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PRESERVING GEOMETRIC PROPERTIES OF THE EXPONENTIAL MATRIX BY BLOCK KRYLOV SUBSPACE METHODS*

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Abstract.

Given a large square real matrix A and a rectangular tall matrix Q, many application problems require the approximation of the operation $\exp(A)Q$. Under certain hypotheses on A, the matrix $\exp(A)Q$ preserves the orthogonality characteristics of Q; this property is particularly attractive when the associated application problem requires some geometric constraints to be satisfied. For small size problems numerical methods have been devised to approximate $\exp(A)Q$ while maintaining the structure properties. On the other hand, no algorithm for large A has been derived with similar preservation properties. In this paper we show that an appropriate use of the block Lanczos method allows one to obtain a structure preserving approximation to $\exp(A)Q$ when A is skew-symmetric or skew-symmetric and Hamiltonian. Moreover, for A Hamiltonian we derive a new variant of the block Lanczos method that again preserves the geometric properties of the exact scheme. Numerical results are reported to support our theoretical findings, with particular attention to the numerical solution of linear dynamical systems by means of structure preserving integrators.

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Key words: matrix exponential, Krylov subspaces, exponential integrators, structure preservation.

1 Introduction.

The approximation of the matrix-vector operation $\exp(A)v$ for a given real $N \times N$ matrix A and a real vector v, is the key ingredient of many exponential integrators for solving systems of ordinary differential equations (ODEs) (see [13, 30, 29]), time-dependent partial differential equations (see [24, 25]) and other application problems ([38, 40]). When N is large, Krylov subspace methods

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represent the de-facto alternative to far more costly procedures for approximating $\exp(A)v$ [37]; this has motivated the study of the convergence properties of Krylov subspace based approaches; see, e.g., [19, 28, 35, 42].

The evaluation of the matrix exponential in the context of geometric integration has recently received significant attention [27]. As an example, let A be skew-symmetric, that is $A = -A^T$ where A^T is the transpose of A, and V be an $N \times N$ orthogonal matrix. Then the product $\exp(A)V$ is still an orthogonal matrix, that is, the matrix exponential operator preserves the geometric property of V. Devising an approximation procedure for $\exp(A)V$ that preserves geometric properties of V is crucial for the effectiveness of certain geometric integration methods. This has lead to the development of methods based on matrix decompositions that comply with this requirement, see, e.g., [11, 12, 16, 32, 47], and references therein.

The structural properties are even richer in case A is skew-symmetric and Hamiltonian, or simply Hamiltonian (cf. Definition 2.1). However, the same structure preservation challenges arise whenever the solution of large dimension problems needs to be approximated.

A situation similar to the one described above arises when V is a *rectangular* $N \times p$ matrix with prescribed properties, such as orthonormal or symplectic columns (cf. Definition 2.1). This is the case, for instance, when one needs to compute geodesics on certain manifolds ([1, 20]), when using structure-based numerical integrators ([15, 22, 14, 39]), or when one needs to compute few Lyapunov exponents of dynamical systems ([10, 17, 34]). In this last application, it is often the case that dynamical systems in the following form need to be solved:

$$Q' = A(Q,t)Q, \quad Q(0) = Q_0, \tag{1.1}$$

where Q_0 is a tall rectangular matrix with orthonormal columns and A is skew-symmetric. A first order discretization leads to the discrete equation $Q^{(k+1)} = \exp(hA(Q^{(k)}, t_k))Q^{(k)}$, where h is the time step. If $\exp(hA)$ is computed accurately, it can be shown that $Q^{(k+1)}$ has orthonormal columns for all k's.

In the case of large N, Krylov subspace methods do not usually preserve structure. Using the same example as above and letting $Q = [q_1, \ldots, q_p]$, the approximation of each $\exp(A)q_i$ in the Krylov subspace $\text{span}\{q_i, Aq_i, \ldots, A^{m-1}q_i\}$ with $m \ll N$, provides unit norm vectors that are not orthogonal to each other, in general. Therefore, unless Q consists of a single vector, the geometric structure is lost when using regular Krylov subspace approximation. We show in this paper that appropriate variants of *block* Krylov subspace methods can completely overcome this problem.

We show that structure preservation is also ensured for A skew-symmetric and Hamiltonian, by making a special selection of the first matrix block that generates the block Krylov subspace.

The situation when A is Hamiltonian but *not* skew-symmetric is more challenging. This is due to the fact that the crucial property that $\exp(A)$ is orthogonal does not hold when A is not skew-symmetric. By generalizing recently devised methods, we propose a block Lanczos approach equipped with an indefinite matricial inner product that again ensures structure preservation.

To support the theoretical results, we report on our numerical experience with the described algorithms, and explore their application to the numerical solution of structure preserving dynamical systems.

2 Notation and preliminaries.

We recall some definitions that we use throughout the text. To this end, we let

$$J_{2n} = \begin{bmatrix} O & I \\ -I & O \end{bmatrix},$$

where I and O are the $n \times n$ identity and zero matrices, respectively. The subscript is omitted when clear from the context, and in particular, whenever J is $N \times N$ with N even. We use the 2-norm for vectors and the induced norm for matrices. Exact arithmetic is assumed throughout.

Our numerical experiments were carried out with Matlab ([36]) and Matlab notation is sometimes used.

DEFINITION 2.1. *Let A be a real $N \times N$ matrix.*

1. *A is skew-symmetric if $A = -A^T$;*
2. *Let N be even. A is Hamiltonian if JA is symmetric;*
3. *Let N be even. A is symplectic if $A^T JA = J$;*
4. *Let N be even. A is ortho-symplectic if A is symplectic and $A^T A = I$.*

The following properties can be readily derived from Definition 2.1. If A is Hamiltonian, then $AJ = -JA^T$, and A has the block form

$$A = \begin{bmatrix} A_1 & A_2 \\ A_3 & -A_1^T \end{bmatrix}, \qquad A_2 = A_2^T, \quad A_3 = A_3^T.$$

If A is ortho-symplectic, then A has the block form

$$A = \begin{bmatrix} A_1 & A_2 \\ A_2 & -A_1 \end{bmatrix}, \qquad A_1^T A_1 + A_2^T A_2 = I, \quad A_1^T A_2 - A_2^T A_1 = 0.$$

When dealing with a rectangular $N \times 2p$ matrix V, we say that V is symplectic if $V^T JV = J_{2p}$.

