Numerische Mathematik (2019) 143:555–582
https://doi.org/10.1007/s00211-019-01065-3

Numerische Mathematik

A structure preserving flow for computing Hamiltonian matrix exponential

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Received: 18 April 2018 / Revised: 24 December 2018 / Published online: 1 August 2019

Abstract
This article focuses on computing Hamiltonian matrix exponential. Given a Hamiltonian matrix $\mathcal{H}$, it is well-known that the matrix exponential $e^{\mathcal{H}}$ is a symplectic matrix and its eigenvalues form reciprocal $(\lambda, 1/\bar{\lambda})$. It is important to take care of the symplectic structure for computing $e^{\mathcal{H}}$. Based on the *structure-preserving flow* proposed by Kuo et al. (SIAM J Matrix Anal Appl 37:976–1001, 2016), we develop a numerical method for computing the symplectic matrix pair $(\mathcal{M}, \mathcal{L})$ which represents $e^{\mathcal{H}}$.

Mathematics Subject Classification 15A22 · 15A24 · 65F30 · 34A12

1 Introduction

We first introduce the algebraic structures that we consider in this paper. Let

$$\mathcal{J}_n = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix},$$

where I_n is the $n \times n$ identity matrix. For convenience, we use $\mathcal{J}$ for $\mathcal{J}_n$ by dropping the subscript "n" if the order of $\mathcal{J}_n$ is clear in the context.

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Definition 1.1 1. A matrix $\mathcal{H} \in \mathbb{C}^{2n\times 2n}$ is Hamiltonian if $\mathcal{H}\mathcal{J} = (\mathcal{H}\mathcal{J})^H$.
2. A matrix $\mathcal{S} \in \mathbb{C}^{2n\times 2n}$ is symplectic if $\mathcal{S}\mathcal{J}\mathcal{S}^H = \mathcal{J}$.
3. A matrix pair $(\mathcal{M}, \mathcal{L})$ with $\mathcal{M}, \mathcal{L} \in \mathbb{C}^{2n\times 2n}$ is symplectic if $\mathcal{M}\mathcal{J}\mathcal{M}^H = \mathcal{L}\mathcal{J}\mathcal{L}^H$.

Denote by $Sp(n)$ the multiplicative group of all $2n \times 2n$ symplectic matrices and by $\mathbb{H}(2n)$ the additive group of all $2n \times 2n$ Hermitian matrices. To study the symplectic pairs, Mehrmann and Poloni [17] showed that for each regular symplectic pair $(\mathcal{M}, \mathcal{L})$ with $\mathcal{M},\ \mathcal{L} \in \mathbb{C}^{2n\times 2n}$, there exist $\mathcal{S}_1, \mathcal{S}_2 \in Sp(n)$ and $X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \in \mathbb{H}(2n)$ such that $(\mathcal{M}, \mathcal{L}) \overset{\text{l.e.}}{\sim} \left(\begin{bmatrix} X_{12} & 0 \\ X_{22} & I \end{bmatrix} \mathcal{S}_2, \begin{bmatrix} I & X_{11} \\ 0 & X_{21} \end{bmatrix} \mathcal{S}_1 \right)$, where $\overset{\text{l.e.}}{\sim}$ means the left equivalent relation of matrix pairs. This provides us a classification for symplectic pairs. Specifically, let $\mathcal{S}_1, \mathcal{S}_2 \in Sp(n)$. We may denote the class of symplectic pairs indexed by $\mathcal{S}_1, \mathcal{S}_2$ as

$$\mathbb{S}_{\mathcal{S}_1,\mathcal{S}_2} = \left\{ \left(\begin{bmatrix} X_{12} & 0 \\ X_{22} & I \end{bmatrix} \mathcal{S}_2, \begin{bmatrix} I & X_{11} \\ 0 & X_{21} \end{bmatrix} \mathcal{S}_1 \right) \mid X = [X_{ij}] \in \mathbb{H}(2n) \right\}. \tag{1.1a}$$

The bijective correspondence between $\mathbb{H}(2n)$ and $\mathbb{S}_{\mathcal{S}_1,\mathcal{S}_2}$ can be constructed by the transformation $T_{\mathcal{S}_1,\mathcal{S}_2} : \mathbb{H}(2n) \to \mathbb{S}_{\mathcal{S}_1,\mathcal{S}_2}$ with

$$T_{\mathcal{S}_1,\mathcal{S}_2}(X) = \left(\begin{bmatrix} X_{12} & 0 \\ X_{22} & I \end{bmatrix} \mathcal{S}_2, \begin{bmatrix} I & X_{11} \\ 0 & X_{21} \end{bmatrix} \mathcal{S}_1 \right). \tag{1.1b}$$

Note that (1.1b) shows that the symplectic pairs in $\mathbb{S}_{\mathcal{S}_1,\mathcal{S}_2}$ can be regarded as the vector space $\mathbb{H}(2n)$. The classification for regular symplectic pairs has been considered in [20].

The Structure-Preserving Doubling Algorithms (SDAs) [1,6,15] are employed for solving the stabilizing solutions of Riccati type equations including discrete-time algebraic Riccati equation (DARE) [11,16] and nonlinear matrix equation (NME) [2]. The sequences of symplectic pairs generated by SDAs for DARE and NME are invariant in the classes of symplectic pairs $\mathbb{S}_1 \equiv \mathbb{S}_{I_{2n},I_{2n}}$ and $\mathbb{S}_2 \equiv \mathbb{S}_{\mathcal{J},-I_{2n}}$, respectively. A flow in certain class $\mathbb{S}_{\mathcal{S}_1,\mathcal{S}_2}$ passing through the iterates generated by SDAs and preserving invariant subspaces has been constructed in [8,10]. This flow is known as the *structure-preserving flow*. This flow is constructed as follows.

Structure-preserving flow [8, Theorem 3.1]. Let $\mathcal{S}_1, \mathcal{S}_2 \in Sp(n)$, $\mathcal{H} \in \mathbb{C}^{2n\times 2n}$ be Hamiltonian and $X_0 \in \mathbb{H}(2n)$. Suppose $X(t)$, for $t \in [0, t_1)$, is the solution of the IVP:

$$\dot{X}(t) = \mathcal{M}(t)\mathcal{H}\mathcal{J}\mathcal{M}(t)^H, \quad X(0) = X_0, \tag{1.2}$$

where $(\mathcal{M}(t), \mathcal{L}(t)) = T_{\mathcal{S}_1,\mathcal{S}_2}(X(t))$. If the pair $(\mathcal{M}_0, \mathcal{L}_0) \equiv (\mathcal{M}(0), \mathcal{L}(0))$ satisfies $\mathcal{M}_0 = \mathcal{L}_0 e^{\mathcal{H}_0}$ for some Hamiltonian $\mathcal{H}_0 \in \mathbb{C}^{2n\times 2n}$, then

$$\mathcal{M}(t) = \mathcal{L}(t) e^{\mathcal{H}_0} e^{\mathcal{H}t} \tag{1.3}$$

for all $t \in [0, t_1)$.

Two important properties. The solution $X(t)$ of IVP (1.2) is Hermitian, i.e., $X(t) \in \mathbb{H}(2n)$, because X_0 and $\mathcal{H}\mathcal{J}$ are Hermitian. This implies that the $(\mathcal{M}(t), \mathcal{L}(t)) = T_{\mathcal{S}_1,\mathcal{S}_2}(X(t))$ shall stay in the class of symplectic pairs $\mathbb{S}_{\mathcal{S}_1,\mathcal{S}_2}$, i.e., $(\mathcal{M}(t), \mathcal{L}(t))$ satisfies *structure-preserving property*. Besides this property, $(\mathcal{M}(t), \mathcal{L}(t))$ also preserves the its deflating subspaces. For the cases $\mathcal{H}_0 = 0$ or $\mathcal{H}_0 = \mathcal{H}$ in (1.3), we see that the structure-preserving flow $(\mathcal{M}(t), \mathcal{L}(t))$ satisfies $\mathcal{M}(t) = \mathcal{L}(t)e^{\mathcal{H}t}$ or $\mathcal{M}(t) = \mathcal{L}(t)e^{\mathcal{H}(t+1)}$, respectively, as t varies. That means $(\mathcal{M}(t), \mathcal{L}(t))$ satisfies *eigenvector-preserving property*.

The domain of the solution $X(t)$ of IVP (1.2) can be extended to the whole $\mathbb{R}$ except some isolated points by Radon's lemma. The extended structure-preserving flow $(\mathcal{M}(t), \mathcal{L}(t)) = T_{\mathcal{S}_1,\mathcal{S}_2}(X(t))$ also satisfies those two important properties mentioned above. This flow links the matrix pairs $(\mathcal{M}_k, \mathcal{L}_k)$ generated by SDAs (see [8]). The asymptotic analysis of the flow is studied in [9].

If we let $\mathcal{S}_1 = \mathcal{S}_2 = I_{2n}$ and $X_0 = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}$ in IVP (1.2), we have that $\mathcal{M}_0 = \mathcal{L}_0 = I_{2n}$ and hence, $\mathcal{H}_0 = 0$. Equation (1.3) turns out to be $\mathcal{M}(t) = \mathcal{L}(t)e^{\mathcal{H}t}$. That is, $(\mathcal{M}(t), \mathcal{L}(t)) \in \mathbb{S}_{I,I}$ is a pair form of the symplectic matrix $e^{\mathcal{H}t}$. On the other hand, $\mathcal{L}(t)^{-1}\mathcal{M}(t)$ is the fundamental matrix solution of the linear Hamiltonian differential equation

$$\dot{y}(t) = \mathcal{H}y(t),$$

provided that $\mathcal{L}(t)$ is invertible. Computing matrix exponentials is an important topic and is widely studied by many researchers [18]. To the best of our knowledge, there is no efficient numerical method for computing the matrix exponential $e^{\mathcal{H}}$ that takes care of the special structures of the Hamiltonian matrix $\mathcal{H}$ as well as the symplectic matrix $e^{\mathcal{H}}$. This motivates us to develop an efficient numerical method for computing $e^{\mathcal{H}}$ in the pair form in $\mathbb{S}_{I,I}$.

Throughout this paper, we shall consider the IVP

$$\dot{X}(t) = \mathcal{M}(t)\mathcal{H}\mathcal{J}\mathcal{M}(t)^H, \quad X(0) = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}, \tag{1.4}$$

where $(\mathcal{M}(t), \mathcal{L}(t)) = T(X(t))$ and the Hamiltonian matrix $\mathcal{H} \in \mathbb{C}^{2n\times 2n}$ is denoted by

$$\mathcal{H} = \begin{bmatrix} -A & G \\ H & A^H \end{bmatrix}. \tag{1.5}$$

Here, $G, H \in \mathbb{H}(n)$ and $T : \mathbb{C}^{2n\times 2n} \to \mathbb{C}^{2n\times 2n} \times \mathbb{C}^{2n\times 2n}$ by

$$T(X) = \left(\begin{bmatrix} X_{12} & 0 \\ X_{22} & I \end{bmatrix}, \begin{bmatrix} I & X_{11} \\ 0 & X_{21} \end{bmatrix}\right),$$

where $X = [X_{ij}]_{1\leqslant i,j\leqslant 2}$ and $X_{ij} \in \mathbb{C}^{n\times n}$. Note that the transformation $T_{\mathcal{S}_1,\mathcal{S}_2}$ with $\mathcal{S}_1 = \mathcal{S}_2 = I_{2n}$ defined in (1.1b) is the restriction of T on $\mathbb{H}(2n)$.

To solve IVP (1.4) numerically, we partition $X(t) = [X_{ij}(t)]_{1\leqslant i,j\leqslant 2} \in \mathbb{H}(2n)$, where $X_{ij}(t) \in \mathbb{C}^{n\times n}$. By extracting (1.4), one can see that $X_{11}(t)$ and $X_{22}(t)$ are the solutions of two different matrix Riccati differential equations (MRDEs). Hence, the structure-preserving flows are governed by MRDEs. For solving MRDE numerically, Schiff and Shnider [19] proposed *Möbius Schemes* to compute the flow. Li and Kahan [13] proposed a family of new anadromic methods for solving MRDEs past singularities. Rather than solving IVP (1.4), the paper [12] proposed a numerical method for solving linear Hamiltonian systems in the sense of QR decomposition which preserves the Hamiltonian eigenstructure.

