

# A QR-LIKE ALGORITHM FOR THE PALINDROMIC EIGENVALUE PROBLEM

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**Abstract.** In this paper we develop a QR-like algorithm for the palindromic eigenvalue problem  $Ax = \lambda A^*x$ . We will discuss the two cases that  $A^*$  denotes the transpose or the conjugate transpose of  $A \in \mathbb{C}^{n,n}$ . It is shown that this so-called palindromic QR iteration is equivalent to applying the standard QR algorithm to  $A^{-*}A$ . Also the concepts of deflation, shifting, and exploiting the invariance of a Hessenberg-type form are adapted. Moreover, we analyze the problem of reducing a general square matrix to the mentioned Hessenberg-type form and establish analogies to the Hamiltonian eigenvalue problem. Finally, we present concrete Hessenberg-type reduction algorithms for special cases.

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**Key words.** palindromic eigenvalue problem, QR algorithm, unitary congruence, canonical form, Hessenberg matrix

**1. Introduction.** A generalized eigenvalue problem of the form

$$Ax = \lambda A^*x \tag{1.1}$$

is called *palindromic eigenvalue problem*. Here,  $A \in \mathbb{C}^{n,n}$  is a complex square matrix,  $\lambda \in \mathbb{C}$  is an eigenvalue, and  $x \in \mathbb{C}^n \setminus \{0\}$  is a corresponding eigenvector. By writing  $A^*$  we denote either the transpose or the complex conjugate transpose of  $A$ , that is  $\star \in \{T, *\}$ . These two cases have similar, though not identical, spectral properties. Whenever possible they are treated in a unified way.

Palindromic eigenvalue problems of the form (1.1) are the linear case of polynomial palindromic eigenvalue problems

$$P(\lambda)x = \left( \sum_{i=0}^k A_i \lambda^i \right) x = 0, \text{ where } A_{n-i}^* = A_i \in \mathbb{C}^{n,n}, i = 1, \dots, k. \tag{1.2}$$

The underlying matrix polynomial  $P(\lambda)$  is invariant under reversing the order of the coefficients and (conjugate-) transposing. This explains the term 'palindromic', as palindromes are words that are invariant under reversing the order of the letters. Well known palindromes are 'mom', 'dad', or 'rotor'. Polynomial palindromic eigenvalue problems were introduced and analyzed in [15] and arise for example in the vibration analysis of rail tracks [10] (T-case) or optimal control problems [17] (\*-case). Under mild conditions, polynomial palindromic problems of the form (1.2) can be linearized to linear palindromic problems of the form (1.1), see [15].

The symmetry in the coefficients of the palindromic eigenvalue problem (1.1) results in a symmetry in the spectrum. Indeed, (conjugate-) transposing equation (1.1) yields

$$x^* A^* = \lambda^* x^* A \Leftrightarrow x^* A = \frac{1}{\lambda^*} x^* A^*.$$

Thus, if  $\lambda \neq 0$  is an eigenvalue (and  $x$  an associated eigenvector) then also  $\frac{1}{\lambda^*}$  is an eigenvalue (and  $x^*$  an associated left eigenvector). Note that for a scalar  $\lambda^*$  means  $\bar{\lambda}$  (if  $\star = T$ ) or  $\bar{\lambda}$ , the complex conjugate of  $\lambda$  (if  $\star = *$ ). This spectral symmetry is called *reciprocal pairing*. Also a zero eigenvalue is paired, with its partner being an infinite eigenvalue and vice versa. In the whole paper we use the conventions  $\frac{1}{0} = \infty$ , and  $\frac{1}{\infty} = 0$ . The reciprocal pairing degenerates for so-called *exceptional eigenvalues* with  $\lambda^* \lambda = 1$ . Exceptional eigenvalues are  $\pm 1$ , if  $\star = T$ , or all numbers on the unit circle, if  $\star = *$ .

Also the number and size of Jordan blocks associated with the eigenvalues  $\lambda$  and  $\frac{1}{\lambda^*}$  coincide. This follows from a structured analogon to the Kronecker canonical form for palindromic pencils

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discussed in [20]. Similar canonical forms were presented in [12, 13, 19], but not in the context of palindromic eigenvalue problems.

Existing methods for the palindromic eigenvalue problem can be divided into two classes based on whether they target the palindromic Schur form (the same condensed form we will be aiming at, see [16] or Theorem 1 below), or not. The first class includes a Jacobi-like method [10] and the structured deflation method, a postprocessing step of the generalized Schur form [16]. Other approaches to the solution of the palindromic eigenvalue problem are based on a URV-type matrix factorization [21] or (for quadratic palindromic problems) on the structured doubling algorithm [7].

This paper is structured as follows. In Section 2 we recall the palindromic Schur form and present the basic palindromic QR algorithm. In Section 3 the technique of shifting is developed as a means to speed up the algorithm. Then, in Section 4 we consider Hessenberg-like matrices that are invariant under palindromic QR steps. In Section 5 we discuss the reduction of a general matrix to this Hessenberg-like form. Finally, we offer some conclusions.

*Notation.* As mentioned before,  $A^\star$  denotes either the transpose or conjugate transpose of  $A$ . Consequently,  $A^{\star\star} := (A^\star)^\star$  denotes either the complex conjugate of  $A$ , or  $A$  itself.

We call a matrix pair  $(A, B)$  a pencil. It refers to the generalized eigenvalue problem  $Ax = \lambda Bx$ . A pencil is called *regular*, if  $A$  and  $B$  are square and  $\det(A - \lambda B) \not\equiv 0$ , otherwise it is called *singular*. The  $i$ -th vector of unity  $e_i$  is the  $i$ -th column of the identity matrix  $I$ . The direct sum of matrices  $A, B$  is defined as

$$A \oplus B = \text{diag}(A, B) = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix}.$$

The term  $\lfloor \alpha \rfloor$  denotes the largest integer that is smaller or equal to  $\alpha$  (known as Gaussian parentheses). Throughout this paper,  $F$  denotes the so-called *flip matrix*

$$F = \begin{bmatrix} 0 & & 1 \\ & \ddots & \\ 1 & & 0 \end{bmatrix}.$$

The name stems from the fact that upon premultiplication by  $F$  a matrix is flipped upside-down, while postmultiplication corresponds to a flip leftside-right.

