A BLOCK J-LANCZOS METHOD FOR HAMILTONIAN MATRICES∗

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Abstract. This work aims to present a structure-preserving block Lanczos-like method. The Lanczos-like algorithm is an effective way to solve large sparse Hamiltonian eigenvalue problems. It can also be used to approximate \( \exp(A)V \) for a given large square matrix \( A \) and a tall-and-skinny matrix \( V \) such that the geometric property of \( V \) is preserved, which interests us in this paper. This approximation is important for solving systems of ordinary differential equations (ODEs) or time-dependent partial differential equations (PDEs). Our approach is based on a block \( J \)-tridiagonalization procedure of a Hamiltonian and skew-symmetric matrix using symplectic similarity transformations.

Key words. block \( J \)-Lanczos method, Hamiltonian matrix, skew-Hamiltonian matrix, symplectic matrix, symplectic reflector, block \( J \)-tridiagonal form, block \( J \)-Hessenberg form

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1. Introduction. The Lanczos method is an efficient tool for computing a few eigenvalues and associated eigenvectors of a large and sparse matrix. In this paper, we introduce a structure-preserving block Lanczos method called block \( J \)-Lanczos algorithm. This algorithm is applied to reduce a large sparse \( 2n \times 2n \) Hamiltonian matrix to a small Hamiltonian block \( J \)-tridiagonal matrix in the form

\[
\begin{bmatrix}
\ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast \\
\end{bmatrix}
\]

where \( \ast \) are matrices of size \( s \times s \). With this structure, we can derive a set of four-six-term recurrence relation of block \( J \)-Lanczos, and find four components of this matrix at the same iteration.

Gerstner and Mehrmann proposed in [8] the reduction of Hamiltonian matrices to Hamiltonian \( J \)-Hessenberg form to solve the real algebraic Riccati equation via the symplectic QR-like algorithm. This form is also used by Benner and Fassbender in [4] to create a family of implicitly restarted Lanczos methods for Hamiltonian and symplectic matrices; see also [5],[8]. It is similar to the basic means used by Ferng, Lin, and Wang ([15],[16]) to construct a \( J \)-Lanczos algorithm for solving large sparse Hamiltonian eigenvalue problems. We refer to [1] for more details on the symplectic Lanczos algorithm for Hamiltonian matrices. The main purpose of

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this paper is to introduce new methods for computing the Hamiltonian block $J$-tridiagonal form. Our approach is based on using $\mathbb{R}^{2s \times 2s}$ as free module on $(\mathbb{R}^{2s \times 2s}, +, \times)$.

We organize this paper as follows. We first introduce some definitions that are related to the $J$-structure matrices. Some notation and terminology are reviewed in Section 2. In Section 3, we propose two different block $J$-Lanczos methods using two types of normalization. An issue related to the $J$-reorthogonalization in the $J$-Lanczos algorithm is also discussed. In Section 4, we give an approximation of $\exp(A)V$ using the block Krylov subspace $K_n(A, V) = \text{blockspan}\{V, AV, ..., A^{n-1}V\}$ (see [14]) generated by the proposed block $J$-Lanczos algorithm. Numerical examples are presented in Section 5 to demonstrate the efficiency of our methods.

2. Terminology, notation, and some basic facts. A ubiquitous matrix in this work is the skew-symmetric matrix $J_{2n} = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix}$, where $I_n$ and $0_n$ denote the $n \times n$ identity and zero matrices, respectively. Note that $J_{2n}^{-1} = J_{2n}^T = -J_{2n}$. In the following, we will drop the subscripts $n$ and $2n$ whenever the dimension is clear from its context. The $J$-transpose of any $2n$-by-$2p$ matrix $M$ is defined by $M^J = J_{2p}^T M^T J_{2n} \in \mathbb{R}^{2p \times 2n}$. A Hamiltonian matrix $M \in \mathbb{R}^{2n \times 2n}$ has the explicit block structure $M = \begin{bmatrix} A & R \\ G & -A^T \end{bmatrix}$, where $A, G, R$ are real $n \times n$ matrices and $G = G^T$, $R = R^T$. By straightforward algebraic manipulation, we can show that a Hamiltonian matrix $M$ is equivalently defined by $M^J = -M$. Likewise, a matrix $M$ is skew-Hamiltonian if and only if $M^J = M$ and it has the explicit block structure $M = \begin{bmatrix} A & R \\ G & A^T \end{bmatrix}$, where $A, G, R$ are real $n \times n$ matrices and $G = -G^T$, $R = -R^T$. Any matrix $S \in \mathbb{R}^{2n \times 2p}$ satisfying $S^T J_{2n} S = J_{2p}$ (or $S^J S = I_{2p}$) is called a symplectic matrix. This property is also called $J$-orthogonality. Symplectic similarity transformations preserve the Hamiltonian and skew-Hamiltonian structure.

**Remark 2.1.** If the matrix $S = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$ is symplectic, then

$$
\tilde{S} = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & H_{11} & 0 & H_{12} \\ 0 & 0 & I & 0 \\ 0 & H_{21} & 0 & H_{22} \end{bmatrix}
$$

is also symplectic.