The following characterizations can be deduced; see, e.g., [6].

COROLLARY 2.1.
If A is skew-symmetric, then $\exp(A)$ *is orthogonal.*
If A is Hamiltonian, then $\exp(A)$ *is symplectic.*
If A is skew-symmetric and Hamiltonian, then $\exp(A)$ *is ortho-symplectic.*

Given a real vector v and a square $N \times N$ real matrix A, we aim to explore geometry-preserving approximations to $\exp(A)v$ from the Krylov space $K_m(A, v)$ and its generalizations. If the matrix W_m is such that Range(W_m)

$= K_m(A, v)$, a common choice is $\exp(A)v \approx W_m \exp(H_m)e_1\beta$, where $\beta = \|v\|$ and H_m is some representation of A onto the Krylov subspace [42]. We refer to the *standard* Krylov method when W_m is such that $W_m^T W_m = I_m$. In this case, $H_m = W_m^T A W_m$.

Given a rectangular $N \times p$ matrix V, a generalization of the subspace above is given by the *block* Krylov subspace defined as

$$\mathbb{K}_m(A, V) = \text{span}\{V, AV, \dots, A^{m-1}V\}. \tag{2.1}$$

A basis of $\mathbb{K}_m(A, V)$ is generated by using the following *block* Lanczos recursion

$$A\mathcal{V}_m = \mathcal{V}_m \mathcal{H}_m + V_{m+1} h_{m+1,m} E_m^T, \tag{2.2}$$

where $\mathcal{V}_m = [V_1, V_2, \dots, V_m] \in \mathbb{R}^{N \times mp}$ with $V_1 = V$, $\mathcal{H}_m$ is an $(mp) \times (mp)$ block tridiagonal matrix, $\mathcal{H}_m = (h_{i,j})$, with $h_{i,j}$ a $p \times p$ block, while V_{m+1} is $N \times p$ and $h_{m+1,m}$ is $p \times p$. Finally, $E_m^T = [O, \dots, O, I_p]$ is a $p \times mp$ matrix; see, e.g., [43]. In the following, we assume that $\dim(\mathbb{K}_m(A, V)) = mp$, where p is the number of columns of V, and we use the notation $\mathcal{V}_{m+1} = [\mathcal{V}_m, V_{m+1}]$; see also Remark 3.1.

The matrix $\mathcal{V}_m$ can be built using (2.2) by imposing an orthogonality condition, from which the structure of $\mathcal{H}_m$ can be deduced. For instance, if M is a nonsingular matrix and $\mathcal{V}_m$ satisfies $\mathcal{V}_{m+1}^T M \mathcal{V}_{m+1} = I_{(m+1)p}$, then $\mathcal{H}_{m+1} = \mathcal{V}_{m+1}^T M A \mathcal{V}_{m+1}$. We use Definition 2.1 to derive different orthogonality conditions, and thus a conveniently structured representation matrix $\mathcal{H}_m$. A natural generalization of the single vector case, amounts to approximating $\exp(A)V$ as

$$\exp(A)V \approx \mathcal{V}_m \exp(\mathcal{H}_m) E_1 \chi_0, \tag{2.3}$$

where $\chi_0 \in \mathbb{R}^{p \times p}$ is such that $V = \mathcal{V}_m E_1 \chi_0$.

3 Preserving geometric properties by structure preservation.

Assume that a rectangular $N \times p$ matrix Q is given, with an orthogonality property such as being an appropriate sub-matrix of an orthogonal, symplectic or ortho-symplectic matrix. Corollary 2.1 ensures that if A has a special structure, then the exponential matrix preserves this property, that is $\exp(A)Q$ has the same orthogonality property as Q. In this section we show that the appropriate selection of the matrix V allows us to derive an approximation to $\exp(A)Q$ in the space $\mathbb{K}_m(A, V)$, that preserves orthogonality properties; in particular, V may have more columns than Q. In the following we also support our theoretical results with numerical experiments. For comparison purposes, we employ small size matrices to be able to compute an accurate approximation to $\exp(A)$. Experiments with larger size problems did not show a significantly different behavior of the proposed approaches.

3.1 The case of A skew-symmetric.

Let A be a real and skew-symmetric matrix, and V be a real $N \times p$ matrix with orthonormal columns, that is V is an element of the Stiefel manifold $\mathcal{S}(N,p)$. Corollary 2.1 ensures that $\exp(A)$ is orthogonal and thus $U = \exp(A)V$ also belongs to $\mathcal{S}(N,p)$. We require an approximation of $\exp(A)V$ to be in $\mathcal{S}(N,p)$ as well. The approximation onto the block Krylov subspace $\mathbb{K}_m(A,V)$ naturally satisfies this requirement.

PROPOSITION 3.1. *Let $V \in \mathcal{S}(N,p)$ and A be skew-symmetric. Let $\mathcal{V}_m$ be generated by the block Lanczos method with $\mathcal{V}_m^T\mathcal{V}_m = I_{mp}$, so that its columns span $\mathbb{K}_m(A,V)$, $\mathcal{H}_m$ be as in (2.2) and also set $E_1^T = [I_p, O_p, \ldots, O_p]$. Then for any $m > 0$, the approximation $U_m = \mathcal{V}_m \exp(\mathcal{H}_m)E_1$ to $U = \exp(A)V$ satisfies $U_m^T U_m = I_p$.*

PROOF. The matrix $\mathcal{H}_m$ is skew-symmetric and thus banded. Indeed, since $\mathcal{V}_{m+1}$ has orthonormal columns and A is skew-symmetric, from (2.2) we have

$$\mathcal{H}_m = \mathcal{V}_m^T A\, \mathcal{V}_m = -\mathcal{V}_m^T A^T \mathcal{V}_m = -\mathcal{H}_m^T.$$

