ON ASYMPTOTIC CONVERGENCE OF NONSYMMETRIC JACOBI ALGORITHMS

CHRISTIAN MEHL*

Abstract. The asymptotic convergence behavior of cyclic versions of the nonsymmetric Jacobi algorithm for the computation of the Schur form of a general complex matrix is investigated. Similar to the symmetric case, the nonsymmetric Jacobi algorithm proceeds by applying a sequence of rotations that annihilate a pivot element in the strict lower triangular part of the matrix until convergence to the Schur form of the matrix is achieved.

In this paper, it is shown that the cyclic nonsymmetric Jacobi method converges locally and asymptotically quadratically under mild hypotheses if special ordering schemes are chosen, namely ordering schemes that lead to so-called northeast directed sweeps. The theory is illustrated by the help of numerical experiments. In particular, it is shown that there are ordering schemes that lead to asymptotic quadratic convergence for the cyclic symmetric Jacobi method, but only to asymptotic linear convergence for the cyclic nonsymmetric Jacobi method. Finally, a generalization of the nonsymmetric Jacobi method to the computation of the Hamiltonian Schur form for Hamiltonian matrices is introduced and investigated.

Key words. Schur form, nonsymmetric Jacobi algorithm, asymptotic convergence, Hamiltonian Jacobi algorithm, Hamiltonian Schur form

AMS subject classification. 65F15

1. Introduction.

Jacobi's method [21] for the diagonalization of a symmetric matrix $A = (a_{ij}) \in \mathbb{R}^{n\times n}$ is a famous, successful, and easy to implement algorithm for the computation of eigenvalues of symmetric matrices. No wonder that this algorithm has been generalized or adapted to many other classes of matrices, see, among other references, [1, 3, 5, 9, 11, 12, 13, 15, 16, 29, 34]. In this paper, we will focus on a particular cyclic Jacobi-like algorithm for the computation of the Schur form of a complex matrix. The basic idea of the algorithm is a direct adaption of Jacobi's method to the nonsymmetric case which has been proposed 1955 by Greenstadt [13] and has later been taken up and modified by various authors [4, 10, 14, 19, 24, 32]. Given a matrix $M = (m_{ij}) \in \mathbb{C}^{n\times n}$, the algorithm selects in each step a pivot element m_{kl}, $k < l$ in the strict lower triangular part. Then a similarity transformation with a rotation $U = (u_{ij}) \in \mathbb{C}^{n\times n}$ is applied to M that annihilates the entry m_{kl} of M:

$$\begin{bmatrix} 1 & & & & & \\ & \overline{u}_{kk} & & & \overline{u}_{lk} & \\ & & 1 & & & \\ & & & 1 & & \\ & \overline{u}_{kl} & & & \overline{u}_{ll} & \\ & & & & & 1 \end{bmatrix} \begin{bmatrix} * & * & * & * & * & * \\ \cdot & * & * & * & * & * \\ \cdot & \cdot & * & * & * & * \\ \cdot & \cdot & \cdot & * & * & * \\ \cdot & m_{kl} & \cdot & \cdot & * & * \\ \cdot & \cdot & \cdot & \cdot & \cdot & * \end{bmatrix} \begin{bmatrix} 1 & & & & & \\ & u_{kk} & & & u_{kl} & \\ & & 1 & & & \\ & & & 1 & & \\ & u_{lk} & & & u_{ll} & \\ & & & & & 1 \end{bmatrix} = \begin{bmatrix} * & * & * & * & * & * \\ \cdot & * & * & * & * & * \\ \cdot & \cdot & * & * & * & * \\ \cdot & \cdot & \cdot & * & * & * \\ \cdot & 0 & \cdot & \cdot & * & * \\ \cdot & \cdot & \cdot & \cdot & \cdot & * \end{bmatrix}$$

Here, U coincides with the identity except for the elements $u_{kk} = u_{ll} = \cos x$, and $u_{kl} = -e^{-i\alpha} \sin x$, $u_{lk} = e^{i\alpha} \sin x$ for some $x, \alpha \in \mathbb{R}$.

Generically, there are two choices for the transformation matrix U and throughout this paper, we will always choose the transformation matrix that is closest to the identity. This corresponds to choosing always the rotation matrix with the smaller rotation angle, a fact that is crucial for the proof of asymptotic quadratic convergence

*Technische Universität Berlin, Institut für Mathematik, Sekretariat MA 4-5, 10623 Berlin, Germany, (mehl@math.tu-berlin.de). Supported by Deutsche Forschungsgemeinschaft through MATHEON, the DFG Research Center *Mathematics for key technologies* in Berlin.

of Jacobi's algorithm for symmetric matrices. Concerning global convergence, this strategy need not be the best. Actually, convergence can be accelerated by sorting the diagonal entries of the occurring 2×2 submatrices, a technique that sometimes requires the application of the rotation corresponding to the larger angle. In this paper, however, we focus on the asymptotic convergence behavior and, therefore, we restrict ourselves to the use of rotations corresponding to the smaller angle.

Cyclic version of Jacobi's algorithm use a fixed sequence of pivot elements to be annihilated in that order. If every element in the strict lower triangular part is annihilated at least once, then the sequence of corresponding Jacobi steps on the matrix is called a *sweep*, and it is repeated until convergence has been achieved.

In contrast to Jacobi's original algorithm, its generalization to general complex matrices has not yet become a well-known and widely-used algorithm, probably mainly for the following two reasons. First, neither global nor local convergence proofs of the method could be given so far, although convergence has been observed in numerical experiments. (In [19], Huang proved convergence of the method for the case $n = 3$, but the case $n > 3$ remains an open problem.) Secondly, the algorithm converges slowly and is expensive. A flop count reveals that three sweeps of the cyclic nonsymmetric Jacobi method are approximately as expensive as a full run of the QR algorithm as implemented in MATLAB. Moreover, the average number of sweeps needed for convergence for a 70×70 matrix is already as high as 30, making the method ten times more expensive then the QR algorithm in that case. Since the average number of sweeps needed for convergence even increases with increasing dimension of the matrix, the algorithm seemed to be out of competition.

However, in recent years there has been renewed interest in nonsymmetric Jacobi methods, because they can easily be adapted to the solution of structured eigenvalue problems, e.g., of Hamiltonian eigenvalue problems [1], for generalized Hermitian eigenvalue problems [27], for palindromic eigenvalue problems [18, 25], and for doubly structured eigenvalue problems [11]. For those eigenvalue problems, a satisfactory generalization of the QR algorithm is not available due to the lack of a corresponding reduction to a structured version of the Hessenberg form in finitely many steps. (This phenomenon is known as "Van Loan's curse" [6]). Thus, the competition for other algorithms is open again. In fact, a variant of the nonsymmetric Jacobi method designed for the solution of the generalized palindromic eigenvalue problem (i.e., the eigenvalue problem $\lambda Ax = A^T x$) has been successfully used in [25] as an ingredient for a structure-preserving eigensolver, where it was applied to the solution of small (i.e., of size $\mathcal{O}(10)$) eigenvalue problems with eigenvalues close to the unit circle.

On the other hand, the nonsymmetric Jacobi method converges fast for matrices that are already close to triangular form, and thus, it has the potential to become a useful tool for the solution of parameter-depending eigenvalue problems. Indeed, assume that $A(\omega)$ is a matrix-valued function that depends continuously on the parameter ω. Once the eigenvalue problem has solved for a specific value of ω, say ω_0, then the transformation that reduces $A(\omega_0)$ to Schur form will transform matrices $A(\omega)$ to a form that is close to being triangular whenever ω is sufficiently close to ω_0. It may then be useful to apply a nonsymmetric Jacobi method to $A(\omega)$ to obtain the Schur form within one or two sweeps. Finally, it was shown in [7] that Jacobi's algorithm for symmetric matrices is more accurate than the QR algorithm if the right stopping criterion is used. Extending this theory to nonsymmetric Jacobi methods may produce a highly accurate algorithm. In this paper, however, we restrict ourselves to the investigation of the asymptotic convergence behavior of the method.

The remainder of the paper is organized as follows. In the following section, we will explain why the convergence theory for nonsymmetric Jacobi algorithms is challenging and different from the theory for the symmetric case. In Section 3, we prove asymptotic quadratic convergence of the cyclic nonsymmetric Jacobi algorithm if so-called northeast directed sweeps are used. In Section 4, we investigate generalizations of the algorithm to the solution of the Hamiltonian eigenvalue problem. In particular, we explain why the Jacobi-like algorithm proposed in [1] does not show asymptotic quadratic convergence and we show how convergence can be accelerated. Finally, we illustrate the theoretical results by the results of numerical experiments in Section 5.

2. Why convergence of nonsymmetric Jacobi algorithms is not obvious. It is well known that Jacobi's classical algorithm as well as many cyclic versions are asymptotically quadratically convergent, see, e.g., [16, 17, 31, 35]. The same is also known for several generalizations; see [20] for a general proof of local quadratic convergence of Jacobi-type methods. However, these results are usually based on the minimization of a particular smooth function in each Jacobi step. For the standard eigenvalue problem with a Hermitian matrix $M = (m_{ij}) \in \mathbb{C}^{n\times n}$ this smooth function is the quantity

$$\operatorname{off}(M) := \sqrt{\sum_{i>j} |m_{ij}|^2} \tag{2.1}$$

that is sometimes called *off-norm*. In contrast to the Hermitian case, the quantity $\operatorname{off}(M)$ need not decrease in a single step of the nonsymmetric Jacobi algorithm. This effect can be explained heuristically with the help of the following sketch:

$$\begin{bmatrix} * & * & * & * & * & * \\ \cdot & \circ & * & * & \circ & * \\ \cdot & \diamond & * & * & \bullet & * \\ \cdot & \cdot & \cdot & * & * & * \\ \cdot & \circ & \cdot & \cdot & \circ & * \\ \cdot & \cdot & \cdot & \cdot & \cdot & * \end{bmatrix}$$

If the pivot element is chosen such that, currently, the 2×2 subproblem indicated by $\circ$ is under investigation, then a very large entry in, e.g., the position marked with $\bullet$ may lead to a temporary increase in $\operatorname{off}(M)$, because the element in the $\diamond$-position will be linearly combined with the element in the $\bullet$-position. It is this effect which makes the convergence analysis of nonsymmetric Jacobi methods so delicate. Indeed, the general results of [20] cannot be applied here, because $\operatorname{off}(M)$ is not minimized in each step.

