A SUBSPACE ITERATION FOR SYMPLECTIC MATRICES

ALEXANDER MALYSHEV†, MILOUD SADKANE‡, AND AHMED SALAM§

Dedicated to Lothar Reichel on the occasion of his 60th birthday

Abstract. We study the convergence behavior of an orthogonal subspace iteration for matrices whose spectrum is partitioned into three groups: the eigenvalues inside, outside, and on the unit circle. The main focus is on symplectic matrices. Numerical experiments are provided to illustrate the theory.

Key words. symplectic matrix, subspace iteration, invariant subspace

AMS subject classifications. 15A21, 65F15

1. Introduction. Every square matrix \( W \in \mathbb{C}^{N \times N} \) can be block-factorized into the form

\[
W = \begin{bmatrix} X_\infty & X_1 & X_0 \end{bmatrix} \begin{bmatrix} W_\infty & W_1 & W_0 \\ W_\infty & W_1 & W_0 \end{bmatrix}^{-1},
\]

where one or two matrices among \( W_\infty, W_1, \) and \( W_0 \) may be empty. The spectrum of \( W \) consists of at most three groups: (i) eigenvalues \( \lambda_1, \ldots, \lambda_{N_\infty} \) of \( W_\infty \) outside the unit circle, (ii) eigenvalues \( \lambda_{N_\infty+1}, \ldots, \lambda_{N_\infty+N_1} \) of \( W_1 \) on the unit circle, and (iii) eigenvalues \( \lambda_{N_\infty+N_1+1}, \ldots, \lambda_{N_\infty+N_1+N_0} \) of \( W_0 \) inside the unit circle. The corresponding invariant subspaces, which we denote by \( X_\infty = \text{range}(X_\infty), X_1 = \text{range}(X_1), \) and \( X_0 = \text{range}(X_0), \) are of particular importance in applications such as optimal control [6, Chapter 14], [8, Chapter 15], and the theory of parametric resonance [5, 14].

Many applications including those mentioned above deal with a symplectic structure. Recall that a matrix \( W \in \mathbb{C}^{N \times N} \) is called \( J \)-symplectic if \( W^*JW = J \), where \( J \in \mathbb{C}^{N \times N} \) is an invertible skew-Hermitian matrix, i.e., \( J^* = -J \). A standard choice for \( J \) is

\[
J = \begin{bmatrix} 0_{N/2} & I_{N/2} \\ -I_{N/2} & 0_{N/2} \end{bmatrix},
\]

where \( N \) is even and \( 0_{N/2} \) and \( I_{N/2} \) are respectively the zero and identity matrices of order \( N/2 \). When \( J \) is given by (1.2), the \( J \)-symplecticity of \( W \) yields the representation \( W^{-1} = -JW^*J \). Moreover, if \( W \) is partitioned as

\[
W = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}, \quad W_{ij} \in \mathbb{C}^{N/2 \times N/2},
\]

then

\[
W^{-1} = \begin{bmatrix} W_{22}^* & -W_{12}^* \\ -W_{21}^* & W_{11}^* \end{bmatrix},
\]

and this formula can be used for an inexpensive computation of \( W^{-1} \); see Algorithm 1.
The symplectic structure of \( W \) implies that \( N_\infty = N_0 = N - N_\infty - N_1 \), and the eigenvalues of \( W_\infty \) and \( W_0 \) in (1.1) are symmetric with respect to the unit circle. When all the blocks \( X_\infty, X_1, \) and \( X_0 \) are nonempty, they satisfy the following \( J \)-orthogonalization properties:

\[
X_\infty^* J X_\infty = 0, \quad X_0^* J X_0 = 0, \quad X_\infty^* J X_1 = 0, \quad X_0^* J X_1 = 0.
\]

Furthermore, the matrices \( X_0^* J X_\infty \) and \( X_1^* J X_1 \) are nonsingular, and the matrix

\[
P_1 = X_1 (X_1^* J X_1)^{-1} X_1^* J
\]

is the projector onto \( \mathcal{X}_1 \) along \( \mathcal{X}_0 + \mathcal{X}_\infty \). More details are found in [14].