Therefore, $\exp(\mathcal{H}_m)$ is orthogonal, and we obtain

$$\begin{aligned} U_m^T U_m &= E_1^T \exp(\mathcal{H}_m)^T \mathcal{V}_m^T \mathcal{V}_m \exp(\mathcal{H}_m) E_1 \\ &= E_1^T \exp(\mathcal{H}_m)^T \exp(\mathcal{H}_m) E_1 = I_p. \end{aligned} \tag{3.1}$$

Hence U_m is in $\mathcal{S}(N,p)$. □

EXAMPLE 3.1. We consider a flow problem as in (1.1), with Q_0 an $N \times 2$ matrix with orthonormal columns, $N = 400$, and A is the skew-symmetric time dependent, $N \times N$ matrix[1]

$$A = \texttt{toeplitz}(c(t), -c(t)) \quad \text{with } c = [0, 10\sin(t), 2\cos(t), -\sin(t), 10, 0, \ldots, 0].$$

Starting with $Q^{(0)} = Q_0$, we consider the iteration

$$Q^{(k)} = \texttt{expm}(hA(t_{k-1}))Q^{(k-1)}, \qquad k = 1, \ldots, 10,$$

with $h = 1/40$, $t_0 = 0$ and $t_k = t_{k-1} + h$. Here `expm` is the Matlab function that numerically approximates the exponential. The same Matlab function is used throughout the text when the matrix exponential is computed "directly"; as a reference approach, we shall refer to this recurrence as the "exact" method. We then compare this solution with the block Lanczos iterate $Y^{(k)}$, obtained at each step k by approximating the action of $\texttt{expm}(hA(t_{k-1}))Y^{(k-1)}$ in the block Krylov subspace $\mathbb{K}_m(A(t_{k-1}), Y^{(k-1)})$ with $m = 5$, with starting matrix $Y^{(0)} = Q_0$ (cf. Proposition 3.1). The departure from orthogonality of $Q^{(k)}$ and of $Y^{(k)}$ is reported in Figure 3.1, where the error norms $\|(Q^{(k)})^T Q^{(k)} - I\|$ and $\|(Y^{(k)})^T Y^{(k)} - I\|$ are displayed. We also report the same quantity for the

[1] We use the notation $A = \texttt{toeplitz}(a,b)$ to denote a Toeplitz matrix whose first column is a and first row is b.

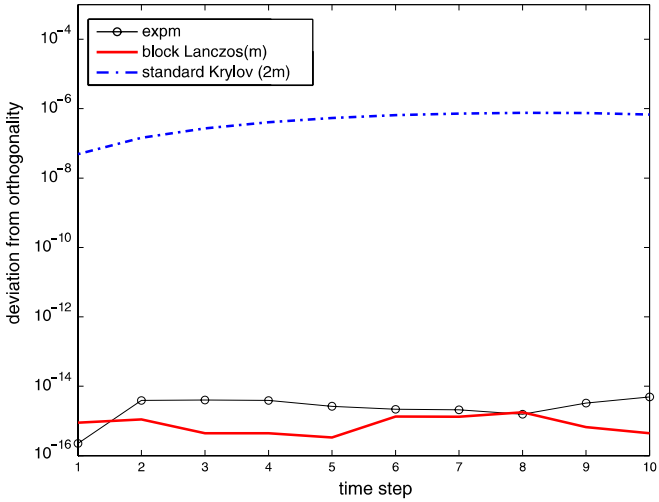

Figure 3.1: Example 3.1. Conservation of orthogonality as time steps proceed.

standard Krylov subspace approach, where the columns of $Z^{(k)} = [z_1^{(k)}, z_2^{(k)}]$ are obtained in $K_m(A(t_{k-1}), z_1^{(k-1)})$ and $K_m(A(t_{k-1}), z_2^{(k-1)})$, respectively, as described in Section 2. As expected, the block method computes an iterate with orthonormal columns with good accuracy, as compared with the standard Krylov approach where orthogonality is completely lost. We also remark that the errors $\|Y^{(k)} - Q^{(k)}\|$ and $\|Z^{(k)} - Q^{(k)}\|$ are comparable for the two approaches, ranging in both cases from $2 \cdot 10^{-5}$ at $k = 1$ to $2 \cdot 10^{-4}$ at $k = 10$.

3.2 The case of A skew-symmetric and Hamiltonian.

Assume now that A is skew-symmetric and also Hamiltonian of size $N = 2n$, that is it has the $2n \times 2n$ form

$$A = \begin{bmatrix} A_1 & A_2 \\ -A_2 & A_1 \end{bmatrix}, \quad A_1 = -A_1^T, \quad A_2 = A_2^T; \tag{3.2}$$

in particular, $AJ = JA$. Corollary 2.1 ensures that $\exp(A)$ is ortho-symplectic so that, given an ortho-symplectic matrix Q, the matrix $\exp(A)Q$ is also ortho-symplectic. Let $Q \in \mathbb{R}^{2n \times 2n}$ be an ortho-symplectic matrix, hence Q has the form

$$Q = \begin{bmatrix} Q_1 & Q_2 \\ Q_2 & -Q_1 \end{bmatrix}.$$

Let $\widehat{Q}$ collect $p \le n$ of its first n columns, and define the $2n \times 2p$ matrix

$$V = [\widehat{Q}, -J\widehat{Q}]. \tag{3.3}$$

Since $JV = VJ_{2p}$, we can show that V is a rectangular ortho-symplectic matrix; indeed, $V^TV = I$, and $V^TJV = V^TVJ_{2p} = J_{2p}$. The following result can thus be established.