At this stage, the reader might stop and ask the question if it would not be advisable to modify the algorithm in such a way that $\operatorname{off}(M)$ decreases monotonically. Indeed, such generalizations have already been considered. For example, Stewart [32] proposed to only use pivot elements from the first subdiagonal. Indeed, this avoid the effect explained in the previous paragraph and it was shown that $\operatorname{off}(M)$ then decreases monotonically. But unfortunately, it turned out that the Jacobi algorithm obtained in this way is characterized by extreme slow convergence: it appears to be almost stagnant. On the other hand, one may also consider variants of nonsymmetric Jacobi algorithm that again allow pivot elements from the whole strict lower triangular part of the matrix, but that minimize $\operatorname{off}(M)$ in each step rather than annihilating the pivot element. This, however, would require the solution of a minimization problem in each step and one would have to take into account "global information", i.e., the knowledge

of all elements in the strict lower triangular part of the matrix would be necessary. In contrast, the transformation annihilating the pivot element can be easily computed from considering the corresponding 2×2 problem only, thus, only taking into account "local information". Consequently, a single Jacobi step of the modified method would be much more expensive than a single Jacobi step of a cyclic nonsymmetric Jacobi method. Thus, although $\mathrm{off}(M)$ does not decrease monotonically in each step, cyclic methods seem to be the cheapest and most reliable variants of nonsymmetric Jacobi algorithms for the general complex eigenvalue problem.

But the non-monotone behavior of the quantity $\mathrm{off}(M)$ is not the only point in which the general case differs from the symmetric case. The asymptotic convergence behavior of a cyclic Jacobi method may be completely different for symmetric matrices on the one hand and general complex matrices on the other hand. As an example let us consider the cyclic Jacobi method using *top-to-bottom column-by-column sweeps* given by the sequence of indices

$$\big((2,1),(3,1),\ldots,(n,1),(3,2),\ldots,(n,2),\ldots,(n,n-1)\big) \tag{2.2}$$

versus the the one using *bottom-to-top column-by-column sweeps* given by

$$\big((n,1),(n-1,1),\ldots,(2,1),(n,2),\ldots,(3,2),\ldots,(n,n-1)\big). \tag{2.3}$$

Both methods appear to be asymptotically quadratically convergent in the symmetric case, while the nonsymmetric case shows quadratic convergence for the "bottom-to-top" variant, but linear convergence for the "top-to-bottom" variant. (See Section 5 for numerical experiments on this topic.) Again this effect can be explained heuristically with the help of a sketch:

$$\Downarrow \text{ top to bottom} \qquad \begin{bmatrix} \circ & * & * & \circ & * & * \\ \diamond & * & * & \bullet & * & * \\ \diamond & \cdot & * & \bullet & * & * \\ \circ & \cdot & \cdot & \circ & * & * \\ \cdot & \cdot & \cdot & \cdot & * & * \\ \cdot & \cdot & \cdot & \cdot & \cdot & * \end{bmatrix} \qquad \Uparrow \text{ bottom to top} \qquad \begin{bmatrix} \circ & * & * & \circ & * & * \\ \cdot & * & * & * & * & * \\ \cdot & \cdot & * & * & * & * \\ \circ & \cdot & \cdot & \circ & * & * \\ \diamond & \cdot & \cdot & \triangle & * & * \\ \diamond & \cdot & \cdot & \triangle & \cdot & * \end{bmatrix}$$

Assume that the matrix under consideration is already close to triangular form so that the algorithm may have reached the expected phase of quadratic convergence. If the pivot element is chosen in such a way that the corresponding 2×2 subproblem under consideration is the one displayed by the symbol $\circ$, then the elements marked by $\diamond$ are the ones that have already been annihilated once in the current sweep. If the top-to-bottom column-by-column sweep is used, then the current Jacobi step linearly combines those elements with possibly large elements from the strict upper triangular part from the matrix marked with the symbol $\bullet$. On the other hand, if the bottom-to-top column-by-column sweep is used, then the current Jacobi step linearly combines the $\diamond$-elements with elements from the strict lower triangular part, marked by the symbol $\triangle$, that are expected to be sufficiently small. Thus, the increase of modulus of elements that have already been annihilated once may be much higher when top-to-bottom column-by-column are used and that is exactly what can be observed in practice. In the symmetric case, however, this observation does not apply, because in this case also the elements in the strict upper triangular part are expected to be sufficiently small.

3. A proof of asymptotic quadratic convergence. Wilkinson's proof [35] of asymptotic quadratic convergence of the classical symmetric Jacobi method makes extensive use of the fact that the offnorm off(M) decreases monotonically over the steps of the algorithm. As pointed out in Section 2, this is no longer true for the nonsymmetric Jacobi method. Thus, we will have to investigate in detail the possible changes in the moduli of the entries in the strict lower triangular part of the matrix in a single Jacobi step. Let us introduce the following notation. Starting with the matrix $M \in \mathbb{C}^{n\times n}$, let us denote by $M_\nu = (m_{ij}^{(\nu)})$ the matrix that we have obtained after performing ν Jacobi steps. (In particular, we have $M_0 = M$.) Moreover, we denote

$$\varrho_\nu := \min_{i\neq j} |m_{i,i}^{(\nu)} - m_{j,j}^{(\nu)}|, \tag{3.1}$$

$$\eta_\nu := \max\Big\{ |m_{ij}^{(\nu)}| \;\Big|\; i,j = 1,\ldots,n \Big\}, \tag{3.2}$$

$$\varepsilon_\nu := \max\Big\{ |m_{ij}^{(\nu)}| \;\Big|\; i > j \Big\}, \tag{3.3}$$

i.e., ϱ_ν is the smallest distance between two diagonal elements of the matrix M_ν, η_ν is the modulus of the largest element in modulus of M_ν, and ε_ν is the modulus of the largest element in modulus of the strict lower triangular part of M_ν. In the following, let ν be fixed and assume we have

$$\varrho_\nu > 0 \quad \text{and} \quad 4\frac{\varepsilon_\nu \eta_\nu}{\varrho_\nu^2} < 1. \tag{3.4}$$

Suppose that the (k,l)-element of M_ν is the pivot element of the current $((\nu+1)$st) step of the algorithm. We then compute the unitary matrix

$$Q = \begin{bmatrix} \cos x & -e^{-i\alpha}\sin x \\ e^{i\alpha}\sin x & \cos x \end{bmatrix}, \quad x, \alpha \in \mathbb{R}$$

that satisfies

$$Q^* \begin{bmatrix} m_{ll}^{(\nu)} & m_{lk}^{(\nu)} \\ m_{kl}^{(\nu)} & m_{kk}^{(\nu)} \end{bmatrix} Q = \begin{bmatrix} m_{ll}^{(\nu+1)} & m_{lk}^{(\nu+1)} \\ 0 & m_{kk}^{(\nu+1)} \end{bmatrix}. \tag{3.5}$$

and that is closest to the identity matrix among all matrices satisfying (3.5). To obtain an estimate for the modulus of $\sin x$, we will use the following lemma that is a special case of Theorem V.2.1 in [33].

LEMMA 3.1. *Let $A \in \mathbb{C}^{2\times 2}$ such that*

$$A = \begin{bmatrix} a & \eta \\ \varepsilon & b \end{bmatrix}, \text{ where } 4\frac{|\varepsilon|\cdot|\eta|}{|a-b|^2} < 1.$$

Then there exists a unique eigenvector v of A satisfying

$$v = \begin{bmatrix} 1 \\ p \end{bmatrix} \quad \text{and} \quad |p| < 2\frac{\varepsilon}{|a-b|}.$$

Using this lemma and taking into account (3.4), it is clear that the parameter x in Q satisfies $|\sin x| < 2\varepsilon_\nu/\varrho_\nu$. If the transformation induced by Q is applied to M_ν then

it only acts on elements in the kth and lth rows and columns of M_ν. For the elements that have been altered in $M_{\nu+1}$, we obtain that

$$\begin{aligned} m_{lj}^{(\nu+1)} &= m_{lj}^{(\nu)} \cos x + m_{kj}^{(\nu)} e^{-i\alpha} \sin x, \\ m_{kj}^{(\nu+1)} &= m_{kj}^{(\nu)} \cos x - m_{lj}^{(\nu)} e^{i\alpha} \sin x, \\ m_{il}^{(\nu+1)} &= m_{il}^{(\nu)} \cos x + m_{ik}^{(\nu)} e^{i\alpha} \sin x, \\ m_{ik}^{(\nu+1)} &= m_{ik}^{(\nu)} \cos x - m_{il}^{(\nu)} e^{-i\alpha} \sin x, \end{aligned}$$

for $i, j = 1, \ldots, n$. Using these identities and Using $|\cos x| \leq 1$ and $|\sin x| < 2\varepsilon_\nu/\varrho_\nu$, we obtain that $|m_{ij}^{(\nu+1)}| \leq w_{ij}$, where w_{ij} is given in the following table:

(3.6)

w_{ij}	$j < l$	$j = l$	$l < j < k$	$j = k$	$k < j$
$i < l$	$\lvert m_{ij}^{(\nu)}\rvert$	$\eta_{\nu+1}$	$\lvert m_{ij}^{(\nu)}\rvert$	$\eta_{\nu+1}$	$\lvert m_{ij}^{(\nu)}\rvert$
$i = l$	$\lvert m_{ij}^{(\nu)}\rvert + 2\frac{\varepsilon_\nu^2}{\varrho_\nu}$	$\eta_{\nu+1}$	$\eta_{\nu+1}$	$\eta_{\nu+1}$	$\eta_{\nu+1}$
$l < i < k$	$\lvert m_{ij}^{(\nu)}\rvert$	$\lvert m_{ij}^{(\nu)}\rvert + 2\frac{\varepsilon_\nu \eta_\nu}{\varrho_\nu}$	$\lvert m_{ij}^{(\nu)}\rvert$	$\eta_{\nu+1}$	$\lvert m_{ij}^{(\nu)}\rvert$
$i = k$	$\lvert m_{ij}^{(\nu)}\rvert + 2\frac{\varepsilon_\nu^2}{\varrho_\nu}$	0	$\lvert m_{ij}^{(\nu)}\rvert + 2\frac{\varepsilon_\nu \eta_\nu}{\varrho_\nu}$	$\eta_{\nu+1}$	$\eta_{\nu+1}$
$k < i$	$\lvert m_{ij}^{(\nu)}\rvert$	$\lvert m_{ij}^{(\nu)}\rvert + 2\frac{\varepsilon_\nu^2}{\varrho_\nu}$	$\lvert m_{ij}^{(\nu)}\rvert$	$\lvert m_{ij}^{(\nu)}\rvert + 2\frac{\varepsilon_\nu^2}{\varrho_\nu}$	$\lvert m_{ij}^{(\nu)}\rvert$

In this table, we can see the effect that has been heuristically explained in Section 2. If we are in the stage that $\varepsilon_\nu \ll \eta_\nu$, i.e., our matrix under consideration is already close to triangular form, then the modulus of entries in the strict lower triangular part in positions (i, j) with $j < l$ or $k < i$ may have increased by $2\varepsilon_\nu^2/\varrho_\nu$ only, while the modulus of entries in positions (i, j) with $l \leq j$ and $i \leq k$ may have increased by $2\eta_\nu\varepsilon_\nu/\varrho_\nu \gg 2\varepsilon_\nu^2/\varrho_\nu$. Thus, the sweep should start from the lower left corner of the lower triangular part and then proceed to the "northeast" in order to guarantee that entries that have been eliminated once are increased by at most $2\varepsilon_\nu^2/\varrho_\nu$. This motivates the following definition.