For the two important properties mentioned above, the structure-preserving property (computed solutions stay in $\mathbb{H}(2n)$) is easy to be preserved, and many known numerical schemes do achieve that, e.g., linear multistep and the Runge-Kutta methods. But preserving the eigenvector-preserving property is a nontrivial task achieved. In this paper, we propose a numerical method for IVP (1.4) such that the computed solution not only stays in $\mathbb{H}(2n)$ but also satisfies the eigenvector-preserving property in the absence of rounding errors. Based on the numerical scheme, we can compute the Hamiltonian matrix exponential in the pair form $(\mathcal{M}, \mathcal{L})$. Due to the eigenvector-preserving property, the truncation error in the numerical method is caused by the eigenvalues of $(\mathcal{M}, \mathcal{L})$. Therefore, we can analyze the truncation error of the numerical method by using Taylor expansion of its eigenvalues. However, solving IVP (1.4) numerically to achieve the Hamiltonian matrix exponential is not efficient. We may employ the SDA for large step size to enhance the computing efficiency.

This paper is organized as follows. In Sect. 2, we propose a numerical method for the IVP (1.4). It can be shown that the computed solutions are Hermitian (Sect. 2.2) and satisfy the eigenvector-preserving property (Sect. 2.3). In Sect. 3, the numerical method introduced in Sect. 2 is combined with the SDA to compute the Hamiltonian matrix exponential. The truncation error analysis is also studied. Some numerical experiments are presented in Sect. 4.

2 An algorithm for the structure-preserving flows

In this section, we consider numerical solution of the structure-preserving flows created by the IVP (1.4). Note that the solution $X(t)$ of (1.4) is Hermitian (*structure-preserving property*) because $\mathcal{H}$ is Hamiltonian and $X(0) = X_0 \in \mathbb{H}(2n)$. In addition, the structure-preserving flow $(\mathcal{M}(t), \mathcal{L}(t)) = T(X(t))$ satisfying $\mathcal{M}(t) = \mathcal{L}(t)e^{\mathcal{H}t}$ preserves invariant subspaces on the whole orbit (*eigenvector-preserving property*). We should prefer numerical methods that preserve those two important properties.

2.1 Numerical method

Consider a one-step of the integration from t to $t+\delta$, where δ is the suitable step-size. Let $X^k \approx X(t)$ be Hermitian, where $X(t)$ is the solution of IVP (1.4). An approximation $X^{k+1} \approx X(t+\delta)$ can be computed by

$$\left(X^{k+\frac{1}{2}}\right)^H = X^k + \frac{\delta}{2}\mathcal{M}_k\mathcal{H}\mathcal{J}\mathcal{M}_{k+\frac{1}{2}}^H, \tag{2.1a}$$

$$X^{k+1} = (X^{k+\frac{1}{2}})^H + \frac{\delta}{2}\mathcal{M}_{k+1}\mathcal{H}\mathcal{J}\mathcal{M}_{k+\frac{1}{2}}^H, \tag{2.1b}$$

where $(\mathcal{M}_{k+\frac{1}{2}}, \mathcal{L}_{k+\frac{1}{2}}) = T(X^{k+\frac{1}{2}})$ and $(\mathcal{M}_{k+1}, \mathcal{L}_{k+1}) = T(X^{k+1})$. This defines a one-step map of a numerical method

$$X^{k+1} = \Phi_\delta(X^k). \tag{2.2}$$

Equation (2.1) is an implicit method. The adjoint method Φ_δ^* of a method Φ_δ is the inverse map of the original method with reversed time step $-\delta$, i.e., $\Phi_\delta^* \equiv \Phi_{-\delta}^{-1}$. In other words, $Y = \Phi_\delta^*(X)$ is defined by $X = \Phi_{-\delta}(Y)$. A method for which $\Phi_\delta = \Phi_\delta^*$ is called symmetric. A symmetric method is also called an anadromic method previously [13]. The following theorem shows that the numerical method (2.2) is a symmetric method.

Theorem 2.1 *The numerical method Φ_δ in (2.2) is symmetric, i.e., $\Phi_\delta = \Phi_{-\delta}^{-1}$.*

Proof Let X be given and $Y = \Theta_{\delta/2}(X)$ be the solution of the linear matrix equation

$$Y = X^H + \frac{\delta}{2}\mathcal{M}_Y\mathcal{H}\mathcal{J}\mathcal{M}_X^H, \tag{2.3}$$

where $(\mathcal{M}_X, \mathcal{L}_X) \equiv T(X)$ and $(\mathcal{M}_Y, \mathcal{L}_Y) \equiv T(Y)$. Since $\mathcal{H}$ is Hamiltonian, $\mathcal{H}\mathcal{J}$ is Hermitian. Using the fact that $X^k \in \mathbb{H}(2n)$, it follows from (2.1) that $X^{k+\frac{1}{2}} = \Theta_{\delta/2}(X^k)$ and $X^{k+1} = \Theta_{\delta/2}(X^{k+\frac{1}{2}})$. Hence, $\Phi_\delta = \Theta_{\delta/2} \circ \Theta_{\delta/2}$.

Taking the conjugate transpose of (2.3), we obtain that $X = Y^H - \frac{\delta}{2}\mathcal{M}_X\mathcal{H}\mathcal{J}\mathcal{M}_Y^H$. That is, $\Theta_{\delta/2}^{-1} = \Theta_{-\delta/2}$. Then $\Phi_\delta^{-1} = \Theta_{\delta/2}^{-1} \circ \Theta_{\delta/2}^{-1} = \Theta_{-\delta/2} \circ \Theta_{-\delta/2} = \Phi_{-\delta}$. Hence, $\Phi_\delta = \Phi_{-\delta}^{-1}$. This completes the proof. □

Remark 2.2 A symmetric method has many attractive properties [3,4,7]. If the numerical method $\Phi_\delta(X)$ is symmetric, then the local error, $\|X(t+\delta) - \Phi_\delta(X(t))\|$, is even order, i.e., $\|X(t+\delta) - \Phi_\delta(X(t))\| = O(\delta^{p+1})$ for some even p. In addition, the expansion of global error contains only even powers of δ

$$\|X(t) - X^k\| = C_p(t)\delta^p + C_{p+2}(t)\delta^{p+2} + \cdots$$

where $X(t)$ is the solution of IVP (1.4) and X^k is given in (2.2) with $X^0 = X(0)$. Later we will show that $p = 2$ in Sect. 3.

We note that the matrix $X^{k+\frac{1}{2}}$ in (2.1a) is not usually a Hermitian matrix even when X^k is Hermitian. In the following, we will show that the numerical method (2.2) preserves the following two important properties: the *structure-preserving property* and the *eigenvector-preserving property*.

2.2 Structure-preserving property

Suppose that $X^k = [X^k_{ij}]_{1\leqslant i,j\leqslant 2}$ is Hermitian, where $X^k_{ij} \in \mathbb{C}^{n\times n}$. Partition $X^{k+\frac{1}{2}} = [X^{k+\frac{1}{2}}_{ij}]$ and $X^{k+1} = [X^{k+1}_{ij}]$ compatibly with X^k. Using the notation of Hamiltonian matrix $\mathcal{H}$ in (1.5), we obtain that $\mathcal{H}\mathcal{J} = \begin{bmatrix} -G & -A \\ -A^H & H \end{bmatrix}$ is a Hermitian matrix. From (2.1), the matrices $X^{k+\frac{1}{2}}$ and X^{k+1} can be achieved, respectively, by solving the following two linear matrix equations

$$\begin{aligned} &\begin{bmatrix} I & \frac{\delta}{2}X^k_{12}G \\ 0 & I+\frac{\delta}{2}(X^k_{22}G+A^H) \end{bmatrix} \begin{bmatrix} {X^{k+\frac{1}{2}}_{11}}^H & {X^{k+\frac{1}{2}}_{21}}^H \\ {X^{k+\frac{1}{2}}_{12}}^H & {X^{k+\frac{1}{2}}_{22}}^H \end{bmatrix} \\ &\quad = \begin{bmatrix} X^k_{11} & X^k_{12} \\ X^k_{21} & X^k_{22} \end{bmatrix} + \frac{\delta}{2}\begin{bmatrix} 0 & -X^k_{12}A \\ 0 & -X^k_{22}A+H \end{bmatrix} \end{aligned} \tag{2.4a}$$

and

$$\begin{aligned} &\begin{bmatrix} X^{k+1}_{11} & X^{k+1}_{12} \\ X^{k+1}_{21} & X^{k+1}_{22} \end{bmatrix} \begin{bmatrix} I & 0 \\ \frac{\delta}{2}G{X^{k+\frac{1}{2}}_{12}}^H & I+\frac{\delta}{2}(G{X^{k+\frac{1}{2}}_{22}}^H+A) \end{bmatrix} \\ &\quad = \begin{bmatrix} {X^{k+\frac{1}{2}}_{11}}^H & {X^{k+\frac{1}{2}}_{21}}^H \\ {X^{k+\frac{1}{2}}_{12}}^H & {X^{k+\frac{1}{2}}_{22}}^H \end{bmatrix} + \frac{\delta}{2}\begin{bmatrix} 0 & 0 \\ -A^H{X^{k+\frac{1}{2}}_{12}}^H & -A^H{X^{k+\frac{1}{2}}_{22}}^H+H \end{bmatrix}. \end{aligned} \tag{2.4b}$$

It is easily seen that X^{k+1} exists if $\delta \in \mathcal{E}^k_+$, where

$$\mathcal{E}^k_+ = \left\{\delta \in \mathbb{R}^+ \mid \det(2I+\delta(A+GX^k_{22})) \neq 0,\ \det(2I+\delta(A^H+X^{k+\frac{1}{2}}_{22}G)) \neq 0\right\}. \tag{2.5}$$

It follows from (2.4a) that the sub-matrix $X^{k+\frac{1}{2}}_{22}$ has the form in term of X^k_{22} as

$$X^{k+\frac{1}{2}}_{22} = \left(X^k_{22} + \frac{\delta}{2}[H, -A^H]\begin{bmatrix} I \\ X^k_{22} \end{bmatrix}\right)\left(I + \frac{\delta}{2}[A, G]\begin{bmatrix} I \\ X^k_{22} \end{bmatrix}\right)^{-1}, \tag{2.6a}$$

if $\delta \in \mathcal{E}^k_+$. Substituting (2.6a) into (2.5), we obtain that the set $\mathcal{E}^k_+$ is whole $\mathbb{R}^+$ except for some isolated points because nonzero analytic function has only isolated roots.

Similarly, it follows from (2.4b) that $X_{22}^{k+\frac{1}{2}}$ has the from in term of X_{22}^{k+1} as

$$X_{22}^{k+\frac{1}{2}} = \left(X_{22}^{k+1^H} - \frac{\delta}{2}[H, -A^H] \begin{bmatrix} I \\ X_{22}^{k+1^H} \end{bmatrix} \right) \left(I - \frac{\delta}{2}[A, G] \begin{bmatrix} I \\ X_{22}^{k+1^H} \end{bmatrix} \right)^{-1}, \tag{2.6b}$$

if $\delta \in \Delta_-^{k+1}$, where

$$\Delta_-^{k+1} = \left\{ \delta \in \mathbb{R}^+ \mid \det(2I - \delta(A + GX_{22}^{k+1^H})) \neq 0 \right\}. \tag{2.7}$$

Note that the set Δ_-^{k+1} is also $\mathbb{R}^+$ except for some isolated points. Equation (2.6) shows that if $\delta \in \mathcal{E}_+^k \cap \Delta_-^{k+1}$ then the column space of $\begin{bmatrix} I \\ X_{22}^{k+\frac{1}{2}} \end{bmatrix}$ can also be spanned by the following matrices:

$$\begin{bmatrix} S^{k+\frac{1}{2}} \\ T^{k+\frac{1}{2}} \end{bmatrix} \equiv \begin{bmatrix} I \\ X_{22}^k \end{bmatrix} + \frac{\delta}{2} \begin{bmatrix} A & G \\ H & -A^H \end{bmatrix} \begin{bmatrix} I \\ X_{22}^k \end{bmatrix}, \tag{2.8a}$$

and

$$\begin{bmatrix} \widehat{S}^{k+\frac{1}{2}} \\ \widehat{T}^{k+\frac{1}{2}} \end{bmatrix} \equiv \begin{bmatrix} I \\ X_{22}^{k+1^H} \end{bmatrix} - \frac{\delta}{2} \begin{bmatrix} A & G \\ H & -A^H \end{bmatrix} \begin{bmatrix} I \\ X_{22}^{k+1^H} \end{bmatrix}. \tag{2.8b}$$

From (2.6) and (2.8), we have $X_{22}^{k+\frac{1}{2}} = T^{k+\frac{1}{2}}(S^{k+\frac{1}{2}})^{-1} = \widehat{T}^{k+\frac{1}{2}}(\widehat{S}^{k+\frac{1}{2}})^{-1}$. Hence,

$$\begin{bmatrix} \widehat{S}^{k+\frac{1}{2}} \\ \widehat{T}^{k+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} S^{k+\frac{1}{2}} \\ T^{k+\frac{1}{2}} \end{bmatrix} W, \tag{2.9}$$

where $W = \left[I + \frac{\delta}{2}(A + GX_{22}^k)\right]^{-1} \left[I - \frac{\delta}{2}(A + GX_{22}^{k+1^H})\right]$.