PROPOSITION 3.2. *Let V be as defined in* (3.3). *Let $\mathcal{V}_m$ be generated by the block Lanczos method with $\mathcal{V}_m^T\mathcal{V}_m = I$, so that its columns span the block Krylov subspace $\mathbb{K}_m(A, V)$. Then the matrix $U_m = \mathcal{V}_m \exp(\mathcal{H}_m)E_1$ with $E_1 \in \mathbb{R}^{mp\times 2p}$, is a rectangular ortho-symplectic matrix.*

PROOF. Since $\mathcal{H}_m = \mathcal{V}_m^T A\ \mathcal{V}_m$ and A is skew-symmetric, $\mathcal{H}_m$ is skew-symmetric (and thus banded), hence $\exp(\mathcal{H}_m)$ is orthogonal. Therefore, from Proposition 3.1 it follows that $U_m^TU_m = I$. Because of the choice of V, we have $\mathrm{Range}(J\mathcal{V}_m) = \mathrm{Range}(\mathcal{V}_m)$; therefore there exists a nonsingular matrix D_m such that

$$J\mathcal{V}_m = \mathcal{V}_m D_m. \tag{3.4}$$

Using the orthogonality of $\mathcal{V}_m$, we have $\mathcal{V}_m^TJ\mathcal{V}_m = D_m$, that is, D_m is skew-symmetric. Relation (3.4) holds for any m, so that it must be

$$J\mathcal{V}_{m+1} = \mathcal{V}_{m+1}D_{m+1} = [\mathcal{V}_m, V_{m+1}] \begin{bmatrix} D_m & D_* \\ O & \tilde{D}_{m+1} \end{bmatrix}.$$

Since D_{m+1} is skew-symmetric, $D_* = O$, so that D_{m+1} is block diagonal, that is $D_{m+1} = \mathtt{blockdiag}(\tilde{D}_1, \ldots, \tilde{D}_m, \tilde{D}_{m+1})$. Thanks to (3.3) we have $\tilde{D}_1 = J_{2p}$. Moreover, since $J^{-1} = J^T$, from (3.4) it follows $\mathcal{V}_m D_m^{-1} = J^T\mathcal{V}_m = -J\mathcal{V}_m$, so that

$$D_m^{-1} = \mathcal{V}_m^T\mathcal{V}_m D_m^{-1} = -\mathcal{V}_m^TJ\mathcal{V}_m = -D_m.$$

Since D_m is skew-symmetric, we can conclude that $D_m^{-T} = D_m$. Therefore, using $JA = AJ$, we have

$$\begin{aligned}\mathcal{H}_m D_m &= \mathcal{V}_m^TA\mathcal{V}_m D_m = \mathcal{V}_m^TJA\mathcal{V}_m \\ &= \left(\mathcal{V}_m D_m^{-1}\right)^T A\mathcal{V}_m = D_m^{-T}\mathcal{V}_m^TA\mathcal{V}_m = D_m\mathcal{H}_m,\end{aligned}$$

from which we also obtain $D_m \exp(\mathcal{H}_m) = \exp(\mathcal{H}_m)D_m$ for any m. Finally,

$$\begin{aligned}U_m^TJU_m &= E_1^T \exp(\mathcal{H}_m)^T\mathcal{V}_m^TJ\mathcal{V}_m \exp(\mathcal{H}_m)E_1 = E_1^T \exp(\mathcal{H}_m)^T D_m \exp(\mathcal{H}_m)E_1 \\ &= E_1^T \exp(\mathcal{H}_m)^T \exp(\mathcal{H}_m)D_m E_1 = \tilde{D}_1 = J_{2p},\end{aligned} \tag{3.5}$$

which completes the proof. ∎

Since the rectangular matrix U_m is partitioned as $U_m = [\widehat{U}_m, -J\widehat{U}_m]$, the explicit computation of the second block of p columns is unnecessary, since it can be easily recovered from the first p columns. The augmented cost given by working with $2p$ rather than with p vectors in V allows us to generate a quasi

J-orthogonal basis (cf. (3.4)), with the matrix D_m having a convenient structure. This constraint conforms with the standard requirements used for building single vector Lanczos-type recurrences that preserve the symplectic structure of the problem [7, 8, 46, 44].

EXAMPLE 3.2. We consider a 200×200 skew-symmetric and Hamiltonian matrix A as in (3.2), with A_2 and A_1 the symmetric and skew-symmetric parts, respectively, of two different matrices with normally distributed random entries (Matlab function `randn`). The condition number of A is $\text{cond}(A) \approx 538$. Matrix $Q = [q_1, \ldots, q_{200}]$ was constructed as $Q = \exp(G)$ with G derived in a way similar to A. We consider $p = 2$ and $p = 6$. The results in Table 3.2 report the error in the preservation of ortho-normality and J-ortho-normality, by means of the two quantities $\|U_m^T U_m - I_{2p}\|$, $\|U_m^T J U_m - J_{2p}\|$, respectively, where $U_m = \mathcal{V}_m \exp(\mathcal{H}_m) E_1$ is the approximation of U in $\mathbb{K}_m(A, V)$ with $V = [q_1, \ldots, q_p, -Jq_1, \ldots, -Jq_p]$ and $m = 1, \ldots, 10$.

Table 3.2 .

p	m	$\|U_m^T J U_m - \widetilde{J}_{2p}\|$	$\|U_m^T U_m - I_{2p}\|$
2	1	2.5249e−14	2.5597e−14
	2	2.2105e−14	2.4717e−14
	3	2.6457e−14	2.8592e−14
	4	2.0475e−14	2.5974e−14
	5	3.2515e−14	3.6217e−14
	6	2.5311e−14	2.7904e−14
	7	2.4948e−14	2.9303e−14
	8	2.6959e−14	3.3816e−14
	9	3.3527e−14	3.9958e−14
	10	2.8564e−14	3.1646e−14
6	1	4.7120e−14	5.1477e−14
	2	4.4224e−14	4.6034e−14
	3	5.5361e−14	5.9217e−14
	4	6.5580e−14	7.1523e−14
	5	5.3517e−14	6.4597e−14
	6	5.7162e−14	7.2058e−14
	7	6.3882e−14	7.7346e−14
	8	5.2415e−14	6.5304e−14
	9	5.5321e−14	6.6984e−14
	10	4.7034e−14	5.4387e−14

The matrix $\mathcal{V}_m$ is computed by using a block Lanczos procedure with local re-orthogonalization. The numbers in the table show that for this example the block Lanczos algorithm provides a satisfactory level of (J)-orthogonality in the approximate solution. Note that for $p = 6$, a block Krylov subspace of dimension as large as 120 is built. Finally, we stress that the level of preservation of the

geometric properties does not depend on the accuracy in the approximation, monitored by the error norm $\|U_m - U\|$.