DEFINITION 3.2. *Let $n \in \mathbb{N}$, $N = \frac{n(n-1)}{2}$, and $S = \big((i_1, j_1), (i_2, j_2) \ldots, (i_N, j_N)\big)$ be a finite sequence (i.e., an N-tuple) of pairs $(i_\nu, j_\nu) \in \{1, 2, \ldots, n\} \times \{1, 2, \ldots, n\}$, where $i_\nu > j_\nu$ for $\nu = 1, \ldots, N$. Then S is called an* northeast directed sweep sequence *if*

$$\nu < \mu \quad \Rightarrow \quad (i_\nu > i_\mu \text{ or } j_\nu < j_\mu)$$

for all $\nu, \mu \in \{1, \ldots, N\}$. A sweep of the nonsymmetric Jacobi algorithm that picks the pivot elements in the order given by a northeast directed sweep sequence is called a northeast directed sweep*.*

Particular example of northeast directed sweep sequences are given by the sequence (2.3) that induces a bottom-to-top column-by-column sweep or by the sequence

$$\big((n, 1), (n-1, 1), (n, 2), (n-2, 1), (n-1, 2), (n, 3), \ldots, (2, 1), (3, 2), \ldots, (n, n-1)\big).$$

We continue by analyzing how the values of ε_ν, η_ν, and ϱ_ν have changed after one Jacobi step (regardless what kind of sweep is used). Since $\varepsilon_\nu \leq \eta_\nu$, we obtain from the discussion above that

$$\varepsilon_{\nu+1} \leq \varepsilon_\nu \left(1 + 2\frac{\eta_\nu}{\varrho_\nu}\right). \tag{3.7}$$

We could also produce a bound for $\eta_{\nu+1}$, but for our purpose it is sufficient to note that η_μ is bounded by $\|M\|_F$ for any $\mu \in \mathbb{N} \cup \{0\}$. It remains to investigate how ϱ_ν has changed. Therefore, we have to investigate in particular the changes on the diagonal of M_ν. Clearly, we have

$$\begin{aligned} m_{ll}^{(\nu+1)} &= m_{ll}^{(\nu)}(1-\sin^2 x) + m_{kl}^{(\nu)} e^{-ia}\sin x\cos x + m_{lk}^{(\nu)} e^{ia}\sin x\cos x + m_{kk}^{(\nu)}\sin^2 x, \\ m_{kk}^{(\nu+1)} &= m_{ll}^{(\nu)}\sin^2 x - m_{kl}^{(\nu)} e^{-ia}\sin x\cos x - m_{lk}^{(\nu)} e^{ia}\sin x\cos x + m_{kk}^{(\nu)}(1-\sin^2)x. \end{aligned}$$

Thus, we obtain $m_{ll}^{(\nu+1)} = m_{ll}^{(\nu)} + \Delta_l$, $m_{kk}^{(\nu+1)} = m_{kk}^{(\nu)} + \Delta_k$, where

$$\begin{aligned} &|\Delta_l| = |\Delta_k| \\ &\le \left|m_{ll}^{(\nu)}\sin^2 x\right| + \left|m_{kl}^{(\nu)} e^{-ia}\sin x\cos x\right| + \left|m_{lk}^{(\nu)} e^{ia}\sin x\cos x\right| + \left|m_{kk}^{(\nu)}\sin^2 x\right| \\ &\le \eta_\nu\cdot 4\frac{\varepsilon_\nu^2}{\varrho_\nu^2} + \varepsilon_\nu\cdot 2\frac{\varepsilon_\nu}{\varrho_\nu} + \eta_\nu\cdot 2\frac{\varepsilon_\nu}{\varrho_\nu} + \eta_\nu\cdot 4\frac{\varepsilon_\nu^2}{\varrho_\nu^2} \\ &\le 2\left(\frac{\varepsilon_\nu^2}{\varrho_\nu} + 4\eta_\nu\frac{\varepsilon_\nu^2}{\varrho_\nu^2} + \eta_\nu\frac{\varepsilon_\nu}{\varrho_\nu}\right). \end{aligned}$$

It follows that $|m_{ii}^{(\nu+1)} - m_{jj}^{(\nu+1)}| \ge |m_{ii}^{(\nu)} - m_{jj}^{(\nu)}| - |\Delta_l| - |\Delta_k|$ for all $i, j = 1, \dots, n$, and thus

$$\varrho_{\nu+1} \ge \varrho_\nu - 4\left(\frac{\varepsilon_\nu^2}{\varrho_\nu} + 4\eta_\nu\frac{\varepsilon_\nu^2}{\varrho_\nu^2} + \eta_\nu\frac{\varepsilon_\nu}{\varrho_\nu}\right). \tag{3.8}$$

Using the above, we will now show that the cyclic nonsymmetric Jacobi method using northeast directed sweeps is quadratically convergent if the matrix under consideration is sufficiently close to triangular form.

THEOREM 3.3. *Let $M = (m_{ij}) \in \mathbb{C}^{n\times n}$, and let $M_\nu = (m_{ij}^{(\nu)})$ denote the matrix that is obtained from M after performing ν Jacobi steps of the cyclic nonsymmetric Jacobi method using northeast directed sweeps. Let δ_0 resp. δ_μ be the largest modulus of an element in the strict lower triangular part of $M = M_0$ resp. of the matrix that is obtained from M after having completed μ sweeps, i.e.,*

$$\delta_\mu := \max\left\{|m_{ij}^{(\mu N)}| \;\middle|\; i > j\right\}, \quad \mu \in \mathbb{N}\cup\{0\}. \tag{3.9}$$

Moreover, set $N := n(n-1)/2$ and

$$\eta := \|M\|_F, \quad \varrho := \frac{1}{2}\min_{i\ne j}|m_{ii} - m_{jj}|, \quad \delta := 2\delta_0\left(1 + 2\frac{\eta}{\varrho}\right)^N, \tag{3.10}$$

If $\varrho > 0$ and if δ_0 is sufficiently small such that

$$\frac{\delta\eta}{\varrho^2} < \frac{1}{4}, \qquad \frac{\delta^2}{\varrho} + 4\eta\frac{\delta^2}{\varrho^2} + \eta\frac{\delta}{\varrho} \le \frac{\varrho_0}{4N}, \qquad 2\frac{N\delta^2}{\varrho} \le \delta_0, \tag{3.11}$$

then for all $\mu \in \mathbb{N}\cup\{0\}$, we have that

$$\delta_{(\mu+1)N} \le \left(1 + 2\frac{\eta}{\varrho}\right)^{2N}\frac{2N}{\varrho}\delta_{\mu N}^2,$$

i.e., the cyclic nonsymmetric Jacobi method using northeast directed sweep converges quadratically over the number of sweeps.

Proof. Let η_ν, ε_ν, and ϱ_ν be defined as in (3.1)–(3.3). Then we have

$$\delta_\mu = \varepsilon_{\mu N} \quad \text{and} \quad \varrho = \frac{\varrho_0}{2}.$$

From (3.7) and (3.8) we obtain that ε_ν (and ϱ_ν, respectively) may increase (or decrease, respectively) in each Jacobi step. We first show by induction that this increase (decrease, respectively) remains under control, i.e., that for $\mu \in \mathbb{N} \cup \{0\}$ and $p = 0, \ldots, N$, we have that

$$\varepsilon_{\mu N} \leq \frac{\delta_0}{2^\mu}, \qquad \varrho_{\mu N} \geq \varrho_0 - \sum_{j=1}^{\mu} \frac{\varrho_0}{2^{j+1}} > \varrho, \quad \text{and} \tag{3.12}$$

$$\varepsilon_{\mu N+p} \leq \varepsilon_{\mu N} \left(1 + 2\frac{\eta}{\varrho}\right)^p, \qquad \varrho_{\mu N+p} \geq \varrho_{\mu N} - p\frac{\varrho_0}{2^{\mu+1}N}. \tag{3.13}$$

'$(\mu, p) = (0, 0)$': There is nothing to prove.

'$(\mu, p) \Rightarrow (\mu, p+1)$': Let $p \leq N$. By the induction hypothesis for (μ, p) and $(\mu, 0)$, we have that

$$\varepsilon_{\mu N+p} \leq \varepsilon_{\mu N} \left(1 + 2\frac{\eta}{\varrho}\right)^p \leq \frac{\delta_0}{2^\mu} \left(1 + 2\frac{\eta}{\varrho}\right)^p \leq \frac{\delta}{2^{\mu+1}} \tag{3.14}$$

using (3.10) and

$$\varrho_{\mu N+p} \geq \varrho_{\mu N} - p\frac{\varrho_0}{2^{\mu+1}N} \geq \varrho_0 - \sum_{j=1}^{\mu} \frac{\varrho_0}{2^{j+1}} - N\frac{\varrho_0}{2^{\mu+1}N} = \varrho_0 - \sum_{j=1}^{\mu+1} \frac{\varrho_0}{2^{j+1}} > \varrho. \tag{3.15}$$