Suppose that $X^k = [X_{ij}^k]$ is Hermitian, so is X_{22}^k. We claim that $X^{k+1} = [X_{ij}^{k+1}]$ is Hermitian. In order to prove this, first we show X_{22}^{k+1} is Hermitian. The method for computing X_{22}^{k+1} in (2.6) is *anadromic numerical method* (see [13]) for MRDEs. It has been proven that anadromic method preserves the "*symmetry property*", i.e., $X_{22}^{k+1} \in \mathbb{H}(n)$. In the following lemma, we show that $X_{22}^{k+1} \in \mathbb{H}(n)$ by using an alternative proof technique.

Lemma 2.3 *If $X^k \in \mathbb{H}(2n)$ and $\delta \in \mathcal{E}_+^k$, then X_{22}^{k+1} is Hermitian, where $\mathcal{E}_+^k$ and $X^{k+1} \equiv [X_{ij}^{k+1}] = \Phi_\delta(X^k)$ are given in (2.2) and (2.5), respectively.*

Proof If $\delta \in \mathcal{E}_+^k$, then $X^{k+1} = \Phi_\delta(X^k)$ exists. Let $\widehat{\mathcal{H}} = \begin{bmatrix} A & G \\ H & -A^H \end{bmatrix}$. Then $\widehat{\mathcal{H}}$ is Hamiltonian. From (2.8) and (2.9), we have $\left(I - \frac{\delta}{2}\widehat{\mathcal{H}}\right)\begin{bmatrix} I \\ X_{22}^{k+1\,H} \end{bmatrix} W^{-1} = \left(I + \frac{\delta}{2}\widehat{\mathcal{H}}\right)\begin{bmatrix} I \\ X_{22}^k \end{bmatrix}$ for $\delta \in \mathcal{E}_+^k \cap \Delta_-^{k+1}$, where Δ_-^{k+1} is defined in (2.7). Let $\Delta_1 = \{\delta \in \mathbb{R}^+ \mid \det(I - \frac{\delta}{2}\widehat{\mathcal{H}}) \neq 0\}$ and $\Delta = \Delta_-^{k+1} \cap \Delta_1$. Then Δ is $\mathbb{R}^+$ except for some isolated points. If $\delta \in \mathcal{E}_+^k \cap \Delta$, then

$$\begin{bmatrix} I \\ X_{22}^{k+1\,H} \end{bmatrix} W^{-1} = \widehat{\mathcal{S}} \begin{bmatrix} I \\ X_{22}^k \end{bmatrix},$$

where $\widehat{\mathcal{S}} = (I - \frac{\delta}{2}\widehat{\mathcal{H}})^{-1}(I + \frac{\delta}{2}\widehat{\mathcal{H}})$. Since $\widehat{\mathcal{S}}$ is the Cayley transform from the Hamiltonian matrix $\widehat{\mathcal{H}}$, it is symplectic. Hence,

$$X_{22}^{k+1\,H} - X_{22}^{k+1} = W^H \left[I, X_{22}^{k\,H}\right] \widehat{\mathcal{S}}^H \mathcal{J} \widehat{\mathcal{S}} \begin{bmatrix} I \\ X_{22}^k \end{bmatrix} W = 0, \text{ for } \delta \in \mathcal{E}_+^k \cap \Delta.$$

Since Δ is $\mathbb{R}^+$ except for some isolated points and $X_{22}^{k+1\,H} - X_{22}^{k+1}$ is continuous on δ, we have X_{22}^{k+1} is Hermitian for $\delta \in \mathcal{E}_+^k$. □

Next, we show that if $\delta \in \mathcal{E}_+^k$, then $X_{12}^{k+1\,H} = X_{21}^{k+1}$, where $X^{k+1} \equiv [X_{ij}^{k+1}] = \Phi_\delta(X^k)$. From (1,2)-block of (2.4a) and (2.4b), we obtain that $X_{21}^{k+\frac{1}{2}\,H} = X_{12}^k \left(I - \frac{\delta}{2}(GX_{22}^{k+\frac{1}{2}\,H} + A)\right)$ and $X_{12}^{k+1} = X_{21}^{k+\frac{1}{2}\,H} \left(I + \frac{\delta}{2}(GX_{22}^{k+\frac{1}{2}\,H} + A)\right)^{-1}$. Hence, we have

$$X_{12}^{k+1} = X_{12}^k \left(I - \frac{\delta}{2}(GX_{22}^{k+\frac{1}{2}\,H} + A)\right)\left(I + \frac{\delta}{2}(GX_{22}^{k+\frac{1}{2}\,H} + A)\right)^{-1}. \tag{2.10}$$

Using the fact that X^k and X_{22}^{k+1} are Hermitian, from (2,1)-block of (2.4a) and (2.4b), we have $X_{12}^{k+\frac{1}{2}} = X_{12}^k \left(I + \frac{\delta}{2}(GX_{22}^k + A)\right)^{-1}$ and $X_{21}^{k+1\,H} = X_{12}^{k+\frac{1}{2}}\Big(I - \frac{\delta}{2} (GX_{22}^{k+1} + A)\Big)$. Hence,

$$X_{21}^{k+1\,H} = X_{12}^k \left(I + \frac{\delta}{2}(GX_{22}^k + A)\right)^{-1}\left(I - \frac{\delta}{2}(GX_{22}^{k+1} + A)\right). \tag{2.11}$$

Lemma 2.4 *If $X^k \in \mathbb{H}(2n)$ and $\delta \in \mathcal{E}_+^k$, then $X_{12}^{k+1} = X_{21}^{k+1\,H}$, where $\mathcal{E}_+^k$ and $X^{k+1} \equiv [X_{ij}^{k+1}] = \Phi_\delta(X^k)$ are given in* (2.2) *and* (2.5)*, respectively.*

Proof If $\delta \in \mathcal{E}_+^k$, then X^{k+1} exists. Hence (2.10) and (2.11) hold. Now we show that $X_{12}^{k+1} = X_{21}^{k+1\,H}$. From (2.10) and (2.11), it suffices to show that

$$\left(I - \frac{\delta}{2}\left(GX_{22}^{k+1} + A\right)\right)\left(I + \frac{\delta}{2}\left(GX_{22}^{k+\frac{1}{2}\,H} + A\right)\right)$$
$$= \left(I + \frac{\delta}{2}\left(GX_{22}^{k} + A\right)\right)\left(I - \frac{\delta}{2}\left(GX_{22}^{k+\frac{1}{2}\,H} + A\right)\right).$$

This is equivalent to the following equation:

$$G\left(X_{22}^k - 2X_{22}^{k+\frac{1}{2}\,H} + X_{22}^{k+1}\right) = \frac{\delta}{2}G\left(X_{22}^k - X_{22}^{k+1}\right)\left(GX_{22}^{k+\frac{1}{2}\,H} + A\right). \quad (2.12)$$

Using the notation of Hamiltonian matrix $\mathcal{H}$ in (1.5), (2.1) can be rewritten as

$$X^k - \frac{\delta}{2}X^k \begin{bmatrix} 0 & 0 \\ GX_{12}^{k+\frac{1}{2}\,H} & GX_{22}^{k+\frac{1}{2}\,H} + A \end{bmatrix}$$
$$= X^{k+\frac{1}{2}\,H} + \frac{\delta}{2}\begin{bmatrix} 0 & 0 \\ A^H X_{12}^{k+\frac{1}{2}\,H} & A^H X_{22}^{k+\frac{1}{2}\,H} - H \end{bmatrix},$$
$$X^{k+1} + \frac{\delta}{2}X^{k+1} \begin{bmatrix} 0 & 0 \\ GX_{12}^{k+\frac{1}{2}\,H} & GX_{22}^{k+\frac{1}{2}\,H} + A \end{bmatrix}$$
$$= X^{k+\frac{1}{2}\,H} - \frac{\delta}{2}\begin{bmatrix} 0 & 0 \\ A^H X_{12}^{k+\frac{1}{2}\,H} & A^H X_{22}^{k+\frac{1}{2}\,H} - H \end{bmatrix}.$$

Summing up the above two equations, we have

$$X^k + X^{k+1} + \frac{\delta}{2}\left(X^{k+1} - X^k\right)\begin{bmatrix} 0 & 0 \\ GX_{12}^{k+\frac{1}{2}\,H} & GX_{22}^{k+\frac{1}{2}\,H} + A \end{bmatrix} = 2X^{k+\frac{1}{2}\,H}.$$

The (2, 2)-block of the last equation is $X_{22}^k + X_{22}^{k+1} - 2X_{22}^{k+\frac{1}{2}\,H} = \frac{\delta}{2}\left(X_{22}^k - X_{22}^{k+1}\right)$ $(GX_{22}^{k+\frac{1}{2}\,H} + A)$. This implies that (2.12) holds. Hence, $X_{12}^{k+1} = X_{21}^{k+1\,H}$. □

In the end of this subsection, we show that $X^{k+1} = \Phi_\delta(X^k)$ is Hermitian if $X^k \in \mathbb{H}(2n)$ and $\delta \in \mathcal{E}_+^k$. Since X^k and X_{22}^k are Hermitian, it follows from (2.1a) that

$$X^{k+\frac{1}{2}}\begin{bmatrix} 0 \\ I \end{bmatrix} = X^{k\,H}\begin{bmatrix} 0 \\ I \end{bmatrix} + \frac{\delta}{2}\mathcal{M}_{k+\frac{1}{2}}\mathcal{H}\mathcal{J}\mathcal{M}_k^H\begin{bmatrix} 0 \\ I \end{bmatrix}$$
$$= X^k\begin{bmatrix} 0 \\ I \end{bmatrix} + \frac{\delta}{2}\mathcal{M}_{k+\frac{1}{2}}\mathcal{H}\mathcal{J}\begin{bmatrix} X_{22}^k \\ I \end{bmatrix}.$$

This implies that $\mathcal{M}_{k+\frac{1}{2}} = \mathcal{M}_k + \frac{\delta}{2}\mathcal{M}_{k+\frac{1}{2}}\mathcal{H}\mathcal{J}\begin{bmatrix} X_{22}^k \\ I \end{bmatrix}\begin{bmatrix} I & 0 \end{bmatrix}$. Hence,

$$\mathcal{M}_{k+\frac{1}{2}}\left(I - \frac{\delta}{2}\mathcal{H}\mathcal{J}\begin{bmatrix} X_{22}^k \\ I \end{bmatrix}\begin{bmatrix} I & 0 \end{bmatrix}\right) = \mathcal{M}_k. \tag{2.13}$$

Similarly, from (2.1b), we have $\mathcal{M}_{k+\frac{1}{2}}\left(I+\frac{\delta}{2}\mathcal{H}\mathcal{J}\begin{bmatrix} X_{22}^{k+1} \\ I \end{bmatrix}\begin{bmatrix} I & 0 \end{bmatrix}\right)=\begin{bmatrix} X_{21}^{k+1\,H} & 0 \\ X_{22}^{k+1\,H} & I \end{bmatrix}$. It follows from Lemmas 2.3 and 2.4 that

$$\mathcal{M}_{k+\frac{1}{2}}\left(I + \frac{\delta}{2}\mathcal{H}\mathcal{J}\begin{bmatrix} X_{22}^{k+1} \\ I \end{bmatrix}\begin{bmatrix} I & 0 \end{bmatrix}\right) = \mathcal{M}_{k+1}. \tag{2.14}$$

Combining (2.13) and (2.14), we obtain that

$$\mathcal{M}_{k+\frac{1}{2}}\left(2I + \frac{\delta}{2}\mathcal{H}\mathcal{J}\begin{bmatrix} X_{22}^{k+1} - X_{22}^k \\ 0 \end{bmatrix}\begin{bmatrix} I & 0 \end{bmatrix}\right) = \mathcal{M}_k + \mathcal{M}_{k+1}. \tag{2.15}$$

Now we are ready to show that $X^{k+1} = \Phi_\delta(X^k)$ is Hermitian.

