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N. Guglielmi, D. Kressner, C. Lubich

http://mathicse.epfl.ch

Phone: +41 21 69 37648

Address:
EPFL - SB - MATHICSE (Bâtiment MA)
Station 8 - CH-1015 - Lausanne - Switzerland

Fax: +41 21 69 32545

COMPUTING EXTREMAL POINTS OF SYMPLECTIC PSEUDOSPECTRA AND SOLVING SYMPLECTIC MATRIX NEARNESS PROBLEMS

NICOLA GUGLIELMI*, DANIEL KRESSNER†, AND CHRISTIAN LUBICH‡

Abstract. We study differential equations that lead to extremal points in symplectic pseudospectra. In a two-level approach, where on the inner level we compute extremizers of the symplectic ε-pseudospectrum for a given ε and on the outer level we optimize over ε, this is used to solve symplectic matrix nearness problems such as the following: For a symplectic matrix with eigenvalues of unit modulus, we aim to determine the nearest complex symplectic matrix such that some or all eigenvalues leave the complex unit circle. Conversely, for a symplectic matrix with all eigenvalues lying off the unit circle, we consider the problem of computing the nearest symplectic matrix that has an eigenvalue on the unit circle.

Key words. Symplectic pseudospectrum, distance to instability, low-rank dynamics, differential equations on Stiefel manifolds.

AMS subject classifications. 15A18, 65K05, 93B36, 93B40, 49N35, 65F15, 93B52, 93C05

1. Introduction.

For a chosen matrix norm $\|\cdot\|$ and a given $\varepsilon > 0$, the ε-pseudospectrum of a matrix $A \in \mathbb{C}^{n\times n}$ is the set

$$\Lambda_\varepsilon(A) = \{\lambda \in \mathbb{C} : \lambda \text{ is an eigenvalue of some } B \in \mathcal{M} \text{ with } \|B - A\| \le \varepsilon\}, \qquad (1.1)$$

where $\mathcal{M} = \mathbb{C}^{n\times n}$. In recent years there has been substantial interest in *structured pseudospectra* [KKK10, Kar11, Ru06], where A is in some linear subspace $\mathcal{M} \subset \mathbb{C}^{n\times n}$ and the perturbed matrices B in (1.1) are restricted to lie in the same subspace $\mathcal{M}$. Cases of particular interest include $\mathcal{M} = \mathbb{R}^{n\times n}$ (real pseudospectra [BRQ98, GL13, Ru06]) and $\mathcal{M} = \mathrm{Ham}(n)$, the space of complex or real Hamiltonian matrices (Hamiltonian pseudospectra [ABKMM11, GKL13]). There are, however, also structures of interest where $\mathcal{M} \subset \mathbb{C}^{n\times n}$ is not a linear space, but a matrix Lie group or, more generally, a matrix manifold. In that case the above definition of the structured ε-pseudospectrum on $\mathcal{M}$ still makes sense, but in addition another notion of pseudospectrum is of interest, in which the distance is not measured in the ambient space of the manifold, but in the tangent space $T_A\mathcal{M}$ at the given matrix A:

$$\begin{aligned}\widetilde{\Lambda}_\varepsilon(A) = \{\lambda \in \mathbb{C} : \lambda &\text{ is an eigenvalue of some } B \in \mathcal{M} \text{ such that} \\ &B = \exp_A(\Omega) \text{ for some } \Omega \in T_A\mathcal{M} \text{ with } \|\Omega\| \le \varepsilon\}.\end{aligned} \qquad (1.2)$$

Here $\exp_A : T_A\mathcal{M} \to \mathcal{M}$ is the exponential map on the manifold $\mathcal{M}$ (see, e.g., [AMS08]). When $\mathcal{M}$ is a matrix Lie group (a subgroup of $\mathrm{GL}(n)$), then $\exp_A(\Omega) = e^{\Omega}A$. For a linear space $\mathcal{M}$, we have $\exp_A(\Omega) = A + \Omega$ and hence the two definitions coincide. For a general manifold, the two pseudospectral sets are $O(\varepsilon^2)$ close for small ε.

For $\mathcal{M} = \mathbb{C}^{n\times n}$ and certain linear structures, computationally tractable characterizations of (1.1) have been derived that allow to decide whether a certain point

*Dipartimento di Matematica Pura ed Applicata, Università degli Studi di L' Aquila, Via Vetoio - Loc. Coppito, I-67010 L' Aquila, Italy. Email: guglielm@univaq.it

†EPFL-SB-MATHICSE-ANCHP, Station 8, CH-1015 Lausanne, Switzerland. Email: daniel.kressner@epfl.ch

‡Mathematisches Institut, Universität Tübingen, Auf der Morgenstelle 10, D–72076 Tübingen, Germany. Email: lubich@na.uni-tuebingen.de

$z \in \mathbb{C}$ is contained in $\Lambda_\varepsilon(A)$, see [KKK10] and the references therein. Little is known in this direction for nonlinear structures, except for the Lie groups of real orthogonal and unitary matrices [Sun97, TG06].

In the present paper we consider the case where $\mathcal{M}$ is the Lie group of symplectic matrices, i.e., all matrices A of even dimension $n = 2d$ that satisfy

$$A^* J A = J, \qquad J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}.$$

The corresponding Lie algebra consists of the set of Hamiltonian matrices, that is, the matrices H satisfying $H^*J + JH = 0$. We recall that the eigenvalues of a symplectic matrix lie symmetric with respect to the unit circle. More precisely, if λ is an eigenvalue of A with right eigenvector y, then $1/\bar{\lambda}$ is an eigenvalue with left eigenvector Jy, see [Fa00] for more properties of symplectic eigenvalue problems.

We will always work with the Frobenius norm in this paper, $\|\cdot\| \equiv \|\cdot\|_F$. We are particularly interested in computing extremal pseudospectral points, i.e., those points in the symplectic ε-pseudospectra (1.1) or (1.2) that have locally maximal absolute value. We will obtain these points and the corresponding extremal matrices as stationary points of a differential equation that we derive; cf. [GL11, GL13] for related differential equations for determining the pseudospectral radius in the case of unstructured complex or real matrices. Combining this approach with an optimization over ε allows us to solve symplectic matrix nearness problems such as the following:

(A) *Given a symplectic matrix with no eigenvalues on the unit circle, find a nearest symplectic matrix having some eigenvalue of unit modulus.*

(B) *Given a symplectic matrix with all eigenvalues on the unit circle, find a nearest symplectic matrix such that arbitrarily close to that matrix there exist symplectic matrices with eigenvalues off the unit circle.*

These problems are the symplectic analogues of matrix nearness problems that were studied for Hamiltonian matrices in [ABKMM11, GKL13]. Here we transfer the two-level approach of [GKL13] to the symplectic case. Related questions have recently been studied in [BPSS13] for linearly structured matrix polynomials arising from the calibration of multivariate ARMA models. Other potential applications include robust solvability of discrete algebraic Riccati equations (see Section 6.1), passivity for discrete-time systems, and robust stability of symplectic integrators (see Section 6.2). The main difference with respect to the Hamiltonian case treated in [GKL13] is that we pass from a linear to a nonlinear manifold, which is more intricate. In particular the proof of the low-rank property of extremal perturbations gets more involved.

The paper is organized as follows. In Section 2 and 3 we characterize extremal perturbations, and derive matrix differential equations that have the extremizers as attractive stationary points. Then, in Section 5 we propose algorithms to compute the desired distances. Finally, in Section 6, we consider two applications: the unique solvability of discrete algebraic Riccati equations and a stability problem of symplectic integrators near elliptic stationary points.

In what follows, we will make frequent use of the following standard perturbation result for eigenvalues. Here and in the following, we denote $\dot{} = d/dt$.

LEMMA 1.1. *Consider the differentiable $n \times n$ matrix valued function $C(t)$ for t in a neighborhood of 0 . Let $\lambda(t)$ be an eigenvalue of $C(t)$ converging to a simple eigenvalue λ_0 of $C_0 = C(0)$ as $t \to 0$. Let x_0 and y_0 be left and right eigenvectors, respectively, of C_0 corresponding to λ_0, that is, $(C_0 - \lambda_0 I)y = 0$ and $x^*(C_0 - \lambda_0 I) = 0$.*

Then, $x_0^* y_0 \neq 0$ and $\lambda(t)$ is differentiable near $t = 0$ with

$$\dot{\lambda}(0) = \frac{x_0^* \dot{C}(0) y_0}{x_0^* y_0}.$$

2. Setting I: Measuring perturbations in the ambient space. In the following we discuss the problem of finding a symplectic matrix such that its distance to the given symplectic matrix A equals ε in the Frobenius norm and its eigenvalue of largest modulus has largest modulus among all such matrices. The general approach is analogous to [GL13] for unstructured real and complex matrices, but it requires nontrivial adaptations to the symplectic case.

Our goal is to construct a family of symplectic matrices $B(t) = A + \varepsilon E(t)$ where $\|E(t)\|_F = 1$ such that $\lim_{t\to\infty} E(t) = E_\infty$ and an eigenvalue of $A + \varepsilon E_\infty$ is a locally extremal point, i.e. with largest modulus, of the symplectic Frobenius-norm ε-pseudospectrum of A. The derivative $\dot{E}(t)$ shall be chosen in a direction that gives the maximum possible increase of $|\lambda(t)|$ for the largest eigenvalue $\lambda(t)$ of $A + \varepsilon E(t)$. Due to the constraint $\|E(t)\|_F^2 = 1$, the derivative must satisfy

$$\frac{d}{dt}\|E(t)\|_F^2 = 0 \quad \Longrightarrow \quad \mathrm{Re}\,\langle E, \dot{E}\rangle = 0,$$

where $\langle X, Y\rangle = \sum_{i,j} \overline{x}_{ij} y_{ij} = \mathrm{trace}(X^* Y)$ is the Frobenius inner product.