Now assume $p < N$. Then we obtain using (3.7), (3.8), (3.14), and (3.15) and the induction hypothesis that

$$\begin{aligned}
\varepsilon_{\mu N+p+1} &\leq \varepsilon_{\mu N+p} \left(1 + 2\frac{\eta_{\mu N+p}}{\varrho_{\mu N+p}}\right) \leq \varepsilon_{\mu N+p} \left(1 + 2\frac{\eta}{\varrho}\right) \leq \varepsilon_{\mu N} \left(1 + 2\frac{\eta}{\varrho}\right)^{p+1}; \\
\varrho_{\mu N+p+1} &\geq \varrho_{\mu N+p} - 4\left(\frac{\varepsilon_{\mu N+p}^2}{\varrho_{\mu N+p}} + 4\eta_{\mu N+p}\frac{\varepsilon_{\mu N+p}^2}{\varrho_{\mu N+p}^2} + \eta_{\mu N+p}\frac{\varepsilon_{\mu N+p}}{\varrho_{\mu N+p}}\right) \\
&\geq \varrho_{\mu N} - p\frac{\varrho_0}{2^{\mu+1}N} - 4\left(\frac{\delta^2}{(2^{\mu+1})^2\varrho} + 4\eta\frac{\delta^2}{(2^{\mu+1})^2\varrho^2} + \eta\frac{\delta}{2^{\mu+1}\varrho}\right) \\
&\geq \varrho_{\mu N} - p\frac{\varrho_0}{2^{\mu+1}N} - \frac{4}{2^{\mu+1}}\left(\frac{\delta^2}{\varrho} + 4\eta\frac{\delta^2}{\varrho^2} + \eta\frac{\delta}{\varrho}\right) \\
&\geq \varrho_{\mu N} - (p+1)\frac{\varrho_0}{2^{\mu+1}N}. \qquad \Big(\text{by (3.11)}\Big)
\end{aligned}$$

'$(\mu, p) \Rightarrow (\mu+1, 0)$': For obtaining a bound for $\varepsilon_{(\mu+1)N}$, let us note that during the $(\mu+1)$st sweep each entry (i, j) in the strict lower triangular part of the current pencil is set to zero at one step. Afterwards, during the remainder of the sweep, it is affected $k < N$ times in the steps, say, $\mu N + \ell_1, \ldots, \mu N + \ell_k$, where k and $\ell_1, \ldots, \ell_k$ depend on i, j. Since a northeast directed sweep is used, we obtain from Table (3.6) that the

modulus of the (i,j)-element of the matrix $M_{((\mu+1)N)}$ obtained after completing the $(\mu+1)$st sweep is bounded by

$$|m_{ij}^{((\mu+1)N)}| \le 2\frac{\varepsilon_{\mu N+\ell_1}^2}{\varrho_{\mu N+\ell_1}} + \cdots + 2\frac{\varepsilon_{\mu N+\ell_k}^2}{\varrho_{\mu N+\ell_k}} \le \sum_{p=1}^{N} 2\frac{\varepsilon_{\mu N+p}^2}{\varrho_{\mu N+p}} \le N\left(\frac{\delta}{2^{\mu+1}}\right)^2 \frac{2}{\varrho}, \tag{3.16}$$

because $k \le N$ and $\varepsilon_{\mu N+p} \le \delta/2^{\mu+1}$ and $\varrho_{\mu N+p} \ge \varrho$ for $p = 0,\dots,N$. Since the right hand side of (3.16) is independent of the indices i and j, we then obtain

$$\varepsilon_{(\mu+1)N} \le N\left(\frac{\delta}{2^{\mu+1}}\right)^2 \frac{2}{\varrho} \le \frac{\delta_0}{(2^{\mu+1})^2} \le \frac{\delta_0}{2^{\mu+2}}. \tag{3.17}$$

This concludes the proof of (3.12) and (3.13). Now observe that (3.13) implies that

$$\varepsilon_{\mu N+p} \le \varepsilon_{\mu N}\left(1+2\frac{\eta}{\varrho}\right)^N = \delta_\mu\left(1+2\frac{\eta}{\varrho}\right)^N$$

for $p = 0,\dots,N$. Using this inequality instead of (3.14), we obtain analogously to (3.17) that

$$\delta_{\mu+1} = \varepsilon_{(\mu+1)N} \le \sum_{p=1}^{N} 2\frac{\varepsilon_{\mu N+p}^2}{\varrho_{\mu N+p}} \le N\delta_\mu^2\left(1+2\frac{\eta}{\varrho}\right)^{2N}\frac{2}{\varrho}$$

which concludes the proof. □

Theorem 3.3 guarantees asymptotic quadratic convergence in terms of the largest modulus ε_ν of subdiagonal entries. Since the so-called offnorm

$$\operatorname{off}(M_\nu) := \sqrt{\sum_{i>j} |m_{ij}^{(\nu)}|^2}$$

is bounded by $\varepsilon_\nu \le \operatorname{off}(M_\nu) \le \sqrt{N}\varepsilon_\nu$, we also obtain asymptotic quadratic convergence in terms of the offnorm.

Remark 3.4. Note that in general the assumption $\varrho > 0$ in Theorem 3.3 cannot be weakened in order to guarantee convergence. Consider, for example, the matrix

$$M = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ \varepsilon & 0 & 1 \end{bmatrix},$$

where $\varepsilon > 0$ is arbitrarily small. Then the sequence of matrices generated by the nonsymmetric Jacobi method becomes periodic as long as exact arithmetic is performed:

$$\begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ \varepsilon & 0 & 1 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 0 & \varepsilon \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & \varepsilon \\ 1 & 0 & 1 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 0 & 1 \\ \varepsilon & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$
$$\rightsquigarrow \begin{bmatrix} 1 & \varepsilon & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & \varepsilon & 1 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ \varepsilon & 0 & 1 \end{bmatrix}$$

However, if finite precision arithmetic is used, then roundoff errors break the periodicity and the algorithm starts to converge. For example, with $\varepsilon = 1/100$ our MATLAB implementation of the algorithm needed eight sweeps for convergence.

4. Hamiltonian Jacobi methods. As pointed out in the introduction, the nonsymmetric Jacobi method may not be competitive in comparison to the highly efficient QR algorithm. However, this changes if one is interested in structure preserving algorithms for the solution of structured eigenvalue problems. As an example, we consider the *Hamiltonian eigenvalue problem*. A matrix $H \in \mathbb{C}^{2n\times 2n}$ is called *Hamiltonian* if

$$H^T J + JH = 0, \quad \text{where } J = J_{2n} = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$$

or, equivalently, if

$$H = (h_{ij}) = \begin{bmatrix} A & C \\ D & -A^T \end{bmatrix}, \quad \text{where } A, C, D \in \mathbb{C}^{n\times n},\ C = C^T,\ D = D^T. \tag{4.1}$$

In some sources, also matrices $H \in \mathbb{C}^{2n\times 2n}$ satisfying $H^*J + JH = 0$ are called Hamiltonian. For the sake of clear distinction, we refer to such matrices as *complex conjugate Hamiltonian matrices*, while we call matrices satisfying (4.1) *complex transpose Hamiltonian matrices*. The real and complex conjugate Hamiltonian eigenvalue problems have been extensively studied in the literature, see, e.g., [22, 28] an the references therein. Also, the complex transpose Hamiltonian eigenvalue problem has attracted some attention in recent years due to its relation to the so-called palindromic eigenvalue problem that arises in an application in the vibration analysis of rail tracks, see [18, 26, 25].

The solution of the Hamiltonian eigenvalue problem is in general tackled by computing condensed forms under unitary symplectic similarity transformations, i.e., transformations of the form $H \mapsto U^{-1}HU$, where $U \in \mathbb{F}^{2n\times 2n}$ is unitary and *symplectic*, i.e., it satisfies $U^\star JU = J$, where $\star = T$ in the real Hamiltonian and complex transpose Hamiltonian case and $\star = *$ in the complex conjugate Hamiltonian case. It is easy to check that unitary symplectic similarity transformations preserve the Hamiltonian structure, i.e., if H is Hamiltonian then so is $U^{-1}HU$. The condensed form one is aiming at is the the *Hamiltonian Schur form*. A Hamiltonian matrix H is said to be in Hamiltonian Schur form if

$$H = \begin{bmatrix} R & B \\ 0 & -R^\star \end{bmatrix}, \tag{4.2}$$

where $\star = T$ or $\star = *$, respectively. This form can always be achieved for complex transpose Hamiltonian matrices. For complex conjugate Hamiltonian matrices, it can be achieved if there are no eigenvalues on the imaginary axis [23].

What makes the Hamiltonian eigenvalue problem challenging is the fact that although a Hamiltonian QR algorithm, i.e., a structure preserving version of the QR algorithm has been developed [2], a preliminary structure-preserving reduction to a Hessenberg-like form is missing – a phenomenon that is known in the literature as "Van Loan's curse" [6, 30]. Thus, the Hamiltonian QR algorithm is in general not efficient, because it is of complexity $\mathcal{O}(n^4)$, and so, the competition is open for other kinds of structure-preserving algorithms.

In [3] and [1] Jacobi-like algorithms for Hamiltonian matrices have been proposed. Both algorithms are based on the solution of 4×4 subproblems in each Jacobi step. Byers [3] follows the idea of Stewart [32] of using only a selected set of pivot elements which results in an extreme slow convergence behavior. Therefore, we omit a detailed discussion of the first algorithm and focus on the algorithm proposed in [1] as well

as on a direct generalization of the nonsymmetric Jacobi method to Hamiltonian matrices which results in a Hamiltonian Jacobi method that is based on the solution of 2×2 subproblems in each step.

We restrict our attention to complex transpose Hamiltonian matrices. (A generalization of the discussion to the case of complex conjugate Hamiltonian matrices is possible, but more involved, because one has to take into account the fact that some of the subproblems may not be solvable. This is due to the fact that the reduction to Hamiltonian Schur form is not always possible in the complex conjugate Hamiltonian case if there are eigenvalues on the imaginary axis.) Our transformation matrices are supposed to be unitary and symplectic, so they must have the form

$$U = \begin{bmatrix} U_1 & -\overline{U}_2 \\ U_2 & \overline{U}_1 \end{bmatrix}, \quad U_1, U_2 \in \mathbb{C}^{n \times n}$$

where $U_1^* U_1 + U_2^* U_2 = I_n$ and $U_2^T U_1 - U_1^T U_2 = 0$.