A matrix  $A \in \mathbb{C}^{n,n}$  is called (*lower*) *skew triangular*, if  $a_{ij} = 0$  whenever  $i + j \leq n$ . Such a matrix will be depicted by  $A = \triangleleft$ . On the other hand, *upper skew triangular* matrices,

depicted by  $A = \triangle$ , are those with  $a_{ij} = 0$  for all  $i + j > n + 1$ . Note that the transpose of a lower skew triangular matrix is also lower skew triangular, while its inverse (if it exists) is upper skew triangular. Moreover, if an upper triangular matrix is flipped upside-down, i.e., if it is premultiplied by  $F$ , it becomes skew triangular. Note further, that the product of an upper skew triangular matrix and a lower skew triangular one is upper triangular, or shorter:  $\triangle \cdot \triangleleft = \square$ .

These properties are summarized in the following table, where  $\square$  depicts a matrix that has no particular zero pattern in general.

$A$	$A^T$	$A^{-1}$	$FA$	$AF$	$A \cdot B, B =$			
					$\triangleleft$	$\triangle$	$\square$	$\square$
$\triangleleft$	$\triangleleft$	$\triangleleft$	$\triangle$	$\triangle$	$\triangleleft$	$\square$	$\square$	$\triangle$
$\triangle$	$\triangle$	$\triangle$	$\triangleleft$	$\triangleleft$	$\square$	$\triangle$	$\triangle$	$\square$
$\square$	$\square$	$\square$	$\square$	$\square$	$\triangle$	$\square$	$\square$	$\triangle$
$\square$	$\square$	$\square$	$\triangle$	$\triangle$	$\square$	$\triangle$	$\triangle$	$\square$

**2. The palindromic QR algorithm.** The palindromic eigenvalue problem is a special case of the generalized eigenvalue problem. Hence it can be solved by standard methods for the generalized eigenvalue problem, e.g., the QZ algorithm [9]. But such general methods do not preserve the palindromic structure of the pencil and thus their results do not (due to rounding errors) conform to the reciprocal pairing. Since in applications this pairing often has a physical meaning, it is desirable to derive a method that preserves palindromic structure and consequently also the reciprocal pairing. Such an algorithm should use only unitary congruence transformations, because congruences preserve the palindromic structure,  $P^\star(A, A^\star)P = (P^\star AP, (P^\star AP)^\star)$ , whereas unitary transformations are essential for achieving numerical backward stability [24].

Since the generalized Schur form is not palindromic (and thus cannot be reached by congruences), the algorithm must target some other condensed form that reveals the eigenvalues of the problem. Such a condensed form is provided by the following two results.

**THEOREM 1.** *For any square matrix  $A \in \mathbb{C}^{n,n}$  there exists a unitary matrix  $Q$  such that*

$$Q^\star A Q = \begin{matrix} & p & & p \\ p & & & A_{13} \\ & A_{22} & & A_{23} \\ p & A_{31} & A_{32} & A_{33} \end{matrix} = \begin{bmatrix} & & & \triangle \\ & & \square & \square \\ \triangle & & \square & \square \end{bmatrix}, \quad (2.1)$$

for some  $p \leq \lfloor \frac{n}{2} \rfloor$  where the pencil  $(A_{22}, A_{22}^\star)$  is regular and has only exceptional eigenvalues with  $\lambda^\star \lambda = 1$ .

*Proof.* For  $\star = T$ , this follows from a stronger result in [16]. The relevant part of the proof given there can be generalized to cover the case  $\star = *$  as well.

It will be shown that if the pencil  $(A, A^\star)$  is singular or has a non-exceptional eigenvalue, then there exists a unitary  $Q \in \mathbb{C}^{n,n}$ , such that

$$Q^\star A Q = \begin{matrix} & 1 & n-2 & 1 \\ 1 & 0 & 0 & \tilde{A}_{13} \\ n-2 & 0 & \tilde{A}_{22} & \tilde{A}_{23} \\ 1 & \tilde{A}_{31} & \tilde{A}_{32} & \tilde{A}_{33} \end{matrix}. \quad (2.2)$$

By applying the same procedure to  $\tilde{A}_{22}$  the matrix is successively reduced to the form (2.1). We consider two cases.

Case 1:  $A$  is singular. Then there exists a vector  $q_1$  of norm 1 such that  $A^\star q_1 = 0$ . Let  $\hat{Q} \in \mathbb{C}^{n,n}$  be unitary, such that  $\hat{Q}e_1 = q_1$ . Then

$$\hat{A} = \hat{Q}^\star A \hat{Q} = \begin{matrix} & 1 & n-2 & 1 \\ 1 & 0 & 0 & 0 \\ n-2 & \hat{A}_{21} & \hat{A}_{22} & \hat{A}_{23} \\ 1 & \hat{A}_{31} & \hat{A}_{32} & \hat{A}_{33} \end{matrix}. \quad (2.3)$$

Now, let  $H \in \mathbb{C}^{n-1, n-1}$  be unitary, such that

$$H^\star \begin{bmatrix} \hat{A}_{21} \\ \hat{A}_{31} \end{bmatrix} = \alpha e_{n-1}$$

with  $\alpha \in \mathbb{C}$ . This could be, e.g., a suitable Householder matrix [9]. Then, with  $Q = \hat{Q}(1 \oplus H)$ , we have

$$Q^\star A Q = \begin{bmatrix} 1 & & & \\ & H & & \\ & & \hat{A} & \\ & & & H \end{bmatrix}^\star \begin{bmatrix} 1 & & & \\ & H & & \\ & & \hat{A} & \\ & & & H \end{bmatrix} = \begin{matrix} & 1 & n-2 & 1 \\ 1 & 0 & 0 & 0 \\ n-2 & 0 & \tilde{A}_{22} & \tilde{A}_{23} \\ 1 & \alpha & \tilde{A}_{32} & \tilde{A}_{33} \end{matrix} \quad (2.4)$$

of the form (2.2).