**Proposition 2.2.** Let $E_i = [e_i, e_{n+i}]$ for $i = 1, \ldots, n$, where $e_i$ denotes the $i$-th unit vector of length $2n$. Then

$$
E_i J_2 = J_{2n} E_i, \quad E_i^J = E_i^T \quad \text{and} \quad E_i^T E_j = \delta_{ij} I_2,
$$

where

$$
E_i^J = J_2^T E_i^T J_{2n} \quad \text{and} \quad \delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}
$$

More generally, given $m, s \in \mathbb{N}$ such that $n = ms$, we define the set $\{F_i\}_{1 \leq i \leq m}$ as

$$
F_i = [e_{(i-1)s+1}, e_{(i-1)s+2}, \ldots, e_{is}], \quad \text{where} \quad e_{is} := e_{n+(i-1)s+1}, e_{n+(i-1)s+2}, \ldots, e_{n+is} \in \mathbb{R}^{2n \times 2s}.
$$

Then we have

$$
F_i J_2 s = J_{2n} F_i, \quad F_i^J = F_i^T \quad \text{and} \quad F_i^T F_j = \delta_{ij} I_{2s},
$$

where
Then $M$ is given by

\[ F^J_i = J^T_2 J^T_2 J_{2n} \] and \[ \delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases} \]

**Proposition 2.3.** Any $2n \times 2s$ real matrix $U$ can be expressed uniquely as a finite linear combination of $(F_i)_{1 \leq i \leq m}$, $U = \sum_{i=1}^{m} F_i C_i$, where

\[
C_i = \begin{bmatrix}
  u(i-1)s+1,1 & \cdots & u(i-1)s+1,s \\
  \vdots & \ddots & \vdots \\
  u_is,i & \cdots & u_is,s \\
  u_{n+i}(i-1)s+1,1 & \cdots & u_{n+i}(i-1)s+1,s \\
  \vdots & \ddots & \vdots \\
  u_{n+i}s,i & \cdots & u_{n+i}s,s \\
\end{bmatrix}
\]

\[ \in \mathbb{R}^{2s \times 2s}. \]

**Proposition 2.4.** Let $M$ be a $2n$-by-$2n$ real matrix, where $n = ms$ with $m, s \in \mathbb{N}$. Then $M$ can be represented uniquely as $M = \sum_{i=1}^{m} \sum_{j=1}^{m} F_i M_{ij} F^T_j$, where $M_{ij} \in \mathbb{R}^{2s \times 2s}$ is given by

\[
\begin{bmatrix}
  \tilde{m}_{(i-1)s+1,(j-1)s+1} & \cdots & \tilde{m}_{(i-1)s+1,j,s} \\
  \vdots & \ddots & \vdots \\
  \tilde{m}_{i,s,j} & \cdots & \tilde{m}_{i,s,j,s} \\
  m_{n+i(s-1)+1,(j-1)s+1} & \cdots & m_{n+i(s-1)+1,j,s} \\
  \vdots & \ddots & \vdots \\
  m_{n+i(s-1)+s,j} & \cdots & m_{n+i(s-1)+s,j,s} \\
\end{bmatrix}
\]

**Proposition 2.5.** The matrix $M$ from the previous proposition is Hamiltonian (respectively, skew-Hamiltonian) if $M_{ij} = -M_{ji}$; respectively, if $M_{ij} = M_{ji}$.

**Proof.** The result is obvious since $M^J = \sum_{i=1}^{m} \sum_{j=1}^{m} F_i M^J_{ij} F^T_j$. \qed

**Definition 2.6.** A matrix $M = \sum_{i=1}^{m} \sum_{j=1}^{m} F_i M_{ij} F^T_j \in \mathbb{R}^{2n \times 2n}$ is said to be in block upper $J$-triangular form if $M_{ij} = 0_{2s}$ for $i > j$ and $M_{ii}$ is upper triangular. It is called in $J$-Hessenberg form if $M_{ij} = 0_{2s}$ for $i > j + 1$, and in block $J$-tridiagonal form if $M_{ij} = 0_{2s}$ when $i < j - 1$ or $i > j + 1$.

**Remark 2.7.** A Hamiltonian block $J$-Hessenberg matrix is in block $J$-tridiagonal form.

**2.1. Symplectic reflector.** We recall that the symplectic reflector on $\mathbb{R}^{2n \times 2}$ is defined in parallel with elementary reflectors as given in the following proposition from [2].

**Proposition 2.8.** Let $U, V$ be $2n$-by-$2$ real matrices satisfying $U^J U = V^J V = I_2$. If the $2$-by-$2$ matrix $C = I_2 + V^J U$ is nonsingular, then $S = (U + V) C^{-1} (U + V)^T - I_{2n}$ is symplectic and transforms $U$ to $V$, hence it is called the symplectic reflector that takes $U$ to $V$.