Let $B(t) = A + \varepsilon E(t)$ with $\|E(t)\|_F = 1$ be a path of symplectic matrices near A. Consider a path $\lambda(t)$ of simple eigenvalues of $B(t)$, with left and right eigenvectors $x(t)$ and $y(t)$, respectively, of unit norm and with $x(t)^* y(t) > 0$. We note, using Lemma 1.1, that (omitting the argument t)

$$\tfrac{1}{2}\,\frac{d}{dt}\,|\lambda(t)|^2 = \mathrm{Re}(\overline{\lambda}\dot{\lambda}) = \mathrm{Re}\frac{(\lambda x)^* \dot{B} y}{x^* y} = \varepsilon \mathrm{Re}\frac{(\lambda x)^* \dot{E} y}{x^* y}. \tag{2.1}$$

Since $B(t)$ is symplectic, we have that

$$\dot{B}B^{-1} \text{ is Hamiltonian.}$$

In first order, maximizing the largest eigenvalues therefore leads to the optimization problem considered in the following lemma. Note that $X_{\mathrm{herm}} := \frac{1}{2}(X + X^*)$ denotes the hermitian part of a matrix X.

LEMMA 2.1. *Let $E, B \in \mathbb{C}^{n\times n}$ be given with $EB^* \neq O$, and let $u, v \in \mathbb{C}^n$ be given vectors with $u \neq 0$, $Bv \neq 0$. Then the unique solution of the optimization problem*

$$Z_\star = \arg\max\{\mathrm{Re}\,(u^*\, ZB\, v) \,:\, Z \text{ Hamiltonian},\ \|ZB\|_F = 1,\ \mathrm{Re}\,\langle E, ZB\rangle = 0\}$$

is given by

$$\mu\, JZ_\star = (Ju(Bv)^*)_{\mathrm{herm}} - \kappa (JEB^*)_{\mathrm{herm}}, \tag{2.2}$$

where

$$\kappa = \frac{\big\langle (JEB^*)_{\mathrm{herm}}, (Ju(Bv)^*)_{\mathrm{herm}} \big\rangle}{\|(JEB^*)_{\mathrm{herm}}\|_F^2} \tag{2.3}$$

and μ is the Frobenius norm of the matrix on the right-hand side.

Proof. Using that J is unitary and JZ hermitian, that the Frobenius product of a hermitian with a skew-hermitian matrix is purely imaginary, and that the Frobenius product of two hermitian matrices is real, we note

$$\begin{aligned}\mathrm{Re}(u^* ZBv) &= \mathrm{Re}\langle u(Bv)^*, Z\rangle = \mathrm{Re}\langle Ju(Bv)^*, JZ\rangle \\ &= \mathrm{Re}\langle (Ju(Bv)^*)_{\mathrm{herm}}, JZ\rangle = \langle (Ju(Bv)^*)_{\mathrm{herm}}, JZ\rangle.\end{aligned}$$

The real part of the inner product of a given nonzero vector (a matrix here) with elements from a subspace is uniquely maximized by orthogonally projecting the vector to that subspace.

The expression in (2.2) is the orthogonal projection of $(Ju(Bv)^*)_{\mathrm{herm}}$ to the space of all Hermitian JZ with

$$\mathrm{Re}\,\langle E, ZB\rangle = \mathrm{Re}\,\langle JE, JZB\rangle = \mathrm{Re}\langle JEB^*, JZ\rangle = \langle (JEB^*)_{\mathrm{herm}}, JZ\rangle = 0.$$

This concludes the proof. ☐

Choosing x and y as left and right eigenvectors of B associated to λ and setting $u = \lambda x$ and $v = y$, as in (2.1), the optimizer in (2.2) becomes

$$\mu\, JZ_\star = |\lambda|^2 \Big((Jxy^*)_{\mathrm{herm}} - \kappa (JEB^*)_{\mathrm{herm}} \Big),$$

where

$$\kappa = \big\langle (JEB^*)_{\mathrm{herm}}, (Jxy^*)_{\mathrm{herm}} \big\rangle / \|(JEB^*)_{\mathrm{herm}}\|_F^2.$$

Therefore the results of Lemmas 1.1 and 2.1 suggest to consider the following steepest ascent differential equation for $|\lambda(t)|$, where we replace Z by $\dot{B}B^{-1}$:

$$J\dot{B}B^{-1} = (Jxy^*)_{\mathrm{herm}} - \kappa (JEB^*)_{\mathrm{herm}}, \tag{2.4}$$

where

$$\varepsilon E = B - A \quad \text{with} \quad \|E\|_F = 1.$$

From the derivation we get immediately the desired monotonicity result for $|\lambda(t)|$.

THEOREM 2.2. *Let the symplectic matrices $B(t)$ satisfy the differential equation (2.4). If $\lambda(t)$ is a simple eigenvalue of $B(t)$, then*

$$\frac{d}{dt}\, |\lambda(t)|^2 \geq 0. \tag{2.5}$$

Proof. Inserting (2.4), we obtain the explicit expression

$$\mathrm{Re}\,(\lambda x)^* \dot{B} y = |\lambda|^2 \Big(\|(Jxy^*)_{\mathrm{herm}}\|_F^2 - \kappa \langle (Jxy^*)_{\mathrm{herm}}, (JEB^*)_{\mathrm{herm}} \rangle \Big). \tag{2.6}$$

Using the definition of κ and introducing the matrix

$$R = (JEB^*)_{\mathrm{herm}} / \|(JEB^*)_{\mathrm{herm}}\|_F$$

of unit norm, (2.6) yields

$$\mathrm{Re}\,(\lambda x)^* \dot{B} y = |\lambda|^2 \Big(\|(Jxy^*)_{\mathrm{herm}}\|^2 - \big\langle (Jxy^*)_{\mathrm{herm}}, R \big\rangle^2 \Big) \geq 0 \tag{2.7}$$

by the Cauchy–Schwarz inequality. Applying (2.1) concludes the proof. ∎

The stationary points of (2.4) are characterized as follows.

Theorem 2.3. *The following statements are equivalent along solutions of* (2.4) *provided that* $|\lambda| \neq 1$*:*

1. $\dfrac{d}{dt}\,|\lambda|^2 = 0$.
2. $\dot{B} = 0$.
3. $(J(B-A)B^*)_{\mathrm{herm}}$ *is a real multiple of* $(Jxy^*)_{\mathrm{herm}}$.

Proof. Assuming $(Jxy^*)_{\mathrm{herm}} \neq 0$ the statement of the theorem follows directly from (2.7) and Lemma 1.1.

Now suppose that $(Jxy^*)_{\mathrm{herm}} = 0$. Then Jx is a scalar multiple of y. However, when x is a left eigenvector of the symplectic matrix B belonging to the eigenvalue λ, then Jx is a right eigenvector belonging to $1/\overline{\lambda}$. Moreover, y is a right eigenvector belonging to the eigenvalue λ. A linear dependence of Jx and y therefore implies $1/\overline{\lambda} = \lambda$, that is, $|\lambda|^2 = 1$ in contradiction to the assumption. ∎

Note that since the eigenvectors Jx and y are linearly independent when $|\lambda| \neq 1$, the matrix

$$(Jxy^*)_{\mathrm{herm}} = \tfrac{1}{2}(Jx, y)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}(Jx, y)^*$$

has rank 2. However, at a stationary point, the rank of $B - A$ is not 2 in general, since only the hermitian part of $J(B-A)B^*$ is restricted to be of rank 2.

Finally we provide the following characterization of extremizers.

Theorem 2.4. *Fix a symplectic matrix* $A \in \mathbb{C}^{n\times n}$ *and* $\varepsilon > 0$. *Let* $B_\star \in \mathbb{C}^{n\times n}$ *be a symplectic matrix such that* $\|B_\star - A\|_F = \varepsilon$. *Let* $\lambda_\star$ *be a simple eigenvalue of* $B_\star$ *satisfying* $|\lambda_\star| \neq 1$ *and consider the corresponding left and right eigenvectors* x *and* y*, respectively, both of unit norm and with* $x^*y > 0$. *Then the following two statements are equivalent:*

1. *Every differentiable path* $(B(t), \lambda(t))$ *such that* $B(t)$ *is symplectic,* $\|B(t) - A\|_F \leq \varepsilon$ *and* $\lambda(t)$ *is an eigenvalue of* $B(t)$*, with* $B(0) = B_\star$ *and* $\lambda(0) = \lambda_\star$*, satisfies* $\frac{d}{dt}\,|\lambda(t)|^2 \leq 0$ *for small* $t \geq 0$.
2. *The hermitian parts of* $J(B_\star - A)B_\star^*$ *and* Jxy^* *are positive multiples of each other.*

Proof. We first show that the negation of *1.* implies the negation of *2.* If there is any path $B(t)$ through $B_\star$ such that $\frac{d}{dt}\,|\lambda|^2(0) > 0$, then the maximization property of Lemma 2.1 shows that the solution path of (2.4) is such a path. Hence $B_\star$ does not determine a stationary point of (2.4), and Theorem 2.3 then yields that $(J(B_\star - A)B_\star^*)_{\mathrm{herm}}$ is not a real multiple of $(Jxy^*)_{\mathrm{herm}}$.

Conversely, if $(J(B_\star - A)B_\star^*)_{\mathrm{herm}}$ is not a real multiple of $(Jxy^*)_{\mathrm{herm}}$, then $B_\star$ does not determine a stationary point of (2.4), and Theorems 2.2 and 2.3 yield that $\frac{d}{dt}\,|\lambda|^2(0) > 0$ along the solution path of (2.4).

