Electronic Transactions on Numerical Analysis.
Volume 52, pp. 26–42, 2020.

ISSN 1068–9613.
DOI: 10.1553/etna_vol52s26

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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

AMS subject classifications. 65F15, 65F30, 65F50

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

$$\left[\begin{array}{cccc|cccc}
* & * & & & * & * & & \\
* & \ddots & \ddots & & * & \ddots & \ddots & \\
 & \ddots & \ddots & * & & \ddots & \ddots & * \\
 & & * & * & & & * & * \\
\hline
* & * & & & * & * & & \\
* & \ddots & \ddots & & * & \ddots & \ddots & \\
 & \ddots & \ddots & * & & \ddots & \ddots & * \\
 & & * & * & & & * & *
\end{array}\right],$$

where * 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

*Received March 11, 2019. Accepted December 10, 2019. Published online on January 29, 2020. Recommended by Wen-Wei Lin.
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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 $\mathbb{R}^{2n\times 2s}$ as free module on $\left(\mathbb{R}^{2s\times 2s}, +, \times\right)$.

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 $K_m(A, V) = \text{blockspan}\{V, AV, ..., A^{m-1}V\}$ (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*

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

where

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

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

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

Then we have

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

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where

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

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*

$$C_i = \left[\begin{array}{ccc|ccc} u_{(i-1)s+1,1} & \cdots & u_{(i-1)s+1,s} & u_{(i-1)s+1,s+1} & \cdots & u_{(i-1)s+1,2s} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ u_{is,1} & \cdots & u_{is,s} & u_{is,s+1} & \cdots & u_{is,2s} \\ \hline u_{n+(i-1)s+1,1} & \cdots & u_{n+(i-1)s+1,s} & u_{n+(i-1)s+1,s+1} & \cdots & u_{n+(i-1)s+1,2s} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ u_{n+is,1} & \cdots & u_{n+is,s} & u_{n+is,s+1} & \cdots & u_{n+is,2s} \end{array}\right] \in \mathbb{R}^{2s \times 2s}.$$

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 $M = \sum_{i=1}^{m} \sum_{j=1}^{m} F_i M_{ij} F_j^T$, where $M_{ij} \in \mathbb{R}^{2s \times 2s}$ is given by*

$$\left[\begin{array}{ccc|ccc} \tilde{m}_{(i-1)s+1,(j-1)s+1} & \cdots & \tilde{m}_{(i-1)s+1,js} & \tilde{m}_{(i-1)s+1,n+(j-1)s+1} & \cdots & \tilde{m}_{(i-1)s+1,n+js} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \tilde{m}_{is,(j-1)s+1} & \cdots & \tilde{m}_{is,js} & \tilde{m}_{is,n+(j-1)s+1} & \cdots & \tilde{m}_{is,n+js} \\ \hline \tilde{m}_{n+(i-1)s+1,(j-1)s+1} & \cdots & \tilde{m}_{n+(i-1)s+1,js} & \tilde{m}_{n+(i-1)s+1,n+(j-1)s+1} & \cdots & \tilde{m}_{n+(i-1)s+1,n+js} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \tilde{m}_{n+is,(j-1)s+1} & \cdots & \tilde{m}_{n+is,js} & \tilde{m}_{n+is,n+(j-1)s+1} & \cdots & \tilde{m}_{n+is,n+js} \end{array}\right].$$

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

Proof. The result is obvious since $M^J = \sum_{i=1}^{m} \sum_{j=1}^{m} F_i M_{ji}^J F_j^T$. □

DEFINITION 2.6. *A matrix $M = \sum_{i=1}^{m} \sum_{j=1}^{m} F_i M_{ij} F_j^T \in \mathbb{R}^{2n \times 2n}$ 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 $S = (U + V) C^{-1} (U + V)^J - I_{2n}$ is symplectic and transforms U to V, hence it is called the symplectic reflector that takes U to V.*

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

$$q(W) = \begin{cases} \sqrt{\alpha} I_2 & \textit{if } \alpha > 0, \\ \sqrt{-\alpha} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & \textit{if } \alpha < 0. \end{cases}$$

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

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

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

$$R = \left[\begin{array}{cccc|cccc} * & * & \dots & * & 0 & * & \dots & * \\ & \ddots & \ddots & \vdots & & \ddots & \ddots & \vdots \\ & & \ddots & * & & & \ddots & * \\ & & & * & & & & 0 \\ \hline 0 & * & \dots & * & * & * & \dots & * \\ & \ddots & \ddots & \vdots & & \ddots & \ddots & \vdots \\ & & \ddots & * & & & \ddots & * \\ & & & 0 & & & & * \end{array}\right].$$

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 $(F_i)_{1\leq i\leq m}$ is given according to the context.