**Lemma 2.9.** Let $W = [w_1 \quad w_2] \in \mathbb{R}^{2n \times 2}$ be a non-isotropic matrix $(\det (W^J W) \neq 0)$, and let $U = W q(W)^{-1}$ be its normalized matrix where, with $\alpha = w_1^T J w_2$,

\[
q(W) = \begin{cases}
\sqrt{\alpha} I_2 & \text{if } \alpha > 0, \\
\sqrt{-\alpha} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & \text{if } \alpha < 0.
\end{cases}
\]
Then there exists a symplectic reflector $S$ that takes $U$ to $E_1$, and therefore $W$ to $E_1 q(W)$. The $2n$-by-$2$ real matrix $SW$ is of the form

$$SW = \begin{bmatrix}
* & 0 \\
0 & 0 \\
\vdots & \vdots \\
0 & 0 \\
0 & 0 \\
\vdots & \vdots \\
0 & 0 \\
\end{bmatrix} \quad \forall n + 1.$$

**Remark 2.10.** Applying symplectic reflectors to a matrix $A \in \mathbb{R}^{2n \times 2n}$, we obtain the factorization $A = SR$, where $S \in \mathbb{R}^{2n \times 2n}$ is symplectic and $R = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} \in \mathbb{R}^{2n \times 2n}$ is upper $J$-triangular (here $s = 1$) and in addition $R_{12}$ is strictly upper triangular. More precisely, the matrix $R$ is of the form

$$R = \begin{bmatrix}
* & * & \cdots & * & 0 & \cdots & * \\
\ddots & \ddots & \vdots & \ddots & \ddots & \vdots & \ddots \\
\ddots & * & \ddots & \ddots & \ddots & \ddots & \ddots \\
\ddots & \ddots & \ddots & * & \ddots & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots & * & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots & \ddots & * \\
0 & 0 & \cdots & \cdots & \cdots & \cdots & * \\
\end{bmatrix}.$$

**3. The block $J$-Lanczos method.** In this section, we propose a block symplectic Lanczos method to compute the reduced Hamiltonian form for $2n$-by-$2n$ real Hamiltonian matrices and construct a block $J$-orthogonal basis of the block Krylov subspace. Recall that the Krylov subspace method is an efficient tool for computing a few eigenvalues and associated eigenvectors of a large and sparse matrix. In the following, the dimension of $(F_t)_{1 \leq t \leq m}$ is given according to the context.

Let for $Q_k := [q_1, \ldots, q_{k+1}, \ldots, q_{2k}] \in \mathbb{R}^{2n \times 2sk}$ be a $2n$-by-$2sk$ symplectic matrix for $k \leq m$, where $q_i \in \mathbb{R}^{2n \times s}$ for $i = 1, 2, \ldots, 2k$, and $n = ms$. Let $H_k$ be a $2sk$-by-$2sk$ Hamiltonian block $J$-tridiagonal matrix (Hamiltonian $J$-Hessenberg form) computed by the $J$-Lanczos recursion such that $MQ_k = Q_k H_k + W_k F_k^{T}$, where $W_k \in \mathbb{R}^{2n \times 2s}$ is $J$-orthogonal to $Q_k$; i.e., $Q_k^T W_k = 0_{2sk \times 2s}$ which also means $q_i^T JW_k = 0_{s \times 2s}$ for $i = 1, 2, \ldots, 2k$. That
is, \( H_k \) is in the form

\[
H_k = \begin{bmatrix}
    a_1 & c_1 & \cdots & c_k \\
    b_1 & a_2 & \cdots & \cdots & \cdots & c_{k-1} \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \gamma_1 & \delta_1 & \cdots & \delta_{k-1} & \beta_k \\
    \delta_1 & \gamma_2 & \cdots & \cdots & \cdots & c_k \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \delta_1 & \gamma_2 & \cdots & \delta_{k-1} & \gamma_k \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
\end{bmatrix}
\]

with blocks \( \alpha_i, \beta_i, \gamma_i, \delta_i, c_i, b_i, c_i, c_i \in \mathbb{R}^{s \times s} \), where \( \beta_i \) and \( \gamma_i \) are symmetric, and \( b_i \neq 0_s \), \( c_i \neq 0_s \), \( \alpha_i \neq 0_s \), and \( \delta_i \neq 0_s \) for \( i = 1, \ldots, k \).

Subsequently, our goal is to use the block Lanczos process to compute the \( 2n \times 2n \) symplectic matrix \( Q_k \) and the \( 2sk \times 2sk \) Hamiltonian block tridiagonal matrix \( H_k \). The block \( J \)-Lanczos method is presented here in two different ways with two normalization methods, one based on the \( SR \) decomposition, and the other one based on the \( R^T R \) decomposition.