A quadratically convergent algorithm was proposed in [2] for computing the invariant subspaces \( \mathcal{X}_\infty, \mathcal{X}_1, \) and \( \mathcal{X}_0 \) of a symplectic matrix \( W \). However, this algorithm necessitates the solution of a \( 3N \times 3N \) linear system at each iteration. In the present paper we propose a cheaper algorithm based on a variant of a subspace iteration suitable for symplectic matrices. It is widely known that (orthogonal) subspace iteration is reliable [9, 10, 11] even though its convergence rate is only linear. In our context, a classical variant of subspace iteration is formally implemented as follows: starting from \( Q_0 = I \), where \( I \) denotes the identity matrix, compute iteratively \( Q_k \) by means of the QR factorizations \( W Q_{k-1} = Q_k R_k \). If

\[
Q_k = \begin{bmatrix} Q_k^{\infty} & Q_k^{(1)} & Q_k^{(0)} \end{bmatrix}
\]

is partitioned such that \( Q_k^{\infty} \in \mathbb{C}^{N \times N_\infty}, Q_k^{(1)} \in \mathbb{C}^{N \times N_1}, \) and \( Q_k^{(0)} \in \mathbb{C}^{N \times N_0} \), then the convergence properties of the subspace iteration method (see, e.g., [10, Chapter 5]) guarantee that for large \( k \), the subspaces range(\( Q_k^{\infty} \)), range(\( Q_k^{(1)} \)), and range(\( Q_k^{(0)} \)) approximate \( \mathcal{X}_\infty, \mathcal{X}_1, \) and \( \mathcal{X}_0 \), respectively. However, the detection of convergence can be nontrivial.

We propose another variant of subspace iteration:

**ALGORITHM 1.**

1. Set \( Q_{0,1} = Q_{0,2} = I \),
2. For \( k = 1, 2, \ldots \),

\[
\begin{bmatrix} W Q_{1,k-1} \\ W^{-1} Q_{2,k-1} \end{bmatrix} = \begin{bmatrix} Q_{1,k} \\ Q_{2,k} \end{bmatrix} R_k.
\]

Here the matrices \( Q_{1,k}, Q_{2,k} \in \mathbb{C}^{N \times N} \) satisfy the identity \( Q_{1,k}^* Q_{1,k} + Q_{2,k}^* Q_{2,k} = I \), and the matrix \( R_k \in \mathbb{C}^{N \times N} \) is upper triangular. Step 2 uses formula (1.3) for a symplectic matrix \( W \). This variant has been used in the context of spectral dichotomy for a general matrix \( [A, B] \), where the identity matrix was used in step 2 instead of \( W^{-1} \). In such a case, Algorithm 1 is twice as slow; see the numerical experiments in Section 4.

We will show that for large \( k \), the subspaces range(\( Q_{1,k} \)) and range(\( Q_{2,k} \)) approximate \( \mathcal{X}_\infty + \mathcal{X}_1 \) and \( \mathcal{X}_0 + \mathcal{X}_1 \), respectively, and that the intersection range(\( Q_{1,k} \)) \cap range(\( Q_{2,k} \)) approximates \( \mathcal{X}_1 \). An orthogonalization process is then applied to extract \( \mathcal{X}_\infty \) and \( \mathcal{X}_0 \) from \( \mathcal{X}_\infty + \mathcal{X}_1 \) and \( \mathcal{X}_0 + \mathcal{X}_1 \).

The convergence behavior of Algorithm 1 is studied in Section 2. Roughly speaking, convergence is fast if the spectra of the blocks \( W_\infty \) and \( W_0 \) are well separated from the unit circle, \( W_1 \) is diagonalizable, and the condition number of \( [X_\infty \quad X_1 \quad X_0] \) is not large.

The following notation and assumptions are used throughout the paper. The matrix \( W_1 \) is assumed to be diagonalizable and hence diagonal due to (1.1). The identity and null matrices of order \( p \) are denoted by \( I_p \) and \( 0_p \) or just \( I \) and \( 0 \) when the order is clear from the context. The 2-norm and Frobenius norm of a matrix \( A \) are denoted by \( \| A \|_2 \) and \( \| A \|_F \). The transpose conjugate of \( A \) is denoted by \( A^* \). A calligraphic letter \( \mathcal{A} \) denotes the subspace range(\( \mathcal{A} \)) corresponding to a matrix \( A \). The singular values of a matrix \( A \) are labeled in decreasing order, i.e., \( \sigma_{\max}(A) = \sigma_1(A) \geq \sigma_2(A) \geq \ldots \geq \sigma_{\min}(A) \). If \( A \) is nonsingular, its condition number \( \sigma_{\max}(A)/\sigma_{\min}(A) \) with respect to the 2-norm is denoted by \( \text{cond}_2(A) \).
2. Convergence theory for Algorithm 1. The columns of the matrix
\[
\begin{bmatrix}
Q_{1,k} \\
Q_{2,k}
\end{bmatrix}
\]
form an orthonormal basis of the linear space spanned by the columns of the matrix
\[
\begin{bmatrix}
W_k \\
W^{-k}
\end{bmatrix}
\]. This fact follows from the following proposition.