It remains to discuss the case $(J(B_\star - A)B_\star^*)_{\mathrm{herm}} = -\beta (Jxy^*)_{\mathrm{herm}}$ with $\beta > 0$. Consider the path $B(t)$ that solves the differential equation

$$J\dot{B}B^{-1} = (Jxy^*)_{\mathrm{herm}}, \qquad B(0) = B_\star.$$

First we note that $\|B(t) - A\|_F$ decreases along the path $B(t)$ in a neighborhood of

$t = 0$. Indeed, at $t = 0$ we have

$$\begin{aligned}\mathrm{Re}\langle B - A, \dot{B}\rangle &= \mathrm{Re}\langle J(B-A)B^*, J\dot{B}B^{-1}\rangle = \mathrm{Re}\langle J(B-A)B^*, (Jxy^*)_{\mathrm{herm}}\rangle \\ &= \langle (J(B-A)B^*)_{\mathrm{herm}}, (Jxy^*)_{\mathrm{herm}}\rangle \\ &= -\beta\langle (Jxy^*)_{\mathrm{herm}}, (Jxy^*)_{\mathrm{herm}}\rangle = -\beta\|(Jxy^*)_{\mathrm{herm}}\|_F^2 < 0.\end{aligned}$$

Moreover,

$$\begin{aligned}\mathrm{Re}\,(\lambda x)^*\dot{B}y &= \mathrm{Re}\langle \lambda xy^*, \dot{B}\rangle = \mathrm{Re}\langle \lambda Jxy^*B^*, J\dot{B}B^{-1}\rangle \\ &= |\lambda|^2\,\mathrm{Re}\langle Jxy^*, (Jxy^*)_{\mathrm{herm}}\rangle = |\lambda|^2\,\|(Jxy^*)_{\mathrm{herm}}\|_F^2 > 0\end{aligned}$$

and hence, by Lemma 1.1, $\frac{d}{dt}|\lambda|^2(0) > 0$ in contradiction to *1.* □

3. Setting II: Measuring perturbations in the tangent space.

3.1. Extremizers in the Lie algebra. In order to preserve the symplecticity of $B(t)$ in the numerical solution of the differential equation (2.4), it is convenient to write

$$B(t) = e^{\Omega(t)}A \tag{3.1}$$

with a Hamiltonian matrix $\Omega(t)$, which is always possible for $B(t)$ sufficiently close to A. We then obtain a differential equation for Ω by noting that (see, e.g., [HLW06, Sect. III.4])

$$\dot{B} = d\exp_\Omega(\dot{\Omega})B, \qquad \text{where} \qquad d\exp_\Omega(H) = \sum_{k\ge 0}\frac{1}{(k+1)!}\,\mathrm{ad}_\Omega^k(H) \tag{3.2}$$

with the iterated commutators $\mathrm{ad}_\Omega^0(H) = H$, $\mathrm{ad}_\Omega(H) = \Omega H - H\Omega$, and $\mathrm{ad}_\Omega^{k+1}(H) = \mathrm{ad}_\Omega(\mathrm{ad}_\Omega^k(H))$.

As in the previous section, we aim to maximize $\frac{d}{dt}|\lambda(t)|^2$ but now under the constraint that $\|\Omega\|_F$ remains constant. In view of Lemma 1.1 we want to maximize, for x and y left and right eigenvectors of B with $x^*y > 0$,

$$\mathrm{Re}\Big((\lambda x)^*\dot{B}y\Big) = \mathrm{Re}\Big((\lambda x)^* d\exp_\Omega(\dot{\Omega})By\Big) = |\lambda|^2\mathrm{Re}(x^* d\exp_\Omega(\dot{\Omega})y).$$

Lemma 3.1. *The solution of the optimization problem*

$$Z_* = \arg\max\{\mathrm{Re}\,(x^* d\exp_\Omega(Z)y) : Z \text{ is Hamiltonian and } \|Z\|_F = 1,\ \mathrm{Re}\,\langle \Omega, Z\rangle = 0\} \tag{3.3}$$

is given by

$$\mu\, JZ_* = \big(J d\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}} - \gamma J\Omega, \tag{3.4}$$

where μ denotes the Frobenius norm of the matrix on the right-hand side and moreover $\gamma = \langle J\Omega, \big(J d\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}\rangle$.

Proof. We first note that

$$\mathrm{Re}(x^* d\exp_\Omega(Z)y) = \mathrm{Re}\langle xy^*, d\exp_\Omega(Z)\rangle = \mathrm{Re}\langle d\exp_{\Omega^*}(xy^*), Z\rangle. \tag{3.5}$$

Here, we have used that the adjoint of $d\exp_\Omega$ is given by $d\exp_{\Omega^*}$. This is a consequence of the identity $\langle \mathrm{ad}_\Omega^k(X), Y\rangle = \langle X, \mathrm{ad}_{\Omega^*}^k(Y)\rangle$ for $X, Y \in \mathbb{C}^{n\times n}$, which can be shown by induction using

$$\langle \mathrm{ad}_\Omega(X), Y\rangle = \langle \Omega X - X\Omega, Y\rangle = \langle X, \Omega^* Y\rangle - \langle X, Y\Omega^*\rangle = \langle X, \mathrm{ad}_{\Omega^*}(Y)\rangle.$$

Using the fact that JZ is Hermitian, we obtain from (3.5) that

$$\mathrm{Re}(x^* d\exp_\Omega(Z)y) = \mathrm{Re}\big\langle \big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}, JZ\big\rangle,$$

which is clearly maximized for a scalar multiple of $JZ = \big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}$. The side constraint $\mathrm{Re}\,\langle \Omega, Z\rangle = \langle \Omega, Z\rangle = 0$ is incorporated by orthogonal projection, yielding (3.4). □

Lemma 3.1 suggests to consider the differential equation

$$\dot{\Omega} = J^{\mathrm{T}}\left(Jd\exp_{\Omega^*}(xy^*)\right)_{\mathrm{herm}} - \gamma\Omega \tag{3.6}$$

with

$$\gamma = \big\langle \big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}, J\Omega\big\rangle / \|\Omega\|_F^2.$$

From a numerical viewpoint, an advantage of (3.6) over (2.4) is that every standard numerical integrator preserves the Hamiltonian structure of $\Omega(t)$, but only specially tailored Lie group integrators [IMNZ00] preserve the symplectic structure of $B(t)$.

We have the following monotonicity result.

LEMMA 3.2. *Let the Hamiltonian matrices* $\Omega(t)$ *of constant Frobenius norm satisfy* (3.6). *If* $\lambda(t)$ *is a simple eigenvalue of* $e^{\Omega(t)}A$, *then* $\frac{d}{dt}|\lambda(t)|^2 \geq 0$.

Proof. By (2.1) and (3.2), we have to prove $\mathrm{Re}(x^* d\exp_\Omega(\dot{\Omega})y) \geq 0$. With a view towards (3.6), we first establish the equalities

$$\begin{aligned}
&\mathrm{Re}\big(x^* d\exp_\Omega(J^T\big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}})y\big)\\
&= \mathrm{Re}\big\langle xy^*, d\exp_\Omega(J^T\big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}\big\rangle\\
&= \mathrm{Re}\big\langle Jd\exp_{\Omega^*}(xy^*), \big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}\big\rangle = \big\|\big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}\|_F^2
\end{aligned}$$

and

$$\mathrm{Re}\big(x^* d\exp_\Omega(\gamma\Omega)y\big) = \gamma\big\langle\big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}, J\Omega\big\rangle.$$

Inserting (3.6) thus gives

$$\mathrm{Re}\big(x^* d\exp_\Omega(\dot{\Omega})y\big) = \big\|\big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}\|_F^2 - \gamma\langle\big(Jd\exp_{\Omega^*}(xy^*)\big)_{\mathrm{herm}}, J\Omega\rangle \geq 0,$$

where the last step follows from the Cauchy-Schwarz inequality. □

A useful reformulation of (3.6) is given in the following lemma.

LEMMA 3.3. *Equation (3.6) is equivalent to*

$$\dot{\Omega} = d\exp_{\Omega^*}\left(J^{\mathrm{T}}\left(Jxy^*\right)_{\mathrm{herm}}\right) - \gamma\Omega \tag{3.7}$$

with

$$\gamma = \langle (Jxy^*)_{\mathrm{herm}}, J\Omega\rangle / \|\Omega\|_F^2. \tag{3.8}$$

Proof. Since Ω is a Hamiltonian matrix, it can be directly shown by induction that

$$J d\exp_{-\Omega}(yx^*)J = d\exp_{\Omega^*}(Jyx^*J),$$

holds. This allows us to rewrite the right-hand side of (3.6) as

$$\begin{aligned} & J^{\mathrm{T}}\left(J d\exp_{\Omega^*}(xy^*)\right)_{\mathrm{herm}} \\ &= \frac{1}{2}\Big(d\exp_{\Omega^*}(xy^*) + J\left(d\exp_{\Omega^*}(xy^*)\right)^* J\Big) - \gamma\Omega \\ &= \frac{1}{2}\Big(d\exp_{\Omega^*}(xy^*) + J d\exp_{-\Omega}(yx^*)J\Big) - \gamma\Omega \\ &= \frac{1}{2}\Big(d\exp_{\Omega^*}(xy^*) + d\exp_{\Omega^*}(Jyx^*J)\Big) - \gamma\Omega, \end{aligned}$$

which coincides with the right-hand side of (3.7). The simplified expression (3.8) for

$$\gamma = \big\langle J d\exp_{\Omega^*}\left(J^{\mathrm{T}}\left(Jxy^*\right)_{\mathrm{herm}}\right), J\Omega\big\rangle / \|\Omega\|_F^2$$

follows from the fact that for any matrix X,

$$\big\langle \mathrm{ad}_{\Omega^*}(X), \Omega\big\rangle = \big\langle X, \mathrm{ad}_{\Omega}(\Omega)\big\rangle = 0.$$

This completes the proof. □

Similarly to [BGMN13] we state the following uniqueness result for sufficiently small ε.