Case 2:  $A$  is non-singular. Then, in particular, the pencil  $(A, A^\star)$  is regular. Let  $(\lambda, x)$  be an eigenpair of  $(A, A^\star)$ , where  $\lambda$  is a non-exceptional eigenvalue, i.e.,  $\lambda^\star \lambda \neq 1$ . If such a pair does not exist, there is nothing to show. But if it exists, then one has

$$x^\star(Ax) = x^\star(\lambda A^\star x) = \lambda(Ax)^\star x = \lambda(\lambda A^\star x)^\star x = \lambda^\star \lambda x^\star Ax, \quad (2.5)$$

i.e.,  $x^\star Ax = 0$ . Let  $q_1$  be the normalized vector  $x$ . Let  $q_2, \dots, q_{n-1}$  be an orthonormal family in the orthogonal complement of  $\text{span}(x, (Ax)^\star)$  and let  $q_n$  be a normalized vector, that is orthogonal to  $q_1, \dots, q_{n-1}$ . Then  $Q = [q_1, \dots, q_n]$  is unitary and

$$\tilde{A} = Q^\star A Q = \begin{matrix} & & 1 & n-2 & 1 \\ & 1 & & & \\ & & 0 & \tilde{A}_{12} & \tilde{A}_{13} \\ & & 0 & \tilde{A}_{22} & \tilde{A}_{23} \\ 1 & & \tilde{A}_{31} & \tilde{A}_{32} & \tilde{A}_{33} \end{matrix},$$

because  $q_1^\star A q_1 = \frac{1}{\|x\|^2} x^\star Ax = 0$  and  $q_j^\star A q_1 = (q_j^\star (A q_1)^\star)^\star = 0$ . Since  $q_1$  is an eigenvector of  $(A, A^\star)$ , the first vector of unity,  $e_1$ , is an eigenvector of  $(\tilde{A}, \tilde{A}^\star)$ . Thus,  $\tilde{A}_{12}$  must be zero as well and hence  $\tilde{A}$  is of the form (2.2). This concludes the proof.  $\square$

From here on, we will assume that  $(A, A^\star)$  is a regular pencil with at most one exceptional eigenvalue. This considerably simplifies the condensed form (2.1).

**COROLLARY 2.** *Let  $A \in \mathbb{C}^{n,n}$  be such that  $(A, A^\star)$  is a regular pencil with at most one exceptional eigenvalue. Then there is a unitary  $Q$  such that*

$$Q^\star A Q = R = \begin{matrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{matrix}.$$

Further, all eigenvalues of  $(A, A^\star)$  can be read off from  $R$ . They are given by the ratios

$$\lambda_i = \frac{r_{n+1-i,i}}{r_{i,n+1-i}^\star}, \quad \text{for } i = 1 \dots n. \quad (2.6)$$

Moreover,  $Q$  can be chosen such that the eigenvalues  $\lambda_1, \lambda_2 \dots \lambda_n$  appear in any order yielding  $\lambda_i^\star = \frac{1}{\lambda_{n+1-i}}$  for  $i = 1, \dots, n$ .

*Proof.* Since  $(A, A^\star)$  has at most one exceptional eigenvalue, the  $A_{22}$  block in the form (2.1) is of size at most 1-by-1. Thus, in this case the form (2.1) reduces to a skew triangular matrix. Since  $(A, A^\star)$  is a regular pencil, it has  $n$  eigenvalues. Considering the determinant of  $R - \lambda R^\star$  the assertion (2.6) follows.

The order of the eigenvalues  $\lambda_1, \dots, \lambda_{\lfloor \frac{n}{2} \rfloor}$  corresponds to the order of the eigenpairs selected in the proof of Theorem 1 in case 2. The other eigenvalues follow from the relation (2.6).  $\square$

**DEFINITION 3.** *Let  $A \in \mathbb{C}^{n,n}$  such that  $(A, A^\star)$  is regular. A matrix  $R \in \mathbb{C}^{n,n}$  is called a palindromic Schur form of  $A$ , if  $R$  is skew triangular and there exists a unitary  $Q \in \mathbb{C}^{n,n}$  such that  $R = Q^\star A Q$ .  $R$  is called ordered, if  $|\lambda_i| \geq |\lambda_{i+1}|$  for  $i = 1, \dots, n-1$  with  $\lambda_i$  as in (2.6).*

**REMARK 4.** The mentioned stronger result in [16] for the case  $\star = T$  states that for every square matrix  $A$  there exists a unitary matrix  $Q$  such that  $Q^T A Q = R = \begin{matrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{matrix}$  is skew triangular. There,  $R$  is called anti-triangular Schur form.