Let for $Q_k := [q_1, \dots, q_k \vdots q_{k+1}, \dots, q_{2k}] \in \mathbb{R}^{2n\times 2sk}$ be a $2n$-by-$2sk$ symplectic matrix for $k \leq m$, where $q_i \in \mathbb{R}^{2n\times s}$ for $i = 1, 2, \cdots, 2k$, 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 $MQ_k = Q_k H_k + W_k F_{k+1}^T$, where $W_k \in \mathbb{R}^{2n\times 2s}$ is J-orthogonal to Q_k; i.e., $Q_k^J W_k = 0_{2sk\times 2s}$ which also means $q_i^T J W_k = 0_{s\times 2s}$ for $i = 1, 2, \dots, 2k$. That

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is, H_k is in the form

$$H_k = \left[\begin{array}{ccccc|ccccc} a_1 & c_1 & & & & \beta_1 & \alpha_1^T & & & \\ b_1 & a_2 & c_2 & & & \alpha_1 & \beta_2 & \alpha_2^T & & \\ & \ddots & \ddots & \ddots & & & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & c_{k-1} & & & \ddots & \ddots & \alpha_{k-1}^T \\ & & & b_{k-1} & a_k & & & & \alpha_{k-1} & \beta_k \\ \hline \gamma_1 & \delta_1^T & & & & -a_1^T & -b_1^T & & & \\ \delta_1 & \gamma_2 & \delta_2^T & & & -c_1^T & -a_2^T & -b_2^T & & \\ & \ddots & \ddots & \ddots & & & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \delta_{k-1}^T & & & \ddots & \ddots & -b_{k-1}^T \\ & & & \delta_{k-1} & \gamma_k & & & & -c_{k-1}^T & -a_k^T \end{array}\right],$$

with blocks α_i, β_i, γ_i, δ_i, a_i, b_i, $c_i \in \mathbb{R}^{s\times s}$, where β_i and γ_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 $2n$-by-$2sk$ symplectic matrix Q_k and the $2sk$-by-$2sk$ Hamiltonian block J-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 $R^J R$ decomposition.

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

$$\begin{cases} Mq_i = q_{i-1}c_{i-1} + q_i a_i + q_{i+1} b_i + q_{k+i-1}\delta_{i-1}^T + q_{k+i}\gamma_i + q_{k+i+1}\delta_i, \\ Mq_{k+i} = q_{i-1}\alpha_{i-1}^T + q_i\beta_i + q_{i+1}\alpha_i - q_{k+i-1}b_{i-1}^T - q_{k+i}a_i^T - q_{k+i+1}c_i^T. \end{cases}$$

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

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

The s-by-s matrix coefficients a_i, γ_i, and β_i can be determined via

$$\begin{cases} a_i = -q_{k+i}^T JMq_i, \\ \gamma_i = q_i^T JMq_i, \\ \beta_i = -q_{k+i}^T JMq_{k+i}, \end{cases}$$

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

$$\begin{cases} \beta_i^T = (-q_{k+i}^T JMq_{k+i})^T = -q_{k+i}^T \underbrace{(JM)^T}_{JM} q_{k+i} = \beta_i, \\ \gamma_i^T = (q_i^T JMq_i)^T = q_i^T \underbrace{(JM)^T}_{JM} q_i = \gamma_i. \end{cases}$$

Set

$$\begin{cases} u_i = Mq_i - q_{i-1}c_{i-1} - q_i a_i - q_{k+i-1}\delta_{i-1}^T - q_{k+i}\gamma_i, \\ v_i = Mq_{k+i} - q_{i-1}\alpha_{i-1}^T - q_i\beta_i - q_{k+i-1}b_{i-1}^T - q_{k+i}a_i^T. \end{cases}$$

Then we get

$$\begin{cases} u_i = q_{i+1} b_i + q_{k+i+1}\delta_i, \\ v_i = q_{i+1}\alpha_i - q_{k+i+1} c_i^T. \end{cases}$$