Lemma 3.4. *Let x_0 and y_0 be unit-norm left and right eigenvectors, respectively, associated to the simple eigenvalue λ_0 of the matrix A.*

If $|\lambda_0| \neq 1$ then, for ε small enough, the system (3.7) *has precisely two stationary points (that correspond to the minimum and the maximum of $|\lambda|$) on $\varepsilon\mathcal{S}_1$, where $\mathcal{S}_1 = \{\Theta \in \mathbb{C}^{n\times n} \colon \|\Theta\|_F = 1\}$.*

Proof. We let $\Theta = \dfrac{1}{\varepsilon}\Omega$ so that $\|\Theta\|_F = 1$, and consider the expansion

$$d\exp_{\Omega^*}\left(J^{\mathrm{T}}\left(Jxy^*\right)_{\mathrm{herm}}\right) = J^{\mathrm{T}}Q_0 + J^{\mathrm{T}}Q(\Theta,\varepsilon)$$

where $Q_0 = (Jx_0y_0^*)_{\mathrm{herm}}$ and the remainder term satisfies

$$\max_{\Theta\in\mathcal{S}_1} \|Q(\Theta,\varepsilon)\|_F = \mathcal{O}(\varepsilon)\ . \tag{3.9}$$

The equation for the equilibria reads $F(\Theta,\varepsilon) = O$, where

$$\begin{aligned} F(\Theta,\varepsilon) &= J^{\mathrm{T}}Q_0 + J^{\mathrm{T}}Q(\Theta,\varepsilon) - \Theta\left\langle Q_0 + Q(\Theta,\varepsilon), J\Theta\right\rangle \\ &= J^{\mathrm{T}}Q_0 - \Theta\left\langle Q_0, J\Theta\right\rangle + J^{\mathrm{T}}Q(\Theta,\varepsilon) - \Theta\left\langle Q(\Theta,\varepsilon), J\Theta\right\rangle. \end{aligned}$$

It is immediate to observe that $F(\Theta,0) = O$ if and only if

$$\Theta = \Theta_\pm^\star = \pm J^{\mathrm{T}}Q_0/\|Q_0\|_F.$$

Moreover, the Jacobian matrix of $F(\Theta,\varepsilon)$ with respect to Θ at the point $(\Theta_\pm^\star, 0)$ is given by the linear operator $\mathcal{L}_\pm \colon \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$, such that

$$\mathcal{L}_\pm B = -\langle Q_0, JB\rangle\Theta_\pm^\star - \langle Q_0, J\Theta_\pm^\star\rangle B\ , \qquad B \in \mathbb{C}^{n\times n}.$$

In order to show invertibility of $\mathcal{L}_\pm$ we recall that

$$\Theta_\pm^\star = \pm J^{\mathrm{T}} Q_0 / \|Q_0\|_F,$$

and observe that the homogeneous equation $\mathcal{L}_\pm B = O$ reads

$$JB = -\frac{\langle Q_0, JB\rangle}{\|Q_0\|_F^2} Q_0,$$

which gives $\langle Q_0, JB\rangle = 0$ and therefore $B = O$.

By the implicit function theorem this implies that there exist $\hat{\varepsilon} > 0$, $r > 0$, and $\Theta_\pm^\varepsilon$ such that $F(\Theta, \varepsilon) = O$ for $\varepsilon \in [0, \hat{\varepsilon}]$ and $\|\Theta - \Theta_\pm^\star\|_F < r$ if and only if $\Theta = \Theta_\pm^\varepsilon$. On the other hand, by (3.9), if $F(\Theta, \varepsilon) = O$ then $\|\Theta - \Theta_+^\star\| = \mathcal{O}(\varepsilon)$ or $\|\Theta - \Theta_-^\star\| = \mathcal{O}(\varepsilon)$. We conclude that $\Theta_\pm^\varepsilon$ are the unique equilibria on the whole hyper-sphere $\mathcal{S}_1$ for ε small enough. Clearly, Θ_+^ε and Θ_-^ε are the maximizer and the minimizer of $|\lambda|$, respectively. ∎

The stationary points of (3.7) are characterized by the following theorem.

Theorem 3.5. *The following statements are equivalent along solutions of* (3.7) *provided that* $|\lambda| \neq 1$*:*

1. $\dfrac{d}{dt}\,|\lambda|^2 = 0$.
2. $\dot{\Omega} = 0$.
3. $J d\exp_{\Omega^*}^{-1}(\Omega)$ *is a real multiple of* $(Jxy^*)_{\mathrm{herm}}$.

Proof. This follows directly from (3.7) and Lemma 1.1, if $(Jxy^*)_{\mathrm{herm}} \neq 0$. The latter can be ensured by the same arguments used in the proof of Theorem 2.3. ∎

At a stationary point of (3.7) it holds

$$\Omega = d\exp_{\Omega^*}\left(\varrho J^{\mathrm{T}} (Jxy^*)_{\mathrm{herm}}\right) \tag{3.10}$$

for positive $\varrho = 1/\gamma$. Observe that (for x_0 and y_0 leading eigenvectors of A, associated to the eigenvalue λ_0 with $|\lambda_0| \neq 1$),

$$\gamma\varepsilon = \|Jx_0 y_0^*\|_F + \mathcal{O}(\varepsilon),$$

which implies

$$\varrho = \mathcal{O}(\varepsilon). \tag{3.11}$$

Finally we provide the following characterization of extremizers.

Theorem 3.6. *Fix a symplectic matrix* $A \in \mathbb{C}^{n\times n}$ *and* $\varepsilon > 0$. *Let* $B_\star \in \mathbb{C}^{n\times n}$ *be a symplectic matrix such that* $B_\star = \mathrm{e}^{\Omega_\star} A$ *with* $\|\Omega_\star\|_F = \varepsilon$. *Let* $\lambda_\star$ *be a simple eigenvalue of* $B_\star$ *with* $|\lambda_\star| \neq 1$, *with left and right eigenvectors* x *and* y, *respectively, both of unit norm and with* $x^* y > 0$. *Then the following two statements are equivalent:*

1. *Every differentiable path* $(B(t), \lambda(t))$ *(for small* $t \geq 0$*) such that* $B(t) = \mathrm{e}^{\Omega(t)} A$ *where* $\Omega(t)$ *is Hamiltonian such that* $\|\Omega(t)\|_F \leq \varepsilon$ *and* $\lambda(t)$ *is an eigenvalue of* $B(t)$, *with* $B(0) = B_\star$ *and* $\lambda(0) = \lambda_\star$, *has* $\frac{d}{dt}\,|\lambda(t)|^2 \leq 0$.
2. $J d\exp_{\Omega^*}^{-1}(\Omega)$ *is a positive multiple of* $(Jxy^*)_{\mathrm{herm}}$.

Proof. The proof is similar to the one given for Theorem 2.4. ∎

3.2. Rank-4 property. We have the following important result.

THEOREM 3.7. *Under the assumptions of Lemma 3.4, the stationary points* Ω *of* (3.7) *have rank at most* 4.

Proof. By Lemma 3.4, there are only two stationary points Ω_- and Ω_+ of (3.7), associated with the minimum and maximum of $|\lambda|$, respectively. We only consider Ω_+; the argument for Ω_- is identical. By a symplectic QR decomposition [Bu86] of $[x_+, y_+, Jx_+, Jy_+]$, there is a matrix $U \in \mathbb{C}^{n\times 4}$ such that

$$\mathcal{R}(U) = \operatorname{span}\{x_+, y_+, Jx_+, Jy_+\}, \quad U^*U = I_4, \quad U^*JU = J_4.$$

where $J_4 = \begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix}$. In particular, this implies $JU = UJ_4$ and the existence of vectors $\tilde{x}, \tilde{y} \in \mathbb{C}^4$ such that $x = U\tilde{x}$, $y = U\tilde{y}$. We apply Lemma 3.4 to conclude that the equation

$$0 = d\exp_{\tilde{\Omega}^*}\left(J_4^{\mathrm{T}}\left(J_4\tilde{x}\tilde{y}^*\right)_{\mathrm{herm}}\right) - \tilde{\gamma}\tilde{\Omega} \tag{3.12}$$

with $\tilde{\gamma} = \langle (J_4\tilde{x}\tilde{y}^*)_{\mathrm{herm}}, J_4\tilde{\Omega}\rangle / \|\tilde{\Omega}\|_F^2$ has a solution $\tilde{\Omega}_+$.

Setting $\bar{\Omega} = U\tilde{\Omega}_+U^*$, we clearly have

$$\langle (Jxy^*)_{\mathrm{herm}}, J\bar{\Omega}\rangle / \|\bar{\Omega}\|_F^2 = \langle (J_4\tilde{x}\tilde{y}^*)_{\mathrm{herm}}, J_4\tilde{\Omega}_+\rangle / \|\tilde{\Omega}_+\|_F^2. \tag{3.13}$$

Moreover, the identity

$$d\exp_{\bar{\Omega}}\left(J^{\mathrm{T}}\left(Jxy^*\right)_{\mathrm{herm}}\right) = U \cdot d\exp_{\tilde{\Omega}_+^*}\left(J_4^{\mathrm{T}}\left(J_4\tilde{x}\tilde{y}^*\right)_{\mathrm{herm}}\right) \cdot U^* \tag{3.14}$$

holds. This can be seen as follows. First, note that

$$\begin{aligned} J^{\mathrm{T}}\left(Jxy^*\right)_{\mathrm{herm}} &= \frac{1}{2}J^{\mathrm{T}}\left(JU\tilde{x}\tilde{y}^*U^* + U\tilde{y}\tilde{x}^*U^*J^T\right) \\ &= \frac{1}{2}U\left(J_4\tilde{x}\tilde{y}^* + \tilde{y}\tilde{x}^*J_4^T\right)U^* = UJ_4^T\left(J_4\tilde{x}\tilde{y}^*\right)_{\mathrm{herm}}U^*. \end{aligned}$$

Combined with the fact that $\mathrm{ad}_{\bar{\Omega}}^{\ell}(U\tilde{H}U^*) = U \cdot \mathrm{ad}_{\tilde{\Omega}_+}^{\ell}(\tilde{H}) \cdot U^*$ holds for any $\tilde{H} \in \mathbb{C}^{4\times 4}$, this establishes the relation

$$\mathrm{ad}_{\bar{\Omega}}^{\ell}(J^{\mathrm{T}}\left(Jxy^*\right)_{\mathrm{herm}}) = U \cdot \mathrm{ad}_{\tilde{\Omega}_+}^{\ell}(J_4^T\left(J_4\tilde{x}\tilde{y}^*\right)_{\mathrm{herm}}) \cdot U^*$$

for every $\ell \geq 0$. Now, (3.14) follows from the definition of $d\exp$.