### 3.1. The first approach

Here, \( 2n \times s \) block vectors instead of single vectors and \( s \times s \) matrix coefficients instead of scalars are used. Since \( MQ_k = Q_k H_k + W_k F_k^T \), by comparing the \( i \)-th and \( (k + i) \)-th block columns on both sides of the equality, we obtain, for \( i = 1, \ldots, k \),

\[
\begin{align*}
MQ_i &= q_i c_i + q_i a_i + q_i b_i + q_{k+i} \delta_i + q_{k+i} \gamma_i + q_{k+i} \beta_i, \\
Mq_{k+i} &= q_i \alpha_i - q_i \delta_i - q_{k+i} \alpha_i - q_{k+i} \beta_i - q_{k+i} \beta_i - q_{k+i} \gamma_i + q_{k+i} \gamma_i.
\end{align*}
\]

Note that \( b_0 = 0_s \), \( c_0 = 0_s \), \( \alpha_0 = 0_s \), and \( \delta_0 = 0_s \). From the symplecticity of the matrix \( Q_k \), we have

\[
q_i^T J q_{k+i} = I_s \quad \text{and} \quad q_i^T J q_j = 0_s \quad \text{for} \quad j \neq k + i.
\]

The \( s \times s \) matrix coefficients \( a_i, \gamma_i, \beta_i \) can be determined via

\[
\begin{align*}
\alpha_i &= -q_{k+i}^T JM q_i, \\
\gamma_i &= q_i^T JM q_i, \\
\beta_i &= -q_{k+i}^T JM q_{k+i},
\end{align*}
\]

for \( i = 1, \ldots, k \). It is well-known that the Hamiltonian matrix \( M \) satisfies \( (JM)^T = JM \). Therefore, the matrix coefficients \( \gamma_i \) and \( \beta_i \) are symmetric. Indeed, we have

\[
\begin{align*}
\beta_i^T &= (-q_{k+i}^T JM q_{k+i})^T = -q_{k+i} (JM)^T q_{k+i} = \beta_i, \\
\gamma_i^T &= (q_i^T JM q_i)^T = q_i^T (JM)^T q_i = \gamma_i.
\end{align*}
\]

Set

\[
\begin{align*}
u_i &= M q_i - q_i - q_i a_i - q_{k+i} \delta_i + q_{k+i} \gamma_i, \\
v_i &= M q_{k+i} - q_i \alpha_i - q_i a_i - q_{k+i} \beta_i - q_{k+i} \gamma_i.
\end{align*}
\]
Then we get
\[
\begin{align*}
\begin{cases}
  u_i = q_{i+1} b_i + q_{k+i+1} \delta_i, \\
  v_i = q_{i+1} \alpha_i - q_{k+i+1} \epsilon_i^T.
\end{cases}
\end{align*}
\]

The $J$-orthogonality condition holds for both $u_i$ and $v_i$, i.e.,
\[
\begin{align*}
\begin{cases}
  q_i^T J u_i = q_i^T J M q_i - \gamma_i = 0_s, \\
  q_{k+i}^T J u_i = q_{k+i}^T J M q_i + a_i = 0_s, \\
  q_{i-1}^T J u_i = q_{i-1}^T J M q_i - \delta_{i-1}^T = - (M q_{i-1})^T J q_i - \delta_{i-1}^T = 0_s, \\
  q_{k+i-1}^T J u_i = q_{k+i-1}^T J M q_i + c_{i-1} = - (M q_{k+i-1})^T J q_i + c_{i-1} = 0_s,
\end{cases}
\end{align*}
\]
and
\[
\begin{align*}
\begin{cases}
  q_i^T J v_i = q_i^T J M q_{k+i} + a_i^T = - (M q_i)^T J q_{k+i} + a_i^T = 0_s, \\
  q_{k+i}^T J v_i = q_{k+i}^T J M q_{k+i} + \beta_i = - (M q_{k+i})^T J q_{k+i} + \beta_i = 0_s, \\
  q_{i-1}^T J v_i = q_{i-1}^T J M q_{k+i} + b_{i-1}^T = - (M q_{i-1})^T J q_{k+i} + b_{i-1}^T = 0_s, \\
  q_{k+i-1}^T J v_i = -q_{k+i-1}^T J M q_{k+i} + \alpha_{i-1}^T = (M q_{k+i-1})^T J q_{k+i} + \alpha_{i-1}^T = 0_s,
\end{cases}
\end{align*}
\]
with $q_j^T J u_i = q_{k+j}^T J u_i = q_j^T J v_i = q_{k+j}^T J v_i = 0_s$ for $j = 1, \ldots, i$.

The $2n$-by-$s$ matrices $q_{i+1}$ and $q_{k+i+1}$ are computed by normalizing the $2n$-by-$2s$ matrix $W_i = [u_i \ v_i]$. Normalization is presented below in two ways. The first one is a normalization based on the $SR$ decomposition by using symplectic reflectors as recalled above (see [2]), and the second one is a normalization based on the symplectic Cholesky $R^T R$ decomposition using the $LU$ $J$-factorization; see [3].

### 3.1.1. Normalization by using the $SR$ decomposition

At step $i$ of the block $J$-Lanczos method given above, we decompose $W_i = [u_i \ v_i] \in \mathbb{R}^{2n \times 2s}$ into a product $W_i = S^i R^i$ by using the $SR$ decomposition based on symplectic reflectors given in Section 2.1, where the matrix $S^i \in \mathbb{R}^{2n \times 2n}$ is symplectic and $R^i = \begin{bmatrix} R_{11}^i & R_{12}^i \\ R_{21}^i & R_{22}^i \end{bmatrix} \in \mathbb{R}^{2n \times 2s}$ is upper $J$-triangular.