**Proposition 2.1.** For the matrices in Algorithm 1, we have
\[
\begin{bmatrix}
W_k \\
W^{-k}
\end{bmatrix} = \begin{bmatrix}
Q_{1,k} \\
Q_{2,k}
\end{bmatrix} \bar{R}_k,
\]
where \( \bar{R}_k = R_k R_{k-1} \ldots R_1 \) is upper triangular, and
\[
Q_{1,k}^* Q_{1,k} + Q_{2,k}^* Q_{2,k} = I.
\]

**Proof.** Apply induction as follows:
\[
\begin{bmatrix}
W_k \\
W^{-k}
\end{bmatrix} = \begin{bmatrix}
W W^{k-1} \\
W^{-1} W^{-k+1}
\end{bmatrix} = \begin{bmatrix}
W Q_{1,k-1} \\
W^{-1} Q_{2,k-1}
\end{bmatrix} \bar{R}_{k-1} = \begin{bmatrix}
Q_{1,k} \\
Q_{2,k}
\end{bmatrix} R_k \bar{R}_{k-1}.
\]

Let us choose the block diagonal factorization
\[
W = X \begin{bmatrix}
W_\infty \\
W_1 \\
W_0
\end{bmatrix} X^{-1}
\]
(2.1)
\[
= [X_\infty \ X_1 \ X_0] \begin{bmatrix}
W_\infty \\
W_1 \\
W_0
\end{bmatrix} [X_\infty \ X_1 \ X_0]^{-1}
\]
so that the columns of \( X_1 \) are eigenvectors of unit length corresponding to the eigenvalues of \( W \) on the unit circle and the orthonormality conditions
\[
X_\infty^* X_\infty = I, \quad X_0^* X_0 = I
\]
(2.2)
hold. Then the norm of \( X \) satisfies the bound \( ||X||_2 \leq \sqrt{2 + N_1} \).

By Proposition 2.1, the linear space spanned by the columns of
\[
\begin{bmatrix}
W_k \\
W^{-k}
\end{bmatrix} = X \begin{bmatrix}
I \\
W_k \\
W^{-k}
\end{bmatrix} X^{-1}
\]
(2.3)
coincides with the linear space spanned by the columns of the matrix \( A_k + E_k \), where
\[
A_k = \begin{bmatrix}
X \begin{bmatrix}
I \\
W_k \\
W^{-k}
\end{bmatrix} \\
X \begin{bmatrix}
0 \\
W^{-k}
\end{bmatrix}
\end{bmatrix}, \quad E_k = \begin{bmatrix}
0 \\
W_{2k} \\
W_{-2k}
\end{bmatrix}.
\]
(2.4)
Convergence of Algorithm 1 is based on the following result from the perturbation theory for the QR factorization.

**Theorem 2.2** (Sun [13]). Consider QR factorizations $A = QR$ and $A + E = \tilde{Q}\tilde{R}$ with the upper triangular factors having positive diagonals for matrices $A$ and $A + E$ of full column rank. If $\|A\|_2\|E\|_2 < 1$, where $A^*$ is the Moore-Penrose pseudoinverse of $A$, then

$$\|\tilde{Q} - Q\|_F \leq \sqrt{2}\|A\|_2\|E\|_F \sqrt{1 - \|A\|_2\|E\|_2}.$$  

To apply this theorem, we need the following lemmas.

**Lemma 2.3.** For all $k \geq 0$, we have

$$\|E_k\|_2 \leq \sqrt{\omega} (1 - \omega^{-1})^k,$$

where $\omega = \max \left\{ \| \sum_{k=0}^\infty W_0^k(W_0^*)^k \|_2, \| \sum_{k=0}^\infty W_\infty^{-k}(W_\infty^*)^k \|_2 \right\} > 1$.