The derived identities (3.12), (3.13), (3.14) imply that the Hamiltonian matrix $\bar{\Omega}$, which has rank at most 4, is a stationary point. Combined with the uniqueness established in Lemma 3.4, this completes the proof. ∎

REMARK 3.1. *In all our numerical experiments we have observed that the computed stationary points of (3.7) have rank* 4*, also for large values of* ε*, a situation which is not covered by Theorem 3.7, as the assumptions of Lemma 3.4 require* ε *to be sufficiently small.*

4. Approximation via low-rank differential equations. To compute the stationary points of the differential equation (3.7), which have rank at most 4 by Theorem 3.7, we use low-rank differential equations with nearby stationary points. The efficient implementation of such an approach requires the efficient computation of $d\exp_Z(Y)$ for low-rank matrices Y, Z. The following result will be helpful for this purpose.

Lemma 4.1. *Let $Y, Z \in \mathbb{C}^{n\times n}$ be such that $\|Z\|_2 \le \varepsilon < 1/2$. Let*

$$E_k := \sum_{\ell=0}^{k-1} \frac{1}{(\ell+1)!}\,\mathrm{ad}_Z^{\ell}(Y).$$

Then

$$\|d\exp_Z(Y) - E_k\|_2 \le e^{2\varepsilon}\frac{(2\varepsilon)^k}{(k+1)!}\|Y\|_2.$$

Proof. We have

$$\left\|\mathrm{ad}_Z^{\ell}(Y)\right\|_2 \le 2\varepsilon\left\|\mathrm{ad}_Z^{\ell-1}(Y)\right\|_2 \le \cdots \le (2\varepsilon)^{\ell}\|Y\|_2,$$

which implies

$$\begin{aligned}\|d\exp_Z(Y) - E_k\|_2 &\le \sum_{\ell=k}^{\infty}\frac{(2\varepsilon)^{\ell}}{(\ell+1)!}\|Y\|_2 = (2\varepsilon)^k\sum_{\ell=0}^{\infty}\frac{(2\varepsilon)^{\ell}}{(\ell+k+1)!}\|Y\|_2\\ &\le \frac{(2\varepsilon)^k}{(k+1)!}\sum_{\ell=0}^{\infty}\frac{(2\varepsilon)^{\ell}}{\ell!}\|Y\|_2 = e^{2\varepsilon}\frac{(2\varepsilon)^k}{(k+1)!}\|Y\|_2.\end{aligned}$$

□

4.1. Low-rank differential equations. Inspired by Lemma 4.1, we make use of

$$d\exp_{Z,k}(Y) := \sum_{\ell=0}^{k}\frac{1}{(\ell+1)!}\,\mathrm{ad}_Z^{\ell}(Y),$$

and consider the following variant of (3.7):

$$\dot\Omega = d\exp_{\Omega^*,k}\left(J^{\mathrm{T}}\left(Jxy^*\right)_{\mathrm{herm}}\right) - \gamma\Omega \tag{4.1}$$

with

$$\gamma = \langle (Jxy^*)_{\mathrm{herm}}, J\Omega\rangle/\|\Omega\|_F^2.$$

The equilibria of (4.1) have rank 2 if $k = 0$ and 4 if $k \ge 1$.

For $k \ge 1$ this leads us to consider the differential equation

$$\dot\Omega = P_\Omega\left(d\exp_{\Omega^*,k}\left(J^{\mathrm{T}}(Jxy^*)_{\mathrm{herm}}\right)\right) - \gamma\Omega, \tag{4.2}$$

where P_Ω is the orthogonal projector onto $T_\Omega\mathcal{M}_4$, the tangent space of

$$\mathcal{M}_4 = \{E \in \mathbb{C}^{n\times n} : \mathrm{rank}(E) = 4,\ JE \text{ is hermitian}\},$$

at Ω.

Equation (4.2) differs from (4.1) only in that $d\exp_{\Omega^*,k}\big(J^T(Jxy^*)_{\mathrm{herm}}\big)$ is replaced by its orthogonal projection to $T_\Omega\mathcal{M}_4$. This also shows that $\mathrm{Re}\,\langle\Omega,\dot\Omega\rangle = 0$, so that the unit norm of Ω is conserved along solutions of (4.2).

Every complex Hamiltonian rank-4 matrix Ω of size $n \times n$ can be written in the form

$$\Omega = J^T V S V^* \tag{4.3}$$

where $V \in \mathbb{C}^{n\times 4}$ has orthonormal columns, i.e., $V^*V = I_4$, and $S \in \mathbb{C}^{4\times 4}$ is nonsingular and hermitian. The eigendecomposition yields S diagonal, but we will not assume a special form of S. The representation (4.3) is not unique: replacing V by $\widetilde{V} = VQ$ with a unitary matrix $Q \in \mathbb{C}^{4\times 4}$ and correspondingly S by $\widetilde{S} = Q^*SQ$ yields the same matrix $\Omega = J^T V S V^* = J^T \widetilde{V}\widetilde{S}\widetilde{V}^*$.

The following lemma is a complex Hamiltonian version of the corresponding real result from [KL07].

LEMMA 4.2. *The orthogonal projection onto the tangent space $T_\Omega\mathcal{M}_4$ at $\Omega = J^T V S V^* \in \mathcal{M}_4$ is given by*

$$P_\Omega(Z) = Z - (I - J^T V V^* J) Z (I - VV^*) \tag{4.4}$$

for $Z \in \mathbb{C}^{n\times n}$.

Based on this result, we can project the differential equation and consider the corresponding low-rank dynamical system.

4.2. Rank-4 differential equation and an iterative correction. The simplest approximation is given by (4.1) with $k = 0$,

$$\dot{\Omega} = J^{\mathrm{T}} \left(Jxy^*\right)_{\mathrm{herm}} - \gamma\Omega \tag{4.5}$$

whose stationary points would have rank 2. The next approximation is obtained for $k = 1$ as:

$$\dot{\Omega} = J^{\mathrm{T}} \left(Jxy^*\right)_{\mathrm{herm}} + \frac{1}{2}\left[J\Omega J, J^{\mathrm{T}} \left(Jxy^*\right)_{\mathrm{herm}}\right] - \gamma\Omega \tag{4.6}$$

with

$$\gamma = \langle \left(Jxy^*\right)_{\mathrm{herm}}, J\Omega\rangle / \|\Omega\|_F^2,$$

which would have rank-4 equilibria and which we consider as starting approximation of (3.7).

4.2.1. Rank-4 projection. In the differential equation (4.6) we replace the vector field by its orthogonal projection to $T_\Omega\mathcal{M}_4$, so that solutions starting with rank 4 will retain rank 4 and their Hamiltonian structure for all times (since $\Omega \in T_\Omega\mathcal{M}_4$, we have that $P_\Omega(\Omega) = \Omega$):

$$\dot{\Omega} = P_\Omega\Big(J^{\mathrm{T}} \left(Jxy^*\right)_{\mathrm{herm}} + \frac{1}{2}\left[J\Omega J, J^{\mathrm{T}} \left(Jxy^*\right)_{\mathrm{herm}}\right]\Big) - \gamma\Omega, \tag{4.7}$$

with

$$\gamma = \langle \left(Jxy^*\right)_{\mathrm{herm}}, J\Omega\rangle / \|\Omega\|_F^2$$

where again $x(t)$ and $y(t)$ are right and left eigenvectors, respectively, to a simple eigenvalue $\lambda(t)$ of $e^{\Omega(t)}A$, both of unit norm and with $x(t)^*y(t) > 0$.

To obtain the differential equation in a form that uses the factors in $\Omega = J^T V S V^*$ rather than the full $n \times n$ matrix Ω, we use the following result.

LEMMA 4.3. *[KL07, Prop. 2.1] For $\Omega = J^T VSV^* \in \mathcal{M}_4$ with nonsingular hermitian $S \in \mathbb{R}^{4\times 4}$ and with $V \in \mathbb{C}^{n\times 4}$ having orthonormal columns, the equation $\dot\Omega = P_\Omega(Z)$ is equivalent to $J\dot\Omega = \dot VSV^* + V\dot SV^* + VS\dot V^*$, where*

$$\begin{aligned}\dot S &= V^* JZV\\ \dot V &= (I - VV^*)(JZ)^* VS^{-1}.\end{aligned}$$

With

$$JZ = (Jxy^*)_{\rm herm} - \frac{1}{2}\Big(\Omega(Jxy^*)_{\rm herm} + (Jxy^*)_{\rm herm}J\Omega J\Big) - \gamma J\Omega,$$

Lemma 4.3 yields that the differential equation (4.6) for $\Omega = J^T VSV^*$ is equivalent to the following system of differential equations. With the notation

$$\begin{aligned}&Y = (Jx, y) \in \mathbb{C}^{n\times 2}, \quad R = V^*Y \in \mathbb{C}^{4\times 2}, \quad P = \tfrac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\\ &T = RPR^* \in \mathbb{C}^{4,4}, \quad W = V^*JV \in \mathbb{C}^{4,4},\end{aligned} \tag{4.8}$$

the differential equations are compactly written as

$$\begin{aligned}\dot S &= T + (WST)_{\rm herm} - \frac{\langle S, T\rangle}{\|S\|_F^2} S \qquad (4.9)\\ \dot V &= \Big(YPR^* + \frac{1}{2}\big(JVSRPR^* - YPR^*SW\big) - VT - V\,(WST)_{\rm herm}\Big)S^{-1}.\end{aligned}$$

Since $\langle S, \dot S\rangle = 0$, the differential equations preserve the unit norm of S.