The J-orthogonality condition holds for both u_i and v_i, i.e.,

$$\begin{cases} q_i^T J u_i = q_i^T J M q_i - \gamma_i & & =0_s, \\ q_{k+i}^T J u_i = q_{k+i}^T J M q_i + a_i & & =0_s, \\ q_{i-1}^T J u_i = q_{i-1}^T J M q_i - \delta_{i-1}^T & = -\left(M q_{i-1}\right)^T J q_i - \delta_{i-1}^T & =0_s, \\ q_{k+i-1}^T J u_i = q_{k+i-1}^T J M q_i + c_{i-1} & = -\left(M q_{k+i-1}\right)^T J q_i + c_{i-1} & =0_s, \end{cases}$$

and

$$\begin{cases} q_i^T J v_i = q_i^T J M q_{k+i} + a_i^T & = -\left(M q_i\right)^T J q_{k+i} + a_i^T & =0_s, \\ q_{k+i}^T J v_i = q_{k+i}^T J M q_{k+i} + \beta_i & = -\left(M q_{k+i}\right)^T J q_{k+i} + \beta_i & =0_s, \\ q_{i-1}^T J v_i = q_{i-1}^T J M q_{k+i} + b_{i-1}^T & = -\left(M q_{i-1}\right)^T J q_{k+i} + b_{i-1}^T & =0_s, \\ q_{k+i-1}^T J v_i = -q_{k+i-1}^T J M q_{k+i} + \alpha_{i-1}^T & = \left(M q_{k+i-1}\right)^T J q_{k+i} + \alpha_{i-1}^T & =0_s, \end{cases}$$

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 $R^J R$ 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,

$$\begin{cases} q_{i+1} = S^i(:, 1:s), \\ q_{k+i+1} = S^i(:, n+1:n+s), \end{cases}$$

and

$$\begin{cases} b_i = R^i(1:s, 1:s), \\ \alpha_i = R^i(1:s, s+1:2s), \\ \delta_i = R^i(n+1:n+s, 1:s), \\ -c_i^T = R^i(n+1:n+s, s+1:2s). \end{cases}$$

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

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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: $b_0 = 0_s$, $c_0 = 0_s$, $\alpha_0 = 0_s$, $\delta_0 = 0_s$, $Q_k(:, 1:s) = q_1$, $Q_k(:, k+1:k+s) = q_{k+1}$.
For $\mathbf{i = 1, 2, \cdots, k-1}$
$a_i = -q_{k+i}^T JMq_i$
$\gamma_i = q_i^T JMq_i$
$\beta_i = -q_{k+i}^T JMq_{k+i}$
$u_i = Mq_i - q_{i-1}c_{i-1} - q_i a_i - q_{k+i-1}\delta_{i-1}^T - q_{k+i}\gamma_i$
$v_i = Mq_{k+i} - q_{i-1}\alpha_{i-1}^T - q_i\beta_i - q_{k+i-1}b_{i-1}^T - q_{k+i}a_i^T$
Normalization step: $\left\{ \begin{array}{l} W_i = [u_i\ v_i] = S^i R^i \ \ (SR \text{ decomposition} \\ \text{by using symplectic reflectors}) \end{array} \right.$
$b_i = R^i(1:s\,, 1:s)$
$c_i = -\left[R^i(n+1:n+s, s+1:2s)\right]^T$
$\alpha_i = R^i(1:s\,, s+1:2s)$
$\delta_i = R^i(n+1:n+s\,, 1:s)$
$q_{i+1} = S^i(:, 1:s)$
$q_{k+i+1} = S^i(:, n+1:n+s)$
End For
Output: The symplectic matrix $Q_k = [q_1, \cdots, q_k \vdots q_{k+1}, \cdots, q_{2k}] \in \mathbb{R}^{2n\times 2ks}$ and the Hamiltonian block J-Hessenberg matrix $H_k \in \mathbb{R}^{2ks\times 2ks}$ such that $Q_k^J M Q_k = H_k$.

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 $W_i = [Q(:, 1:is), u_i \vdots Q(:, k+1:k+is), v_i] \in \mathbb{R}^{2n\times 2(i+1)s}$ instead of taking $W_i = [u_i\ v_i]$. Then we obtain

$$\left\{ \begin{array}{l} b_i = R^i(is+1:(i+1)s, is+1:(i+1)s), \\ c_i = -\left[R^i(n+is+1:n+(i+1)s, (2i+1)s:2(i+1)s)\right]^T, \\ \alpha_i = R^i(is+1:(i+1)s, (2i+1)s:2(i+1)s), \\ \delta_i = R^i(n+is+1:n+(i+1)s, is+1:(i+1)s), \end{array} \right.$$

and

$$\left\{ \begin{array}{c} Q(:, is+1:(i+1)s) = S(:, is+1:(i+1)s), \\ Q(:, k+is+1:k+(i+1)s) = S(:, n+is+1:n+(i+1)s). \end{array} \right.$$

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 $W_i^J W_i = R_i^J R_i$ where $W_i = [u_i\ \ v_i] \in \mathbb{R}^{2n\times 2s}$, thus $[q_{i+1}, q_{k+i+1}] = W_i R_i^{-1}$. 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., $X^J MX = \alpha I_2$, 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, $x_1^T Jx_2 \neq 0$)), and let $M = LU$ be its LU J-factorization. The matrix $R = (LD)^J$,* *where D is a diagonal matrix defined by*

$$D = \sum_{i=1}^{n} E_i \begin{pmatrix} \sqrt{sign(u_{ii})u_{ii}} & 0 \\ 0 & sign(u_{ii})\sqrt{sign(u_{ii})u_{ii}} \end{pmatrix} E_i^T$$

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 $M = R^J R$.