We set, using Matlab notation,
\[
\begin{align*}
\begin{cases}
  q_{i+1} = S^i(:, \ 1 : s), \\
  q_{k+i+1} = S^i(:, \ n + 1 : n + s),
\end{cases}
\end{align*}
\]
and
\[
\begin{align*}
\begin{cases}
  b_i = R^i(1 : s, 1 : s), \\
  \alpha_i = R^i(1 : s, s + 1 : 2s), \\
  \delta_i = R^i(n + 1 : n + s, 1 : s), \\
  -\epsilon_i^T = R^i(n + 1 : n + s, s + 1 : 2s).
\end{cases}
\end{align*}
\]

This leads to the block $J$-Lanczos algorithm in Algorithm 1.
Algorithm 1 The block J-Lanczos method

**Input:** Hamiltonian matrix $M \in \mathbb{R}^{2n \times 2n}$ and symplectic matrix $V_1 = [q_1 \, q_{k+1}] \in \mathbb{R}^{2n \times 2s}$ with $n = ms$ and $k \leq m$.

**Initialize:** $b_0 = 0_s$, $c_0 = 0_s$, $\alpha_0 = 0_s$, $\delta_0 = 0_s$, $Q_k (\cdot, 1 : k + s) = q_1$.

For $i = 1, 2, \ldots, k - 1$

\begin{align*}
a_i &= -q_{k+i}^T J M q_i \\
\gamma_i &= q_i^T J M q_i \\
\beta_i &= q_{k+i}^T J M q_{k+i} \\
u_i &= M q_i - q_{i-1} c_{i-1} - q_i a_i - q_{k+i-1} \delta_{i-1} - q_{k+i} \gamma_i \\
v_i &= M q_{k+i} - q_{i-1} \alpha_{i-1} - q_i \beta_i - q_{k+i-1} \beta_{i-1} - q_{k+i} \alpha_i^T \\
\text{Normalization step:} & \quad \begin{cases} 
W_i = [u_i \, v_i] = S^i R^i \quad (SR \text{ decomposition by using symplectic reflectors}) 
\end{cases}
\end{align*}

\begin{align*}
b_i &= R^i (1 : s, 1 : s) \\
c_i &= -[R^i (n + 1 : n + s, s + 1 : 2s)]^T \\
\alpha_i &= R^i (1 : s, s + 1 : 2s) \\
\delta_i &= R^i (n + 1 : n + s, 1 : s) \\
q_{i+1} &= S^i (\cdot, 1 : s) \\
q_{k+i+1} &= S^i (\cdot, n + 1 : n + s)
\end{align*}

**End For**

**Output:** The symplectic matrix $Q_k = [q_1, \ldots, q_k \, q_{k+1}, \ldots, q_{2k}] \in \mathbb{R}^{2n \times 2ks}$ and the Hamiltonian block J-Hessenberg matrix $H_k \in \mathbb{R}^{2ks \times 2ks}$ such that $Q_k^T M Q_k = H_k$.

**Remark 3.1.** In order to prevent the loss of $J$-orthogonality in the block $J$-Lanczos type Algorithm 1, we do $J$-reorthogonalization by computing the $SR$ decomposition of $W_i = [Q(\cdot, 1 : is), u_i ; Q(\cdot, k + 1 : k + is), v_i] \in \mathbb{R}^{2n \times 2(i+1)s}$ instead of taking $W_i = [u_i \, v_i]$. Then we obtain

\begin{align*}
\begin{cases} 
b_i &= R^i (is + 1 : (i + 1)s, is + 1 : (i + 1)s), \\
c_i &= -[R^i (n + is + 1 : n + (i + 1)s, (2i + 1)s : 2(i + 1)s)]^T, \\
\alpha_i &= R^i (is + 1 : (i + 1)s, (2i + 1)s : 2(i + 1)s), \\
\delta_i &= R^i (n + is + 1 : n + (i + 1)s, is + 1 : (i + 1)s), \\
\end{cases}
\end{align*}

and

\begin{align*}
\begin{cases} 
Q(\cdot, is + 1 : (i + 1)s) = S(\cdot, is + 1 : (i + 1)s), \\
Q(\cdot, k + is + 1 : k + (i + 1)s) = S(\cdot, n + is + 1 : n + (i + 1)s). 
\end{cases}
\end{align*}

**3.1.2. Normalization by using the $R^j R$ decomposition.** At step $i$ of the block $J$-Lanczos algorithm given above, we compute $R_i \in \mathbb{R}^{2s \times 2s}$ such that $W_i^T W_i = R_i^T R_i$ where $W_i = [u_i \, v_i] \in \mathbb{R}^{2n \times 2s}$, thus $[q_1 \, q_{k+i+1}] = W_i R_i^{-1}$. The square matrix $R_i \in \mathbb{R}^{2s \times 2s}$ is derived from the $LU$ $J$-decomposition with the pivoting strategy as presented in the following theorem. See [3] for more details on the $LU$ $J$-decomposition.