The reason why 4×4 subproblems instead of 2×2 problems are considered in the algorithm proposed in [1] becomes obvious from the following sketch.

$$\left[\begin{array}{cccc|cccc} * & * & * & * & * & * & * & * \\ \cdot & \bullet & \bullet & * & * & \bullet & \bullet & * \\ \cdot & \diamond & \bullet & * & * & \bullet & \bullet & * \\ \cdot & \cdot & \cdot & * & * & * & * & * \\ \hline \cdot & \cdot & \cdot & \cdot & * & \cdot & \cdot & \cdot \\ \cdot & \circ & \circ & \cdot & * & \bullet & \circ & \cdot \\ \cdot & \circ & \circ & \cdot & * & \bullet & \bullet & \cdot \\ \cdot & \cdot & \cdot & \cdot & * & * & * & * \end{array}\right]$$

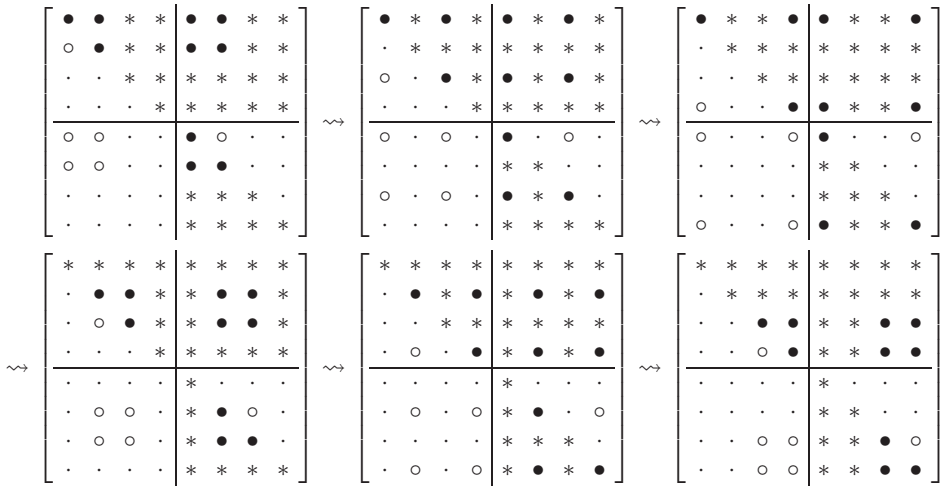
If the element displayed by $\diamond$ has been chosen as pivot element, then the 4×4 submatrix displayed by the symbols $\circ$ and $\bullet$ is the smallest Hamiltonian submatrix that contains the pivot element. (Here, $\circ$ refers to elements in the subproblem that are annihilated while $\bullet$ stands for entries that may remain large in norm.) For details concerning the solution of the 4×4 subproblem, we refer the reader to [1]. (The discussion there involves complex conjugate Hamiltonian matrices only, but the generalization to the complex transpose Hamiltonian case is straightforward.) Among all possible transformation matrices, we once again choose the one that is closest to the identity in order to enable asymptotic quadratic convergence.

A sweep of the Hamiltonian Jacobi algorithm as proposed in [1] is then given by the following sequence of indices, where the quadrupel of indices (i, j, k, l) refers to the 4×4 subproblem consisting of the rows and columns i, j, k, l:

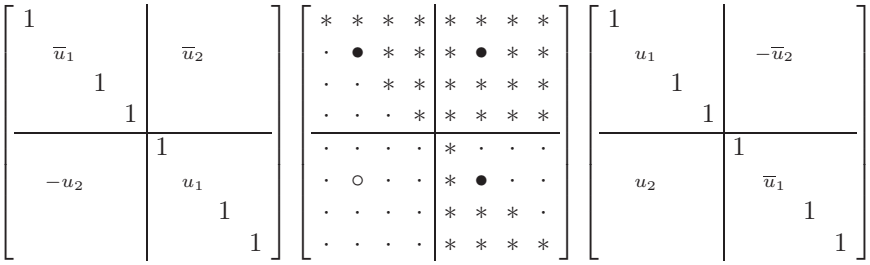
$$\begin{aligned} &(1, 2, n+1, n+2), (1, 3, n+1, n+3), \ldots, (1, n, n+1, 2n) \\ &(2, 3, n+2, n+3), (2, 4, n+2, n+4), \ldots, (n-1, n, 2n-1, 2n) \end{aligned} \tag{4.3}$$

Indeed, one easily checks that each pivot element is eliminated at least once during the sweep. On the other hand, the elements in the $(j, n+j)$ positions are annihilated $n-1$ times in each sweep, a fact that cannot be avoided when Hamiltonian 4×4 subproblems are considered. In the following, we will refer to the cyclic Hamiltonian Jacobi algorithm as proposed in [1] as *Hamiltonian* 4*-Jacobi* when sweeps based on the sequence of indices (4.3) are used. As an example, we display such a sweep for an

8×8 Hamiltonian matrix in the sketch below.



Next we consider a Jacobi-like algorithm for Hamiltonian matrices that is based on the solution of 2×2 subproblems. (This algorithm is related to the algorithm JIGH2 in [27] that was designed for the solution of the generalized Hermitian eigenvalue problem.) In this algorithm, we have to distinguish between pivot elements that are on the diagonal of C in (4.1) and those that are not. Indeed, if we select a pivot element $h_{n+k,k}$ from the diagonal of C, then there is a corresponding Hamiltonian 2×2 subproblem that contains this element as indicated in the following sketch.



This 2×2 subproblem can be solved as in the nonsymmetric Jacobi method for general complex matrices by choosing $x, \alpha \in \mathbb{R}$ such that

$$Q = \begin{bmatrix} u_1 & -\overline{u}_2 \\ u_2 & \overline{u}_1 \end{bmatrix} = \begin{bmatrix} \cos x & -e^{-i\alpha} \sin x \\ e^{i\alpha} \sin x & \cos x \end{bmatrix}$$

annihilates the pivot element $h_{n+k,k}$ and is the matrix that is closest to the identity among all matrices that do so. If the matrix U is then obtained from the $2n \times 2n$ identity matrix by substituting $u_{kk} = u_{n+k,n+k} = u_1$, and $u_{k,n+k} = -\overline{u}_2$, $u_{n+k,k} = u_2$, we find that U is not only unitary, but also symplectic and thus, the transformation with U will preserve the Hamiltonian structure of H.

The situation is different when the pivot element is not on the diagonal of C as then there is no Hamiltonian 2×2 subproblem that contains the given pivot element. To be specific, let $h_{k\ell}$ be a pivot element satisfying $\ell < k \leq n$ or $n + \ell < k \leq 2n$, i.e., the pivot element is in the strict lower triangular part of either the block A or the

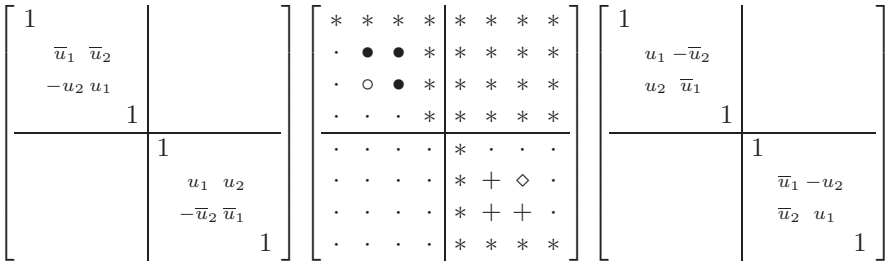
block C in (4.1). As in the previous we then compute the matrix

$$Q = \begin{bmatrix} u_1 & -\overline{u}_2 \\ u_2 & \overline{u}_1 \end{bmatrix} = \begin{bmatrix} \cos x & -e^{-i\alpha}\sin x \\ e^{i\alpha}\sin x & \cos x \end{bmatrix} \tag{4.4}$$

that triangularizes the 2×2 submatrix $\hat{H}$ consisting of the elements $h_{\ell\ell}$, $h_{\ell k}$, $h_{k\ell}$, and h_{kk}, and that is closest to the identity among all matrices of the form (4.4) that do so. Note that Q is not only unitary, but also symplectic. However, when embedding Q into an $2n\times 2n$ matrix U by setting U to be the identity matrix except for the elements $u_{\ell\ell} = u_1$, $u_{\ell k} = -\overline{u}_2$, $u_{k\ell} = u_2$, $u_{kk} = \overline{u}_1$, then the resulting matrix U is unitary, but not symplectic, so we have to set $u_{n+\ell,n+\ell} = \overline{u}_1$, $u_{n+\ell,p} = -u_2$, $u_{p,n+\ell} = \overline{u}_2$, and $u_{p,p} = u_1$, where $p = n + k$ if $k \le n$ and $p = k - n$ if $n + \ell < k \le 2n$ to make it unitary *and* symplectic. Let us investigate this in detail. Denote $A = (a_{ij})$, $C = (c_{ij})$, $D = (d_{ij})$, where the submatrices A, C, D are given as in (4.1), and consider first the case $k \le n$, i.e., we have

$$\hat{H} = \begin{bmatrix} a_{\ell\ell} & a_{\ell k} \\ a_{k\ell} & a_{kk} \end{bmatrix}$$

and thus, the pivot element is from the strict lower triangular part of A. The situation is depicted in the following sketch, where the pivot element is displayed with the symbol $\circ$ and the subproblem $\hat{H}$ is marked with the symbols $\circ$ and $\bullet$.



Due to the special structure of U, we find that a second 2×2 subproblem given by

$$\widetilde{H} = \begin{bmatrix} h_{n+\ell,n+\ell} & h_{n+\ell,n+k} \\ h_{n+k,n+\ell} & h_{n+k,n+k} \end{bmatrix} = \begin{bmatrix} -a_{\ell\ell} & -a_{k\ell} \\ -a_{\ell k} & -a_{kk} \end{bmatrix} = -\hat{H}^T$$

is solved as well. This subproblem is depicted in the sketch above by the symbols $+$ and $\diamond$, where the symbol $\diamond$ display the element that will be annihilated by the transformation with U. Indeed, $\widetilde{H}$ will be transformed as

$$\begin{bmatrix} u_1 & u_2 \\ -\overline{u}_2 & \overline{u}_1 \end{bmatrix} \widetilde{H} \begin{bmatrix} \overline{u}_1 & -u_2 \\ \overline{u}_2 & u_1 \end{bmatrix} = -Q^T \hat{H}^T \overline{Q} = -(Q^* \hat{H} Q)^T = \begin{bmatrix} * & 0 \\ * & * \end{bmatrix}.$$

We have a similar situation for the case $n + \ell < k \le 2n$, i.e., when the pivot element is from the strict lower triangular part of C. Again, besides

$$\hat{H} = \begin{bmatrix} a_{\ell\ell} & c_{\ell k} \\ d_{k\ell} & -a_{kk} \end{bmatrix},$$

a second subproblem $\widetilde{H}$ is solved when the transformation with U is applied. Here, we have

$$\widetilde{H} = \begin{bmatrix} h_{k-n,k-n} & h_{k-n,n+\ell} \\ h_{n+\ell,k-n} & h_{n+\ell,n+\ell} \end{bmatrix} = \begin{bmatrix} a_{kk} & c_{\ell k} \\ d_{k\ell} & -a_{\ell\ell} \end{bmatrix} = -J_2^T \hat{H}^T J_2, \quad J_2 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

since $c_{k\ell} = c_{\ell k}$ and $d_{k\ell} = d_{\ell k}$. Then, $\widetilde{H}$ will be transformed as

$$Q^*\widetilde{H}Q = (J_2^T Q^T J_2)(-J_2^T \hat{H}^T J_2)(J_2^T \overline{Q} J_2) = -J_2^T (Q^* \hat{H} Q)^T J_2 = \begin{bmatrix} * & * \\ 0 & * \end{bmatrix},$$

where we used that Q is both unitary and symplectic, i.e., $Q = J_2^T Q^{-T} J_2 = J_2^T \overline{Q} J_2$. The situation is depicted in the sketch below, where $\hat{H}$ is displayed by the symbols $\circ$ and $\bullet$ and $\widetilde{H}$ is displayed by the symbols $\diamond$ and $+$.