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

$$\begin{cases} Mq_i = q_{i-1}c_{i-1} + q_i a_i + q_{i+1}b_i + q_{k+i-1}\delta_{i-1}^T + q_{k+i}\gamma_i + q_{k+i+1}\delta_i, \\ Mq_{k+i} = q_{i-1}\alpha_{i-1}^T + q_i\beta_i + q_{i+1}\alpha_i - q_{k+i-1}b_{i-1}^T - q_{k+i}a_i^T - q_{k+i+1}c_i^T, \end{cases}$$

we can combine the two equations into

$$M\,[q_i \ q_{k+i}] = [q_{i-1} \ q_{k+i-1}] \underbrace{\begin{bmatrix} c_{i-1} & \alpha_{i-1}^T \\ \delta_{i-1}^T & -b_{i-1}^T \end{bmatrix}}_{h_{i-1,i}} + [q_i \ q_{k+i}] \underbrace{\begin{bmatrix} a_i & \beta_i \\ \gamma_i & -a_i^T \end{bmatrix}}_{h_{i,i}} + [q_{i+1} \ q_{k+i+1}] \underbrace{\begin{bmatrix} b_i & \alpha_i \\ \delta_i & -c_i^T \end{bmatrix}}_{h_{i+1,i}}.$$

Let

$$\begin{cases} V_{i-1} &= \begin{bmatrix} q_{i-1} & q_{k+i-1} \end{bmatrix}, \\ V_i &= \begin{bmatrix} q_i & q_{k+i} \end{bmatrix}, \\ V_{i+1} &= \begin{bmatrix} q_{i+1} & q_{k+i+1} \end{bmatrix}, \end{cases}$$

and

$$\begin{cases} h_{i,i} = T_i & = \begin{bmatrix} a_i & \beta_i \\ \gamma_i & -a_i^T \end{bmatrix}, \\ h_{i+1,i} = C_i = h_{i,i+1}^J & = \begin{bmatrix} b_i & \alpha_i \\ \delta_i & -c_i^T \end{bmatrix}, \\ h_{i-1,i} = -C_{i-1}^J & = \begin{bmatrix} c_{i-1} & \alpha_{i-1}^T \\ \delta_{i-1}^T & -b_{i-1}^T \end{bmatrix}. \end{cases}$$

$$\left(C_{i-1} = \begin{bmatrix} b_{i-1} & \alpha_{i-1} \\ \delta_{i-1} & -c_{i-1}^T \end{bmatrix} \Longleftrightarrow C_{i-1}^J = \begin{bmatrix} b_{i-1} & \alpha_{i-1} \\ \delta_{i-1} & -c_{i-1}^T \end{bmatrix}^J = -\begin{bmatrix} c_{i-1} & \alpha_{i-1}^T \\ \delta_{i-1}^T & -b_{i-1}^T \end{bmatrix} \right).$$

Hence, $MV_i = -V_{i-1}C_{i-1}^J + V_iT_i + V_{i+1}C_i$. 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 $k \le m$.
Initialize: $V_0 = 0_{2n\times 2s}$, $h_{0,1} = C_0 = 0_{2s}$, $V_1 \in \mathbb{R}^{2n\times 2s}$ such that $V_1^J V_1 = I_{2s}$.
For $\mathbf{i = 1, 2, \ldots, k-1}$
$h_{i,i} = T_i = V_i^J M V_i$
$\Lambda_i = MV_i + V_{i-1}C_{i-1}^J - V_i T_i$.
Normalization step: $\begin{cases} \Lambda_i = S^i R^i \ (SR \text{ decomposition} \\ \text{by using symplectic reflectors}) \end{cases}$
$V_{i+1} = S^i F_1$ and $h_{i+1,i} = C_i = h_{i,i+1}^J = F_1^T R^i$ (such that $\Lambda_i = V_{i+1}C_i$).
End For
$Q_k = \sum_{i=1}^{k} V_i F_i^T$ and $H_k = \sum_{j=1}^{k} \sum_{i=\min(j-1,1)}^{\min(j+1,k)} F_i h_{ij} F_j^T$.