Theorem 2.5 *If $X^k \in \mathbb{H}(2n)$ and $\delta \in \mathcal{E}_+^k$, then $X^{k+1} = \Phi_\delta(X^k) \in \mathbb{H}(2n)$.*

Proof If $\delta \in \mathcal{E}_+^k$, then $X^{k+1} = \Phi_\delta(X^k)$ exists and (2.15) holds. Now, we show that $X^{k+1} \in \mathbb{H}(2n)$. From (2.1), we have

$$X^{k+1} = X^k + \frac{\delta}{2}(\mathcal{M}_k + \mathcal{M}_{k+1})\mathcal{H}\mathcal{J}\mathcal{M}_{k+\frac{1}{2}}^H. \tag{2.16}$$

Since $X^k \in \mathbb{H}(2n)$, it suffices to show that $(\mathcal{M}_k + \mathcal{M}_{k+1})\mathcal{H}\mathcal{J}\mathcal{M}_{k+\frac{1}{2}}^H \in \mathbb{H}(2n)$. Denote $\triangle X_{22} = X_{22}^{k+1} - X_{22}^k$, then $\triangle X_{22} \in \mathbb{H}(n)$ by Lemma 2.3. From (2.15), we have

$$\begin{aligned}(\mathcal{M}_k + \mathcal{M}_{k+1})\mathcal{H}\mathcal{J}\mathcal{M}_{k+\frac{1}{2}}^H &= \mathcal{M}_{k+\frac{1}{2}}\left(2I + \frac{\delta}{2}\mathcal{H}\mathcal{J}\begin{bmatrix} \triangle X_{22} \\ 0 \end{bmatrix}\begin{bmatrix} I & 0 \end{bmatrix}\right)\mathcal{H}\mathcal{J}\mathcal{M}_{k+\frac{1}{2}}^H \\ &= \mathcal{M}_{k+\frac{1}{2}}\left(2\mathcal{H}\mathcal{J} + \frac{\delta}{2}\mathcal{H}\mathcal{J}\begin{bmatrix} \triangle X_{22} & 0 \\ 0 & 0 \end{bmatrix}\mathcal{H}\mathcal{J}\right)\mathcal{M}_{k+\frac{1}{2}}^H.\end{aligned}$$

Since $\mathcal{H}\mathcal{J}$ and $\triangle X_{22}$ are Hermitian, we obtain that $(\mathcal{M}_k + \mathcal{M}_{k+1})\mathcal{H}\mathcal{J}\mathcal{M}_{k+\frac{1}{2}}^H \in \mathbb{H}(2n)$. From (2.16), we obtain that X^{k+1} is Hermitian directly. □

Next, we develop a structure-preserving algorithm to compute the solution of IVP (1.4). Since the initial matrix $X^0 = X(0)$ is Hermitian, Theorem 2.5 shows that the sequence $\{X^k\}_{k=0}^\infty$ generated by (2.1) guarantees a sequence of Hermitian matrices and hence $(\mathcal{M}_k, \mathcal{L}_k) = T(X^k)$ is symplectic pair for each k.

Algorithm 1

Input:	A Hamiltonian matrix $\mathcal{H}$, positive time step δ, initial $X^0 = X(0)$ in (1.4) and $k = 0$;
Output:	A sequence of Hermitian matrices $\{X^k\}_{k=0}^{\infty}$ which is approximate solution of IVP (1.4).
	For $k = 0, 1, 2, \ldots,$
	`Compute` $X^{k+\frac{1}{2}}$ by solving (2.1a);
	`Compute` the Hermitian matrix X^{k+1} by solving (2.1b);
	End

Here, we note that Algorithm 1 works if $\delta \in \mathcal{E}_+^k$. Consequently, rounding errors may be significantly accumulated if δ is close to the critical points. The number of flops for the first iteration of Algorithm 1 is roughly $\frac{53}{3}n^3$ flops. For the other iterations, it requires about $\frac{71}{3}n^3$ flops, where a flop denotes a multiplication or an addition in complex arithmetic. A more detailed counting is given in Table 1.

2.3 Eigenvector-preserving property

In the following, we will show that the matrix pairs $(\mathcal{M}_k, \mathcal{L}_k) = T(X^k)$ preserve the eigenvectors for each k, where the sequence $\{X^k\}_{k=0}^{\infty}$ is generated by Algorithm 1. Suppose that $(\mathcal{M}_k, \mathcal{L}_k)$ is a regular matrix pair and the column space of U, denoted by $\mathcal{R}(U)$, is an eigenspace of the regular pair $(\mathcal{M}_k, \mathcal{L}_k) = T(X^k)$ corresponding to eigenvalue matrix Λ, i.e., $\mathcal{M}_k U = \mathcal{L}_k U \Lambda$ holds. We shall prove that $\mathcal{R}(U)$ is also an eigenspace of $(\mathcal{M}_{k+1}, \mathcal{L}_{k+1}) = T(X^{k+1})$.

Table 1 Operation counts for the kth iteration in Algorithm 1

Equation	Computation	Flops for $k = 0$	Flops for $k \geqslant 1$
(2.4a)	`Compute` $X_{22}^k G$, $X_{22}^k A$	0	$4n^3$
	`LU decomp. of` $I + \frac{\delta}{2}(X_{22}^k G + A^H)$	$\frac{2}{3}n^3$	$\frac{2}{3}n^3$
	`Solve` $X_{22}^{k+\frac{1}{2}}$, $X_{12}^{k+\frac{1}{2}}$	$4n^3$	$4n^3$
	`Compute` $G{X_{12}^{k+\frac{1}{2}}}^H$, $X_{11}^{k+\frac{1}{2}}$	$2n^3$	$4n^3$
(2.4b)	`Compute` $G{X_{22}^{k+\frac{1}{2}}}^H$, $A^H {X_{22}^{k+\frac{1}{2}}}^H$, $A^H {X_{12}^{k+\frac{1}{2}}}^H$	$6n^3$	$6n^3$
	`LU decomp. of` $I + \frac{\delta}{2}(G{X_{22}^{k+\frac{1}{2}}}^H + A)$	$\frac{2}{3}n^3$	$\frac{2}{3}n^3$
	`Solve` X_{22}^{k+1} (Hermitian)	$\frac{4}{3}n^3$	$\frac{4}{3}n^3$
	`Solve` X_{21}^{k+1}	$2n^3$	$2n^3$
	`Solve` X_{11}^{k+1} (Hermitian)	n^3	n^3
	Total	$\frac{53}{3}n^3$	$\frac{71}{3}n^3$

Let $\mathcal{H}$ with the form in (1.5) be a Hamiltonian matrix and $X = [X_{ij}]$ be Hermitian. Consider the iteration

$$\widehat{X} = X + \delta \widehat{\mathcal{M}} \mathcal{H} \mathcal{J} \mathcal{M}^H, \tag{2.17}$$

where $(\mathcal{M}, \mathcal{L}) = T(X)$ and $(\widehat{\mathcal{M}}, \widehat{\mathcal{L}}) = T(\widehat{X})$. Equation (2.17) can be written as

$$\widehat{X} \begin{bmatrix} I & 0 \\ \delta G X_{21} & I + \delta(G X_{22} + A) \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} - \delta A^H X_{21} & X_{22} + \delta(-A^H X_{22} + H) \end{bmatrix}.$$

Hence, the matrix $\widehat{X}$ of (2.17) exists if $\delta \in \mathcal{E}$, where

$$\mathcal{E} = \{\delta \in \mathbb{R} \mid \det(I + \delta(G X_{22} + A)) \neq 0\}. \tag{2.18}$$

Note that the set $\mathcal{E}$ is whole $\mathbb{R}$ except for some isolated points.

Remark 2.6 The iterations (2.1a) and (2.1b) can be rewritten as the iteration (2.17). For the case (2.1a), X^k and $\mathcal{H}\mathcal{J}$ are Hermitian. Taking the conjugate transpose of (2.1a), we obtain that the iteration (2.17) is consistent with the iteration (2.1a) in which X^k, $X^{k+\frac{1}{2}}$ and $\frac{\delta}{2}$ are replaced by X, $\widehat{X}$ and δ, respectively. For the case (2.1b), we know that X^{k+1} is Hermitian by Theorem 2.5. The iteration (2.1b) can be rewritten as $X^{k+\frac{1}{2}} = X^{k+1} - \frac{\delta}{2} \mathcal{M}_{k+\frac{1}{2}} \mathcal{H} \mathcal{J} \mathcal{M}_{k+1}^H$. Hence, the iteration (2.17) is consistent with the iteration (2.1b) in which X^{k+1}, $X^{k+\frac{1}{2}}$ and $\frac{\delta}{2}$ are replaced by X, $\widehat{X}$ and $-\delta$, respectively.

The following lemma can be obtained by direct calculations.

Lemma 2.7 *Let $X \in \mathbb{C}^{2n \times 2n}$, $(\mathcal{M}, \mathcal{L}) = T(X)$ and $U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$, where $U_1, U_2 \in \mathbb{C}^{n \times \ell}$. Then $\mathcal{M}U = \mathcal{L}U\Lambda$ if and only if $X \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} = \begin{bmatrix} U_1\Lambda \\ -U_2 \end{bmatrix}$.*

Next, we will show that if $X \in \mathbb{H}(2n)$ and $\delta \in \mathcal{E}$, then the matrix pairs $(\mathcal{M}, \mathcal{L}) = T(X)$ and $(\widehat{\mathcal{M}}, \widehat{\mathcal{L}}) = T(\widehat{X})$ have the same invariant subspaces.

Theorem 2.8 *Let $\mathcal{H}$ have the form in (1.5) and the column space of U be an eigenspace of $\mathcal{H}$ corresponding to eigenvalue matrix Λ_H, i.e., $\mathcal{H}U = U\Lambda_H$. Suppose that $X \in \mathbb{H}(2n)$, $\delta \in \mathcal{E}$ in (2.18) and $\widehat{X}$ satisfies (2.17). Let $(\mathcal{M}, \mathcal{L}) = T(X)$ and $(\widehat{\mathcal{M}}, \widehat{\mathcal{L}}) = T(\widehat{X})$. Then*

(i) if $\mathcal{M}U = \mathcal{L}U\Lambda$ and $I - \delta\Lambda_H$ is invertible then $\widehat{\mathcal{M}}U = \widehat{\mathcal{L}}U\hat{\Lambda}$, where $\hat{\Lambda}$ satisfies

$$\Lambda = \hat{\Lambda}(I - \delta\Lambda_H); \tag{2.19}$$

(ii) if $\widehat{\mathcal{M}}U = \widehat{\mathcal{L}}U\hat{\Lambda}$ and $I - \delta(\widehat{X}_{22}G + A^H)$ is invertible, then $\mathcal{M}U = \mathcal{L}U\Lambda$, where Λ satisfies (2.19) and G, A are given in (1.5).

Proof Suppose that $\mathcal{M}U = \mathcal{L}U\Lambda$ and $U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$. From Lemma 2.7, we have

$$X \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} = \begin{bmatrix} U_1\Lambda \\ -U_2 \end{bmatrix}. \tag{2.20}$$

Since X is Hermitian, we have $\mathcal{M}^H \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} = \begin{bmatrix} X_{21} & X_{22} \\ 0 & I \end{bmatrix} \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} = \begin{bmatrix} -U_2 \\ U_1 \end{bmatrix}$. Here the second equality follows from (2.20). Then

$$\begin{aligned} \widehat{\mathcal{M}}\mathcal{H}\mathcal{J}\mathcal{M}^H \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} &= \widehat{\mathcal{M}}\mathcal{H}\mathcal{J} \begin{bmatrix} -U_2 \\ U_1 \end{bmatrix} = \widehat{\mathcal{M}}\mathcal{H} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} \\ &= \begin{bmatrix} \widehat{X}_{12} & 0 \\ \widehat{X}_{22} & I \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} \Lambda_H = \begin{bmatrix} \widehat{X}_{12} \\ \widehat{X}_{22} \end{bmatrix} U_1\Lambda_H + \begin{bmatrix} 0 \\ U_2 \end{bmatrix} \Lambda_H. \end{aligned}$$

From (2.17) and (2.20), we obtain that

$$\widehat{X} \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} = \begin{bmatrix} U_1\Lambda \\ -U_2 \end{bmatrix} + \delta \begin{bmatrix} \widehat{X}_{12} \\ \widehat{X}_{22} \end{bmatrix} U_1\Lambda_H + \delta \begin{bmatrix} 0 \\ U_2 \end{bmatrix} \Lambda_H. \tag{2.21}$$

Hence, $\widehat{X} \begin{bmatrix} -U_2\Lambda \\ U_1(I - \delta\Lambda_H) \end{bmatrix} = \begin{bmatrix} U_1\Lambda \\ -U_2(I - \delta\Lambda_H) \end{bmatrix}$. Since $I - \delta\Lambda_H$ is invertible, denote $\hat{\Lambda} = \Lambda(I - \delta\Lambda_H)^{-1}$. Then we have $\widehat{X} \begin{bmatrix} -U_2\hat{\Lambda} \\ U_1 \end{bmatrix} = \begin{bmatrix} U_1\hat{\Lambda} \\ -U_2 \end{bmatrix}$. It follows from Lemma 2.7 that $\widehat{\mathcal{M}}U = \widehat{\mathcal{L}}U\hat{\Lambda}$. This prove assertion (i).