4.2.2. Correction through higher truncation. We consider the solution of (4.9) as long as $|\lambda(t)|$ is monotonically increasing. Let $\bar t$ be a local maximum point for $|\lambda(t)|$ and consider the corresponding matrix $\Omega_1 = J^T V(\bar t)S(\bar t)V(\bar t)^*$.

Afterwards we can solve (4.1) (or (4.2)) with $k = 2$ and with initial datum $\Omega(0) = \Omega_1$. We can further project the r.h.s. onto $T_\Omega\mathcal{M}_4$ and compute the solution of (4.2) in a maximal interval of monotonicity. Iterating this idea we can solve (4.2) with $k = 3, 4, \ldots$ and indicate as Ω_k the solution at the instant $\bar t$ to which corresponds a turning point of $|\lambda(t)|$. This procedure is sketched in Algorithm 1. For $k = O(1)$, the expression $d\exp_{\Omega^*,k}\left(J^{\rm T}\,(Jxy^*)_{\rm herm}\right)$ required in Algorithm 1 can be evaluated in $O(n)$ operations.

4.3. Illustrative example. Consider the symplectic matrix $A = {\rm e}^H$, where the Hamiltonian matrix

$$H = \frac{1}{10}\begin{pmatrix}
1-i & -1-i & 1-i & 1 & 1+i & -2 & -2+i & 1 & -3-2i & 0+i\\
2-3i & 2-i & -1+i & 0 & 1-i & -2-i & -2 & -1-i & -3-i & 0-i\\
2-i & 2 & -1+2i & 4+i & 2-2i & 1 & -1+i & 0 & -2-4i & -1-3i\\
1-3i & 0-i & 2+2i & 0+i & 1-i & -3+2i & -3+i & -2+4i & -2 & -2-2i\\
2+3i & 1 & 3 & 1+3i & 2 & 0-i & 0+i & -1+3i & -2+2i & 0\\
2 & -1 & 0 & 3 & 0 & -1-i & -2-3i & -2-i & -1-3i & -2+3i\\
-1 & 4 & 1 & -1 & 1-3i & 1-i & -2-i & -2 & 0-i & -1\\
0 & 1 & 0 & 1 & 1-3i & -1-i & 1+i & 1+2i & -2+2i & -3\\
3 & -1 & 1 & -2 & 2 & -1 & 0 & -4+i & 0+i & -1+3i\\
0 & 1+3i & 1+3i & 2 & 2 & -1+i & -1-i & -2-2i & -1-i & -2
\end{pmatrix}$$

is such that it has spectral radius $\rho(A) = 2.164638002457682$, and set $\varepsilon = 0.25$.

We first solve numerically the full rank system of differential equations (3.7) and get the spectral radius

$$\rho({\rm e}^{\Omega_\star}A) = 2.763848551977566$$

Algorithm 1: Basic correction iteration

Data: Ω_1, x, y, K and tol with x, y leading eigenvectors of $\mathrm{e}^{\Omega_1}A$
Result: k, Ω_k
begin
- Set P_Ω the orthogonal projector onto $T_\Omega\mathcal{M}_4$
- **for** $k \leftarrow 2$ **to** K **do**
  - Solve $\dot{\Omega} = P_\Omega\left(d\exp_{\Omega^*,k}\left(J^{\mathrm{T}}\left(Jxy^*\right)_{\mathrm{herm}}\right)\right) - \gamma\Omega$
  - with initial datum $\Omega(0) = \Omega_{k-1} \in \mathcal{M}_4$ (such that $\|\Omega(0)\|_F = \varepsilon$)
  - Set Ω_k the extremal point and λ_k the leading eigenvalue of $\mathrm{e}^{\Omega_k}A$
  - **if** $|\lambda_k - \lambda_{k-1}| \leq$ tol **then**
    - **return**
  - **else**
    - Compute leading eigenvectors x and y of $\mathrm{e}^{\Omega_k}A$
- Print *K-th expansion of $d\exp$ does not provide required tolerance.*

at the computed stationary point $\Omega_\star$.

We then run Algorithm 1, implemented with variable stepsize. We obtain the results summarized in Table 4.1, where we denote by Ω_k the computed extremal matrix obtained by integrating (4.2) .

k	$\rho(\mathrm{e}^{\Omega_k}A)$	err
0^*	2.761609008013191	$2.2395e-3$
1	2.763836218931326	$1.2333e-5$
2	2.763848512990621	$3.8976e-8$
3	2.763848551858705	$1.0744e-10$

Table 4.1
Computed spectral radii $\rho(\mathrm{e}^{\Omega_k}A)$ for the considered example.

Note that we have started with $k = 0$ which gives a rank-2 differential equation. The final matrix is further transformed as $d\exp_{\Omega_0^*,1}(\varrho J^{\mathrm{T}}(Jxy^*)_{\mathrm{herm}})$, where ϱ is the normalization factor, to give a rank-4 initial value for the next differential equation corresponding to the choice $k = 1$.

5. Stability distances. Let A be a symplectic matrix with all eigenvalues of modulus different from one. We address first the problem of finding the closest symplectic matrix with an eigenvalue of unit modulus. We recall that for a symplectic matrix the eigenvalues λ and $1/\overline{\lambda}$ come in pairs so that we can confine our search to the interior of the unit disk.

We consider the following symplectic matrix nearness problem:

Given a symplectic matrix A with no eigenvalues on the unit circle and $\delta \geq 0$, find a symplectic matrix $B = \mathrm{e}^{\Omega}A$ with Hamiltonian matrix Ω of minimal Frobenius norm such that some eigenvalue λ of B is of modulus $\mathrm{e}^{-\delta}$.

Recalling the definition (1.2) of the symplectic ε-pseudospectrum, we thus aim to devise an algorithm to compute

$$\varepsilon_\delta = \inf\{\varepsilon \geq 0 : \widetilde{\Lambda}_\varepsilon^{\mathrm{symp}}(A) \cap S_\delta \neq \emptyset\}, \tag{5.1}$$

where $S_\delta = \{z \in \mathbb{C} : \ e^{-\delta} \le |z| \le e^{\delta}\}$.

5.1. The inner ε-pseudospectral radius of a symplectic matrix. In order to compute the value of ε_δ defined in (5.1), we make use of the following definition: The *inner ε-pseudospectral radius* of a symplectic matrix A is

$$\rho_\varepsilon(A) = \max\{|\lambda| : \lambda \in \widetilde{\Lambda}_\varepsilon^{\mathrm{symp}}(A),\ |\lambda| \le 1\}. \tag{5.2}$$

We call $\lambda \in \widetilde{\Lambda}_\varepsilon^{\mathrm{symp}}(A)$ an *inner maximum point* if $|\lambda| < 1$ and the above maximum is attained at λ. Similarly, we call λ an *inner local maximum point* if $|\lambda| < 1$ and there is a complex neighborhood of λ such that λ has maximum modulus among all points of $\widetilde{\Lambda}_\varepsilon^{\mathrm{symp}}(A)$ within this neighborhood.

Starting from $\varepsilon > 0$ such that $\rho_\varepsilon(A) < 1$, we want to compute a root ε_δ of the equation

$$\rho_\varepsilon(A) = e^{-\delta}.$$

We make the following generic assumption for all ε near ε_δ.

ASSUMPTION 1. *If $\lambda(\varepsilon)$ is an inner local maximum point in the symplectic ε-pseudospectrum $\widetilde{\Lambda}_\varepsilon^{\mathrm{symp}}(A)$, then $\lambda(\varepsilon)$ is a* simple *eigenvalue of the corresponding perturbed matrix $\mathrm{e}^{\Omega(\varepsilon)}A$ with a Hamiltonian extremizer $\Omega(\varepsilon)$ of Frobenius norm ε.*

Under Assumption 1, inner local maximum points $\lambda(\varepsilon)$ are smooth functions of ε and the same holds for suitably normalized eigenvectors $x(\varepsilon)$ and $y(\varepsilon)$. The inner global maximum point is then piecewise smooth in ε. In order to derive an equation for ε to approximate $\varepsilon^\star$, we can compute the derivative of $\rho_\varepsilon(A)$ with respect to ε.

THEOREM 5.1. *Let $\lambda(\varepsilon)$, $\varepsilon \in [\underline{\varepsilon}, \overline{\varepsilon})$, be a smooth branch of inner maximum points in the symplectic ε-pseudospectrum $\widetilde{\Lambda}_\varepsilon^{\mathrm{symp}}(A)$, such that $\rho_\varepsilon(A) = |\lambda(\varepsilon)| < 1$ for all ε, and Assumption 1 holds. Let $x(\varepsilon)$ and $y(\varepsilon)$ be left and right eigenvectors of $\mathrm{e}^{\Omega(\varepsilon)}A$ to the eigenvalue $\lambda(\varepsilon)$, where the Hamiltonian matrix $\Omega(\varepsilon)$ of Frobenius norm ε is an extremizer. We then have*

$$\frac{d\rho_\varepsilon(A)}{d\varepsilon} = \rho_\varepsilon(A)\,\mathrm{Re}\,\frac{x(\varepsilon)^*\hat{\Omega}(\varepsilon)y(\varepsilon)}{x(\varepsilon)^*y(\varepsilon)} \ge 0, \tag{5.3}$$

where $\varepsilon\hat{\Omega}(\varepsilon) = \Omega(\varepsilon)$ (i.e. $\|\hat{\Omega}(\varepsilon)\|_F \equiv 1$).