This does not hold in the  $\star = *$  case. For example, the identity matrix  $I_2$  cannot be skew triangularized by unitary  $*$ -congruence. Indeed,  $Q^\star I Q = I$  is not skew triangular for any unitary  $Q$ . In the T-case, however, with  $Q = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -i \\ i & -1 \end{bmatrix}$  we have  $Q^\star Q = I_2$ ,  $Q^T I Q = -i \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{matrix} & & & \\ & & & \\ & & & \\ & & & \end{matrix}$ .  $\square$

The palindromic eigenvalue problem can be solved by transforming  $A$  in (1.1) to palindromic Schur form. Thus, we are looking for a unitary matrix  $Q$  such that  $Q^\star A Q$  is skew triangular. This situation is similar to the standard eigenvalue problem, where we want to find a unitary matrix  $Q$  such that  $Q^\star A Q$  is upper triangular. A commonly used method to compute such a  $Q$  is the QR iteration [9]. A basic step of the iteration consists of performing a QR factorization  $A = QR$  and then forming the  $A_+ = RQ = Q^\star A Q$ . Because of the mentioned similarity between the reduction

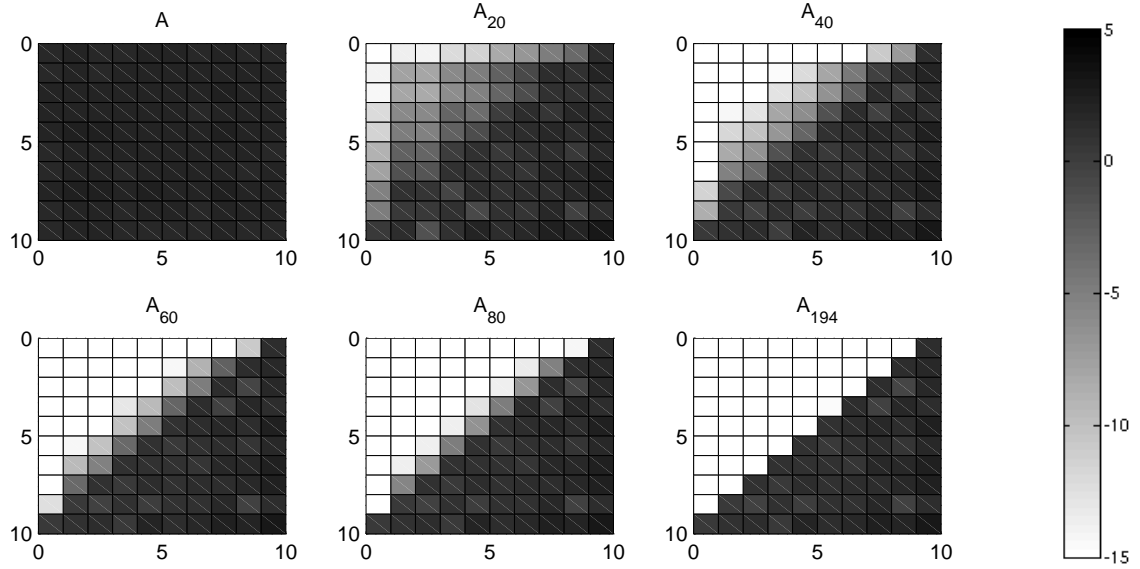


FIG. 2.1. Convergence history of the palindromic QR iteration. We plot the elementwise common logarithm. The lighter an element is the smaller it is in magnitude. The color bar to the right is labeled logarithmically.

to standard and palindromic Schur form, it is natural to come up with the *palindromic QR iteration* consisting of repeatedly applying the following *palindromic QR step*.

ALGORITHM 1. Palindromic QR step

- 1:  $A \rightarrow QR$  (skew QR factorization, i.e.,  $R = \begin{smallmatrix} \triangle \\ \triangle \end{smallmatrix}$ )
- 2:  $A_1 \leftarrow RQ^{\star\star}$

Note, that  $A_1$  is unitarily  $\star$ -congruent to  $A$ , as  $A_1 = RQ^{\star\star} = Q^{\star}AQ^{\star}$ . Here,  $Q^{\star\star}$  is a somewhat cryptic notation for  $Q$  (if  $\star = *$ ) or  $\bar{Q}$  ( $\star = T$ ), respectively.

EXAMPLE 1. As an example, we have applied the palindromic QR iteration to a  $(10 \times 10)$  real matrix,  $A$ , defined as follows:  $A = XDX^T$  where  $X$  is a  $(10 \times 10)$  random matrix (generated by the MATLAB command `rand(10)`) with condition number  $\text{cond}(X) \approx 100$ .  $D$  was set to  $\begin{bmatrix} & & & & & & & & & 10 \\ & & & & & & & & & \cdot \\ & & & & & & & & & \cdot \\ & & & & & & & & & \cdot \\ & & & & & & & & & \cdot \\ & & & & & & & & & \cdot \\ & & & & & & & & & \cdot \\ & & & & & & & & & \cdot \\ & & & & & & & & & \cdot \\ 1 & & & & & & & & & \cdot \end{bmatrix}$ . Hence, the eigenvalues of  $(A, A^T)$  are  $\frac{1}{10}, \frac{2}{9}, \frac{3}{8}, \frac{4}{7}, \frac{5}{6}, \frac{6}{5}, \frac{7}{4}, \frac{8}{3}, \frac{9}{2}$  and  $\frac{10}{1}$ .

In Figure 2.1 the results of every 20th step are plotted. It can be observed that it takes 80 iterations for the first eigenvalue pair to converge. In  $A_{80}$  (lower center plot) the ratio  $\frac{a_{1,10}}{a_{10,1}}$  equals 0.1 to an accuracy of 15 digits. After 194 iterations the matrix has converged to a skew triangular form.  $\square$

The palindromic QR iteration converged for the preceding example. In order to analyze the convergence behavior the following result relates the palindromic QR iteration to the standard QR iteration applied to the standard eigenvalue problem  $A^{-\star}Ax = \lambda x$ , that arises if (1.1) is premultiplied by  $A^{-\star}$  and thus has the same eigenvalues and (right) eigenvectors as (1.1).