REMARK 3.1. In practical situations, the generated block basis $\mathcal{V}_m$ may lose rank, so that $\dim(\mathbb{K}_m(A,V)) < mp$. When A is symmetric, effective implementations of the block Lanczos algorithm that allow one to purge redundant columns in $\mathcal{V}_m$ have been proposed; see [26, 5] and also [4, Section 4.6]. Since the block Lanczos method remains unchanged for A skew-symmetric or for A skew-symmetric and Hamiltonian, these approaches can be readily used, and the corresponding properties of $\mathcal{H}_m := \mathcal{V}_m^T A \mathcal{V}_m$ are preserved.

3.3 The case of A Hamiltonian.

In the proof of Proposition 3.2 the fact that A was skew-symmetric played a crucial role. In fact, relaxing the skew-symmetry property makes the structure preservation problem more challenging, so that the basic block Lanczos procedure needs to be adapted.

Let $\widehat{Q} \in \mathbb{R}^{N\times p}$ be a symplectic matrix. Given a Hamiltonian matrix A, Corollary 2.1 ensures that $U = \exp(A)\widehat{Q}$ is still a symplectic matrix. For a specifically chosen V, we wish to determine a symplectic approximation U_m in $\mathbb{K}_m(A,V)$ to U. To completely reproduce the characteristics of the original problem within the space $\mathbb{K}_m(A,V)$, we need to construct a symplectic basis $\mathcal{V}_m$ and a Hamiltonian representation matrix $\mathcal{H}_m$.

The generation of a symplectic basis for a Krylov subspace has recently received considerable attention, at least in the single vector case, namely $\widehat{Q} = q$. This is due to the impact that structure preservation has on the accuracy and stability properties of eigenvalue computation and on the solution of equations in several applications; see, e.g., [9]. In the single vector case, the construction of a symplectic basis can be carried out by means of a non-symmetric Lanczos recurrence, using the properties of the Hamiltonian matrix A introduced in Definition 2.1; see [23]. Further developments include the derivation of a Hamiltonian matrix $\mathcal{H}_m$ to effectively approximate eigenvalues of a Hamiltonian matrix A; see [7, 8, 46]. A more recent implementation of the Gram–Schmidt algorithm for the construction of a symplectic basis for $p = 1$ is given in [44], and expanded in [45] to devise a symplectic 'block-style' Lanczos method for the eigenvalue problem again for $p = 1$.

In our setting, we wish to construct a symplectic basis for the block Krylov subspace $\mathbb{K}_m(A,V)$ with the $N \times 2p$ matrix V properly chosen, for $p \geq 1$. To this end, we propose a new algorithm that stems from the single vector (i.e., $p = 1$) symplectic Lanczos process in [45]. We adapt the idea in [45] to work in the case of a general *block* Lanczos process with $p \geq 1$, equipped with a specific orthogonalization procedure, yielding a basis that is "logically" symplectic, together with a Hamiltonian representation matrix $\mathcal{H}_m$. Let $\widetilde{Q}$ consist of $2p$ columns of a symplectic matrix, so that $\widetilde{Q}^T J \widetilde{Q} = J_{2p}$. Let us introduce the $2kp \times 2kp$ permutation matrix $P_k = [I_{:,1:p:2kp}, I_{:,2:p:2kp}, \ldots, I_{:,p:p:2kp}]$; for instance, for $p = 2$, we get $P_k = [e_1, e_3, e_5, e_{2kp-1}, e_2, e_4, \ldots, e_{2kp}]$.

Hence, we define the starting matrix V as $V = \widetilde{Q}P$, so that V satisfies

$$V^T J V = \widetilde{J}_{2p}, \qquad \text{where} \quad \widetilde{J}_{2p} := \mathtt{blockdiag}(J_2, J_2, \dots, J_2) \in \mathbb{R}^{2p\times 2p}. \tag{3.6}$$

Therefore, V is logically (upon permutation) symplectic. Note that $P_1^T \widetilde{J}_{2p} P_1 = J_{2p}$. This permutation is commonly performed for algorithmic and notational convenience also in the single vector case, i.e. for $p = 1$.

The algorithm proceeds by using the block Lanczos recurrence (2.2) and requiring, upon permutation, the basis vectors to be symplectic. More precisely, the matrix $\mathcal{V}_m$ is constructed from (2.2) with

$$\mathcal{V}_m^T J \mathcal{V}_m = \widetilde{J}_{2mp} \qquad \text{or, equivalently} \quad (\mathcal{V}_m P_m)^T J (\mathcal{V}_m P_m) = J_{2mp}. \tag{3.7}$$

Multiplying (2.2) from the left by $\widetilde{J}_{2mp}^{-1}\mathcal{V}_m^T J$ we obtain $\mathcal{H}_m = \widetilde{J}_{2mp}^{-1}\mathcal{V}_m^T J A\, \mathcal{V}_m$. Using the fact that JA is symmetric, we deduce that $\widetilde{J}_{2mp}\mathcal{H}_m = \mathcal{V}_m^T JA\, \mathcal{V}_m$ is also symmetric. Finally, writing

$$P_m^T \widetilde{J}_{2mp} \mathcal{H}_m P_m = P_m^T \widetilde{J}_{2mp} P_m P_m^T \mathcal{H}_m P_m = J_{2mp}\big(P_m^T \mathcal{H}_m P_m\big),$$

we conclude that $P_m^T \mathcal{H}_m P_m$ is Hamiltonian. Since $\mathcal{H}_m$ is banded with bandwidth $2p$, the permuted matrix has the form

$$P_m^T \mathcal{H}_m P_m = \begin{bmatrix} \mathtt{H}_1 & \mathtt{H}_2 \\ \mathtt{H}_3 & -\mathtt{H}_1^T \end{bmatrix}, \qquad \mathtt{H}_2 = \mathtt{H}_2^T, \quad \mathtt{H}_3 = \mathtt{H}_3^T,$$

with $\mathtt{H}_i$, $i = 1, 2$ banded with semi-bandwidth equal to p, while $\mathtt{H}_3$ has semi-bandwidth equal to $p - 1$.