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

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 $\Lambda_i^J \Lambda_i = R_i^J R_i$, where $\Lambda_i = MV_i + V_{i-1}C_{i-1}^J - V_i T_i \in \mathbb{R}^{2n\times 2s}$. We then obtain $C_i = R_i$ and $V_{i+1} = \Lambda_i R_i^{-1}$. Otherwise, in order to prevent loss of J-orthogonality, we normalize

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

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

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 $K_m(A, V) = \text{blockspan}\{V, AV, ..., A^{m-1}V\}$, 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 Λ_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 each other, i.e.,

$$V_i^J V_i = I_{2s} \text{ and } V_i^J V_j = 0_{2s}, \text{ for } i, j = 1, \ldots, m;\ i \neq j.$$

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

$$AQ_m = Q_m H_m + V_{m+1} h_{m+1,m} F_m^T.$$

Then

$$Q_m^J A Q_m = H_m.$$

The matrix H_m is in $2ms \times 2ms$ block J-Hessenberg form, $h_{ij} = 0_{2s}$ for $i > j+1$. Therefore,

$$AV = AQ_m F_1 D_1 = Q_m H_m F_1 D_1 + V_{m+1} h_{m+1,m} \underbrace{F_m^T F_1}_{\mathbf{0}} D_1.$$

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

$$\begin{aligned} A^2 V &= AQ_m H_m F_1 D_1 \\ &= Q_m H_m^2 F_1 D_1 + V_{m+1} h_{m+1,m} \underbrace{F_m^T H_m F_1}_{0} D_1. \end{aligned}$$

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

$$\exp(A)V \simeq Q_m \exp(H_m) F_1 D_1.$$

5. Numerical examples. The numerical examples given below demonstrate the effectiveness of the proposed block J-Lanczos method using the block symplectic SR and $R^J R$-factorizations. By using the Frobenius norm, we compute the accuracy of the resulting symplectic matrix Q_k (i.e., $\|I_{2ks} - Q_k^J Q_k\|_F$) and the Hamiltonian J-Hessenberg $2ks$-by-$2ks$ matrix H_k (i.e., $\|H_k - Q_k^J M Q_k\|_F$). 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 $2n$-by-$2s$ 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.

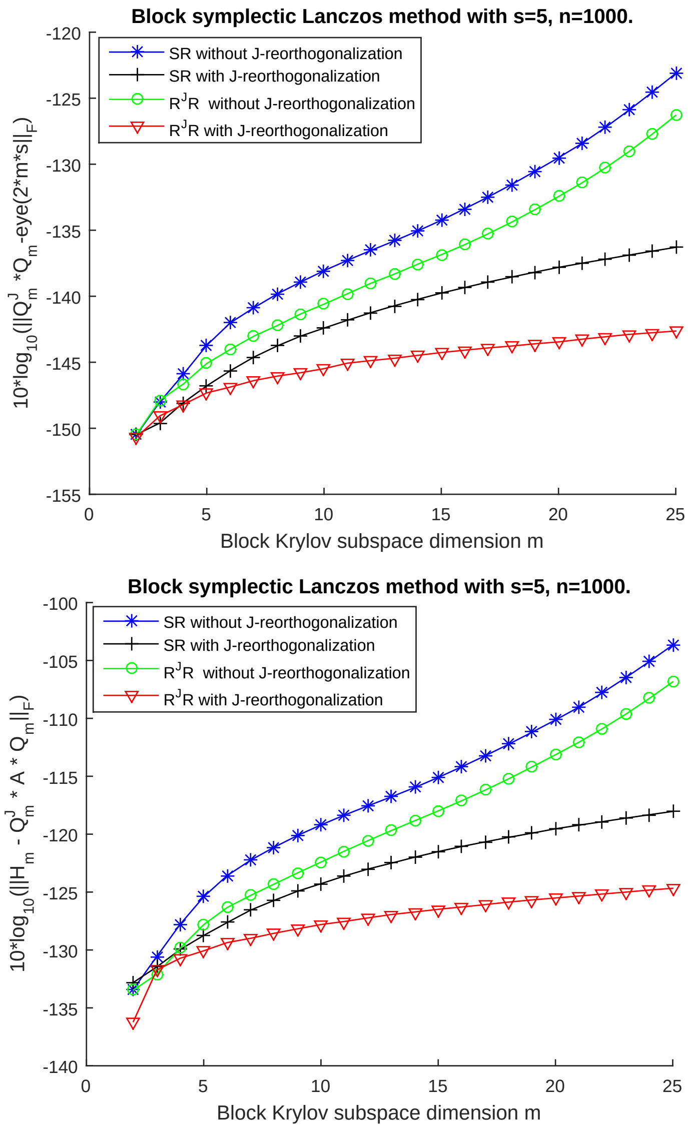

FIG. 5.1. *Example 5.1: $s = 5$, $k = 1, \ldots, 25$.*

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.