$$\left[\begin{array}{cccc|cccc}
1 & & & & & & & \\
 & \overline{u}_1 & & & & & \overline{u}_2 & \\
 & & \overline{u}_1 & & & \overline{u}_2 & & \\
 & & & 1 & & & & \\
\hline
 & & & & 1 & & & \\
 & & -u_2 & & & u_1 & & \\
 & -u_2 & & & & & u_1 & \\
 & & & & & & & 1
\end{array}\right]
\left[\begin{array}{cccc|cccc}
* & * & * & * & * & * & * & * \\
\cdot & \bullet & * & * & * & * & \bullet & * \\
\cdot & \cdot & + & * & * & + & * & * \\
\cdot & \cdot & \cdot & * & * & * & * & * \\
\hline
\cdot & \cdot & \cdot & \cdot & * & \cdot & \cdot & \cdot \\
\cdot & \cdot & \diamond & \cdot & * & + & \cdot & \cdot \\
\cdot & \circ & \cdot & \cdot & * & * & \bullet & \cdot \\
\cdot & \cdot & \cdot & \cdot & * & * & * & *
\end{array}\right]
\left[\begin{array}{cccc|cccc}
1 & & & & & & & \\
 & u_1 & & & & & -\overline{u}_2 & \\
 & & u_1 & & & -\overline{u}_2 & & \\
 & & & 1 & & & & \\
\hline
 & & & & 1 & & & \\
 & & u_2 & & & \overline{u}_1 & & \\
 & u_2 & & & & & \overline{u}_1 & \\
 & & & & & & & 1
\end{array}\right]$$

(Again, $\circ$ and $\diamond$ stand for the elements that are annihilated by the transformation with U.)

It becomes clear from this discussion that it is sufficient to annihilate all elements in the strict lower triangular parts of A and C during one sweep. But how should a sweep be organized? The answer follows by noting that the Hamiltonian matrix H as in (4.2) is in Hamiltonian Schur form if and only if the matrix

$$\mathcal{F}H\mathcal{F} = \begin{bmatrix} R & BF_n \\ 0 & -F_n R^T F_n \end{bmatrix}, \quad \mathcal{F} = \begin{bmatrix} I_n & 0 \\ 0 & F_n \end{bmatrix}, \quad F_n = \begin{bmatrix} 0 & & 1 \\ & \iddots & \\ 1 & & 0 \end{bmatrix} \tag{4.5}$$

is in Schur form. Here, F_n denotes the *flip matrix*, i.e., the matrix with ones on the southeast northwest diagonal and zeros elsewhere. (It is straightforward to check that a matrix L is lower triangular if and only if $F_n L F_n$ is upper triangular.) If we then carry out a *Hamiltonian sweep* given by the sequence of indices

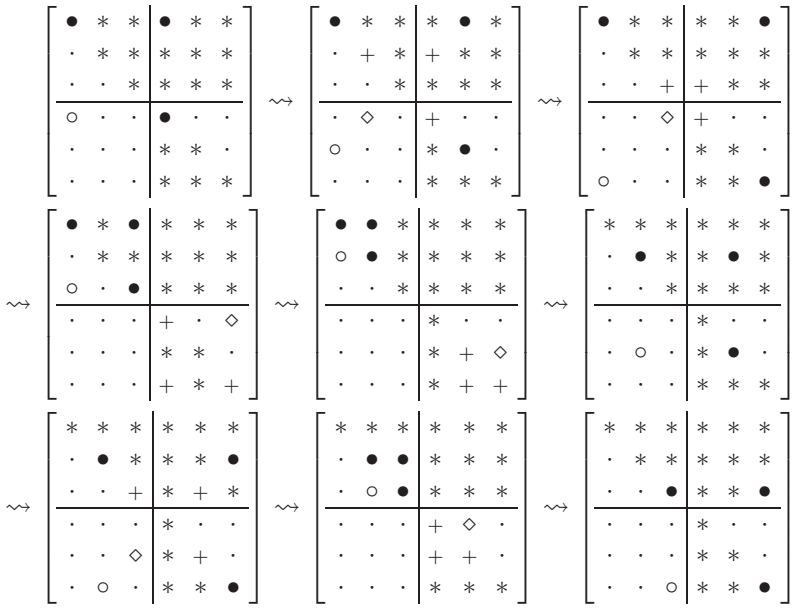
$$((n+1,1),(n+2,1),\ldots,(2n,1),(n,1),(n-1,1),\ldots,(2,1),(n+2,2),(n+3,2),\ldots,(2n,n)),$$

then given the fact that most of the times two elements are annihilated during a single Jacobi step, we find that the elements are annihilated in the order

$$\begin{aligned}
&((n+1,1),(n+2,1),(n+1,2),(n+3,1),(n+1,3),\ldots,(2n,1),(n+1,n)\\
&(n,1),(n+1,2n),(n-1,1),(n+1,2n-1),\ldots,(2,1),(n+1,n+2),\\
&(n+2,2),(n+3,2),(n+2,3),\ldots,(2n,n)).
\end{aligned}$$

It is then straightforward to check that this corresponds to a northeast directed sweep on the matrix $\mathcal{F}H\mathcal{F}$, and thus, the Hamiltonian Jacobi algorithm for H using a Hamiltonian sweep corresponds to the nonsymmetric Jacobi algorithm for $\mathcal{F}H\mathcal{F}$ using a special northeast directed sweep. Therefore, by Theorem 3.3 we expect asymptotic quadratic convergence for the Hamiltonian Jacobi algorithm when Hamiltonian sweeps are used and this is exactly what can be observed in numerical experiments. We depict

one Hamiltonian sweep for the case $n = 3$.



The Hamiltonian Jacobi algorithm based on the solution of 2×2 subproblems will be referred to as *Hamiltonian* 2*-Jacobi* if Hamiltonian sweeps are used.

Let us return to the Hamiltonian 4-Jacobi. Surprisingly, only linear asymptotic convergence of the method can be observed as we will see in Section 5. This behavior can be explained by looking at the order in which the pivot elements are annihilated. One easily finds that, for example, the pivot element in the $(2,1)$-position is annihilated in the step preceding the annihilation of the element in the $(3,1)$-position. Thus, the sweep given by the sequence of indices (4.3) *does not correspond to a northeast directed sweep* on the matrix $\mathcal{F}H\mathcal{F}$. In order to ensure this, we have to modify the sequence of indices as

$$
\begin{aligned}
&(1,2,n{+}1,n{+}2),(1,3,n{+}1,n{+}3),\dots,(1,n{-}1,n{+}1,2n{-}1),(1,n,n{+}1,2n),\\
&(1,n{-}1,n{+}1,2n{-}1),\dots,(1,3,n{+}1,n{+}3),(1,2,n{+}1,n{+}2),\\
&(2,3,n{+}2,n{+}3),\dots,(2,n,n{+}2,2n),\dots,(2,3,n{+}2,n{+}3),\dots,(n{-}1,n,2n{-}1,2n)
\end{aligned}
\tag{4.6}
$$

Here, the majority of pivot elements is annihilated at least twice during a sweep, but the order in which the pivot elements are annihilated the last time during a sweep is now

$$((n{+}1,1),(n{+}2,1),\dots,(2n,1),(n,1),(n{-}1,1),\dots,(2,1),(n{+}2,2),(n{+}3,2),\dots,(2n,n)),$$

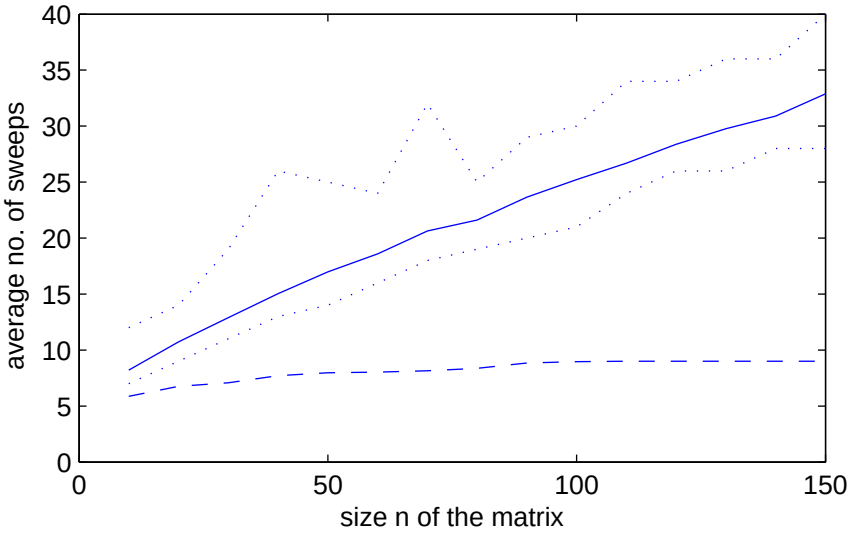
which corresponds to a northeast directed sweep on the matrix $\mathcal{F}H\mathcal{F}$. We refer to the Hamiltonian Jacobi method based on the solution of 4×4 subproblems using sweeps given by the sequence of indices (4.6) as *improved Hamiltonian* 4*-Jacobi*. By the discussion above, we now expect asymptotic quadratic convergence of the method and this is what can be observed in experiments, see Section 5.

Concerning the computational effort, one can roughly say that one sweep of the improved Hamiltonian 4-Jacobi is approximately twice as expensive as the Hamiltonian 4-Jacobi. On the other hand, one sweep of the Hamiltonian 2-Jacobi needs approximately 80% of the number of flops (floating point operations) of one sweep of the Hamiltonian 4-Jacobi (and thus about 40% of the number of flops of one sweep of the improved Hamiltonian 4-Jacobi).

5. Numerical experiments. We implemented the cyclic nonsymmetric Jacobi algorithm in MATLAB Version 7 and run it on a PC with a Pentium III processor (800 MHz). As a stopping criterion we used $\text{maxoff}(A) := \max_{i>j} |a_{ij}| < 10\texttt{eps}$.