A structure-preserving approximation to $U = \exp(A)V$ is thus given by $U_m = \mathcal{V}_m P_m \exp(P_m^T \mathcal{H}_m P_m)(\mathcal{V}_m P_m)^T JV$. Since $\exp(P_m^T \mathcal{H}_m P_m) = P_m^T \exp(\mathcal{H}_m) P_m$, it follows that the approximation above is equivalent to

$$U_m = \mathcal{V}_m \exp(\mathcal{H}_m)\mathcal{V}_m^T JV = \mathcal{V}_m \exp(\mathcal{H}_m) E_1 \widetilde{J}_{2p},$$

and the approximate solution is also symplectic, upon permutation.

PROPOSITION 3.3. *Let V satisfy* (3.6). *Let $\mathcal{V}_m$ be generated by the block Lanczos method with $\mathcal{V}_m^T J \mathcal{V}_m = \widetilde{J}_{2mp}$, so that its columns span the block Krylov subspace $\mathbb{K}_m(A, V)$, and let $\mathcal{H}_m = \widetilde{J}_{2mp}^{-1}\mathcal{V}_m^T JA\, \mathcal{V}_m$. Then the matrix $U_m = \mathcal{V}_m \exp(\mathcal{H}_m) E_1 \widetilde{J}_{2p}$ with $E_1 \in \mathbb{R}^{mp\times 2p}$, is a symplectic matrix after permutation with P_1.*

PROOF. Let $\widehat{\mathcal{H}}_m = P_m^T \mathcal{H}_m P_m$, $\widehat{\mathcal{V}}_m = \mathcal{V}_m P_m$, so that we can write

$$U_m = \widehat{\mathcal{V}}_m \exp(\widehat{\mathcal{H}}_m) P_m^T E_1 \widetilde{J}_{2p}.$$

We also recall that $\widehat{\mathcal{H}}_m$ Hamiltonian implies that $\exp(\widehat{\mathcal{H}}_m)$ is symplectic. Therefore,

$$\begin{aligned} U_m^T J U_m &= \widetilde{J}_{2p}^T E_1^T P_m \exp(\widehat{\mathcal{H}}_m)^T \widehat{\mathcal{V}}_m^T J \widehat{\mathcal{V}}_m \exp(\widehat{\mathcal{H}}_m) P_m^T E_1 \widetilde{J}_{2p} \\ &= \widetilde{J}_{2p}^T E_1^T P_m \exp(\widehat{\mathcal{H}}_m)^T J_{2mp} \exp(\widehat{\mathcal{H}}_m) P_m^T E_1 \widetilde{J}_{2p} \\ &= \widetilde{J}_{2p}^T E_1^T P_m J_{2mp} P_m^T E_1 \widetilde{J}_{2p} = \widetilde{J}_{2p}. \end{aligned} \tag{3.8}$$

Hence, $(U_m P_1)^T J (U_m P_1) = P_1^T \widetilde{J}_{2p} P_1 = J_{2p}$, and the proof is completed. ∎

3.3.1 Computational aspects.

A possible implementation of the procedure outlined above is as follows, where V is a given symplectic matrix.

Algorithm: Symplectic block Lanczos.
Input: scalar m
matrices A of size $2n \times 2n$, and $V = [q_1, \hat{q}_1, q_2, \hat{q}_2, \dots]$ of size $2n \times 2p$
Output: $\mathcal{V}_m$ of size $2n \times 2mp$, $\mathcal{H}_m$ of size $2mp \times 2mp$
$X = V$
$\ell = 1$
for $i = 1, \dots, m$
  $\widehat{X} = A\,X$
  % Enforce symplecticity w.r.t. previous blocks
  $k = 2pi$
  $j_0 = \max\{1, k - 2(2p) + 1\}$
  for $j = j_0 : 2 : i \cdot 2p$,
    $H_{j:j+1,\ell:\ell+2p-1} = J_2^T\, V_{:,j:j+1}^T\, J\, \widehat{X}$
    $\widehat{X} = \widehat{X} - V_{:,j:j+1} H_{j:j+1,\ell:\ell+2p-1}$
  end
  % Enforce symplecticity within block
  $[X, H_{k+1:k+2p,\ell:\ell+2p-1}] = \texttt{mbsgs}(\widehat{X})$
  $V = [V, X]$
  $\ell = \ell + 2p$
end
$\mathcal{V}_m = V_{:,1:2mp}$, $\mathcal{H}_m = H_{1:2mp,1:2mp}$

The routine $\texttt{mbsgs}(\widehat{X})$ orthogonalizes the columns of $\widehat{X}$ so as to maintain symplecticity. The corresponding algorithm was proposed in [44] and its Matlab-style implementation is reproduced in the Appendix for completeness.

Our algorithm is based on the "block" indefinite inner product

$$[X, Y]_J = J_2^T X^T J Y, \qquad X, Y \in \mathbb{R}^{2n \times 2},$$

therefore, it may happen that $[X, X]_J$ is singular with X full column rank. In this case, breakdown occurs in the symplectic block Gram–Schmidt method (function `mbsgs`) and the symplectic block Lanczos method cannot proceed. A similar situation is encountered in the non-symmetric block Lanczos process. In there, some form of look-ahead strategy has been developed (see, e.g., [2]) to overcome the occurrence of near singularity, that is, quasi-breakdown. It is not clear whether a look-ahead strategy could be devised in this case without destroying the underlying symplectic structure. In fact, it should be noticed that a similar (but not equal!) recurrence to the one proposed here, could be obtained by using the non-symmetric block Lanczos algorithm with starting auxiliary matrix equal to $P = J^T V J_{2p}$; an implementation of the non-symmetric block Lanczos method that includes safeguard strategies is proposed in [3]; see also [4, Sections 7.8, 7.9].