LEMMA 5. Let  $A \in \mathbb{C}^{n,n}$  be non-singular and let  $A_2$  be the result of two palindromic QR steps applied to  $A$ . Further, let  $B = A^{-\star}A$  and let  $B_+$  be the result of one standard QR step applied to  $B$ . Then there is a unitary diagonal matrix  $D$  such that  $B_+ = D^*A_2^{-\star}A_2D$ .

*Proof.* Carrying out two palindromic QR steps on  $A$  yields

$$\begin{aligned} A &:= Q_1R_1, \text{ with } R_1 = \begin{smallmatrix} \triangle \\ \triangle \end{smallmatrix}, & A_1 &:= Q_1^*AQ_1^{\star}, \\ A_1 &:= Q_2R_2, \text{ with } R_2 = \begin{smallmatrix} \triangle \\ \triangle \end{smallmatrix}, & A_2 &:= Q_2^*A_1Q_2^{\star}. \end{aligned}$$

It follows that  $R_1 = Q_1^* A$  and  $R_2 = Q_2^* Q_1^* A Q_1^{*\star}$ . Let  $Q := (Q_1 Q_2)^{*\star}$  and  $R := R_2^{-\star} R_1 = \begin{smallmatrix} \diagup & & \\ & \diagdown & \\ & & \triangle \end{smallmatrix} = \begin{smallmatrix} \diagdown & & \\ & \diagup & \\ & & \triangle \end{smallmatrix}$ . Then we have

$$QR = (Q_1 Q_2)^{*\star} (Q_2^* Q_1^* A Q_1^{*\star})^{-\star} Q_1^* A = A^{-\star} A,$$

i.e.,  $QR$  forms a standard QR-decomposition of  $A^{-\star} A$ . So, applying a standard QR step with this QR-decomposition to  $A^{-\star} A$  yields

$$\begin{aligned} Q^* A^{-\star} A Q &= Q_2^* Q_1^* A^{-\star} (Q_1 Q_2 Q_2^* Q_1^*) A Q_1^{*\star} Q_2^{*\star} \\ &= (Q_2^* Q_1^* A Q_1^{*\star} Q_2^{*\star})^{-\star} (Q_2^* Q_1^* A Q_1^{*\star} Q_2^{*\star}) \\ &= (Q_2^* A_1 Q_2^{*\star})^{-\star} (Q_2^* A_1 Q_2^{*\star}) \\ &= A_2^{-\star} A_2. \end{aligned}$$

Since the QR-factorization of a non-singular matrix is unique up to a unitary diagonal factor [9] the assertion follows.  $\square$

REMARK 6. In Lemma 5  $A$  was assumed to be non-singular. This is not necessary for the basic palindromic QR iteration to work. In fact, if  $A$  is singular then two steps of Algorithm 1 implement the procedure used in case 1 of the proof of Theorem 1. It is easy to check that (in the generic case that the kernel of  $A$  is not orthogonal to  $e_n$ )  $A_1$  is of the form (2.3) and  $A_2$  is of the form (2.4).  $\square$

The following result relates the Schurform of  $A^{-\star} A$  to the palindromic Schur form of  $A$ .

LEMMA 7. *Let  $A \in \mathbb{C}^{n,n}$  be non-singular such that all eigenvalues of  $(A, A^{\star})$  are of geometric multiplicity 1 and there is at most one exceptional eigenvalue. Assume further that  $T := A^{-\star} A$  is in Schur form, with  $\frac{1}{t_{ii}^{\star}} = t_{n+1-i, n+1-i}$  for  $i = 1, \dots, n$ . Then  $A$  is in palindromic Schur form.*

*Proof.* By Corollary 2 there is a palindromic Schur decomposition  $A = Q^{*\star} R Q^*$  of  $A$  such that  $\frac{r_{n+1-i, i}}{r_{i, n+1-i}^{\star}} = t_{ii}$  for  $i = 1, \dots, \lfloor \frac{n}{2} \rfloor$ . Set  $\tilde{T} := R^{-\star} R = \begin{smallmatrix} \diagdown & & \\ & \diagup & \\ & & \triangle \end{smallmatrix}$  and note that  $\frac{1}{\tilde{t}_{ii}^{\star}} = \tilde{t}_{n+1-i, n+1-i}$  for  $i = 1, \dots, n$ . We have

$$T = A^{-\star} A = (Q^{*\star} R Q^*)^{-\star} (Q^{*\star} R Q^*) = Q R^{-\star} R Q^* = Q \tilde{T} Q^*. \quad (2.7)$$

So,  $T$  and  $\tilde{T}$  are both Schur forms of  $A^{-\star} A$  with the eigenvalues occurring in the same order. Moreover,  $T$  and  $\tilde{T}$  are unitarily similar. Since all eigenvalues are of geometric multiplicity 1, the Schur form is essentially unique. So,  $Q$  must be a unitary diagonal matrix. Thus,  $A = Q^{*\star} R Q^*$  is skew triangular.  $\square$

Lemmas 5 and 7 indicate that the palindromic QR iteration converges to a palindromic Schur form under the assumptions that there is at most one exceptional eigenvalue, all eigenvalues are non-derogatory and that the standard basic QR iteration converges when applied to  $A^{-\star} A$ .

At this point, the basic palindromic QR iteration has been introduced. The remainder of the paper is about how to speed up the algorithm by strategies like deflation (Section 2.2), shifting (Section 3) or the use of Hessenberg-like structures (Section 4).

**2.1. The real case.** Many palindromic problems arising in practice are real. In this case one would like to keep all computations real as real operations are faster by a factor of 4 than complex operations. Furthermore, in this case the eigenvalues occur in quadruples of the form  $(\lambda, \bar{\lambda}, \frac{1}{\bar{\lambda}}, \frac{1}{\lambda})$ , and exceptional eigenvalues are those on the unit circle.

