-1} \left[ I - b_1 B_2^k \right]^{-1} \left[ I + \sum_{j=1}^{\tilde{r}} a_j B_2^k \right] R_i \Delta W^i_{n,k},$$

with $\Delta W^i_{n,k} = W^i(nh + (k + 1)h') - W^i(nh + kh')$. 

Where $\tilde{r}$ is the modified time step, $b_1$ is a constant, and $a_j$ are coefficients relating to the scheme's properties.
Approximating $e^{B_1}$ by $P(\hat{r},\hat{s})(B_1)$, we get

$$Z_{n+1} = \left[I + \sum_{j=1}^{\hat{s}} b_j(-B_1)\right]^{-1}\left[I + \sum_{j=1}^{\hat{r}} a_j(B_1)\right]Z_n$$

$$+ \sum_{i=1}^{m} \sum_{k=0}^{N'-1} \left[I - b_1B_2^k\right]^{-1}\left[I + \sum_{j=1}^{\hat{r}} a_j(B_2^k)\right]R_i\Delta W_{n,k}. \tag{3.1}$$
Approximating \( \int_{t_n}^{t_{n+1}} e^{B_2(\theta)} R_i dW^i(\theta) \) by the left-rectangle formula and \( P_{(1,1)}(hJ^{-1} \tilde{C}^0) \), we obtain

\[
Z_{n+1} = \left[ I + \sum_{j=1}^{\hat{s}} b_j (-B_1)^j \right]^{-1} \left[ I + \sum_{j=1}^{\hat{r}} a_j (B_1)^j \right] Z_n \\
+ \sum_{i=1}^{m} \left[ I - \frac{1}{2} B_1 \right]^{-1} \left[ I + \frac{1}{2} B_1 \right] R_i \Delta W^i_n.
\]  

(3.2)

- (3.2) is symplectic if \( \hat{r} = \hat{s} \);
- (3.2) is of mean-square order 1.
The convergence of numerical schemes $Z_n$

**Theorem (L. Sun and L. Wang, arXiv)**

The numerical method

$$Z_{n+1} = \left[ I + \sum_{j=1}^{\hat{s}} b_j (-B_1)^j \right]^{-1} \left[ I + \sum_{j=1}^{\hat{r}} a_j (B_1)^j \right] Z_n$$

$$+ \sum_{i=1}^{m} \sum_{k=0}^{N'-1} \left[ I - b_1 B_2^k \right]^{-1} \left[ I + \sum_{j=1}^{\hat{r}} a_j (B_2^k)^j \right] R_i \Delta W_{n,k}$$

is of mean-square order $\hat{r} + 2$, where $N' = \left[ \frac{1}{h^{\hat{r}+2}} \right] + 1$ and $\hat{r} + \hat{s} = \hat{r} + 3$. 

Liying Sun (UCAS)
The symplecticity of numerical methods $Z_n$

**Theorem (L. Sun and L. Wang, arXiv)**

If $\hat{r} = \hat{s}$, the numerical method

$$Z_{n+1} = \left[ I + \sum_{j=1}^{\hat{s}} b_j (-B_1)^j \right]^{-1} \left[ I + \sum_{j=1}^{\hat{r}} a_j (B_1)^j \right] Z_n$$

$$+ \sum_{i=1}^{m} \sum_{k=0}^{N'-1} \left[ I - b_1 B_2^k \right]^{-1} \left[ I + \sum_{j=1}^{\hat{r}} a_j (B_2^k)^j \right] R_i \Delta W_{i,n,k}^i$$

is symplectic.
Outline

1. Introduction

2. Symplectic schemes for LSHS I

3. Symplectic schemes for LSHS II

4. Numerical experiments
Kubo Oscillator

The 2-dim SDE:

\[ dP = -aQ \, dt - \sigma Q \, dW(t), \quad P(0) = p, \]
\[ dQ = aP \, dt + \sigma P \, dW(t), \quad Q(0) = q, \]

has an exact solution

\[ P(t) = p \cos(at + \sigma W(t)) - q \sin(at + \sigma W(t)), \]
\[ Q(t) = p \sin(at + \sigma W(t)) + q \cos(at + \sigma W(t)). \]
Denoting by $\bar{B}_i = (ah + \sigma \sqrt{h}\zeta_i)J$ and $M_i^i = \sqrt{4i|h|}$, $i = 1, 2, 3, 4$, we have