Proof. Indicating by $'$ differentiation with respect to ε, we have

$$B(\varepsilon) = \mathrm{e}^{\Omega(\varepsilon)}A \quad \Longrightarrow \quad B'(\varepsilon) = d\exp_{\Omega(\varepsilon)}\left(\hat{\Omega}(\varepsilon) + \varepsilon\hat{\Omega}'(\varepsilon)\right)B(\varepsilon).$$

We obtain

$$\begin{aligned}
&\frac{1}{2}\frac{d}{d\varepsilon}|\lambda(\varepsilon)|^2 = \mathrm{Re}(\lambda'(\varepsilon)\overline{\lambda}(\varepsilon)) = \mathrm{Re}\frac{(\lambda(\varepsilon)x(\varepsilon))^*B'(\varepsilon)y(\varepsilon)}{x(\varepsilon)^*y(\varepsilon)}\\
&= \mathrm{Re}\frac{(\lambda(\varepsilon)x(\varepsilon))^*d\exp_{\Omega(\varepsilon)}\big(\hat{\Omega}(\varepsilon) + \varepsilon\hat{\Omega}'(\varepsilon)\big)B(\varepsilon)y(\varepsilon)}{x(\varepsilon)^*y(\varepsilon)}\\
&= |\lambda(\varepsilon)|^2\mathrm{Re}\frac{x(\varepsilon)^*d\exp_{\Omega(\varepsilon)}\big(\hat{\Omega}(\varepsilon)\big)y(\varepsilon) + \varepsilon x(\varepsilon)^*d\exp_{\Omega(\varepsilon)}\big(\hat{\Omega}'(\varepsilon)\big)y(\varepsilon)}{x(\varepsilon)^*y(\varepsilon)}.
\end{aligned}$$

Next we make use of the same argument used in [GKL13] to prove that

$$x(\varepsilon)^*d\exp_{\Omega(\varepsilon)}\big(\hat{\Omega}'(\varepsilon)\big)y(\varepsilon) = 0 \quad \forall\varepsilon.$$

Exploiting $d\exp_{\Omega(\varepsilon)}(\hat{\Omega}(\varepsilon)) = \hat{\Omega}(\varepsilon)$ and

$$\frac{d}{d\varepsilon}\,|\lambda(\varepsilon)| = \frac{1}{2|\lambda(\varepsilon)|}\frac{d}{d\varepsilon}\,|\lambda(\varepsilon)|^2$$

we complete the proof. □

5.2. The algorithm. When an eigenvalue $\lambda(\varepsilon)$ reaches the unit disk it coalesces with another eigenvalue. Motivated by this and Theorem 5.2 of [GKL13] (which treats the related situation when an eigenvalue of a Hamiltonian matrix approaches the imaginary axis), close to the imaginary axis we make use of the second order expansion

$$\varepsilon \approx \varepsilon^\star - \gamma(\rho_\varepsilon(A) - 1)^2 \tag{5.4}$$

where $\varepsilon^\star$ denote the limit of ε_δ (see (5.1)) as $\delta \to 0^+$ and $\gamma > 0$. Given ε_ℓ, we use Theorem 5.1 and estimate γ and $\varepsilon^\star$ by γ_ℓ and $\varepsilon_\ell^\star$ using the formulæ (the first of which is obtained by differentiating (5.4) with respect to ε and using Theorem 5.1),

$$\gamma_\ell = \frac{x^*(\varepsilon_\ell)y(\varepsilon_\ell)}{2\rho_{\varepsilon_\ell}(A)|\rho_{\varepsilon_\ell}(A) - 1|\,\mathrm{Re}\left(x^*(\varepsilon_\ell)\hat{\Omega}(\varepsilon_\ell)y(\varepsilon_\ell)\right)}$$

$$\varepsilon_\ell^\star = \varepsilon_\ell + \gamma_\ell(\rho_{\varepsilon_\ell}(A) - 1)^2$$

and then compute

$$\varepsilon_{\ell+1} = \varepsilon_\ell^\star - \gamma_\ell\left(e^{-\delta} - 1\right)^2.$$

This results in Algorithm 2, where tol is a tolerance controlling the desired accuracy of the computed optimal ε. (Note that tol cannot be too small due to the fact that (5.4) is not exact.)

Since values $\varepsilon > \varepsilon^\star$ lead to rejected steps, it is necessary to choose a starting value $\varepsilon_0 < \varepsilon^\star$ and possibly underestimate the initial predicted values for ε_k. A good choice for ε_0 is the unstructured distance from the unit circle, that is the norm of the smallest unstructured matrix Ω such that $\mathrm{e}^{\Omega}A$ has an eigenvalue on the unit circle (this can be done by a variant of the method discussed in [GL11]).

Example 5.1. Consider the symplectic matrix

$$A = \mathrm{e}^H, \quad H = \begin{pmatrix} 4 & 1 & 3-\mathbf{i} & -2 & -2+2\mathbf{i} & 1-\mathbf{i} \\ \mathbf{i} & -1-\mathbf{i} & 1+2\mathbf{i} & -2-2\mathbf{i} & 0 & 1+\mathbf{i} \\ -2+\mathbf{i} & 1-\mathbf{i} & -1+2\mathbf{i} & 1+\mathbf{i} & 1-\mathbf{i} & 0 \\ -4 & -3 & -1+\mathbf{i} & -4 & \mathbf{i} & 2+\mathbf{i} \\ -3 & -2 & -1-2\mathbf{i} & -1 & 1-\mathbf{i} & -1-\mathbf{i} \\ -1-\mathbf{i} & -1+2\mathbf{i} & 0 & -3-\mathbf{i} & -1+2\mathbf{i} & 1+2\mathbf{i} \end{pmatrix}$$

where H is Hamiltonian. We have $\rho_0(A) = 0.488903507469143$.

We set $\delta = 10^{-2}$, so that $e^{-\delta} = 0.990049833749168$ and $\varepsilon_0 = 0.1$. Table 5.1 illustrates the behavior of Algorithm 2. Five steps have been rejected, which means that the estimated value of ε exceeded the stability distance.

The method shows local quadratic convergence.

Algorithm 2: Basic algorithm for computing the nearest symplectic matrix with an eigenvalue of modulus $e^{-\delta}$.

Data: δ, tol and ε_0 (such that $\rho_{\varepsilon_0}(A) < 1$)
Result: ε_f
begin
  Set Reject = False and $k = 0$
  while $|\rho_{\varepsilon_\ell}(A) - e^{-\delta}| \geq$ tol **do**
    if Reject = False **then**
      Store ε_ℓ and ρ_{ε_ℓ} into the memory
      Compute γ_ℓ and $\varepsilon_\ell^\star$
      Set $\varepsilon_{\ell+1} = \varepsilon_\ell^\star - \gamma_\ell (e^{-\delta} - 1)^2$
      Set $\ell = \ell + 1$
    else
      Set $\varepsilon_\ell = \dfrac{\varepsilon_\ell + \varepsilon_{\ell-1}}{2}$
    Integrate (3.7) (or (4.1)) with initial datum $\varepsilon_\ell \hat{\Omega}(\varepsilon_{\ell-1})$ (for $\ell \geq 1$), by following the $(n/2-1)$-th eigenvalue (the ordering is considered with respect to the modulus in descending order)
    Compute ρ_{ε_ℓ}.
    if $|\rho_{\varepsilon_k}(A) - 1| \leq$ tol *(with tolerance tol)* **then**
      Set Reject = True
    else
      Set Reject = False
  Set $\varepsilon_f = \varepsilon_\ell$

k	ε_k	ρ_{ε_k}
0	0.1	0.680778818253031
1	0.125043323898556	0.786311841363729
2	0.134101923158280	0.853262279387085
3	0.137872622506389	0.897911116485599
4	0.139554993045362	0.**9**28323984372156
5	0.140336072028250	0.**9**49224240903257
6	0.141079473114967	0.**99**4112370360526
7	0.141061471987975	0.**9900**60569442100
8	0.141061411881051	0.**990049833**828471
		0.**990049833749168**

TABLE 5.1
Computed values of ε and ρ_ε for Example 5.1.

5.3. Distance to instability. Let A be a symplectic matrix with all eigenvalues of modulus one and $\delta > 0$ be fixed. We address the second problem of finding the closest symplectic matrix with an eigenvalue of modulus larger than one. For brevity, we just give the main idea because the algorithm is based on similar ideas to those of Algorithm 2.

The idea is to start with an initial perturbation Ω_0 of norm ε_0 such that some eigenvalue of $e^{\Omega_0} A$ has modulus larger than one. Then we decrease ε by using formulæ based on the second order expansion

$$\varepsilon \approx \varepsilon^\star + \gamma(\rho_\varepsilon(A) - 1)^2 \tag{5.5}$$

and generate a sequence ε_ℓ until we determine ε_{ℓ^*} such that the largest eigenvalue of $\mathrm{e}^{\Omega_{\ell^*}} A$ has modulus e^δ. An analogous algorithm for the distance to instability of the flow of a Hamiltonian matrix has been given in [GKL13].

6. Some applications. We consider here two applications, namely the solvability of discrete algebraic Riccati equations and the stability of symplectic integrators.