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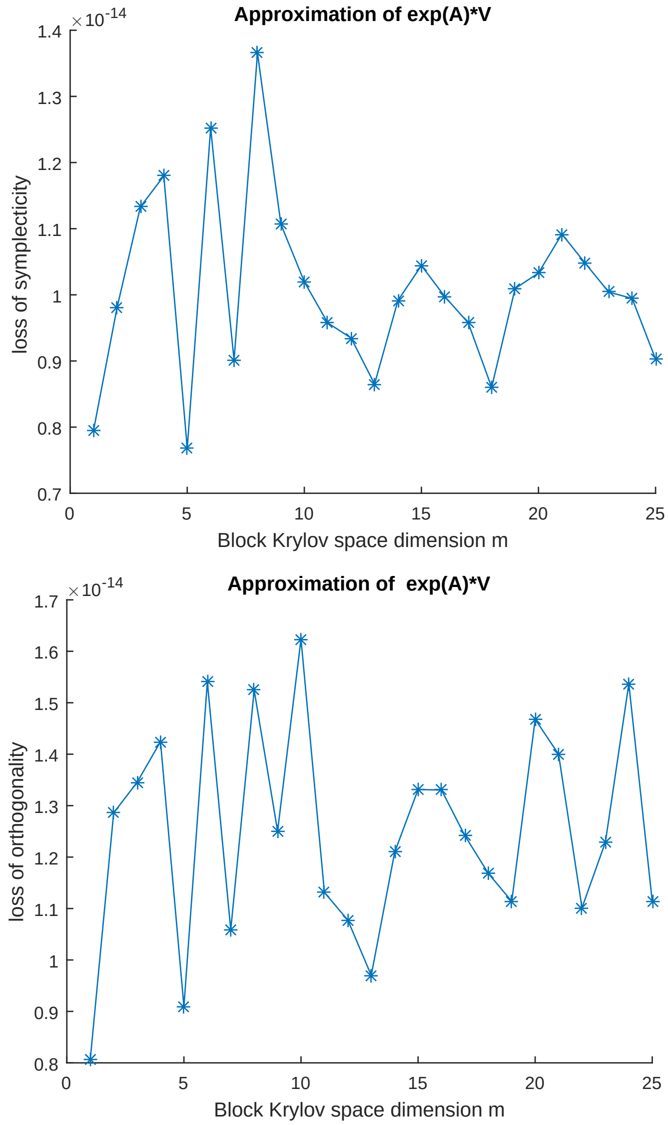

FIG. 5.2. *Example 5.1:* $s = 5$, $m = 1, \ldots, 25$.

EXAMPLE 5.2. In this example, we consider a 2000×2000 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 $A_2 = gallery('ris', n)$ is a 1000×1000 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.