- $\bar{X}_{n+1}^{(1,1)} = \bar{X}_n^{(1,1)} + \frac{1}{2} \bar{B}_1(\bar{X}_n^{(1,1)} + \bar{X}_{n+1}^{(1,1)})$;
- $\bar{X}_{n+1}^{(2,2)} = \bar{X}_n^{(2,2)} + \frac{1}{2} \bar{B}_2(\bar{X}_n^{(2,2)} + \bar{X}_{n+1}^{(2,2)}) + \frac{1}{12} \bar{B}_2^2(\bar{X}_n^{(2,2)} - \bar{X}_{n+1}^{(2,2)})$;
- $\bar{X}_{n+1}^{(3,3)} = \bar{X}_n^{(3,3)} + (\frac{1}{2} \bar{B}_3 + \frac{1}{120} \bar{B}_3^3)(\bar{X}_n^{(3,3)} + \bar{X}_{n+1}^{(3,3)}) + \frac{1}{10} \bar{B}_3^2(\bar{X}_n^{(3,3)} - \bar{X}_{n+1}^{(3,3)})$;
- $\bar{X}_{n+1}^{(4,4)} = \bar{X}_n^{(4,4)} + (\frac{1}{2} \bar{B}_4 + \frac{1}{84} \bar{B}_4^3)(\bar{X}_n^{(4,4)} + \bar{X}_{n+1}^{(4,4)}) + (\frac{1}{24} \bar{B}_4^2 + \frac{1}{1680} \bar{B}_4^4)(\bar{X}_n^{(4,4)} - \bar{X}_{n+1}^{(4,4)})$. 
Kubo Oscillator

The figures depict the log of mean squared error (ms-error) as a function of log(h) for different methods and error comparisons. The lines represent:

- Red: the error between the exact solution and numerical method $x^{(1,1)}$
- Dotted red: the reference line with slope 1
- Green: the error between the exact solution and numerical method $x^{(2,2)}$
- Green dash-dotted: the reference line with slope 2
- Blue: the error between the exact solution and numerical method $x^{(3,3)}$
- Blue dotted: the reference line with slope 3
- Pink: the error between the exact solution and numerical method $x^{(4,4)}$
- Pink dotted: the reference line with slope 4

The graphs illustrate how the error decreases as the step size $h$ decreases, with different slopes indicating different rates of convergence.
Kubo Oscillator

Symplectic schemes for some LSHSs
Linear stochastic oscillator

The 2-dim SDE:

\[ dp = -q dt + \sigma dW(t), \quad p(0) = 0, \]
\[ dq = pdt, \quad q(0) = 1, \]

has an exact solution

\[ p(t) = p_0 \cos t + q_0 \sin t + \sigma \int_0^t \sin(t - s)dW(s), \]
\[ q(t) = -p_0 \sin t + q_0 \cos t + \sigma \int_0^t \cos(t - s)dW(s), \]

- The second moment \( \mathbb{E}(p(t)^2 + q(t)^2) = 1 + \sigma^2 t; \)
- (Markus and Weerasinghe) \( p(t) \) has infinitely many zeros, all simple, on each half line \([t_0, \infty)\) for every \( t_0 \geq 0, \) a.s.
Let \( \hat{r} = \hat{s} = 2 \) and \( \hat{r} = 1 \), we get

\[
Z_{n+1} = \left( I - \frac{h}{2} J + \frac{h^2}{12} J^2 \right)^{-1} \left( I + \frac{h}{2} J + \frac{h^2}{12} J^2 \right) Z_n
\]

\[
+ \sum_{k=0}^{N'-1} \left( I - \frac{h - kh'}{2} J \right)^{-1} \left( I + \frac{h - kh'}{2} J \right) \begin{pmatrix} \sigma \\ 0 \end{pmatrix} \Delta W_{n,k}.
\]

(4.1)
Linear stochastic oscillator

- The numerical scheme vs the reference line with slope 3
- The exact solution vs the numerical scheme
- Sample average of $P^2+Q^2$
- $P(t)$ vs time $t$

Liying Sun (UCAS)
Let $\hat{r} = \hat{s} = \check{r} = 1$, we get

\[ Z_{n+1} = \left( I - \frac{h}{2} J \right)^{-1} \left[ I + \frac{h}{2} J \right] Z_n \\
+ \left( I - \frac{h}{2} J \right)^{-1} \left[ I + \frac{h}{2} J \right] \begin{pmatrix} \sigma \\ 0 \end{pmatrix} \Delta W_{n,k}. \]

(4.2)
Linear stochastic oscillator

- Logarithmic error plot
- Phase space trajectory
- Sample average of $P(t)$
- Sample average of $Q(t)$

Liying Sun (UCAS)
Symplectic schemes for some LSHSs
Main references


Thank you!