THEOREM 8. *Let  $A \in \mathbb{R}^{n,n}$ . Then, there is an orthogonal matrix  $Q \in \mathbb{R}^{n,n}$  such that*

$$Q^T A Q = \begin{matrix} & p & & p \\ p & \begin{bmatrix} & & A_{13} \\ & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} & & \\ & & & \end{matrix} \quad (2.8)$$

for some  $p \leq \lfloor \frac{n}{2} \rfloor$  where  $A_{13}$  is skew triangular,  $A_{31}$  is quasi skew triangular (i.e., with 1-by-1 and 2-by-2 blocks on the skew diagonal) and  $(A_{22}, A_{22}^T)$  has only exceptional eigenvalues.

*Proof.* The proof is analogous to that of Theorem 1. Case 1 holds without changes. All that remains to be shown in case 2 is the analogon of relation (2.5). So, assume that  $X \in \mathbb{R}^{n,2}$  spans a deflating subspace corresponding to a complex conjugate pair of non-exceptional eigenvalues, i.e.,  $AX = A^T X L$  with  $L \in \mathbb{R}^{2,2}$ ,  $\lambda(L) = \{\lambda, \bar{\lambda}\}$ , and  $|\lambda| \neq 1$ . We have to show that  $X^T A X = 0$ . This is indeed the case as

$$X^T (AX) = X^T (A^T X L) = (AX)^T X L = (A^T X L)^T X L = L^T X^T A X L.$$

So,  $(L^T \otimes L^T - I) \text{vec}(X^T A X) = 0$ , where  $\text{vec}$  denotes the vectorization operator and  $\otimes$  the Kronecker product, see [11]. The spectrum of  $\tilde{L} := L^T \otimes L^T$  is given by  $\{\lambda_i \lambda_j | \lambda_i, \lambda_j \in \lambda(L)\}$ . So every eigenvalue  $\mu$  of  $\tilde{L}$  is of modulus  $|\mu| = |\lambda^2| \neq 1$ . Thus,  $L^T \otimes L^T - I$  is non-singular, and hence  $X^T A X = 0$ .  $\square$

If the palindromic QR algorithm is applied to a real matrix  $A$ , the whole iteration will stay real. Moreover, Lemma 5 and a straightforward generalization of Lemma 7 still hold. So, what we have said about the convergence of the iteration also applies to the real case. An example was given in Example 1, as the matrix considered there was chosen real.

**2.2. Deflation.** If during the course of the iteration, the matrix  $A$  has the form

$$A = \begin{matrix} & \begin{matrix} p & n-2p & p \end{matrix} \\ \begin{matrix} p \\ n-2p \\ p \end{matrix} & \begin{bmatrix} 0 & 0 & A_{13} \\ 0 & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \end{matrix}, \quad (2.9)$$

for some integer  $p \leq \lfloor \frac{n}{2} \rfloor$ , then the first  $p$  vectors of unity span a deflating subspace of the pencil  $(A, A^*)$ , and the spectrum decomposes into three subsets,  $\lambda(A, A^*) = \lambda(A_{13}, A_{31}^*) \cup \lambda(A_{22}, A_{22}^*) \cup \lambda(A_{31}, A_{13}^*)$ .

The first and last subsets can be computed simultaneously by transforming  $(A_{13}, A_{31}^*)$  into generalized Schur form, i.e., by determining two unitary matrices  $Q, Z \in \mathbb{C}^{p,p}$ , such that

$$Q A_{13} Z = R_1 = \begin{bmatrix} \diagdown \\ \square \end{bmatrix}, \quad Q A_{31}^* Z = R_2 = \begin{bmatrix} \square \\ \diagdown \end{bmatrix}.$$

For example, the QZ algorithm [9] can compute such matrices  $Q$  and  $Z$ . Let  $\tilde{Q} = F Q^* \oplus I \oplus Z$ . Then we have

$$\tilde{Q}^* A \tilde{Q} = \begin{matrix} & \begin{matrix} p & n-2p & p \end{matrix} \\ \begin{matrix} p \\ n-2p \\ p \end{matrix} & \begin{bmatrix} 0 & 0 & F R_1 \\ 0 & A_{22} & \tilde{A}_{23} \\ R_2^* F & \tilde{A}_{32} & \tilde{A}_{33} \end{bmatrix} \end{matrix} = \begin{matrix} & \begin{matrix} p & n-2p & p \end{matrix} \\ \begin{matrix} p \\ n-2p \\ p \end{matrix} & \begin{bmatrix} 0 & 0 & \begin{bmatrix} \diagdown \\ \square \end{bmatrix} \\ 0 & \square & \square \\ \begin{bmatrix} \diagdown \\ \square \end{bmatrix} & \square & \square \end{bmatrix} \end{matrix}.$$

Then, the palindromic QR iteration can be continued on  $A_{22}$ , yielding the remaining set  $\lambda(A_{22}, A_{22}^*)$ . The subsequent iterations will be computationally less expensive, because  $A_{22}$  is of smaller size than  $A$ .

In practice, the blocks  $A_{11}, A_{12}, A_{21}$  generally do not vanish as in (2.9). Rather they are set to zero if they are neglectable, for instance, if  $\|[A_{11}, A_{12}, A_{21}^T]\|_F < 10^{-16} \|A\|_F$ .

**3. Shifting.** In general, the palindromic QR iteration converges very slowly (as in Example 1). However, if  $(0, \infty)$  is an eigenvalue pair, it is discovered within only two steps of the iteration. If  $(0, \infty)$  is not an exact, but an approximate eigenvalue pair, then it can still be expected to be found within only a few iterations.