6.1. Discrete Algebraic Riccati Equations (DARE). Consider the following algebraic Riccati equation:

$$F^*XF - X - F^*XG_1\left(G_2 + G_1^*XG_1\right)^{-1}G_1^*XF + H = 0 \tag{6.1}$$

where $F, H, X \in \mathbb{C}^{n,n}$, $G_1 \in \mathbb{C}^{n,m}$ $(m < n)$, $G_2 \in \mathbb{C}^{m,m}$ and $H = H^*$ is positive semidefinite, $G_2 = G_2^*$ is positive definite.

A well-known result (see e.g. [Da04, La79]) states that if (F, G_1) is stabilizable and (C, F) is detectable (where $H = C^*C$) and F is invertible, the symplectic matrix

$$Z = \begin{pmatrix} F + GF^{-*}H & -GF^{-*} \\ -F^{-*}H & F^{-*} \end{pmatrix} \qquad \text{with} \quad G = G_1 G_2^{-1} G_1^*, \tag{6.2}$$

has no eigenvalues on the unit circle, a condition which guarantees the existence of a unique Hermitian positive semidefinite discrete-stabilizing solution X to (6.1).

Let us now suppose that (6.1) is such that Z (see (6.2)) has no eigenvalues on the unit circle. If we consider small perturbations in the entries of the matrices, it is possible that a pair of eigenvalues of Z reaches the unit circle; as a consequence the solvability of (6.1) in terms of a unique Hermitian positive semidefinite discrete-stabilizing solution X is not guaranteed anymore.

We can compute, by Algorithm 2, the nearest symplectic matrix that has a pair of eigenvalues on the unit circle and interpret its distance from Z as a distance of (6.1) to unsolvability.

EXAMPLE 6.1. We consider the following equation from [AB99]:

$$F = \begin{pmatrix} 0.9980 & 0.0670 & 0 & 0 \\ -0.0670 & 0.9980 & 0 & 0 \\ 0 & 0 & 0.9980 & 0.1530 \\ 0 & 0 & -0.1530 & 0.9980 \end{pmatrix},$$

$$H = \begin{pmatrix} 1.8700 & 0 & 0 & -0.2440 \\ 0 & 0.7440 & 0.2050 & 0 \\ 0 & 0.2050 & 0.5890 & 0 \\ -0.2440 & 0 & 0 & 1.0480 \end{pmatrix},$$

$$G_1 = \begin{pmatrix} 0.0033 & 0.0200 \\ 0.1000 & -0.0007 \\ 0.0400 & 0.0073 \\ -0.0028 & 0.1000 \end{pmatrix}$$

$$G_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The resulting symplectic matrix Z of (6.2) reads (we represent it by using 5 digits)

$$\begin{pmatrix} 0.9982 & 0.0672 & 0.0001 & 0.0020 & -0.0004 & -0.0003 & 0.0000 & -0.0020 \\ -0.0677 & 1.0063 & 0.0044 & 0.0004 & 0.0004 & -0.0100 & -0.0040 & -0.0003 \\ -0.0002 & 0.0033 & 0.9997 & 0.1539 & -0.0000 & -0.0040 & -0.0015 & -0.0009 \\ 0.0013 & -0.0003 & -0.1536 & 1.0079 & -0.0020 & 0.0002 & 0.0009 & -0.0099 \\ -1.8653 & -0.0498 & -0.0137 & 0.2434 & 0.9975 & 0.0670 & 0 & 0 \\ 0.1252 & -0.7421 & -0.2045 & -0.0163 & -0.0670 & 0.9975 & 0 & 0 \\ 0.0366 & -0.2007 & -0.5766 & -0.1573 & 0 & 0 & 0.9790 & 0.1501 \\ 0.2389 & 0.0308 & 0.0884 & -1.0260 & 0 & 0 & -0.1501 & 0.9790 \end{pmatrix}$$

which has eigenvalues:

$$1.0604 \pm 0.1562\mathbf{i},\ 1.0682 \pm 0.0801\mathbf{i},\ 0.9230 \pm 0.1359\mathbf{i},\ 0.9309 \pm 0.0698\mathbf{i},$$

of moduli $1.0719, 1.0712, 0.9330, 0.9335$, respectively.

Applying Algorithm 2 with $\delta = 10^{-4}$ yields a perturbation Ω

$$10^{-3} \left(\begin{matrix} -0.0045 + 0.0438\mathbf{i} & -0.0777 + 0.0050\mathbf{i} & -0.0162 - 0.0031\mathbf{i} & -0.0012 - 0.0369\mathbf{i} \\ -0.0258 - 0.0037\mathbf{i} & -0.0012 - 0.0460\mathbf{i} & 0.0022 - 0.0095\mathbf{i} & 0.0218 + 0.0002\mathbf{i} \\ 0.0053 + 0.0004\mathbf{i} & 0.0009 + 0.0093\mathbf{i} & -0.0003 + 0.0020\mathbf{i} & -0.0044 + 0.0003\mathbf{i} \\ -0.0002 - 0.0002\mathbf{i} & 0.0003 - 0.0004\mathbf{i} & 0.0001 - 0.0001\mathbf{i} & 0.0002 + 0.0002\mathbf{i} \\ -0.0007 & -0.0002 - 0.0013\mathbf{i} & 0.0000 - 0.0003\mathbf{i} & 0.0006 - 0.0001\mathbf{i} \\ -0.0002 + 0.0013\mathbf{i} & -0.0023 & -0.0005 - 0.0001\mathbf{i} & 0.0000 - 0.0011\mathbf{i} \\ 0.0000 + 0.0003\mathbf{i} & -0.0005 + 0.0001\mathbf{i} & -0.0001 & -0.0001 - 0.0002\mathbf{i} \\ 0.0006 + 0.0001\mathbf{i} & 0.0000 + 0.0011\mathbf{i} & -0.0001 + 0.0002\mathbf{i} & -0.0005 \end{matrix} \right.$$

$$\left. \begin{matrix} 2.6360 & -0.0614 - 1.5557\mathbf{i} & -0.0087 + 0.3178\mathbf{i} & -0.0124 - 0.0133\mathbf{i} \\ -0.0614 + 1.5557\mathbf{i} & 0.9195 & -0.1873 - 0.0125\mathbf{i} & 0.0082 - 0.0070\mathbf{i} \\ -0.0087 - 0.3178\mathbf{i} & -0.1873 + 0.0125\mathbf{i} & 0.0383 & -0.0016 + 0.0015\mathbf{i} \\ -0.0124 + 0.0133\mathbf{i} & 0.0082 + 0.0070\mathbf{i} & -0.0016 - 0.0015\mathbf{i} & 0.0001 \\ 0.0045 + 0.0438\mathbf{i} & 0.0258 - 0.0037\mathbf{i} & -0.0053 + 0.0004\mathbf{i} & 0.0002 - 0.0002\mathbf{i} \\ 0.0777 + 0.0050\mathbf{i} & 0.0012 - 0.0460\mathbf{i} & -0.0009 + 0.0093\mathbf{i} & -0.0003 - 0.0004\mathbf{i} \\ 0.0162 - 0.0031\mathbf{i} & -0.0022 - 0.0095\mathbf{i} & 0.0003 + 0.0020\mathbf{i} & -0.0001 - 0.0001\mathbf{i} \\ 0.0012 - 0.0369\mathbf{i} & -0.0218 + 0.0002\mathbf{i} & 0.0044 + 0.0003\mathbf{i} & -0.0002 + 0.0002\mathbf{i} \end{matrix} \right)$$

of Frobenius norm $\varepsilon^\star = 0.003597659294944$. This determines two eigenvalues of Ze^{Ω},

$$\lambda_1 = 0.997155929660901 + 0.074027508000265\mathbf{i}$$
$$\lambda_2 = 0.997355380791263 + 0.074042314983335\mathbf{i}$$

of modulus $0.99990000\ldots$ and $1.00010000\ldots$ respectively.

This indicates that the problem is quite close to an unsolvability condition.

We remark that, by the approach we consider, it is in general not possible to express the final perturbation of (6.2) in terms of perturbations of the matrices F, H, G_1 and G_2. Dealing with this additional structure appears to be a very challenging problem.

6.2. Application to the stability of symplectic integrators.. Consider a Hamiltonian differential equation $\dot{u} = J^{-1}\nabla\mathcal{H}(u)$ that has an elliptic (linearly stable) stationary point u_*, that is, the Hamiltonian matrix $H = J^{-1}\mathrm{Hess}\,\mathcal{H}(u_*)$ has all eigenvalues on the imaginary axis. Consider now the application of a symplectic integration method to the Hamiltonian system, say of Runge–Kutta type. This method preserves the stationary point u^*, and there arises the question for which step sizes h the stationary point is linearly stable also for the discretization.

The linearized time-h flow of the Hamiltonian system has the propagation matrix e^{hH} which is symplectic, that of the numerical method has the symplectic matrix $R(hH)$. One can then ask: For which bound ε on the local error $\|R(hH)-e^{hH}\|_F \leq \varepsilon$ is it guaranteed that the numerical method is linearly stable? This is answered by the distance to instability measured in the ambient space, which is computed using the above iterative approach with the differential equation of Section 2.

On the other hand, in the spirit of backward analysis of differential equations we can write, for sufficiently small h, that $R(hH) = e^{h\widetilde{H}}$ with the Hamiltonian matrix $h\widetilde{H} = \log R(hH)$, or written differently, $R(hH) = e^{\Omega(h)}e^{hH}$ with $\Omega(h) = h\widetilde{H} - hH$. With the algorithm of this section we can find a bound ε of $\|h\widetilde{H} - hH\|_F \leq \varepsilon$ that guarantees that the numerical method is linearly stable.

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The Matlab codes implementing the described algorithms are made available on the website `http://univaq.it/~guglielm/`

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