Now we prove assertion (ii). The proof is the reverse argument of (i). Suppose that $\widehat{\mathcal{M}}U = \widehat{\mathcal{L}}U\hat{\Lambda}$, we have $\widehat{X} \begin{bmatrix} -U_2\hat{\Lambda} \\ U_1 \end{bmatrix} = \begin{bmatrix} U_1\hat{\Lambda} \\ -U_2 \end{bmatrix}$ by Lemma 2.7. Letting $\Lambda = \hat{\Lambda}(I - \delta\Lambda_H)$, Eq. (2.21) holds, and hence,

$$\widehat{X} \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} = \begin{bmatrix} U_1\Lambda \\ -U_2 \end{bmatrix} + \delta\widehat{\mathcal{M}}\mathcal{H}\mathcal{J} \begin{bmatrix} -U_2 \\ U_1 \end{bmatrix}. \tag{2.22}$$

Multiplying $\begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix}$ from the right of (2.17) and combing the resulting equation and (2.22), we have

$$X \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} - \begin{bmatrix} U_1\Lambda \\ -U_2 \end{bmatrix} = \delta\widehat{\mathcal{M}}\mathcal{H}\mathcal{J} \left(\begin{bmatrix} -U_2 \\ U_1 \end{bmatrix} - \mathcal{M}^H \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} \right). \tag{2.23}$$

Let $E = X_{12}^H U_2 \Lambda - X_{22} U_1 - U_2$. Using the fact that X is Hermitian and the notation of $\mathcal{H}$ in (1.5), the second row of (2.23) can be rewritten as

$$-E = \delta[\widehat{X}_{22}, I] \begin{bmatrix} -A & G \\ H & A^H \end{bmatrix} \mathcal{J} \begin{bmatrix} E \\ 0 \end{bmatrix}.$$

That is, $(I - \delta(\widehat{X}_{22}G + A^H))E = 0$. Since $I - \delta(\widehat{X}_{22}G + A^H)$ is invertible, we conclude that $E = 0$. The right-hand side of (2.23) vanishes, hence $X \begin{bmatrix} -U_2\Lambda \\ U_1 \end{bmatrix} = \begin{bmatrix} U_1\Lambda \\ -U_2 \end{bmatrix}$. This implies that $\mathcal{M}U = \mathcal{L}U\Lambda$. □

Note that the condition, "$I - \delta(\widehat{X}_{22}G + A^H)$ is invertible", in Theorem 2.8 (ii) is also the necessary condition for solving matrix X in (2.17) when $\widehat{X}$ is given. If the symplectic matrix pair $(\mathcal{M}, \mathcal{L})$ and the Hamiltonian matrix $\mathcal{H}$ have the same invariant subspace $\mathcal{R}(U)$, it is shown in Theorem 2.8 that the matrix pair $(\widehat{\mathcal{M}}, \widehat{\mathcal{L}})$ preserves the invariant subspace $\mathcal{R}(U)$. The following theorem shows that Algorithm 1 has the eigenvector-preserving property.

Theorem 2.9 *Suppose that $\delta > 0$ is a suitable time step such that $\{(\mathcal{M}_k, \mathcal{L}_k)\}_{k=0}^{\infty}$ generated by Algorithm 1 is well-defined. Then the symplectic matrix pairs $(\mathcal{M}_k, \mathcal{L}_k)$ have common invariant subspaces with the Hamiltonian matrix $\mathcal{H}$.*

Proof Since $\mathcal{M}_0 = \mathcal{L}_0 = I_{2n}$, the statement is true for $k = 0$. Suppose that $(\mathcal{M}_k, \mathcal{L}_k)$ and $\mathcal{H}$ have the same invariant subspaces. Since $\delta \in \mathcal{E}_+^k$ in (2.5), it follows from Theorem 2.8 and Remark 2.6 that the matrix pairs $(\mathcal{M}_k, \mathcal{L}_k)$ and $(\mathcal{M}_{k+1}, \mathcal{L}_{k+1})$ have the same invariant subspaces. This theorem follows from the inductive argument. □

2.4 Remarks on the truncation error of eigenvalues

It is shown in Sect. 2.3 that Algorithm 1 has the eigenvector-preserving property. In this subsection, we shall analyze the truncation error of eigenvalues for Algorithm 1. In the following remark we describe the variation of eigenvalues for each iteration.

Remark 2.10 Suppose that $(\lambda_H, \mathbf{v})$ is an eigenpair of Hamiltonian matrix $\mathcal{H}$ and $\delta \in \mathbb{R}^+$ such that $1 - \frac{\delta}{2}\lambda_H \neq 0$.

(i) Let $X^k \in \mathbb{H}(2n)$ and $\mathcal{M}_k\mathbf{v} = \lambda\mathcal{L}_k\mathbf{v}$, where $(\mathcal{M}_k, \mathcal{L}_k) = T(X^k)$ is a symplectic pair. Suppose that $X^{k+\frac{1}{2}}$, X^{k+1} are generated by (2.1). Let $(\mathcal{M}_{k+\frac{1}{2}}, \mathcal{L}_{k+\frac{1}{2}}) = T(X^{k+\frac{1}{2}})$ and $(\mathcal{M}_{k+1}, \mathcal{L}_{k+1}) = T(X^{k+1})$. From Remark 2.6 and Theorem 2.8, we have

$$\mathcal{M}_{k+\frac{1}{2}}\mathbf{v} = \frac{2\lambda}{2 - \delta\lambda_H}\mathcal{L}_{k+\frac{1}{2}}\mathbf{v} \text{ and } \mathcal{M}_{k+1}\mathbf{v} = \lambda\left(\frac{2 + \delta\lambda_H}{2 - \delta\lambda_H}\right)\mathcal{L}_{k+1}\mathbf{v}. \tag{2.24}$$

(ii) Suppose that $\{X^k\}_{k=0}^{\infty}$ is generated by Algorithm 1. Then $(\mathcal{M}_k, \mathcal{L}_k) = T(X^k)$ is symplectic for each $k = 0, 1, 2, \ldots$. From (2.24), we obtain that

$$\mathcal{M}_k \mathbf{v} = \left(\frac{2+\delta\lambda_H}{2-\delta\lambda_H}\right)^k \mathcal{L}_k \mathbf{v}$$

Denote $\rho = \frac{2+\delta\lambda_H}{2-\delta\lambda_H}$. We have $|\rho| < 1$ if $\lambda_H \in \mathbb{C}_< \equiv \{a+bi \in \mathbb{C} | a < 0\}$ and $|\rho| > 1$ if $\lambda_H \in \mathbb{C}_> \equiv \{a+bi \in \mathbb{C} | a > 0\}$. Suppose that the sequence $\{(\mathcal{M}_k, \mathcal{L}_k)\}_{k=0}^{\infty}$ converges to a regular pair $(\mathcal{M}_*, \mathcal{L}_*)$ as $k \to \infty$. Then $\mathbf{v}$ is a null vector of $\mathcal{M}_*$ (or $\mathcal{L}_*$) if $\lambda_H \in \mathbb{C}_<$ (or $\lambda_H \in \mathbb{C}_>$).

We know that the solution $X(t)$ of IVP (1.4) satisfies $\mathcal{M}(t) = \mathcal{L}(t)e^{\mathcal{H}t}$, where $(\mathcal{M}(t), \mathcal{L}(t)) = T(X(t))$ is symplectic matrix pair. In particular, $(\mathcal{M}(1), \mathcal{L}(1))$ is the symplectic matrix pair that represents the Hamiltonian matrix exponential $e^{\mathcal{H}}$. The approximation symplectic pair $(\mathcal{M}_m, \mathcal{L}_m) = T(X^m)$ can be computed by Algorithm 1 with time step $\delta = 1/m$. In the following, we will analyze the local and global errors of eigenvalues.

Remark 2.11 **Local error of eigenvalues**. Suppose that λ and λ_H are eigenvalues of $(\mathcal{M}_k, \mathcal{L}_k) = (\mathcal{M}(t_0), \mathcal{L}(t_0))$ and $\mathcal{H}$, respectively, where t_0 is given. It follows from (2.24) that

$$\hat{\lambda} = \lambda \frac{2+\delta\lambda_H}{2-\delta\lambda_H} = \lambda + \lambda(\delta\lambda_H) + \frac{\lambda}{2}(\delta\lambda_H)^2 + \frac{\lambda}{2^2}(\delta\lambda_H)^3 + O(\delta^4)$$

is an eigenvalue of $(\mathcal{M}_{k+1}, \mathcal{L}_{k+1})$ which is computed by (2.1). We have that $\lambda e^{\delta\lambda_H}$ is an eigenvalue of the matrix pair $(\mathcal{M}(t_0+\delta), \mathcal{L}(t_0+\delta))$ and

$$\lambda e^{\delta\lambda_H} = \lambda + \lambda(\delta\lambda_H) + \frac{\lambda}{2!}(\delta\lambda_H)^2 + \frac{\lambda}{3!}(\delta\lambda_H)^3 + O(\delta^4).$$

Hence, the local error admits the bound $|\hat{\lambda} - \lambda e^{\delta\lambda_H}| \leqslant C\delta^3$.

Global error of eigenvalues. We analyze the difference of eigenvalue of computed matrix pair $(\mathcal{M}_m, \mathcal{L}_m)$ and symplectic matrix $e^{\mathcal{H}}$. Suppose that λ_H is an eigenvalue of $\mathcal{H}$. We have that $\lambda_S \equiv \left(\frac{2+\delta\lambda_H}{2-\delta\lambda_H}\right)^m$ and e^{λ_H} are eigenvalues of $(\mathcal{M}_m, \mathcal{L}_m)$ and $e^{\mathcal{H}}$, respectively. Then

$$\begin{aligned} e^{\lambda_H} - \lambda_S &= e^{\lambda_H} - \exp\left[m\left(\ln(1+\frac{1}{2m}\lambda_H) - \ln(1-\frac{1}{2m}\lambda_H)\right)\right] \\ &= e^{\lambda_H} - \exp\left[\lambda_H + \frac{1}{12}\lambda_H^3\delta^2 + \frac{1}{80}\lambda_H^5\delta^4 + \cdots\right]. \end{aligned}$$

Denote $d(\delta) = \frac{1}{12}\lambda_H^3\delta^2 + \frac{1}{80}\lambda_H^5\delta^4 + \cdots$. Note that $d(\delta)$ contains only even powers of δ. Then we obtain

$$\begin{aligned} e^{\lambda_H} - \lambda_S &= -e^{\lambda_H}\left[d(\delta) + \frac{1}{2!}(d(\delta))^2 + \frac{1}{3!}(d(\delta))^3 + \cdots\right] \\ &\equiv C_2(\lambda_H)\delta^2 + C_4(\lambda_H)\delta^4 + \cdots, \end{aligned}$$

where the leading coefficient is $C_2(\lambda_H) = \frac{-e^{\lambda_H}\lambda_H^3}{12}$. This coincides with Remark 2.2. Consequently, the relative error has the form

$$R_{\lambda_S} \equiv \frac{\left|e^{\lambda_H} - \lambda_S\right|}{|e^{\lambda_H}|} = \frac{|\lambda_H|^3}{12}\delta^2 + O(\delta^4). \tag{2.25}$$

3 Computing Hamiltonian matrix exponential

Given a Hamiltonian matrix $\mathcal{H} \in \mathbb{C}^{2n\times 2n}$, it is well-known that the matrix exponential, $e^{\mathcal{H}}$, is a symplectic matrix. It is important to take care of the symplectic structure of the computed matrix exponential $e^{\mathcal{H}}$. Note that the symplectic matrix $e^{\mathcal{H}}$ may be ill-conditioned even if $\mathcal{H}$ is well-conditioned. Based on the structure-preserving flow, a structure-preserving method (Algorithm 1) for computing the symplectic matrix pair $(\mathcal{M}, \mathcal{L}) \in \mathbb{S}_{I,I}$ which represents $e^{\mathcal{H}}$ has been developed in Sect. 2. However, Algorithm 1 is not efficient to achieve the Hamiltonian matrix exponential. To overcome this issue, we propose a numerical method that combines Algorithm 1 with the SDA. We will introduce the detailed properties of the SDA in the following subsection.