**Proof.** The norms of the matrix powers $W_0^{2k}$ and $W_\infty^{-2k}$, $k \geq 0$, decay as follows (see, e.g., [4]):

$$\|W_0^{2k}\|_2 \leq \|H_0\|_2 \left(1 - \frac{1}{\|H_0\|_2}\right)^k, \quad \|W_\infty^{-2k}\|_2 \leq \|H_\infty\|_2 \left(1 - \frac{1}{\|H_\infty\|_2}\right)^k,$$

where $H_0 = \sum_{k=0}^\infty W_0^k(W_0^*)^k$ and $H_\infty = \sum_{k=0}^\infty W_\infty^{-k}(W_\infty^*)^k$. Furthermore, from (2.2) and (2.4) we obtain $\|E_k\|_2^2 = \max \left\{ \|W_0^{2k}\|_2^2, \|W_\infty^{-2k}\|_2^2 \right\}$. \hfill \Box

**Lemma 2.4.** The Moore-Penrose pseudoinverse of $A_k$ satisfies the bound

$$\|A_k^*\|_2 \leq \|X^{-1}\|_2^2.$$  

**Proof.** From the properties of the singular values [12] and the matrix $W_1$, we have

$$\sigma_{\min}(A_k) \geq \sigma_{\min} \left( \begin{bmatrix} I & W_1^k \\ 0 & \hat{W}_1^{-k} \end{bmatrix} \right) \sigma_{\min}(X) = \sigma_{\min}(X),$$

which yields the desired bound. \hfill \Box

Lemmas 2.3 and 2.4 show that $A_k$ has full rank and $A_k + E_k$ has full rank for large $k$. To apply Theorem 2.2 for sufficiently large $k$, consider the QR decompositions

$$A_k = Q_kR_k, \quad A_k + E_k = \tilde{Q}_k\tilde{R}_k.$$  

From (2.3) and (2.4) we know that $\tilde{Q}_k = \begin{bmatrix} Q_{1,k} \\ Q_{2,k} \end{bmatrix}$. Let $Q_k = \begin{bmatrix} Q_{1,k} \\ Q_{2,k} \end{bmatrix}$. Then with the help of Lemmas 2.3, 2.4, and Theorem 2.2, we arrive at the following convergence estimate

$$\max \left\{ \|Q_{1,k} - Q_{1,1}\|_2, \|Q_{2,k} - Q_{2,1}\|_2 \right\} \leq \sqrt{2}\sqrt{N}\|X^{-1}\|_2 \sqrt{\omega(1 - \omega^{-1})^k}. $$

From this estimate and the fact that $Q_{1,k} = X_\infty + X_1$ and $Q_{2,k} = X_1 + X_0$, we obtain the following result.
PROPOSITION 2.5. Algorithm 1 is linearly convergent, and
\[
\lim_{k \to \infty} Q_{1,k} = X_\infty + X_1, \quad \lim_{k \to \infty} Q_{2,k} = X_1 + X_0.
\]

The above convergence analysis shows that convergence mainly depends on the condition number of the matrix \( X \) from the block-diagonalization (2.1) and on the decay of the powers of \( W_0 \) and \( W^{-1}_\infty \).

The next theorem characterizes the singular values of \( Q_{1,k} \) and \( Q_{2,k} \). For large \( k \), this theorem and the estimate (2.6) characterize the singular values of \( Q_{1,k} \) and \( Q_{2,k} \). Such a characterization will be useful mainly for numerical purposes; see Section 4.

THEOREM 2.6. The matrix \( Q_{1,k} \) has \( N_\infty \) singular values equal to 1, \( N_0 \) singular values equal to 0, and \( N_1 \) singular values in the interval \([s, \sqrt{1-s^2}]\), where \( s = \frac{1}{\sqrt{2 \text{cond}(X)}} \). The singular values \( \sigma_i(Q_{2,k}) \) equal \( \sqrt{1 - \sigma_{N-i+1}^2(Q_{1,k})} \).

Proof. Since \( Q_{1,k}^* Q_{1,k} + Q_{2,k}^* Q_{2,k} = I \), it is clear that \( \sigma_i^2(Q_{1,k}) + \sigma_{N-i+1}^2(Q_{2,k}) = 1 \).

Also, since from (2.4) and (2.5) it follows that
\[
Q_{1,k} = X \left[ \begin{array}{c} I \\ W_1^k \end{array} \right] B_k^{-1}, \quad Q_{2,k} = X \left[ \begin{array}{c} 0 \\ W_1^{-k} \\ I \end{array} \right] B_k^{-1},
\]

it is clear that \( \sigma_i(Q_{1,k}) = 0 \) for \( i > N_\infty + N_1 \) and \( \sigma_i(Q_{2,k}) = 0 \) for \( i > N_0 + N_1 \), and therefore, \( \sigma_i(Q_{1,k}) = 1 \) for \( 1 \leq i \leq N_\infty \) and \( \sigma_i(Q_{2,k}) = 1 \) for \( 1 \leq i \leq N_0 \).