First, the nonsymmetric Jacobi method was run for 100 random complex matrices (generated with the MATLAB command `randn`) of size $n \times n$, where $n = 10, 20, \ldots, 150$, after normalization to spectral norm equal to one, see Figure 5.1.

FIG. 5.1. *Test for* 100 *random matrices of different sizes.*



The solid line in Figure 5.1 displays the average number of sweeps needed for convergence for random complex matrices while the dashed line displays the corresponding number for Hermitian matrices. Thus, the method runs much faster for Hermitian matrices than for general complex matrices, an effect that had already been observed by Eberlein [10]. The dotted lines display the maximal and minimal number of sweeps that were needed for convergence for random complex matrices. E.g., for $n = 100$ the algorithm needed between 21 and 30 sweeps. The distribution of the number of sweeps for the tests on 100×100 matrices is shown in Figure 5.2.

FIG. 5.2. *Distribution of number of sweeps needed for convergence.*

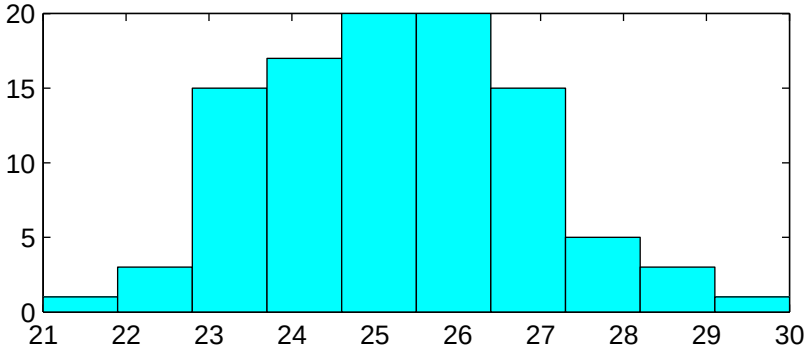
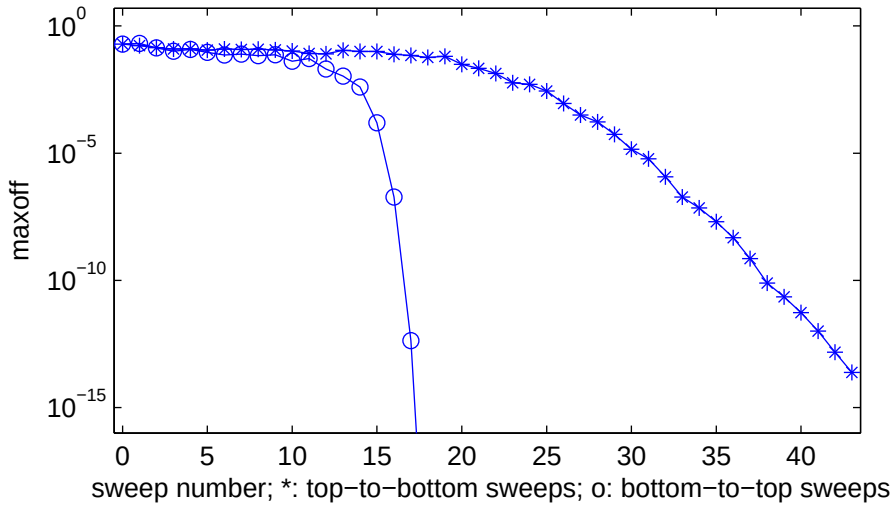


Figure 5.3 displays the typical convergence behavior of the nonsymmetric Jacobi algorithm for a random complex matrix of size 50×50 using top-to-bottom sweeps versus using bottom-to-top sweeps.

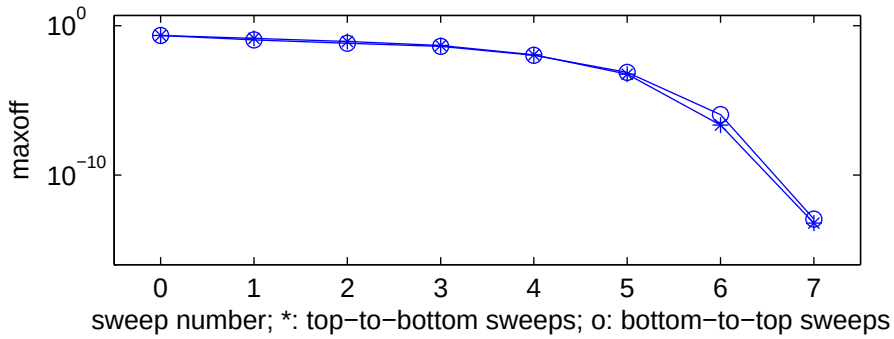
FIG. 5.3. *Typical convergence behavior for general matrices*



In both cases, the algorithm starts with a phase of "sorting elements" that is characterized by almost stagnation. As expected, it can be observed that maxoff(A) does not decrease monotonically over the number of sweeps. The phase of almost stagnation is followed by the phase of convergence. As predicted by the theory, the convergence rate becomes asymptotically quadratic in the case of bottom-to-top sweeps. However, the convergence rate appears to be only linear in the case of top-to-bottom sweeps.

The situation is completely different, when the algorithm is applied to a Hermitian matrix. Figure 5.4 shows the typical convergence behavior of the nonsymmetric Jacobi algorithm for a 50×50 Hermitian matrix. There is hardly any difference in the convergence behavior of the algorithm when using bottom-to-top sweeps compared to using top-to-bottom sweeps and both methods show asymptotic quadratic convergence.

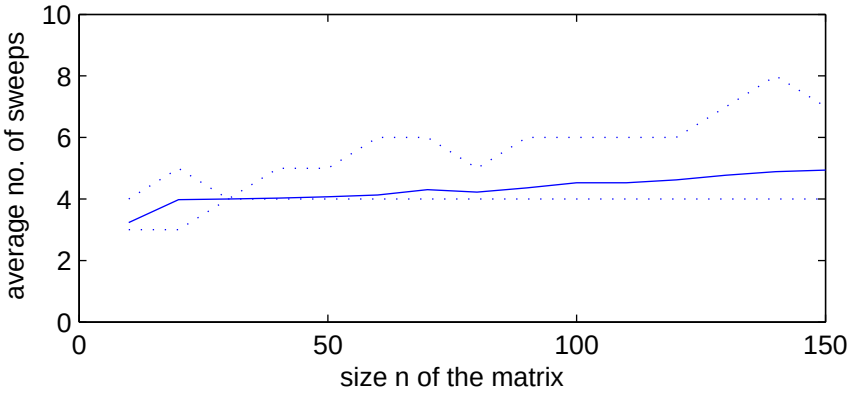
FIG. 5.4. *Typical convergence behavior for Hermitian matrices*



A second test has been run for 100 matrices close to Schur form. For this, 100 random complex $n \times n$ matrices have been generated and normalized to norm one.

Then, the Schur form has been computed by using the MATLAB function `schur` and a random perturbation of norm 1/100 has been added. Then the nonsymmetric Jacobi algorithm has been run on the perturbed Schur form. The results are displayed in Figure 5.5.

FIG. 5.5. *Test for* 100 *matrices close to Schur form.*



Once again, the solid line displays the average number of sweeps that were needed for convergence, while the dotted lines display the maximal and minimal number of needed sweeps. Even for matrices of size 150×150, the algorithm only needs about five sweeps for convergence, because the entries in the strict lower triangular part of the matrices are of magnitude of order 1/100 compared to the entries in the upper triangular part and thus, the hypothesis of Theorem 3.3 is very likely to be satisfied so that we may have a quadratic rate of convergence right from the beginning.

FIG. 5.6. *Typical convergence behavior for matrices close to Schur form*

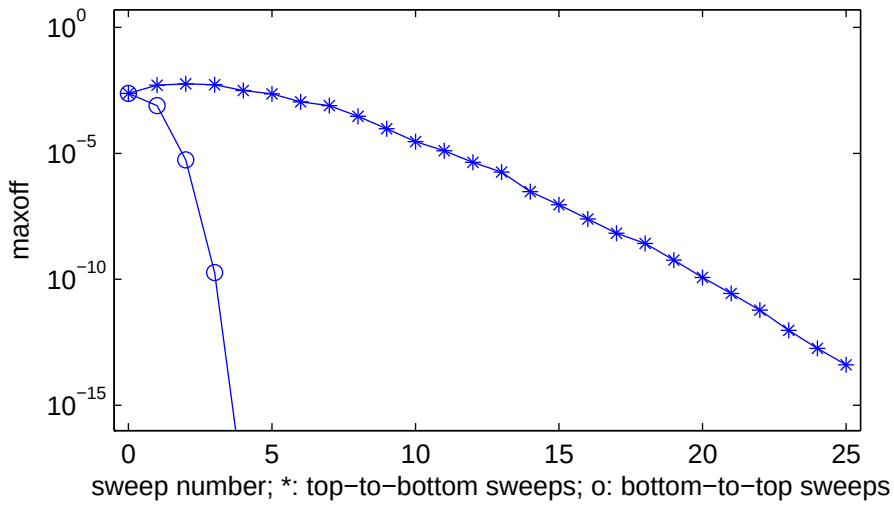


Figure 5.6 displays the typical convergence behavior of the nonsymmetric Jacobi algorithm for a matrix of size 50×50 that is close to Schur form. While the algorithm almost immediately enters the phase of quadratic convergence when using bottom-to-top sweeps, the convergence rate appears once again to be only linear when using top-to-bottom sweeps. Next, we tested the performance of the Hamiltonian Jacobi

algorithms described in Section 4 for 100 random Hamiltonian matrices normalized to spectral norm equal to one for the sizes $2n = 10, 20, \ldots, 100$.

FIG. 5.7. *Test for* 100 *random Hamiltonian matrices of different sizes.*

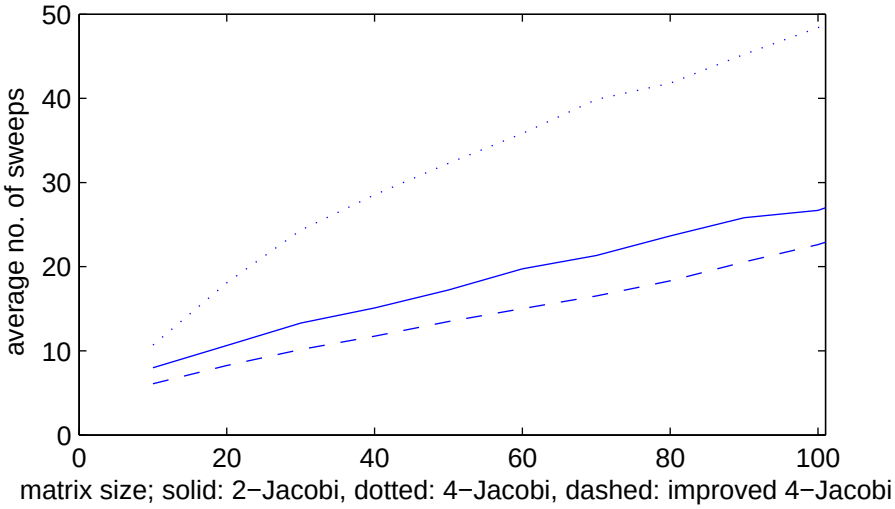


Figure 5.7 displays the average number of sweeps that was needed for convergence. The Hamiltonian 2-Jacobi performs similarly to the nonsymmetric Jacobi algorithm for general complex matrices as expected. On the other hand, the Hamiltonian 4-Jacobi needs a much larger number of sweeps. This changes drastically when passing to the improved Hamiltonian 4-Jacobi.