An alternative way for improving the stability properties of the method, that has been proposed in the single vector case consists in (implicitly) restarting the symplectic Lanczos process [8]. In [45] the authors report a numerical example where the symplectic Lanczos method breaks down, whereas their algorithm (corresponding to ours for $p = 1$) successfully completes the computation.

None of these strategies has been specifically designed towards the approximation of the matrix exponential, hence further analysis is required to assess their effectiveness in this context.

3.3.2 Numerical experiments for A Hamiltonian.

In the following we explore the numerical performance of the proposed block algorithm when A is Hamiltonian.

EXAMPLE 3.3. We consider a 2000×2000 Hamiltonian matrix A as in Definition 2.1. The blocks A_2, A_3 were taken as the symmetric parts of two matrices with sparse random entries uniformly distributed, with sparsity ratio 0.1 and condition number 10 (Matlab function `sprand`). The block A_1 was taken as a sparse random matrix, with the same parameters as before. Matrix $Q = [q_1, \dots, q_{2000}]$ was constructed as $Q = \exp(G)$, with G generated following the same steps as for A. In the table below we report the error norms $\|U - U_m\|$ and $\|U_m^T J U_m - \widetilde{J}_p\|$ as the Krylov subspace $\mathbb{K}_m(A, V)$ grows, with $V = [q_1, q_{1001}, q_2, q_{1002}]$ and $m = 1, \dots, 10$. The condition number of the generated basis $\mathcal{V}_m$ and the dimension of the Krylov subspace, $2mp$, are also listed.

m	$2mp$	$\mathrm{cond}(\mathcal{V}_m)$	$\|U_m - U\|$	$\|U_m^T J U_m - \widetilde{J}_p\|$
1	4	$1.08 \cdot 10^{0}$	$6.24 \cdot 10^{-1}$	$9.99 \cdot 10^{-15}$
2	8	$1.05 \cdot 10^{3}$	$3.74 \cdot 10^{0}$	$1.00 \cdot 10^{-12}$
3	12	$8.78 \cdot 10^{5}$	$1.65 \cdot 10^{-1}$	$1.25 \cdot 10^{-10}$
4	16	$1.47 \cdot 10^{6}$	$5.26 \cdot 10^{-2}$	$1.25 \cdot 10^{-10}$
5	20	$1.75 \cdot 10^{6}$	$1.19 \cdot 10^{-3}$	$1.25 \cdot 10^{-10}$
6	24	$1.84 \cdot 10^{6}$	$7.62 \cdot 10^{-5}$	$1.25 \cdot 10^{-10}$
7	28	$2.40 \cdot 10^{6}$	$4.02 \cdot 10^{-6}$	$1.25 \cdot 10^{-10}$
8	32	$2.53 \cdot 10^{6}$	$1.13 \cdot 10^{-6}$	$1.25 \cdot 10^{-10}$
9	36	$2.75 \cdot 10^{6}$	$9.25 \cdot 10^{-9}$	$1.25 \cdot 10^{-10}$
10	40	$2.84 \cdot 10^{6}$	$1.18 \cdot 10^{-9}$	$1.25 \cdot 10^{-10}$

EXAMPLE 3.4. We consider the following linear Hamiltonian system:

$$\begin{cases} q' = A\, q \\ q(0) = q_0 \end{cases}$$

with $q = q(t)$, $A = J^{-1}S$ and S a 400×400 constant, symmetric diagonal matrix of uniformly distributed values between 1 and 100, so that A is Hamiltonian. The starting vector is $q_0 = \widehat{Q} e_1$, where $\widehat{Q}$ is a 400×400 symplectic matrix generated

as in the previous example and the auxiliary symplectic vector is $\widehat{q} = \widehat{Q}e_{201}$, so that the matrix $V = [q_0, \widehat{q}]$ is symplectic, that is it holds $V^T JV = J_2$. The energy function of the system is given by $E(q(t)) = q(t)^T Sq(t)$ which remains constant for all $t > 0$. In this test, we are interested in evaluating the preservation of the system energy after discretization. More precisely, starting with $q^{(0)} = q_0$ and $r = 0$, we apply a symplectic exponential integrator to solve our Hamiltonian system, that is $q^{(r+1)} = \exp(hA)q^{(r)}$, with $h = 1/40$ and $r \geq 0$. If $\exp(hA)$ is determined exactly, then the energy norm $E(q^{(r)})$ remains constant for all $r \geq 0$. By approximating the action of $\exp(hA)$ on $q^{(r)}$ with a standard Krylov subspace approach, the energy associated with the approximate iterate is no longer constant, unless $\exp(hA)q^{(r)}$ is obtained at high accuracy. On the other hand, the Hamiltonian Lanczos method allows us to maintain constant energy with good accuracy irrespective of the solution accuracy, at a price of some extra computation. The left plot of Figure 3.2 shows the error $|E(q^{(r+1)}) - E(q_0)|$. The curve with symbol "-o-" refers to the case when the iterate is obtained by using the Matlab function `expm` to evaluate $\exp(hA)$ at each iteration. The solid curve is given by time stepping with the solution obtained with $m = 5$ iterations of the Hamiltonian Lanczos, whereas the dash-dotted curve depicts the energy behavior when the iterate is obtained with $2m = 10$ iterations of the regular Krylov subspace method. Note that this subspace dimension requires approximately the same amount of space as five iterations of the new Hamiltonian Lanczos method, for $p = 1$.