From (2.4) and (2.5),
\[
R_k^* R_k = \left[ \begin{array}{c} I \\ W_1^k \\ 0 \end{array} \right] X^* X \left[ \begin{array}{c} I \\ W_1^k \\ 0 \end{array} \right] + \left[ \begin{array}{c} 0 \\ W_1^{-k} \\ I \end{array} \right] X^* X \left[ \begin{array}{c} 0 \\ W_1^{-k} \\ I \end{array} \right],
\]

which yields \( \| R_k \|_2 \leq \sqrt{2} \| X \|_2 \).

Now, for \( i \leq N_\infty + N_1 \),
\[
1 = \sigma_i \left[ \begin{array}{c} I \\ W_1^k \end{array} \right] \leq \sigma_i(Q_{2,k}) \| X^{-1} \|_2 \| R_k \|_2 \leq \sigma_i(Q_{1,k}) \sqrt{2} \text{cond}(X).
\]

Hence, \( \sigma_i(Q_{1,k}) \geq \frac{1}{\sqrt{2 \text{cond}(X)}} \) for \( i \leq N_\infty + N_1 \). Similarly, \( \sigma_i(Q_{2,k}) \geq \frac{1}{\sqrt{2 \text{cond}(X)}} \) for \( i \leq N_0 + N_1 \).

3. Algorithmic aspects. In this section we discuss some important issues that arise when implementing Algorithm 1, namely the approximation of the invariant subspaces \( X_\infty \), \( X_0 \), and \( X_\infty \) from the matrices \( Q_{1,k} \) and \( Q_{2,k} \) and the stopping criterion.

3.1. Computation of \( X_\infty \), \( X_0 \), and \( X_\infty \). The subspace \( X_1 \) is the intersection of the subspaces \( X_\infty + X_1 \) and \( X_1 + X_0 \). From Proposition 2.5, the natural way to obtain such an intersection, once the iteration has been stopped, is to compute the intersection of the subspaces \( Q_{1,k} \) and \( Q_{2,k} \). This can be obtained from the SVDs of \( Q_{1,k} \) and \( Q_{2,k} \) [7, Chapter 12]. Let \( Q_{1,k} \) and \( Q_{2,k} \) be matrices whose columns form orthonormal bases of \( Q_{1,k} \) and \( Q_{2,k} \). Then the intersection can be obtained as the left or right singular vectors associated with the singular values of \( Q_{2,k} Q_{1,k} \) that are equal to 1.
Let \( \tilde{X}_1 \) be the matrix whose columns are formed by these singular vectors. Then we have \( \tilde{X}_1 \approx X_1 \), and \( \tilde{P}_1 = \tilde{X}_1(\tilde{X}_1^*J\tilde{X}_1)^{-1}\tilde{X}_1^*J \) is an approximation of the projector \( P_1 \) given in (1.5). The \( J \)-orthogonalization properties (1.4) allow us to conclude that

\[
\tilde{X}_\infty \equiv \text{range} \left( (I - \tilde{P}_1)Q_{1,k} \right) \approx X_\infty \quad \text{and} \quad \tilde{X}_0 \equiv \text{range} \left( (I - \tilde{P}_1)Q_{2,k} \right) \approx X_0.
\]

If needed, the approximate projectors onto \( X_\infty \) and \( X_0 \) can be constructed as follows: since by construction, the matrices \( (I - \tilde{P}_1)Q_{1,k} \) and \( (I - \tilde{P}_1)Q_{2,k} \) have only \( N_\infty = N_0 \) non-negligible singular values, the SVDs of \( (I - \tilde{P}_1)Q_{1,k} \) and \( (I - \tilde{P}_1)Q_{2,k} \) yield matrices \( \tilde{X}_\infty \) and \( \tilde{X}_0 \) of \( N_\infty = N_0 \) orthonormal columns (left singular vectors associated with the larger singular values) which form an approximate basis of \( X_\infty \) and \( X_0 \). The desired projectors are then given by \( P_\infty = \tilde{X}_\infty(\tilde{X}_\infty^*J\tilde{X}_\infty)^{-1}\tilde{X}_\infty^*J \) and \( P_0 = \tilde{X}_0(\tilde{X}_0^*J\tilde{X}_0)^{-1}\tilde{X}_0^*J \).