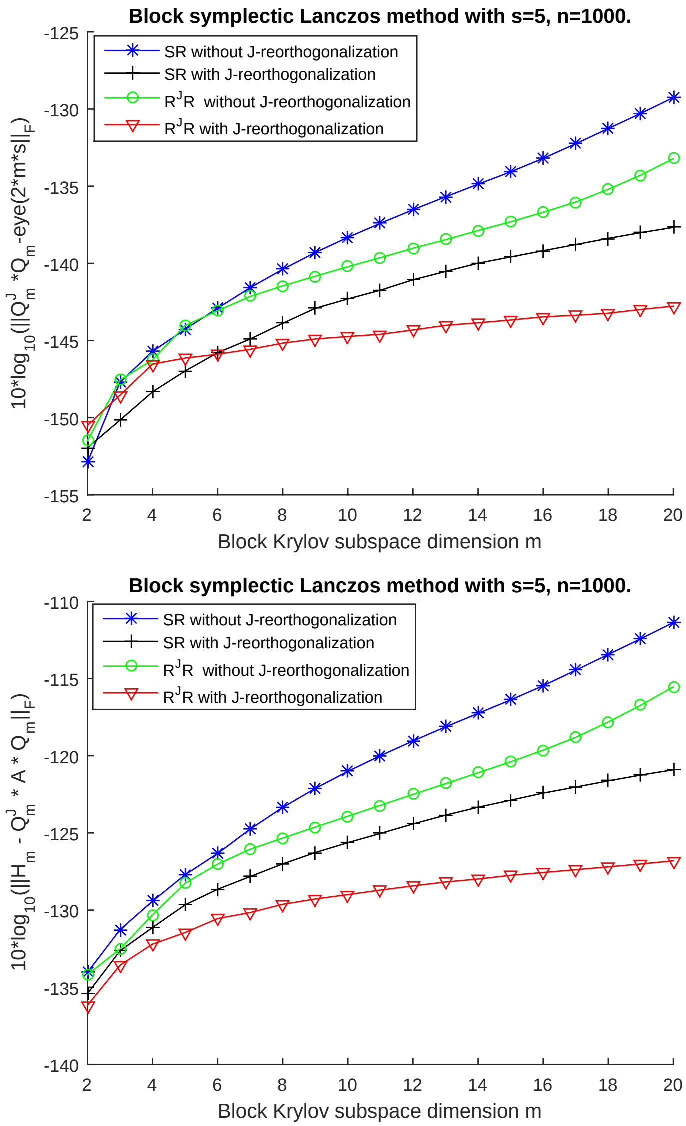

FIG. 5.3. *Example 5.2:* $s = 5$, $k = 1, \ldots, 20$.

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.

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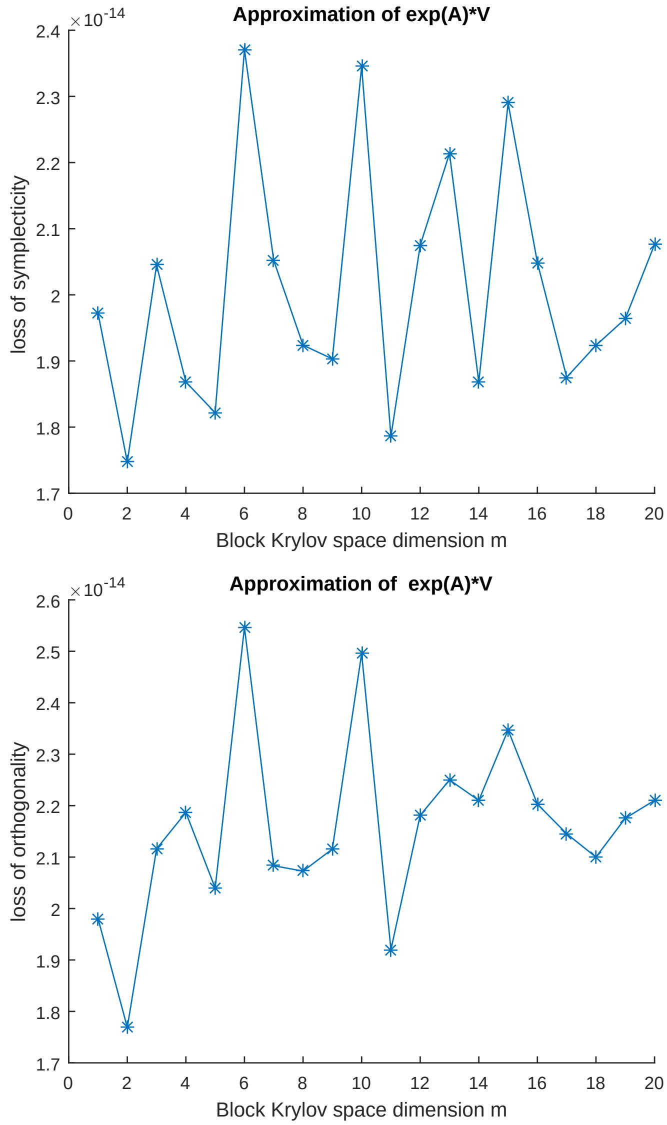

FIG. 5.4. *Example 5.2:* $s = 5$, $k = 1, \ldots, 20$.