The basic idea behind shifting for the QR algorithm is to shift the original matrix to another one with some eigenvalues near zero, so that the iterations can speed up. Here, we follow the same idea. We will shift the pencil  $(A, A^*)$  to another palindromic pencil  $(\tilde{A}, \tilde{A}^*)$ . The choice

$$\tilde{A} = A - \kappa A^*. \quad (3.1)$$

is natural (as it is the analogon of the choice  $\tilde{A} = A - \kappa B$  used by the shifted QZ iteration). If  $\kappa$  is close to an eigenvalue it is reasonable to assume that this choice of  $\tilde{A}$  is close to singular. We now analyze how the eigenvalues and eigenvectors of the so-called shifted system are related to those of the original problem.

LEMMA 9. *Let  $A \in \mathbb{C}^{n,n}$  such that  $(A, A^\star)$  is a regular pencil, and  $\kappa \in \mathbb{C}$  with  $\kappa^\star \kappa \neq 1$ . Set  $\tilde{A} = A - \kappa A^\star$ . Then  $(\tilde{A}, \tilde{A}^\star)$  is regular.*

*Further, let  $(\lambda, x)$  be an eigenpair of  $(A, A^\star)$ . Then  $(\tilde{\lambda}, x)$  is an eigenpair of  $(\tilde{A}, \tilde{A}^\star)$  with*

$$\tilde{\lambda} = f_\kappa(\lambda) = \frac{\lambda - \kappa}{1 - \kappa^\star \lambda} \quad (3.2)$$

*In particular, if  $\kappa = \lambda$  then  $\tilde{\lambda} = 0$  and if  $\kappa = \frac{1}{\lambda^\star}$  then  $\tilde{\lambda} = \infty$ .*

*Proof.* Suppose that  $y := A^\star x \neq 0$ , then  $(A - \kappa A^\star)x = (\lambda - \kappa)y$  and  $(A - \kappa A^\star)^\star x = (1 - \kappa^\star \lambda)y$ , thus,  $\tilde{A}x = \frac{\lambda - \kappa}{1 - \kappa^\star \lambda} \tilde{A}^\star x$ .

If  $A^\star x = 0$ , the result follows by exchanging the roles of  $A$  and  $A^\star$ .  $\square$

Note, that the requirement  $\kappa^\star \kappa \neq 1$  in Lemma 9 is important. If a value  $\kappa$  with  $\kappa^\star \kappa = 1$  is used as shift, all eigenvalues are mapped to the same value,  $\tilde{\lambda} = -\kappa$  for all  $\lambda$ . This can also be seen from the shifted system matrix  $\tilde{A}$ . It satisfies

$$\tilde{A}^\star = (A - \kappa A^\star)^\star = A^\star - \kappa^\star A = \frac{-1}{\kappa} (-\kappa A^\star + \kappa^\star \kappa A) = \frac{-1}{\kappa} \tilde{A}.$$

Thus, every vector would be an eigenvector (associated with the eigenvalue  $-\kappa$ ) of the pencil  $(\tilde{A}, \tilde{A}^\star)$  and no information could be drawn from the shifted pencil.

The *shifted palindromic QR step* proceeds by applying a palindromic QR step to the shifted system matrix  $\tilde{A}$  to get  $\tilde{A}_1 = Q^\star \tilde{A} Q^{\star\star}$ , where  $Q$  stems from the skew QR factorization of  $\tilde{A}$ . Afterwards,  $\tilde{A}_1$  has to be 'unshifted'. The formula  $\tilde{A}_1 = A_1 - \kappa A_1^\star$  can be solved for  $A_1$  (again, under the assumption that  $\kappa^\star \kappa \neq 1$ ) yielding

$$A_1 = \frac{1}{1 - \kappa^\star \kappa} (\tilde{A}_1 + \kappa \tilde{A}_1^\star). \quad (3.3)$$

Another way is to directly apply  $Q$  to  $A$ , i.e. setting  $A_1 = Q^\star A Q^{\star\star}$ . The latter is more expensive, but could be numerically preferable, since then possible cancellation errors in (3.1) and (3.3) do not carry over to  $A_1$ .

Summarizing the discussion above, a shifted palindromic QR step looks as follows:

ALGORITHM 2. Shifted palindromic QR step

- 1: choose  $\kappa$
- 2:  $\tilde{A} \leftarrow A - \kappa A^\star$
- 3:  $\tilde{A} \rightarrow QR$  with  $R = \begin{array}{|c} \hline \triangle \\ \hline \end{array}$
- 4:  $A_1 \leftarrow Q^\star A Q^{\star\star}$

It remains to find an eigenvalue approximation  $\kappa$  from  $A$ . One possible choice is

$$\kappa_1 = \frac{a_{1,n}}{a_{n,1}^\star}. \quad (3.4)$$

This is a good approximation if the first row and column of  $A$  are close to a multiple of the last vector of unity, i.e., if  $A$  is close to the form (2.9) for  $p = 1$ .

Another possibility is to partition  $A$  as follows

$$A = \begin{array}{ccc} & 2 & n-4 & 2 \\ & 2 & \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} & \\ & 2 & & \end{array}$$

and to chose  $\kappa$  as the eigenvalue of the pencil  $(A_{13}, A_{31}^\star)$  that is nearest to  $\kappa_1$  as of (3.4).