### 3.2. Stopping criterion

An important and difficult task is the choice of an effective criterion to stop the iteration of Algorithm 1. We have seen in Section 2 that the subspaces \( Q_{1,k} \) and \( Q_{2,k} \) converge to \( X_\infty + X_1 \) and \( X_1 + X_0 \), respectively. In particular, for large \( k \), the matrices \( Q_{1,k} \) and \( Q_{2,k} \) become singular, the \( N_0 = N_\infty \) smallest singular values of \( Q_{1,k} \) and \( Q_{2,k} \) converge to 0, the \( N_\infty = N_0 \) largest singular values converge to 1, and the remaining \( N_1 \) singular values oscillate in the open interval \((0, 1)\). This fact can be used as a stopping criterion.

For example, if the eigenvalues of \( W \) are all on the unit circle (i.e., \( N_\infty = N_0 = 0 \)), then \( Q_{1,k} \) and \( Q_{2,k} \) converge to \( X_1 \). Actually, in this case, (1.1) reduces to \( W = X_1 W_1 X_1^{-1} \). It can easily be shown that then \( Q_{1,k} = Q_{2,k} = X_1 \) for all \( k \geq 1 \). In other words, Algorithm 1 converges at the first iteration. In practice, if the singular values of \( Q_{1,k} \) or \( Q_{2,k} \) oscillate in \((0, 1)\), we may conclude that the eigenvalues of \( W \) are all on the unit circle. Then \( \tilde{X}_0 = \tilde{X}_\infty = 0 \), and \( \tilde{X}_1 \) can be computed as explained above.

If \( W \) has no eigenvalue on the unit circle, i.e., \( N_\infty = N_0 = N/2 \), then \( Q_{1,k} \) converges to \( X_\infty \) and \( Q_{2,k} \) converges to \( X_0 \). For large \( k \), \( Q_{1,k} \) and \( Q_{2,k} \) have \( N/2 \) singular values close to 0 and \( N/2 \) singular values close to 1. A stopping criterion is obtained by monitoring the decrease to 0 of the \( (\frac{N}{2} + 1) \)-st largest singular value of \( Q_{1,k} \). Another stopping criterion can be derived from the property \( \lim_{k \to \infty} \sigma_i(Q_{1,k}Q_{2,k}) = 0 \) for all \( i \), and thus, the stopping criterion consists of checking if the norm \( \|Q_{1,k}Q_{2,k}\| \) is less than some fixed threshold \( \text{tol} \).

In the general case when there are eigenvalues inside, on, and outside the unit circle, for large \( k \), \( Q_{1,k} \) has \( N_\infty \) singular values close to 1, \( N_0 = N_\infty \) singular values close to 0, and \( N_1 = N - 2N_\infty \) singular values that oscillate in the open interval \((0, 1)\). The numerical experiments show that in general the convergence to 1 and 0 is fast when there is a sufficiently large gap between the eigenvalues on the unit circle and those outside or inside of it. A stopping criteria is obtained by monitoring the larger singular values of \( Q_{1,k} \) (which must converge to 1). The iterations are stopped when the number of ones stabilizes to a value, say, \( \tilde{N}_\infty \), and \( \sigma_{N-\tilde{N}_\infty+1}(Q_{1,k}) < \text{tol} < \sigma_{N-\tilde{N}_\infty}(Q_{1,k}) \), where \( \text{tol} \) is some prescribed tolerance. Then we set \( N_\infty = \tilde{N}_\infty \). To keep the cost as small as possible, the computation of the singular values is carried out periodically, for example, every 10th iteration. Once the iteration is stopped, the matrices \( \tilde{X}_\infty \), \( \tilde{X}_1 \), and \( \tilde{X}_0 \) can be computed as explained in Section 3.1. Note that these matrices must satisfy approximately the properties (1.4) and (1.5), which can be used as an a posteriori verification of the accuracy of the computed matrices.

### 4. Numerical experiments

In this section we report some numerical experiments illustrating the convergence behavior of Algorithm 1. In all tests, the matrix \( J \) has the form (1.2). We also present comparisons with Algorithm 2 which consists of replacing, in step 2 of Algorithm 1, the matrix \( W^{-1} \) by the identity matrix.
and converges at the first iteration (and especially in line 4 of Section 3.2).