**Theorem 3.2.** [3] Let $M$ be a $2n$-by-$2n$ real skew-Hamiltonian, $J$-definite matrix (i.e., $X^T M X = \alpha I_2$, where $\alpha \neq 0$ for each matrix $X = [x_1 \, x_2] \in \mathbb{R}^{2n \times 2}$ that is not $J$-isotropic (that is, $x_1^T J x_2 \neq 0$)), and let $M = LU$ be its $LU$ $J$-factorization. The matrix $R = (LD)^J$, where $LD$ is the $LU$ factorization of $M$ with $D$ being a diagonal $J$-definite matrix, is $J$-orthogonal.
where \( D \) is a diagonal matrix defined by
\[
D = \sum_{i=1}^{n} E_i \begin{pmatrix}
\sqrt{\text{sign}(u_{ii})} u_{ii} & 0 \\
0 & \text{sign}(u_{ii}) \sqrt{\text{sign}(u_{ii})} u_{ii}
\end{pmatrix} E_i^T
\]
with \( u_{ii} = e_i^T U e_i \) and \( E_i = [e_i \ e_{n+i}] \in \mathbb{R}^{2n \times 2} \), is lower \( J \)-triangular. It holds that \( M = R^T R \).

Remark 3.3. In the same manner as in the previous remark, to avoid the loss of \( J \)-orthogonality, we normalize \( W_i = [Q(:, 1 : is), u_i; Q(:, k + 1 : k + is), v_i] \in \mathbb{R}^{2n \times 2(i+1)s} \) instead of taking \( W_i = [u_i \ v_i] \).

3.2. The second approach. Here, \( 2n \)-by-\( 2s \) blocks of vectors instead of single vectors and \( 2s \)-by-\( 2s \) matrix coefficients instead of scalars are used. Since at iteration \( i \) we have, for \( i = 1, \ldots, k \),
\[
\begin{align*}
M q_i &= q_i - c_{i-1} q_{i-1} + q_i a_i + q_{i+1} b_i + q_{k+i-1} \delta_{i-1}^T + q_{k+i} \gamma_i + q_{k+i+1} \delta_i, \\
M q_{k+i} &= q_i a_i + q_{k+1} a_i - q_{k+i-1} b_i + q_{k+i} b_i - q_{k+i+1} c_i^T,
\end{align*}
\]
we can combine the two equations into
\[
M [q_i \ q_{k+i}] = [q_i - c_{i-1} q_{i-1} - q_{k+i-1}] \begin{pmatrix}
\alpha_{i-1}^T & \alpha_i^T \\
\delta_{i-1}^T & -\beta_i^T
\end{pmatrix} + [q_i \ q_{k+i}] \begin{pmatrix}
\alpha_i & \beta_i \\
\gamma_i & -\alpha_i^T
\end{pmatrix},
\]
\[
= [q_i + q_{k+i+1}] \begin{pmatrix}
b_i & \alpha_i \\
\delta_i & -c_i^T
\end{pmatrix}.
\]

Let
\[
\begin{align*}
V_{i-1} &= [q_i \ q_{k+i-1}] , \\
V_i &= [q_i \ q_{k+i}] , \\
V_{i+1} &= [q_{i+1} \ q_{k+i+1}] ,
\end{align*}
\]
and
\[
\begin{align*}
h_{i,i} &= T_i = \begin{pmatrix}
a_i & \beta_i \\
\gamma_i & -\alpha_i^T
\end{pmatrix}, \\
h_{i+1,i} &= C_i = h_{i,i+1} = \begin{pmatrix}
b_i & \alpha_i \\
\delta_i & -c_i^T
\end{pmatrix}, \\
h_{i-1,i} &= -C_{i-1}^T = \begin{pmatrix}
c_{i-1} & \alpha_{i-1} \\
\delta_{i-1} & -c_{i-1}^T
\end{pmatrix}.
\end{align*}
\]
\[
\left(
\begin{pmatrix}
c_{i-1} = \begin{pmatrix}
b_{i-1} & \alpha_{i-1} \\
\delta_{i-1} & -c_{i-1}^T
\end{pmatrix} \iff C_i^J = \begin{pmatrix}
b_{i-1} & \alpha_{i-1} \\
\delta_{i-1} & -c_{i-1}^T
\end{pmatrix}^J = -\begin{pmatrix}
c_{i-1} & \alpha_{i-1}^T \\
\delta_{i-1} & -c_{i-1}^T
\end{pmatrix} \right).
\]

Hence, \( MV_i = -V_{i-1} C_{i-1}^J + V_i T_i + V_{i+1} C_i \). This leads to Algorithm 2.
Algorithm 2 The compact block $J$-Lanczos method.

**Input:** Hamiltonian matrix $M \in \mathbb{R}^{2n \times 2n}$ and symplectic matrix $V_1 = [q_1 \ q_{k+1}] \in \mathbb{R}^{2n \times 2s}$ with $n = ms$ and $k \leq m$.