3.1 Structure-preserving Doubling Algorithms

Suppose that $(\mathcal{M}_k, \mathcal{L}_k) = \left(\begin{bmatrix} E_k & 0 \\ -H_k & I \end{bmatrix}, \begin{bmatrix} I & G_k \\ 0 & E_k^H \end{bmatrix}\right) \in \mathbb{S}_{I,I}$ is a symplectic pair, where E_k is invertible and $G_k, H_k \in \mathbb{H}(2n)$. The iteration of the SDA is given as follows

$$\begin{aligned} E_{k+1} &= E_k(I + G_kH_k)^{-1}E_k, \\ G_{k+1} &= G_k + E_kG_k(I + H_kG_k)^{-1}E_k^H, \\ H_{k+1} &= H_k + E_k^H(I + H_kG_k)^{-1}H_kE_k. \end{aligned} \tag{3.1}$$

If $I+G_kH_k$ is invertible, then the iteration is well-defined. We denote $(\mathcal{M}_{k+1}, \mathcal{L}_{k+1}) = \left(\begin{bmatrix} E_{k+1} & 0 \\ -H_{k+1} & I \end{bmatrix}, \begin{bmatrix} I & G_{k+1} \\ 0 & E_{k+1}^H \end{bmatrix}\right)$. It has been shown in [1,15] that

(i) $(\mathcal{M}_{k+1}, \mathcal{L}_{k+1}) \in \mathbb{S}_{I,I}$ is a regular symplectic pair;
(ii) if $\mathcal{M}_k = \mathcal{L}_k e^{t\mathcal{H}}$, then $\mathcal{M}_{k+1} = \mathcal{L}_{k+1}e^{2t\mathcal{H}}$.

Note that items (i) and (ii) mean that the SDA has the *structure-preserving property* and the *eigenvector-preserving property*, respectively. Furthermore, item (ii) implies

Table 2 Operation counts for the kth iteration of SDA

Computation	Flops
`LU decomp.` of $I + G_k H_k$	$(2 + \frac{2}{3})n^3$
`Compute` $(I + G_k H_k)^{-1} E_k$	$2n^3$
`Compute` E_{k+1},	$2n^3$
`Compute` H_{k+1}, G_{k+1} (Hermitian)	$3n^3$ (for H_{k+1})+$5n^3$ (for G_{k+1})
Total	$\frac{44}{3}n^3$

that $(\mathcal{M}_{k+1}, \mathcal{L}_{k+1})$ is the squaring of the pair $(\mathcal{M}_k, \mathcal{L}_k)$. In addition, the SDA requires about $\frac{44}{3}n^3$ flops for each iteration. A more detailed counting is given in Table 2. Note that the squaring of a $2n \times 2n$ matrix requires about $2(2n)^3 = 16n^3$ flops, which is larger than $\frac{44}{3}n^3$ flops required for SDA.

3.2 An efficient algorithm for Hamiltonian matrix exponential

The main idea of the algorithm for computing Hamiltonian matrix exponential is as follows. We combine Algorithm 1 with the SDA. The first, we employ Algorithm 1 to compute the approximation solution $T(X^m) \approx (\mathcal{M}(1/2^s), \mathcal{L}(1/2^s))$ of IVP (1.4) with time step $\delta = 1/(m2^s)$. Here s and m are positive integers to be determined in Theorem 3.1. The next, the approximation solution $T(X^m)$ is used for the initial of the SDA to compute approximations of

$$(\mathcal{M}(1/2^{s-1}), \mathcal{L}(1/2^{s-1})),\ (\mathcal{M}(1/2^{s-2}), \mathcal{L}(1/2^{s-2})), \ldots,\ (\mathcal{M}(1), \mathcal{L}(1)).$$

The following is the algorithm.

Algorithm 2

Input: A Hamiltonian matrix $\mathcal{H}$, positive integers m, s, initial $X^0 = X(0)$ in (1.4) and $\delta = \frac{1}{2^s m}$;

Output: A symplectic matrix pair $(\mathcal{M}, \mathcal{L}) \in \mathbb{S}_{I,I}$ which represents $e^{\mathcal{H}}$.

For $k = 0, 1, \ldots, m-1$,
  `Compute` the Hermitian matrix X^{k+1} by solving (2.1);
End
Set $E_0 = X^m_{12}$, $G_0 = X^m_{11}$ and $H_0 = -X^m_{22}$;
For $k = 0, 1, \ldots, s-1$,
  `Run` (3.1);
End
Denote $\mathcal{M} = \begin{bmatrix} E_s & 0 \\ -H_s & I \end{bmatrix}$ and $\mathcal{L} = \begin{bmatrix} I & G_s \\ 0 & E_s^H \end{bmatrix}$;

Equations (2.1) and (2.4) are equivalent. Therefore, (2.1) is solvable for $k = 0$ if $\delta = \frac{1}{2^s m} < 2\min\{\|X^k_{22}G + A^H\|^{-1}, \|G{X^{k+\frac{1}{2}}_{22}}^H + A\|^{-1}\}$. In the end of this subsection, we shall see that the optimal choice for m is $m = 1$ with respect to the cost. For running (3.1), rounding errors may be accumulated if $I + G_k H_k$ is nearly singular. Note that Algorithm 2 satisfies the eigenvector-preserving property in the absence of rounding errors. We shall analyze the truncation error of eigenvalues in the following.

Truncation error bound of eigenvalues: Suppose that λ_H is an eigenvalue of $\mathcal{H}$. The symplectic matrix pair $T(X^m)$ in Algorithm 2 has eigenvalue

$$\left(\frac{2+\frac{1}{2^s m}\lambda_H}{2-\frac{1}{2^s m}\lambda_H}\right)^m = \exp\left[m\left(\ln(1+\frac{\lambda_H}{2^{s+1}m}) - \ln(1-\frac{\lambda_H}{2^{s+1}m})\right)\right]$$
$$= \exp\left[\frac{\lambda_H}{2^s} + \frac{\lambda_H}{3\times 2^s}\left(\frac{\lambda_H}{2^{s+1}m}\right)^2 + \frac{\lambda_H}{5\times 2^s}\left(\frac{\lambda_H}{2^{s+1}m}\right)^4 + \cdots\right].$$

Hence, the output symplectic matrix pair $(\mathcal{M}, \mathcal{L})$ has eigenvalue

$$\lambda_S \equiv \left[\left(\frac{2+\frac{1}{2^s m}\lambda_H}{2-\frac{1}{2^s m}\lambda_H}\right)^m\right]^{2^s} = e^{\lambda_H}\exp\left[\frac{\lambda_H}{3}\left(\frac{\lambda_H}{2^{s+1}m}\right)^2 + \frac{\lambda_H}{5}\left(\frac{\lambda_H}{2^{s+1}m}\right)^4 + \cdots\right]$$

which approximates the eigenvalue e^{λ_H} of symplectic matrix $e^{\mathcal{H}}$. Let $\kappa = \frac{|\lambda_H|}{2^{s+1}m}$. Using the inequality $|e^x - 1| = |x + \frac{x^2}{2!} + \cdots| \leqslant |x| + \frac{|x|^2}{2!} + \cdots = e^{|x|} - 1$, the relative error is

$$R_{\lambda_S} \equiv \frac{|\lambda_S - e^{\lambda_H}|}{|e^{\lambda_H}|} = \left|\exp\left[\frac{\lambda_H}{3}\left(\frac{\lambda_H}{2^{s+1}m}\right)^2 + \frac{\lambda_H}{5}\left(\frac{\lambda_H}{2^{s+1}m}\right)^4 + \cdots\right] - 1\right|$$
$$\leqslant \exp\left[\frac{|\lambda_H|}{3}(\kappa^2 + \kappa^4 + \cdots)\right] - 1 = \exp\left[\frac{|\lambda_H|}{3}\left(\frac{\kappa^2}{1-\kappa^2}\right)\right] - 1. \tag{3.2}$$

Now we have the following theorem.

Theorem 3.1 *For a given ε with $0 < \varepsilon < 1$, if $4^s m^2 \geqslant \frac{|\lambda_H|^3}{6\varepsilon(2-\varepsilon)} + |\lambda_H|^2$, then $R_{\lambda_S} < \varepsilon$.*

Proof If $\lambda_H = 0$ then $R_{\lambda_S} = 0 < \varepsilon$ by (3.2). When $\lambda_H \neq 0$, using $\kappa = \frac{|\lambda_H|}{2^{s+1}m}$ and $4^s m^2 > |\lambda_H|^2$, we have $\frac{1-\kappa^2}{\kappa^2} = \frac{2^{2s+2}m^2 - |\lambda_H|^2}{|\lambda_H|^2} > 0$. Then

$$\frac{|\lambda_H|^3}{6\varepsilon(2-\varepsilon)} \leqslant \frac{1}{4}(4^{s+1}m^2 - 4|\lambda_H|^2) < \frac{1}{4}(2^{2s+2}m^2 - |\lambda_H|^2) = \frac{|\lambda_H|^2}{4}\frac{1-\kappa^2}{\kappa^2}.$$

This implies $\frac{|\lambda_H|}{3}\frac{\kappa^2}{1-\kappa^2} < \varepsilon - \frac{\varepsilon^2}{2}$ because $\frac{1-\kappa^2}{\kappa^2} > 0$ and $0 < \varepsilon < 1$. Using the fact that $\varepsilon - \frac{\varepsilon^2}{2} < \ln(1+\varepsilon)$, we have $\frac{|\lambda_H|}{3}\frac{\kappa^2}{1-\kappa^2} < \ln(1+\varepsilon)$. Hence, $\exp\left[\frac{|\lambda_H|}{3}\left(\frac{\kappa^2}{1-\kappa^2}\right)\right] < 1+\varepsilon$. It follows from (3.2) that $R_{\lambda_S} < \varepsilon$. □

Remark 3.2 Suppose that m and s are given in Algorithm 2. It follows from Theorem 3.1 that

$$R_{\lambda_S} \leqslant 1 - \sqrt{1 - \frac{|\lambda_H|^3}{6(m^2 4^s - |\lambda_H|^2)}} \equiv \hat{R}_{\lambda_S}. \tag{3.3}$$

This shows that the relative *truncation* error of eigenvalue $\lambda_S \approx e^{\lambda_H}$ depends on the magnitude of λ_H. Roughly speaking, in the absence of rounding errors, the eigenvalue λ_S of matrix pair $(\mathcal{M}, \mathcal{L})$ has a better accuracy whenever λ_H is closed to the origin. Rather than Algorithm 2 using the pair form of $e^{\mathcal{H}}$, traditional numerical methods for computing $e^{\mathcal{H}}$ have a better accuracy whenever λ_H has a larger real part (see [5,18]).

Optimal choice of steps m and s: Algorithm 2 requires

$$f(m, s) = \frac{53}{3}n^3 + \frac{71(m-1)}{3}n^3 + \frac{44s}{3}n^3 \tag{3.4}$$

flops for computing the symplectic matrix pair $(\mathcal{M}, \mathcal{L})$. For a given tolerance ε with $0 < \varepsilon < 1$, we set $\tau = (\frac{|\lambda_H|^3}{6\varepsilon(2-\varepsilon)} + |\lambda_H|^2)^{1/2}$ and consider the optimization problem

$$\min_{2^s m \geqslant \tau} f(m, s). \tag{3.5}$$

Note that the $m, s \in \mathbb{R}$ in (3.5). Since $f(m, s)$ is linear, it is well-known that the optimizer $(m_*, s_*) \in \mathbb{R}^2$ will satisfy $2^{s_*} m_* = \tau$. Substituting $m = \tau 2^{-s}$ into (3.4), we have $f(s) = \frac{53}{3}n^3 + \frac{71(\tau 2^{-s}-1)}{3}n^3 + \frac{44s}{3}n^3$. Then $f'(s) = \frac{44}{3}n^3 - \frac{71\tau 2^{-s}\ln 2}{3}n^3$. Since $m = \tau 2^{-s}$ the optimizer

$$m_* = \frac{44}{71 \ln 2} \approx 0.8941 \text{ and } s_* = \log_2(\tau/m_*).$$

It is well-known that $|\lambda_H| \leqslant \|\mathcal{H}\|$ for each eigenvalue λ_H of $\mathcal{H}$. Since the numbers m and s in Algorithm 2 should be positive integers, we suggest that $m = 1$ and $s = \lceil \frac{1}{2}\log_2(\frac{\|\mathcal{H}\|^3}{6\varepsilon(2-\varepsilon)} + \|\mathcal{H}\|^2)\rceil$, where $\lceil\cdot\rceil$ is ceiling function.