Table 4.1

<table>
<thead>
<tr>
<th>Iteration $k$</th>
<th>$1$</th>
<th>$50$</th>
<th>$100$</th>
<th>$150$</th>
<th>$190$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_1(Q_{1,k})$</td>
<td>$9.983 \times 10^{-1}$</td>
<td>$1$</td>
<td>$1$</td>
<td>$1$</td>
<td>$1$</td>
</tr>
<tr>
<td>$\sigma_{10}(Q_{1,k})$</td>
<td>$7.794 \times 10^{-1}$</td>
<td>$1$</td>
<td>$1$</td>
<td>$1$</td>
<td>$1$</td>
</tr>
<tr>
<td>$\sigma_{11}(Q_{1,k})$</td>
<td>$7.002 \times 10^{-1}$</td>
<td>$1.356 \times 10^{-3}$</td>
<td>$9.844 \times 10^{-8}$</td>
<td>$7.142 \times 10^{-12}$</td>
<td>$2.400 \times 10^{-15}$</td>
</tr>
<tr>
<td>$\sigma_{20}(Q_{1,k})$</td>
<td>$5.805 \times 10^{-2}$</td>
<td>$4.770 \times 10^{-21}$</td>
<td>$3.741 \times 10^{-39}$</td>
<td>$2.814 \times 10^{-66}$</td>
<td>$3.659 \times 10^{-78}$</td>
</tr>
</tbody>
</table>

Example 4.1. This example shows that Algorithm 1 converges at the first iteration when the eigenvalues of $W$ are all on the unit circle. The matrix $W$ is chosen block diagonal as $W = \text{blockdiag}(Q_1, Q)$, where $Q$ is a $10 \times 10$ orthogonal matrix constructed with the MATLAB function \texttt{orth}.

At the first iteration of Algorithm 1 ($k = 1$), the singular values of the matrix $Q_{1,k}$ are all equal to $7.0711 \times 10^{-1}$ and remain the same during all iterations. From the discussion in Section 3.2, we conclude that the eigenvalues of $W$ are all on the unit circle. The algorithm computes $\tilde{X}_1$ being of order 20 satisfying $\| W \tilde{X}_1 - \tilde{X}_1 \left( \tilde{X}_1^* W \tilde{X}_1 \right) \| = 1.5504 \times 10^{-15}$ and $\tilde{P}_1$ satisfying $\| \tilde{P}_1 - I_{20} \| = 1.3545 \times 10^{-15}$.

Example 4.2. This example shows that when $W$ has no eigenvalues on the unit circle ($N = N_0 = N_\infty$), then the $N_0$ largest (smallest) singular values of $Q_{1,k}$ and $Q_{2,k}$ converge to 1 (0). The matrix $W$ is given by $W = \text{blockdiag}(A, (A^{-1})^*)$, where $A$ is a $10 \times 10$ upper triangular matrix whose strictly upper triangular part is chosen randomly in $(0, 1)$ and the diagonal elements are such that $A(k, k) = 1 + k/10$, $k = 1, \ldots, 10$. Therefore $W$ has $N_0 = 10$ eigenvalues inside the unit circle and $N_\infty = 10$ eigenvalues outside of it. Following the discussion in Section 3.2, we show in Figure 4.1 and Table 4.1 (and especially in line 4 of this table) the convergence to 0 of the 11-th largest singular value of $Q_{1,k}$. With the stopping criterion discussed in Section 3.2 and $\texttt{tol} = 10^{-14}$, Algorithm 1 necessitates 190 iterations. The figure also exhibits the results of Algorithm 2. At iteration 431, $\sigma_{11}(Q_{1,k})$ computed by Algorithm 2 stagnates at $1.4681 \times 10^{-14}$.