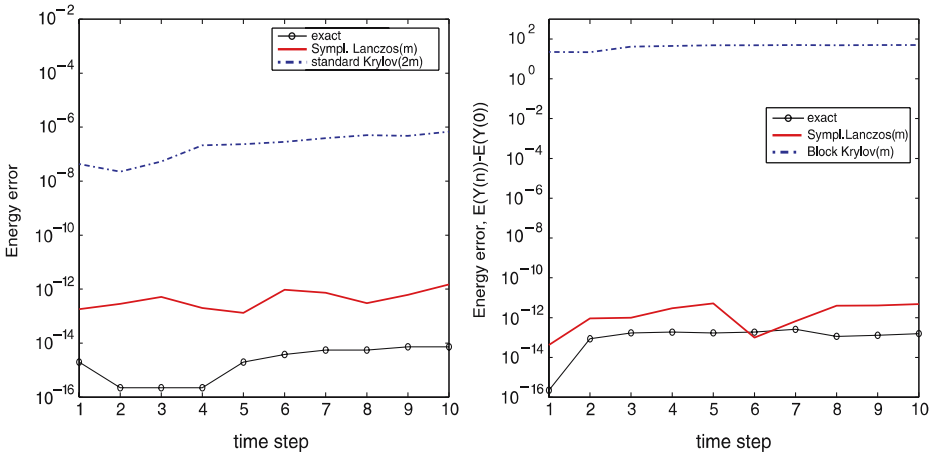

Figure 3.2: Example 3.4. Conservation of energy. Left plot: $|E(q^{(r)}) - E(q_0)|$ for the exact, Hamiltonian and Krylov methods, for $p = 1$. Right plot: $\|E(Q^{(r+1)}) - E(Q_0)\|$, where $Q_0 = Q[e_1, e_{n+1}]$ for the exact, Hamiltonian and block Krylov methods..

Not surprisingly, the error in the energy preservation occurring in the standard Krylov subspace approach (cf. left plot of Figure 3.2) is of the same order of magnitude as the error in the iterate. We refer to [21] for similar experiments in the single vector case. The accuracy in the evaluation of the sys-

tem energy is much higher in the structure preserving method. This fact is particularly apparent if one is interested in evaluating the energy of the flow obtained by iterating with both q_0 and the auxiliary vector $\widehat{q}$. In this case, the quantity $E(Q^{(r)}) = (Q^{(r)})^T S Q^{(r)}$ should stay constant in norm, where $Q^{(r+1)} = \exp(hA)Q^{(r)}$ and $Q^{(0)} = Q_0 = [q_0, \widehat{q}]$. The right plot of Figure 3.2 shows the energy error for the exact iterates, for the Hamiltonian Lanczos iterates after $m = 5$ iterations, and for the iterates obtained after $m = 5$ steps of the *block* version of the standard Krylov process (cf. (2.3)) started with $Q^{(0)}$. The discrepancy between the two Krylov subspace-based methods can be further appreciated. Note that m iterations of the block Krylov method provide a less accurate approximation than $2m$ iterations of the regular Krylov approach. This explains the larger error in the energy conservation than in the left plot.

4 Conclusions.

In this paper we have shown that Krylov subspace methods can be naturally adapted to preserve geometric properties of the exponential operator when the matrix is skew-symmetric or also Hamiltonian. In the case of a Hamiltonian matrix, we have proposed a new variant of the block Lanczos algorithm that again allows one to preserve the geometric structure of the operator. Assuming exact arithmetic, the derived strategies completely address the question of how to maintain structure properties in geometric integrators when dealing with problems of large dimension whose (exponential) iterate need to be approximated (cf. [47]).

Finally, we observe that the main results of this paper hold for functions different from the exponential. Indeed, it was shown in [11] that geometric properties may also be preserved by diagonal Padé rational functions $P_{\nu,\nu}(z)$, which play an important role for two reasons. Firstly they represent a reliable and feasible computational device to accurately approximate the exponential of small matrices and it is routinely implemented in standard software (cf., e.g., function `expm` in Matlab [36]). Secondly, due to the aforementioned geometric properties, low order Padé functions can efficiently replace $\exp(A)$ in the numerical integration of ODEs on manifolds, see, e.g., [41, 18, 31].

Several questions remain open and deserve further investigations. In particular, very little is known about the convergence properties of the Hamiltonian (block) Lanczos method, and about the role of the conditioning of the generated basis on the accuracy of the approximate solution. To this end, the inherent matrix structure should be fully taken into account; see, e.g., [33].

Although our experiments did not seem to be significantly affected by finite precision computation, this should be taken into account. More precisely, stability problems and loss of symplecticity (or of rank) may destroy the Hamiltonian structure, if no safeguard strategies are developed. Some strategies have been devised in [7] for the single vector case, but a complete analysis is still lacking. Methods that address similar problems in the general non-symmetric block Lanczos methods may provide additional insight.

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Appendix.

In this appendix we reproduce a Matlab-style algorithm for the modified Symplectic Gram–Schmidt algorithm described in [44].

```
function [w,h]=mbsgs(v,J);

J2=[0 1;-1  0]; [n,p2]=size(v); p =p2/2;

\% First block
  w = v;

  v0 = w(:,1);
  h(1,1) = norm(v0);
  w(:,1) = v0/h(1,1);
  h(1,2) = w(:,1)'*w(:,2);
  w(:,2) = w(:,2) - w(:,1)*h(1,2);
  h(2,2) = w(:,1)'*J*w(:,2);
  w(:,2) = w(:,2)/h(2,2);

\% Subsequent blocks
  for j=3:2:p2,
     w(:,j:j+1)=w(:,j:j+1);
     for i=1:2:j-1
        h(i:i+1,j:j+1) = J2'*w(:,i:i+1)'*J*w(:,j:j+1);
        w(:,j:j+1) = w(:,j:j+1) - w(:,i:i+1)*h(i:i+1,j:j+1);
     end

\% Last block
     v0 = w(:,j);
     h(j,j) = norm(v0);
     w(:,j) = v0/h(j,j);
     h(j,j+1) = w(:,j)'*w(:,j+1);
     w(:,j+1) = w(:,j+1) - w(:,j)*h(j,j+1);
     h(j+1,j+1) = w(:,j)'*J*w(:,j+1);
     w(:,j+1) = w(:,j+1)/h(j+1,j+1);
   end

end
```

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