4 Numerical results

In this section, all numerical experiments are carried out using MATLAB R2014a with IEEE double-precision floating-point arithmetic. We show some numerical experiments to demonstrate that (i) Algorithm 1 preserves the *eigenvector-preserving property*; and (ii) how Algorithms 1 and 2 work for computing Hamiltonian matrix exponential. Suppose that $\mathbf{v}_\ell$ for $\ell = 1, \ldots, 2n$ are eigenvectors of Hamiltonian matrix $\mathcal{H}$. To verify the eigenvector-preserving property of computed iteration pair $(\mathcal{M}_k, \mathcal{L}_k)$ corresponding to eigenvectors $\mathbf{v}_\ell$, we use

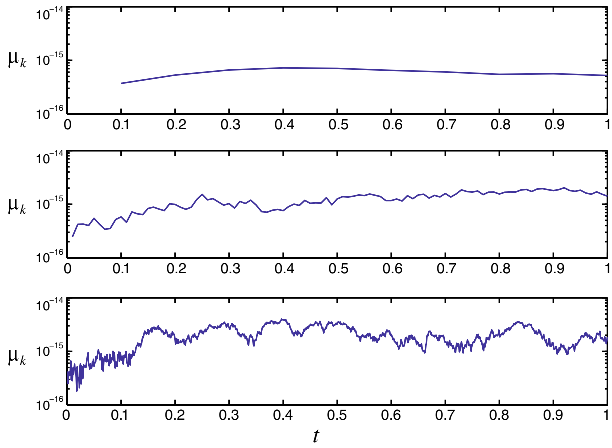

Fig. 1 The values μ_k varies $t_k = k\delta$, $k = 0, 1, \ldots, m$, for cases $\delta = 0.1$ (top), 0.01 (middle) and 0.001 (bottom)

$$\mu_k = \max_{1 \leqslant \ell \leqslant 2n} \sigma_{\min}\left(\left[\mathcal{M}_k \frac{\mathbf{v}_\ell}{\|\mathbf{v}_\ell\|}, \mathcal{L}_k \frac{\mathbf{v}_\ell}{\|\mathbf{v}_\ell\|}\right]\right),$$

where $\sigma_{\min}(\cdot)$ denotes the minimal singular value.

To illustrate the relative errors of eigenvalues, we assume $e^{\mathcal{H}}$ has reciprocal eigenvalues e^{λ_H} and $1/e^{\lambda_H}$ with $|e^{\lambda_H}| \leqslant 1$. Since the computed pair $(\mathcal{M}, \mathcal{L})$ that approximates $e^{\mathcal{H}}$ is a symplectic pair, the approximate eigenvalues are $(1+\epsilon)e^{\lambda_H}$ and $1/((1+\epsilon)e^{\lambda_H})$, where $0 < |\epsilon| \ll 1$. It is easily seen that the relative errors of these two approximate eigenvalues have the form $|\epsilon|$ and $|\epsilon| + O(|\epsilon|^2)$. That is, they have the same leading coefficient in terms of error $|\epsilon|$. Therefore, in the following examples, we only show the relative errors for eigenvalues inside the unit circle.

Example 4.1 Consider the Hamiltonian Jordan canonical form [14] $\mathfrak{J} = \left[\begin{array}{c|c} R & 0 \\ \hline 0 & -R^H \end{array}\right] \in \mathbb{R}^{4\times 4}$, where $R = \begin{bmatrix} -1 & 0 \\ 0 & -5 \end{bmatrix}$. We construct the Hamiltonian matrix $\mathcal{H} = \left[\begin{array}{c|c} -A & G \\ \hline H & A^H \end{array}\right] = \mathcal{S}\mathfrak{J}\mathcal{S}^{-1} \in \mathbb{R}^{4\times 4}$, where $\mathcal{S}$ is a randomly generated symplectic matrix. Note that $\mathcal{S}^{-1} = \mathcal{J}\mathcal{S}^H\mathcal{J}^H$. We let $\mathbf{v}_\ell = \mathcal{S}(:, \ell)$, for $\ell = 1, \ldots, 4$. Their corresponding eigenvalues are $\lambda_{H,1} = -1$, $\lambda_{H,2} = -5$, $\lambda_{H,3} = 1$ and $\lambda_{H,4} = 5$. Note that $e^{\lambda_{H,1}} = 0.36788$ and $e^{\lambda_{H,2}} = 6.7379 \times 10^{-3}$ are eigenvalues of $e^{\mathcal{H}}$ inside the unit circle.

First, we divide the time domain [0, 1] into m subintervals, i.e., the length of each subinterval is $\delta = 1/m$. Taking $t_k = k\delta$, $k = 0, 1, \ldots, m$, Algorithm 1 is employed to compute a sequence of Hermitian matrices $\{X^k\}_{k=0}^m$ and let $(\mathcal{M}_k, \mathcal{L}_k) = T(X^k)$. We choose $\delta = 0.1$, $\delta = 0.01$ and $\delta = 0.001$. The numerical results are shown in Fig. 1 and Table 3. Figure 1 shows that Algorithm 1 preserves the eigenvectors well as shown in Theorem 2.9, for cases $\delta = 0.1, 0.01$ and 0.001. The nonzero values of μ_k are caused

Table 3 Numerical results for Example 4.1

	$e^{\lambda_{H,1}} = 0.36788$			$e^{\lambda_{H,2}} = 6.7379 \times 10^{-3}$		
	$\lambda_{S,1}$	$R_{\lambda_{S,1}}$	$\lvert\lambda_{H,1}\rvert^3\delta^2/12$	$\lambda_{S,2}$	$R_{\lambda_{S,2}}$	$\lvert\lambda_{H,2}\rvert^3\delta^2/12$
$\delta = 0.1$	3.6757e−01	8.3424e−04	8.3333e−04	6.0466e−03	1.0260e−01	1.0417e−01
$\delta = 0.01$	3.6788e−01	8.3334e−06	8.3333e−06	6.7309e−03	1.0415e−03	1.0417e−03
$\delta = 0.001$	3.6788e−01	8.3333e−08	8.3333e−08	6.7379e−03	1.0417e−05	1.0417e−05

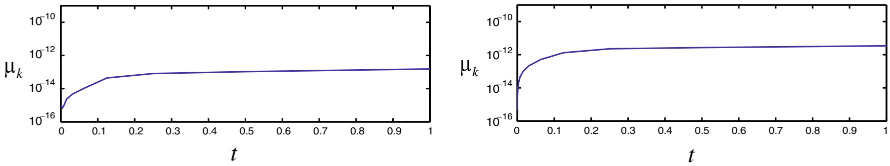

Fig. 2 The values μ_k varies $t \in [0, 1]$ for case 1: Algorithm 2 with $m = 1, s = 10$ (left) and for case 2: Algorithm 2 with $m = 1, s = 15$ (right)

by rounding errors. We see that the value of μ_k increases as the step size δ decreases. Let $(\mathcal{M}_m, \mathcal{L}_m) = T(X^m)$ be the computed matrix pair that approximates $e^{\mathcal{H}}$. Suppose that $\lambda_{S,1}$ and $\lambda_{S,2}$ with $|\lambda_{S,2}| < |\lambda_{S,1}| < 1$ are eigenvalues of $(\mathcal{M}_m, \mathcal{L}_m)$. Table 3 shows the numerical results of this example including the computed eigenvalues $\lambda_{S,\ell}$, their relative errors $R_{\lambda_{S,\ell}}$ and the leading term of relative error for $\ell = 1, 2$. Here, the leading term of relative error for eigenvalue $\lambda_{S,\ell}$ is $\frac{|\lambda_{H,\ell}|^3}{12}\delta^2$ as showed in (2.25).

In next example, Algorithm 2 is employed to compute a matrix pair form of $e^{\mathcal{H}}$, where $\mathcal{H}$ is a Hamiltonian matrix.

Example 4.2 We construct a Hamiltonian matrix $\mathcal{H} \in \mathbb{R}^{24\times 24}$ which has eigenpairs $\{(\lambda_{H,\ell}, \mathbf{v}_\ell)\}_{\ell=1}^{24}$, where $\lambda_{H,\ell} = -3(\ell-1)$ and $\lambda_{H,12+\ell} = 3(\ell-1)$ for $\ell = 1, \ldots, 12$. Here, $e^{\lambda_{H,\ell}}$ are inside the closed unit circle for $\ell = 1, \ldots, 12$.

We compute a matrix pair that approximates $e^{\mathcal{H}}$ by Algorithm 2 with the following cases: for case 1, $m = 1$ and $s = 10$; and for case 2, $m = 1$ and $s = 15$. The numerical results are shown in Fig. 2 and Table 4.

Figure 2 shows that Algorithm 2 preserves the eigenvectors in each case. The $O(10^{-13})$ error in case 1 and the $O(10^{-12})$ error in case 2 are caused by rounding errors. Table 4 shows that the numerical results of this example including the computed eigenvalues $\{\lambda_{S,\ell}\}_{\ell=1}^{12}$, their relative errors $\{R_{\lambda_{S,\ell}}\}_{\ell=1}^{12}$ and upper bounds $\{\hat{R}_{\lambda_{S,\ell}}\}_{\ell=1}^{12}$ of relative *truncation* errors given in (3.3). In Table 4, the relative error increases as $|\lambda_{H,\ell}|$ increases, as shown in Remark 3.2. For the data given in italics, we can see $\hat{R}_{\lambda_{S,\ell}}$ provides a good upper bound for the relative error $R_{\lambda_{S,\ell}}$. For the rest cases, we see that the relative errors $R_{\lambda_{S,\ell}} > \hat{R}_{\lambda_{S,\ell}}$. Here, only truncation errors are involved in the estimation of $\hat{R}_{\lambda_{S,\ell}}$, but rounding errors are absent. Hence, the computed relative error $R_{\lambda_{S,\ell}}$ may be larger than the value $\hat{R}_{\lambda_{S,\ell}}$ because of the accumulated rounding errors.

In the following example, we show the numerical results for Algorithm 2 when the Hamiltonian matrix $\mathcal{H}$ is deflective.

Example 4.3 Consider the Hamiltonian Jordan canonical form [14] $\mathfrak{J} = \left[\begin{array}{c|c} R & D \\ \hline G & -R^H \end{array}\right] \in \mathbb{C}^{12\times 12}$, where $\alpha_1, \alpha_2, \ \beta, \ \gamma, \ \tau \in \mathbb{R}$ and

$$R = \begin{bmatrix} \alpha_1 + i\alpha_2 & 1 & 0 \\ 0 & \alpha_1 + i\alpha_2 & 1 \\ 0 & 0 & \alpha_1 + i\alpha_2 \end{bmatrix} \oplus \left[\, i\beta \,\right] \oplus \begin{bmatrix} i\gamma & -\frac{\sqrt{2}}{2} \\ 0 & \frac{i}{2}(\gamma+\tau) \end{bmatrix},$$