At iteration $k = 190$, Algorithm 1 computes matrices $\tilde{X}_0$ and $\tilde{X}_\infty$ each of size $20 \times 10$ whose columns are orthonormal and satisfy $\| W \tilde{X}_0 - \tilde{X}_0 \left( \tilde{X}_0^* W \tilde{X}_0 \right) \| = 8.3316 \times 10^{-16}$ and $\| W \tilde{X}_\infty - \tilde{X}_\infty \left( \tilde{X}_\infty^* W \tilde{X}_\infty \right) \| = 1.7496 \times 10^{-15}$. The computed projectors $\tilde{P}_0$, $\tilde{P}_\infty$ sat-
The singular values of the matrix \( W = \text{blockdiag} \left( A, (A^{-1})^* \right) \) with \( A = \text{blockdiag} \left( A_0, A_1 \right) \) where \( A_0 \) is a \( 6 \times 6 \) Jordan block corresponding to the eigenvalue 0.9 and \( A_1 \) is a \( 4 \times 4 \) orthogonal matrix constructed with the MATLAB function \text{orthog}. Therefore, \( W \) has \( N_0 = 6 \) eigenvalues inside the unit circle, \( N_\infty = 6 \) eigenvalues outside the unit circle, and \( N_1 = 8 \) eigenvalues on the unit circle. The singular values \( \sigma_1, \sigma_16, \ldots, \sigma_20 \) should converge to 0. The stopping criterion discussed in Section 3.2 is used with \( tol = 10^{-10} \). Algorithm 1 required 250 iterations while Algorithm 2 required 500 iterations. The convergence behavior of both algorithms is shown in Figure 4.2. Table 4.2 illustrates the convergence of the singular values of \( Q_{1,k} \) computed by Algorithm 1.

**Example 4.3.** This example reveals the convergence behavior when \( W \) has eigenvalues inside, on, and outside the unit circle. The matrix \( W \) is given by \( W = \text{blockdiag} \left( A, (A^{-1})^* \right) \) with \( A = \text{blockdiag} \left( A_0, A_1 \right) \) where \( A_0 \) is a \( 6 \times 6 \) Jordan block corresponding to the eigenvalue 0.9 and \( A_1 \) is a \( 4 \times 4 \) orthogonal matrix constructed with the MATLAB function \text{orthog}. Therefore, \( W \) has \( N_0 = 6 \) eigenvalues inside the unit circle, \( N_\infty = 6 \) eigenvalues outside the unit circle, and \( N_1 = 8 \) eigenvalues on the unit circle. The singular values \( \sigma_1, \sigma_16, \ldots, \sigma_20 \) should converge to 0. The stopping criterion discussed in Section 3.2 is used with \( tol = 10^{-10} \). Algorithm 1 required 250 iterations while Algorithm 2 required 500 iterations. The convergence behavior of both algorithms is shown in Figure 4.2. Table 4.2 illustrates the convergence of the singular values of \( Q_{1,k} \) computed by Algorithm 1.

**Table 4.2**

<table>
<thead>
<tr>
<th>( Q_{1,k} )</th>
<th>( k )</th>
<th>( 1 )</th>
<th>( 50 )</th>
<th>( 100 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_1 )</td>
<td>( \sigma_6 )</td>
<td>( \sigma_7 )</td>
<td>( \sigma_{14} )</td>
<td>( \sigma_{15} )</td>
</tr>
<tr>
<td>1</td>
<td>9.991 ( 10^{-1} )</td>
<td>7.268 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
</tr>
<tr>
<td>50</td>
<td>8.10 -1</td>
<td>7.071 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
</tr>
<tr>
<td>100</td>
<td>9.496 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( Q_{1,k} )</th>
<th>( k )</th>
<th>( 150 )</th>
<th>( 200 )</th>
<th>( 250 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_1 )</td>
<td>( \sigma_6 )</td>
<td>( \sigma_7 )</td>
<td>( \sigma_{14} )</td>
<td>( \sigma_{15} )</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>200</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>250</td>
<td>7.071 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
<td>7.071 ( 10^{-1} )</td>
</tr>
<tr>
<td>3.020 ( 10^{-8} )</td>
<td>( 8.380 \times 10^{-14} )</td>
<td>( 1.409 \times 10^{-23} )</td>
<td>( 1.638 \times 10^{-19} )</td>
<td></td>
</tr>
</tbody>
</table>
is unpredictable. We consider the preceding example where $A_0$ is a $4 \times 4$-Jordan block for the eigenvalue 1. Table 4.3 displays the singular values of $Q_{1,k}$.

It seems that, during the iterations, the 8 eigenvalues on the unit circle moved off the unit circle preserving the symmetry of the spectrum. See the singular values $\sigma_i(Q_{1,k})$, $i = 7, 8, \ldots, 14$, in Table 4.3, where we observe that 4 eigenvalues moved out of the unit circle and 4 moved inside of it.

5. Conclusions. We have studied the behavior of a variant of a subspace iteration suited for symplectic matrices. The study reveals the parameters responsible for the convergence rate. The algorithm is attractive due to its simplicity and the low cost of a single iteration.

REFERENCES