**Initialize:** $V_0 = 0_{2n \times 2s}, h_{0,1} = C_0 = 0_{2s}, V_1 \in \mathbb{R}^{2n \times 2s}$ such that $V_1^T V_1 = I_{2s}$.

**For** $i = 1, 2, \ldots, k - 1$

$h_{i,i} = T_i = V_i^T M V_i$

$\Lambda_i = M V_i + V_{i-1} C_{i-1}^T - V_i T_i$.

Normalization step: $\{ \Lambda_i = S^T R^i \text{ (SR decomposition)} \}$

$V_{i+1} = S^T F_1$ and $h_{i+1,i} = C_i = h_{i,i+1} = F_i^T R^i$ (such that $\Lambda_i = V_{i+1} C_i$).

**End For**

$Q_k = \sum_{i=1}^{k} V_i F_i^T$ and $H_k = \sum_{j=1}^{\min(j+1,k)} \sum_{i=\min(j-1,1)}^{k} F_i h_{ij} F_j^T$.

**Output:** The symplectic matrix $Q_k = [q_1, \ldots, q_k \ : \ q_{k+1}, \ldots, q_{2s}] \in \mathbb{R}^{2n \times 2ks}$ and the Hamiltonian block $J$-Hessenberg matrix $H_k \in \mathbb{R}^{2ks \times 2ks}$ such that $Q_k^T M Q_k = H_k$.

**Remark 3.4.** In the normalization step of the compact block $J$-Lanczos algorithm, instead of using the SR decomposition one can use the LU $J$-decomposition with the pivoting strategy presented in [3] to compute $R_i \in \mathbb{R}^{2s \times 2s}$ such that $\Lambda_i^T \Lambda_i = R_i^T R_i$, where $\Lambda_i = M V_i + V_{i-1} C_{i-1}^T - V_i T_i \in \mathbb{R}^{2n \times 2s}$. We then obtain $C_i = R_i$ and $V_{i+1} = \Lambda_i$. Otherwise, in order to prevent loss of $J$-orthogonality, we normalize

$$W_i = \sum_{j=1}^{i} V_j F_j^T + \Lambda_i F_i^T \in \mathbb{R}^{2n \times 2(i+1)s}$$

instead of taking $W_i = \Lambda_i$. By using the SR decomposition, we obtain $V_{i+1} = S^T F_i + 1$ and $C_i = F_i^T R_i F_{i+1}$. When we use the $R^T J R$ decomposition to compute $Z = W_i R_{i-1}^T$, where $R_i \in \mathbb{R}^{2(i+1)s \times 2(i+1)s}$ such that $W_i^T W_i = R_i^T R_i$, we then get $V_{i+1} = Z F_{i+1}$ and $h_{i,i} = C = F_{i+1}^T R_i F_i + 1$.

4. **Exponential block approximation method.** The approximation of $\exp(A)V$ for a given tall matrix $V$ and a square matrix $A$ is recommended in many applications. It is the key element of many exponential integrators to solve systems of ODEs or time-dependent PDEs [6]. The use of Krylov subspace approaches in this context has been proposed in the literature; see [9], [10], [12], [13], [16], [17] [20]. The approximation procedure for $\exp(A)V$ that preserves structural properties of $V$ is more efficient and accurate in the case when $A$ is Hamiltonian and skew-symmetric or simply Hamiltonian. The preservation of geometric properties is necessary for the effectiveness of certain geometric integration methods; see [11], [19]. Structure-preserving methods can be used, for example, to calculate Lyapunov exponents of dynamical systems and geodesics; see [7], [10]. Our goal in this section is to present a structure-preserving block Krylov method for approximating the matrix-matrix product $\exp(A)V$ using the block Krylov subspace $K_m(A, V) = \text{blockspan}\{V, AV, \ldots, A^{m-1}V\}$, for a given $2n$-by-$2n$ Hamiltonian, skew-symmetric matrix $A$ and a $2n$-by-$2s$ rectangular matrix $V$ where $s << n$.

The algorithm may suffer from breakdown if the matrix $\Lambda_i$ computed in the algorithm is isotropic at a certain step $i$. Suppose that the algorithm goes until the iteration $m$. By construction, the matrices $V_i$ generated by the algorithm are symplectic and $J$-orthogonal to
The matrix 
\[ V_i^TV_i = I_{2s} \text{ and } V_i^TV_j = 0_{2s}, \text{ for } i, j = 1, \ldots, m; i \neq j. \]

Let \( Q_m = \sum_{i=1}^{m} V_i F_i^T \) and \( H_m = \sum_{i=1}^{m} \sum_{j=\max(i-1,1)}^{m} F_i h_{ij} F_j^T \), where \( h_{ij} \in \mathbb{R}^{2s \times 2s} \).