FIG. 5.8. *Typical convergence behavior for Hamiltonian matrices.*

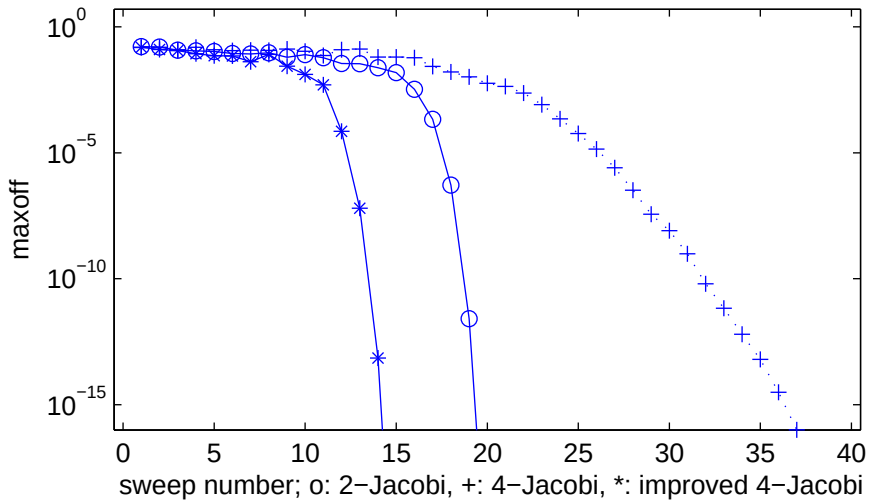


Figure 5.8 displays the typical convergence behavior of the Hamiltonian Jacobi methods. As expected, the Hamiltonian 2-Jacobi and the improved Hamiltonian 4-Jacobi show asymptotic quadratic convergence. On the other hand, the asymptotic convergence rate of the Hamiltonian 4-Jacobi appears to be only linear which ex-

plains the large average number of sweeps that is needed for convergence. Although the improved Hamiltonian 4-Jacobi method needs the least number of sweeps for convergence in general, the Hamiltonian 2-Jacobi turns out to be the most efficient version of the Hamiltonian Jacobi methods due to the fact that the cost of one sweep of the Hamiltonian 2-Jacobi is only about 40% of the cost of one sweep of the improved Hamiltonian 4-Jacobi..

6. Conclusions. We have revisited the nonsymmetric Jacobi algorithm for the computation of the Schur form of a general complex matrix. In particular, asymptotic quadratic convergence of the cyclic version of the method can be proved if northeast directed sweeps are used. Other sweeps, in turn, seem to lead to a linear convergence rate only. Based on this convergence theory, we were able to explain why the convergence behavior of the Hamiltonian Jacobi algorithm proposed in [1] is less satisfactory than expected and what can be done to overcome this inconvenience.

Still, there are many aspects that have not yet been investigated. First of all, a proof of global convergence is still missing. Then, the convergence behavior of the algorithm is not yet optimal, because the initial phase of almost stagnation is very long and the phase of quadratic convergence is entered rather late. Therefore, preconditioning methods should be introduced and investigated in order to improve the convergence, for example, like it has been done for a Jacobi algorithm for computing the singular value decomposition, see [8]. Another important issue is parallelization. Since the solution of 2×2 subproblems only requires local information, it is possible to implement parallel version of Jacobi-like algorithms, like it has already been considered in [10]. However, the discussion in Section 2 shows that further investigation is necessary as a naive parallel implementation of the algorithm may lead to a loss of the property of asymptotic quadratic convergence.

Acknowledgment. I would like to thank Heike Faßbender for valuable discussions and for giving helpful comments on an earlier draft of the paper.

REFERENCES

[1] A. Bunse-Gerstner and H. Fassbender, *A Jacobi-like method for solving algebraic Riccati equations on parallel computers*, IEEE Trans. Automat. Control, 42 (1997), pp. 1071–1084.
[2] R. Byers, *A Hamiltonian QR-algorithm*, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 212–229.
[3] ———, *A Hamiltonian Jacobi algorithm*, IEEE Trans. Automat. Control, 35 (1990), pp. 566–570.
[4] R. Causey, *Computing eigenvalues of non-Hermitian matrices by methods of Jacobi type*, J. Soc. Indust. Appl. Math., 6 (1958), pp. 172–181.
[5] J. Charlier and P. van Dooren, *A Jacobi-like algorithm for computing the generalized schur form of a regular pencil*, J. Comput. Appl. Math., 27 (1989), pp. 17–36.
[6] D. Chu, X. Liu, and V. Mehrmann, *A numerically strongly stable method for computing the Hamiltonian schur form*, preprint 2004/24, Institut für Mathematik, TU Berlin, 2004. Submitted.
[7] J. Demmel and K. Veselić, *Jacobi's method is more accurate than QR*, SIAM J. Matrix Anal. Appl., 13 (1992), pp. 1204–1245.
[8] Z. Drmač, *A posteriori computation of the singular vectors in a preconditioned Jacobi SVD algorithm*, IMA J. Numer. Anal., 19 (1999), pp. 191–213.
[9] P. Eberlein, *A Jacobi-like method for the automatic computation of eigenvalues and eigenvectors of an arbitrary matrix*, J. Soc. Indust. Appl. Math., 10 (1962), pp. 74–88.
[10] ———, *On the Schur decomposition of a matrix for parallel computation*, IEEE Trans. Comp., 36 (1987), pp. 167–174.
[11] H. Fassbender, D. S. Mackey, and N. Mackey, *Hamiltonian and Jacobi come full circle: Jacobi algorithms for structured Hamiltonian eigenproblems*, Linear Algebra Appl., 332–334 (2001), pp. 37–80.

[12] H. Goldstine and L. Horwitz, *A procedure for the diagonalization of normal matrices*, J. Assoc. Comput. Mach., 6 (1959), pp. 176–195.
[13] J. Greenstadt, *A method for finding roots of arbitrary matrices*, Math. Tables Aids Comput., 9 (1955), pp. 47–52.
[14] ———, *Some numerical experiments in triangularizing matrices*, Numer. Math., 4 (1962), pp. 187–195.
[15] D. Hacon, *Jacobi's method for skew-symmetric matrices*, SIAM J. Matrix Anal. Appl., 14 (1993), pp. 619–628.
[16] V. Hari, *A Jacobi-like eigenvalue algorithm for general real matrices*, Glasnik Mar. Ser. III, 11 (31) (1976), pp. 367–378.
[17] P. Henrici, *On the speed of convergence of cyclic and quasicyclic Jacobi methods for computing the eigenvalues of hermitian matrices*, J. Soc. Indust. Appl. Math, 6 (1958), pp. 144–162.
[18] A. Hilliges, C. Mehl, and V. Mehrmann, *On the solution of palindromic eigenvalue problems*, in Proceedings of the 4th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Jyväskylä, Finland, 2004. CD-ROM.
[19] C. P. Huang, *A jacobi-type method for triangularizing an arbitrary matrix*, SIAM J. Numer. Anal., 4 (1975), pp. 566–570.
[20] K. Hüper, *A calculus approach to matrix eigenvalue algorithms*. Habilitationsschrift, Universität Würzburg, Würzburg, Germany, 2002.
[21] C. G. J. Jacobi, *Über ein leichtes Verfahren, die in der Theorie der Säcularströmungen vorkommenden Gleichungen numerisch aufzulösen*, J. Reine Angew. Math., 30 (1846), pp. 51–95.
[22] P. Lancaster and L. Rodman, *Algebraic Riccati Equations*, Clarendon Press, Oxford, 1995.
[23] W.-W. Lin, V. Mehrmann, and H. Xu, *Canonical forms for Hamiltonian and symplectic matrices and pencils*, Linear Algebra Appl., 302/303 (1999), pp. 469–533.
[24] M. Lotkin, *Characteristic values of arbitrary matrices*, Quart. Appl. Math., 14 (1956), pp. 267–275.
[25] D. S. Mackey, N. Mackey, C. Mehl, and V. Mehrmann, *Numerical solution of palindromic eigenvalue problems*. In preparation, 2006.
[26] ———, *Structured polynomial eigenvalue problems: Good vibrations from good linearizations*, SIAM Matrix Anal. Appl., 28 (2006), pp. 1029–1051.
[27] C. Mehl, *Jacobi-like algorithms for the indefinite generalized Hermitian eigenvalue problem*, SIAM J. Matrix Anal. Appl., 25 (2004), pp. 964–985.
[28] V. Mehrmann, *The Autonomous Linear Quadratic Control Problem, Theory and Numerical Solution*, no. 163 in Lecture Notes in Control and Information Sciences, Springer-Verlag, Heidelberg, July 1991.
[29] M. H. C. Paardekooper, *An eigenvalue algorithm for skew-symmetric matrices*, Numer. Math., 17 (1971), pp. 189–202.
[30] C. Paige and C. Van Loan, *A Schur decomposition for Hamiltonian matrices*, Linear Algebra Appl., 14 (1981), pp. 11–32.
[31] A. Schönhage, *Zur quadratischen Konvergenz des Jacobi-Verfahrens*, Numer. Math., 6 (1964), pp. 410–412.
[32] G. W. Stewart, *A Jacobi-like algorithm for computing the Schur decomposition of a non-Hermitian matrix*, SIAM J. Sci. Statist. Comput., 6 (1985), pp. 853–864.
[33] G. W. Stewart and J. Sun, *Matrix perturbation theory*, Academic Press, Inc., Boston, 1990.
[34] K. Veselić, *A Jacobi eigenreduction algorithm for definite matrix pairs*, Numer. Math., 64 (1993), pp. 241–269.
[35] J. H. Wilkinson, *Note on the quadratic convergence of the cyclic Jacobi process*, Numer. Math, 4 (1962), pp. 296–300.