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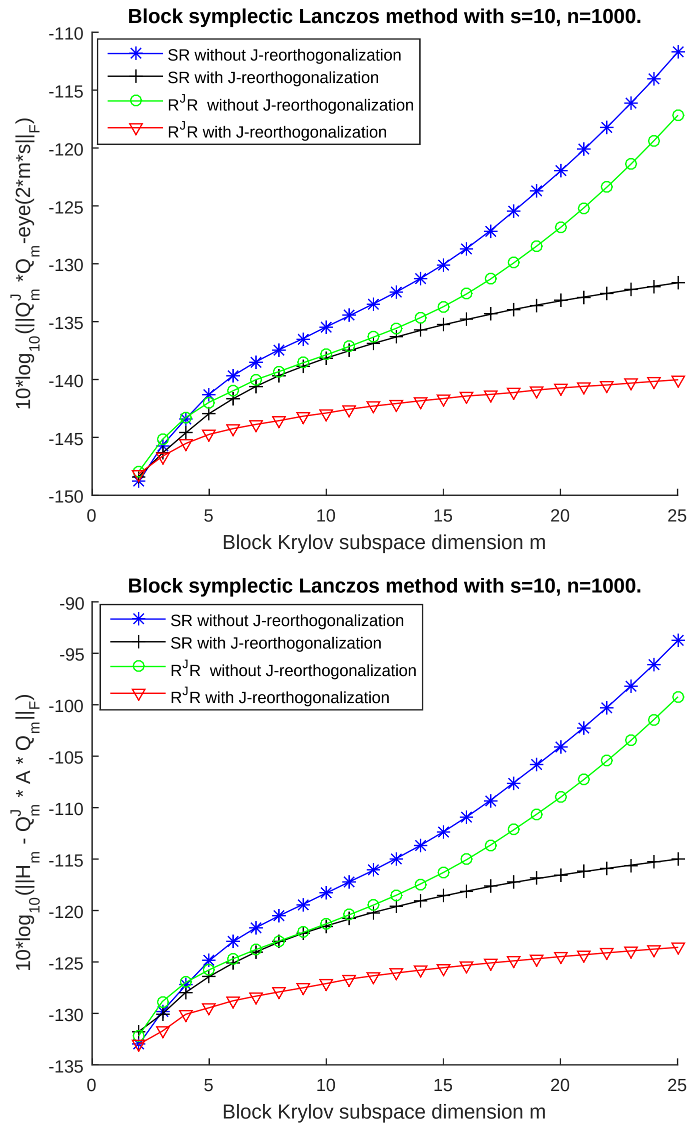

FIG. 5.5. *Example 5.2: $n = 1000$, $s = 10$, $k = 1, \ldots, 25$.*

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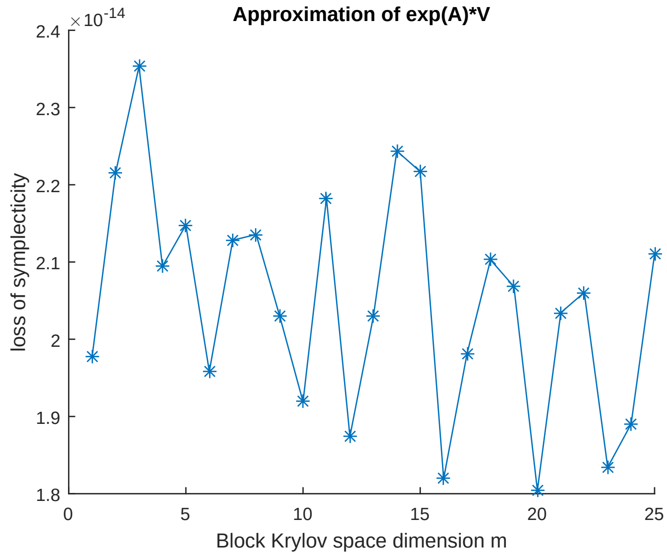

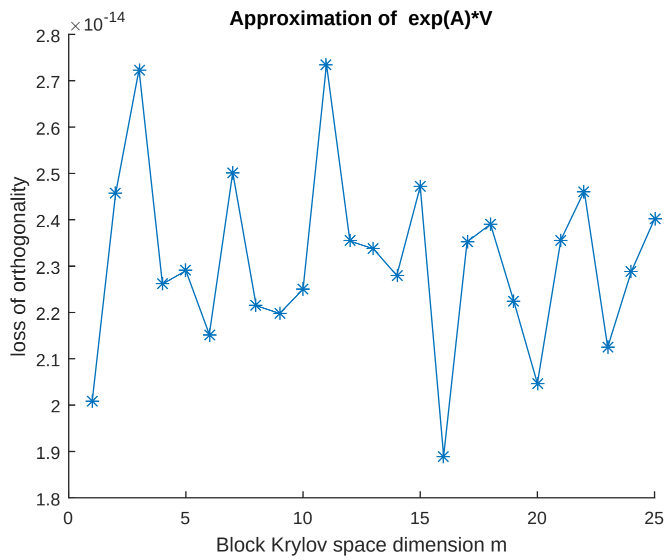

FIG. 5.6. *Example 5.2:* $n = 1000$, $s = 10$, $k = 1, \ldots, 25$.

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