From Algorithm 2 we can easily obtain
\[
AQ_m = Q_m H_m + V_{m+1} h_{m+1,m} F_{m+1}^T.
\]

Then
\[
Q_m^T AQ_m = H_m.
\]

The matrix \( H_m \) is in \( 2ms \times 2ms \) block \( J \)-Hessenberg form, \( h_{ij} = 0_{2s} \) for \( i > j + 1 \). Therefore,
\[
AV = AQ_m F_1 D_1 = Q_m H_m F_1 D_1 + V_{m+1} h_{m+1,m} F_{m+1}^T F_1 D_1.
\]

The \( 2s \)-by-\( 2s \) real matrix \( D_1 \) defined above satisfies \( D_1^T D_1 = V^T V \), which comes from the normalization of \( V \) using the decomposition \( R^T R \), and since \( H_m \) is in block \( J \)-Hessenberg form (i.e., \( h_{ij} = 0_{2s} \) for \( i > j + 1 \)), we have
\[
A^2 V = AQ_m H_m F_1 D_1
= Q_m H_m^2 F_1 D_1 + V_{m+1} h_{m+1,m} F_{m+1}^T H_m F_1 D_1.
\]

By induction this implies that \( p_{m-1}(A)V = \Lambda_m p_{m-1}(H_m) F_1 D_1 \) for all polynomials \( p_{m-1} \) of degree \( \leq m - 1 \). This relation suggests using the approximation
\[
\exp(A)V \approx Q_m \exp(H_m) F_1 D_1.
\]

5. Numerical examples. The numerical examples given below demonstrate the effectiveness of the proposed block \( J \)-Lanczos method using the block symplectic \( SR \) and \( R^T R \)-factorizations. By using the Frobenius norm, we compute the accuracy of the resulting symplectic matrix \( Q_k \) (i.e., \( \| I_{2ks} - Q_k^T Q_k \|_F \)) and the Hamiltonian \( J \)-Hessenberg \( 2k_s \times 2k_s \) matrix \( H_k \) (i.e., \( \| H_k - Q_k^T M Q_k \|_F \)). We show the error as the dimension \( k \) increases. We also show the error obtained when approximating \( \exp(A)V \) by \( Q_m \exp(H_m) F_1 D_1 \), and we examine the error of the symplecticity and orthogonality preserving property of the exponential approximation. We display the error as the dimension \( m \) increases. The \( 2n \times 2s \) matrix \( V \) is given by \( V = [U, -JU] \), where \( U = \exp(G) I_{2n \times s} \), with \( G \) being a \( 2n \)-by-\( 2n \) skew-symmetric and Hamiltonian matrix derived in a way similar to \( A \). Here, \( I_{2n \times s} \) consists of the first \( s \) columns of the identity matrix \( I_{2n} \). Since \( G \) is a skew-symmetric and Hamiltonian matrix, \( V = [U, -JU] \) is ortho-symplectic. We remark that an ortho-symplectic matrix \( V \)
satisfies \( VJ = JV \). The matrices in Example 5.1 are constructed in a way similar to the matrices of [18, Example 3.2] by L. Lopez and V. Simoncini. All numerical experiments are performed in Matlab 2015a.
EXAMPLE 5.1. We consider a 2000-by-2000 skew-symmetric and Hamiltonian matrix defined as

$$A = \begin{bmatrix} A_1 & A_2 \\ -A_2 & A_1 \end{bmatrix},$$

where $A_1$ and $A_2$ are the $n$-by-$n$ skew-symmetric and symmetric parts, respectively. For $s = 5$, varying $m$ from 1 to 25, we obtain the error displayed in Figure 5.1 and Figure 5.2.
EXAMPLE 5.2. In this example, we consider a $2000 \times 2000$ skew-symmetric and Hamiltonian matrix $A$ constructed as

$$A = \begin{bmatrix} A_1 & A_2 \\ -A_2 & A_1 \end{bmatrix}.$$ 

The blocks $A_1$ and $A_2$ are the $n$-by-$n$ skew-symmetric and symmetric parts, respectively. $A_1$ is taken as a random matrix with normally distributed numbers and $A_2 = \text{gallery}('ris', n)$ is a $1000 \times 1000$ symmetric Hankel matrix, with elements $A(i, j) = 0.5/(n - i - j + 1.5)$ for $i, j = 1, \ldots, n$.

For $s = 5$, varying $k$ from 1 to 20, we obtain Figure 5.3 and Figure 5.4. For $n = 1000$ and $s = 10$, varying $k$ from 1 to 25, the results are displayed in Figure 5.5 and Figure 5.6.
6. Conclusion. The block $J$-Lanczos method is well adapted to compute a preserving geometric structure approximation of the exponential operator matrix-matrix product $\exp(A)V$. The presented numerical examples show the efficiency of the proposed algorithms. The $J$-reorthogonality seems to be promising to get higher accuracy.

REFERENCES


Fig. 5.4. Example 5.2: $s = 5, k = 1, \ldots, 20$.


Block symplectic Lanczos method with s=10, n=1000.

Block symplectic Lanczos method with s=10, n=1000.

Fig. 5.5. Example 5.2: n = 1000, s = 10, k = 1, . . . , 25.


Fig. 5.6. Example 5.2: \( n = 1000, s = 10, k = 1, \ldots, 25. \)