Table 4 Numerical results for Example 4.2

$e^{\lambda_{H,\ell}}$	Algorithm 2: $m = 1$ and $s = 10$			Algorithm 2: $m = 1$ and $s = 15$		
	$\lambda_{S,\ell}$	$R_{\lambda_{S,\ell}}$	$\hat{R}_{\lambda_{S,\ell}}$	$\lambda_{S,\ell}$	$R_{\lambda_{S,\ell}}$	$\hat{R}_{\lambda_{S,\ell}}$
$e^{0} = 1.0000$	1.0000	1.6498e−13	0	1.0000	2.2627e−12	0
$e^{-3} = 4.9787e{-}02$	*4.9787e−02*	*2.1458e−06*	*2.1458e−06*	*4.9787e−02*	*2.0955e−09*	*2.0955e−09*
$e^{-6} = 2.4788e{-}03$	*2.4787e−03*	*1.7166e−05*	*1.7167e−05*	*2.4788e−03*	*1.6760e−08*	*1.6764e−08*
$e^{-9} = 1.2341e{-}04$	*1.2340e−04*	*5.7935e−05*	*5.7942e−05*	*1.2341e−04*	*5.6577e−08*	*5.6578e−08*
$e^{-12} = 6.1442e{-}06$	*6.1434e−06*	*1.3732e−04*	*1.3736e−04*	*6.1442e−06*	*1.3412e−07*	*1.3412e−07*
$e^{-15} = 3.0590e{-}07$	*3.0582e−07*	*2.6819e−04*	*2.6831e−04*	*3.0590e−07*	*2.6181e−07*	*2.6193e−07*
$e^{-18} = 1.5230e{-}08$	*1.5223e−08*	*4.6341e−04*	*4.6374e−04*	*1.5230e−08*	*4.5062e−07*	*4.5262e−07*
$e^{-21} = 7.5826e{-}10$	*7.5770e−10*	*7.3580e−04*	*7.3658e−04*	*7.5826e−10*	*5.9797e−07*	*7.1875e−07*
$e^{-24} = 3.7751e{-}11$	*3.7710e−11*	*1.0974e−03*	*1.0998e−03*	3.7751e−11	3.5452e−06	1.0729e−06
$e^{-27} = 1.8795e{-}12$	*1.8797e−12*	*9.9602e−05*	*1.5666e−03*	1.8795e−12	2.9494e−05	1.5276e−06
$e^{-30} = 9.3576e{-}14$	9.3341e−14	2.5093e−03	2.1499e−03	9.3587e−14	1.1165e−04	2.0955e−06
$e^{-33} = 4.6589e{-}15$	4.0266e−15	1.3573e−01	2.8631e−03	4.6339e−15	5.3639e−03	2.7891e−06

$$D = 0_{3\times 3} \oplus \left[\, 1 \,\right] \oplus \begin{bmatrix} 0 & -\frac{\sqrt{2}}{2}i \\ \frac{\sqrt{2}}{2}i & \frac{\gamma-\tau}{2} \end{bmatrix}, \quad G = 0_{3\times 3} \oplus 0_{3\times 3} \oplus \begin{bmatrix} 0 & 0 \\ 0 & -\frac{\gamma-\tau}{2} \end{bmatrix}.$$

We construct the Hamiltonian matrix $\mathcal{H} = \mathcal{S}\mathfrak{J}\mathcal{S}^{-1} \in \mathbb{C}^{12\times 12}$, where $\mathcal{S}$ is a randomly generated symplectic matrix. $\mathcal{H}$ has eigenvalues $\alpha_1 + i\alpha_2, -\alpha_1 + i\alpha_2, i\beta, i\gamma$ and $i\tau$ with multiplicities 3, 3, 2, 3 and 1, respectively. The sizes of Jordan blocks corresponding to eigenvalues $\alpha_1 + i\alpha_2$, $-\alpha_1 + i\alpha_2$ and $i\gamma$ are 3 and the size of other Jordan block corresponding to eigenvalue $i\beta$ is 2. Let $J(\alpha_1 + i\alpha_2)$, $J(-\alpha_1 + i\alpha_2)$, $J(i\gamma) \in \mathbb{C}^{3\times 3}$, $J(i\beta) \in \mathbb{C}^{2\times 2}$ and $J(i\tau) \in \mathbb{C}$ denote the Jordan blocks. Let $U_{\alpha_1+i\alpha_2}$, $U_{-\alpha_1+i\alpha_2}$, $U_{i\gamma} \in \mathbb{C}^{12\times 3}$, $U_{i\beta} \in \mathbb{C}^{12\times 2}$ and $U_{i\tau} \in \mathbb{C}^{12\times 1}$ be of full column rank such that

$$\mathcal{H}U_{\lambda_H} = U_{\lambda_H} J(\lambda_H),$$

where $\lambda_H = \pm\alpha_1 + i\alpha_2,\ i\beta,\ i\gamma,\ i\tau$. To measure the accuracy of the computed $(\mathcal{M}, \mathcal{L})$ we use the relative residual

$$RRes_{\lambda_H} = \frac{\|\mathcal{M}U_{\lambda_H} - \mathcal{L}U_{\lambda_H} e^{J(\lambda_H)}\|}{\|\mathcal{M}U_{\lambda_H}\| + \|\mathcal{L}U_{\lambda_H} e^{J(\lambda_H)}\|},$$

where $\|\cdot\|$ is the spectral norm.

Let $\alpha_1 = 15$, $\alpha_2 = 10$, $\beta = 5$, $\gamma = 10$ and $\tau = 15$. We compute a matrix pair that approximates $e^{\mathcal{H}}$ by Algorithm 2 with case 1: $m = 1$ and $s = 10$ and case 2: $m = 1$ and $s = 10$. The numerical results are shown in Table 5. This demonstrates Algorithm 2 preserves invariant subspaces even if the corresponding eigenvalue has Jordan blocks. For $\lambda_H = i\beta,\ i\gamma$ and $i\tau$ and $s = 15$, we can see that the eigenvalues of $e^{J(\lambda_H)}$ are on the unit circle and the relative residual, $RRes_{\lambda_H}$, are inside $O(10^{-7})$.

For a given Hamiltonian matrix $\mathcal{H}$, we can compute the matrix $\texttt{expm}(\mathcal{H})$ by using the $\texttt{Matlab}$ function $\texttt{expm}$ and the matrix pair $(\mathcal{M}, \mathcal{L})$ by Algorithm 2. Some numerical comparisons including eigenvalues, $e^{\mathcal{H}}b$ and $(e^{\mathcal{H}})^{-1}b$ are shown in the following example.

Example 4.4 Let $\mathfrak{J} = \left[\begin{array}{c|c} R & 0 \\ \hline 0 & -R^H \end{array}\right] \in \mathbb{R}^{4\times 4}$ be Hamiltonian canonical form, where $R = \begin{bmatrix} -1 & 0 \\ 0 & -\alpha \end{bmatrix}$. The Hamiltonian matrix is constructed by $\mathcal{H} = \mathcal{S}\mathfrak{J}\mathcal{S}^{-1} \in \mathbb{R}^{4\times 4}$, where $\mathcal{S}$ is a randomly generated symplectic matrix.

We compute $\texttt{expm}(\mathcal{H})$ by using the $\texttt{Matlab}$ function $\texttt{expm}$ and the matrix pair $(\mathcal{M}, \mathcal{L})$ by Algorithm 2 with $m = 1$ and $s = 15$ for $\alpha = 5,\ 10,\ 15$ and 20. It is easily seen that $\lambda_H \in \{\pm 1, \pm\alpha\}$ is an eigenvalue of $\mathcal{H}$ and hence, $e^{\lambda_H} \in \{e^{\pm 1}, e^{\pm\alpha}\}$ is the exact eigenvalue of matrix $e^{\mathcal{H}}$. Table 6 shows the relative errors $R_{\lambda_S} = \frac{|\lambda_S - e^{\lambda_H}|}{|e^{\lambda_H}|}$, where λ_S is computed eigenvalue of $\texttt{expm}(\mathcal{H})$ or $(\mathcal{M}, \mathcal{L})$. We see that $\texttt{expm}(\mathcal{H})$ has good relative errors for the largest eigenvalue e^{α} in all cases. But it has poor relative error for the smallest eigenvalue $e^{-\alpha}$ when $\alpha = 15$ and 20. The matrix $\texttt{expm}(\mathcal{H})$ seems not symplectic because of the lack of the reciprocal structure of

Table 5 Numerical results for Example 4.3

λ_H	e^{λ_H}	Algorithm 2: $m = 1, s = 10$	Algorithm 2: $m = 1, s = 15$
		$RRes_{\lambda_H}$	$RRes_{\lambda_H}$
$\alpha_1 + i\alpha_2 = 15 + 10i$	$-2.7429\text{e}{+}06 - 1.7784\text{e}{+}06i$	2.4077e−04	4.4981e−07
$-\alpha_1 + i\alpha_2 = -15 + 10i$	$-2.5667\text{e}{-}07 - 1.6642\text{e}{-}07i$	2.3482e−04	2.4248e−07
$i\beta = 5i$	$2.8366\text{e}{-}01 - 9.5892\text{e}{-}01i$	5.9590e−06	5.8855e−09
$i\gamma = 10i$	$-8.3907\text{e}{-}01 - 5.4402\text{e}{-}01i$	1.4148e−04	1.2190e−07
$i\tau = 15i$	$-7.5969\text{e}{-}01 + 6.5029\text{e}{-}01i$	3.9736e−05	3.8805e−08

Table 6 Relative error of eigenvalues of $\texttt{expm}(\mathcal{H})$ computed by using $\texttt{Matlab}$ and $(\mathcal{M}, \mathcal{L})$ computed by Algorithm 2 (Example 4.4)

α	λ_H	e^{λ_H}	$\texttt{Matlab}$: $\texttt{expm}(\mathcal{H})$	Algorithm 2: $m = 1, s = 15$	
			R_{λ_S}	R_{λ_S}	$\hat{R}_{\lambda_S}$
5	−1 (1)	0.3679 (2.718)	2.943e−14 (3.921e−15)	9.360e−11 (9.359e−11)	7.761e−11
	−5 (5)	6.738e−03 (1.484e+02)	1.116e−12 (3.447e−15)	9.712e−09 (9.712e−09)	9.701e−09
10	−1 (1)	0.3679 (2.718)	1.427e−11 (2.655e−12)	7.870e−11 (7.870e−11)	7.761e−11
	−10 (10)	4.540e−05 (2.203e+04)	3.907e−08 (1.321e−15)	7.761e−08 (7.761e−08)	7.761e−08
15	−1 (1)	0.3679 (2.718)	2.069e−11 (6.723e−13)	7.331e−11 (7.331e−11)	7.761e−11
	−15 (15)	3.059e−07 (3.269e+06)	1.365e−04 (1.425e−16)	2.620e−07 (2.618e−07)	2.619e−07
20	−1 (1)	0.3679 (2.718)	2.509e−08 (1.971e−09)	7.811e−11 (7.813e−11)	7.761e−11
	−20 (20)	2.061e−09 (4.852e+08)	3.352 (4.791e−15)	3.456e−07 (7.959e−08)	6.209e−07

Table 7 Relative errors $RRes_x = \|x - x_e\|/\|x_e\|$ and $RRes_y = \|y - y_e\|/\|y_e\|$ (Example 4.4)

α	`Matlab` function: `expm`($\mathcal{H}$)		Alg. 2: $m = 1, s = 15$	
	$RRes_x$	$RRes_y$	$RRes_x$	$RRes_y$
5	9.0305e−16	1.3479e−12	9.9050e−09	9.7559e−09
10	1.1907e−15	2.3975e−08	7.7609e−08	7.7617e−08
15	1.0218e−15	7.8515e−05	2.6196e−07	2.6191e−07
20	4.3737e−15	1.8545e−01	6.8425e−08	1.8692e−07

eigenvalues. The symplectic pair $(\mathcal{M}, \mathcal{L})$ has better relative error for eigenvalues $e^{\pm 1}$ which demonstrate the results in Remark 3.2.

Let $b \in \mathbb{R}^4$ be randomly generated, $x = e^{\mathcal{H}} b$ and $y = (e^{\mathcal{H}})^{-1} b$. We compute $x = \texttt{expm}(\mathcal{H}) * b$ ($x = \mathcal{L} \backslash (\mathcal{M} * b)$) and $y = \texttt{expm}(\mathcal{H}) \backslash b$ ($y = \mathcal{M} \backslash (\mathcal{L} * b)$) to approximate the vectors $x = e^{\mathcal{H}} b$ and $y = (e^{\mathcal{H}})^{-1} b$ by each method, respectively. To measure the accuracy of the computed solution, we use the relative errors $RRes_x = \frac{\|x - x_e\|}{\|x_e\|}$ and $RRes_y = \frac{\|y - y_e\|}{\|y_e\|}$, where $x_e = \mathcal{S} e^{\mathfrak{J}} \mathcal{J} \mathcal{S}^H \mathcal{J}^H b$ and $y_e = \mathcal{S} e^{-\mathfrak{J}} \mathcal{J} \mathcal{S}^H \mathcal{J}^H b$. The numerical results are shown in Table 7. We see that it has high accuracy for the computed vector x by using $x = \texttt{expm}(\mathcal{H}) * b$, but poor relative error for the computed vector y by using $y = \texttt{expm}(\mathcal{H}) \backslash b$ when α is large. The relative errors $RRes_x$ and $RRes_y$ for Algorithm 2 are stable and are inside $O(10^{-7})$.

Acknowledgements We thank the Editor, Professor Volker Mehrmann, and the anonymous referees for their careful reading, valuable comments and suggestions on the manuscript.

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