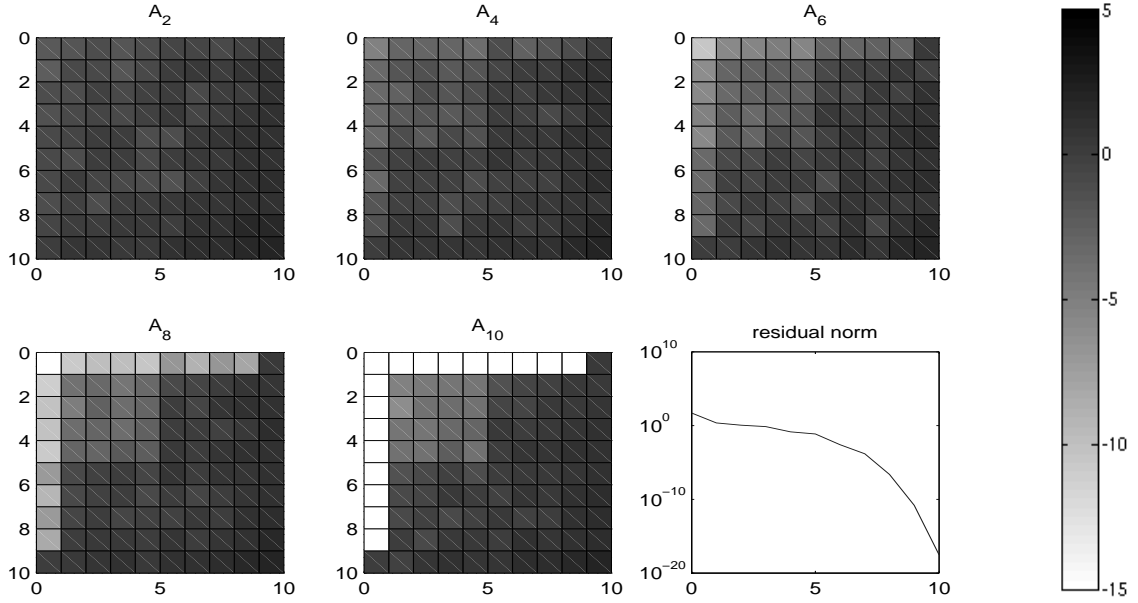


FIG. 3.1. Convergence history of the shifted palindromic QR iteration. The plotted residual was computed as  $r = \|[A(1, 1 : 9), A(2 : 9, 1)^T]\|$ .

EXAMPLE 2. The shifted palindromic QR iteration with shift (3.4) is applied to the matrix from Example 1. As shown in Figure 3.1, the first eigenvalue pair converges within 10 iterations.

After deflation it takes 6 further steps for the next pair and all together only 28 steps for the whole matrix to converge.

Note, that the lower right plot of the residual norm indicates quadratic convergence.  $\square$

In order to explain the observed quadratic convergence, we now give a result that connects the shifted palindromic QR iteration with the rational QZ iteration described in [23]. Recall, that a rational QZ step with numerator shift  $\mu$  and denominator shift  $\theta$  applied to a pencil  $(B, C)$  consists of a QZ step with shift  $\mu$  followed by a ZQ step with shift  $\theta$ . The standard choices for the shifts are  $\mu = \frac{b_{nn}}{c_{nn}}$  and  $\theta = \frac{b_{11}}{c_{11}}$ . For this choice, the rational QZ algorithm is observed to converge quadratically.

LEMMA 10. Let  $A \in \mathbb{C}^{n,n}$  be non-singular and assume that  $\kappa = \frac{a_{1n}}{a_{n1}^*}$  is not an exact eigenvalue of  $(A, A^*)$ . Let  $A_2$  be the result of two shifted palindromic QR steps applied to  $A$ , both steps using  $\kappa$  as shift. Set  $S = A_2^{-*} A_2$ .

Further, define  $B = FA$ , and  $C = FA^*$ ,  $\mu = \frac{b_{nn}}{c_{nn}}$ ,  $\theta = \frac{b_{11}}{c_{11}}$ . Let  $B_2, C_2$  be the result of a rational QZ step applied to  $(B, C)$  using the standard shifts  $\mu, \theta$ . Set  $T = C_2^{-1} B_2$ .

Then there exists a unitary, diagonal matrix  $D$  such that  $S = DTD^*$ .

*Proof.* The QZ step starts by forming the QR factorization

$$B - \mu C = Q_1 R_1, \text{ with } R_1 = \begin{array}{c} \diagdown \\ \diagup \end{array},$$

followed by the RQ factorization  $Q_1^* C = C_1 Z_1$ , where  $C_1$  is upper triangular. The results of the QZ step are  $B_1 = Q_1^* B Z_1^*$  and  $C_1 = Q_1^* C Z_1^*$ . The following ZQ step proceeds by forming the RQ factorization

$$B_1 - \theta C_1 = R_2 Z_2, \text{ with } R_2 = \begin{array}{c} \diagdown \\ \diagup \end{array},$$

followed by the QR factorization  $C_1 Z_2^* = Q_2 C_2$ , where  $C_2$  is upper triangular. This results in  $B_2 = Q_2^* B_1 Z_2^*$ ,  $C_2 = Q_2^* C_1 Z_2^*$ . Thus, with  $Q := Z_2 Z_1$ , we have  $T = C_2^{-1} B_2 = Z_2 Z_1 A^{-*} A Z_1^* Z_2^* = Q A^{-*} A Q^*$ .

On the other hand, two palindromic QR steps proceed as follows

$$\begin{aligned} A - \kappa A^\star &= \tilde{Q}_1 \tilde{R}_1, \quad \text{with } \tilde{R}_1 = \begin{array}{|c} \triangle \\ \hline \end{array}, \\ A_1 &= \tilde{Q}_1^\star A \tilde{Q}_1^{\star\star}, \\ A_1 - \kappa A_1^\star &= \tilde{Q}_2 \tilde{R}_2, \quad \text{with } \tilde{R}_2 = \begin{array}{|c} \triangle \\ \hline \end{array}, \\ A_2 &= \tilde{Q}_2^\star A_1 \tilde{Q}_2^{\star\star}. \end{aligned}$$

Thus, with  $\tilde{Q} := \tilde{Q}_2^\star \tilde{Q}_1^\star$  it follows that  $S = A_2^{-\star} A_2 = \tilde{Q}_2^\star \tilde{Q}_1^\star A^{-\star} A \tilde{Q}_1^{\star\star} \tilde{Q}_2^{\star\star} = \tilde{Q} A^{-\star} A \tilde{Q}^\star$ .

In the following, we show, that both matrices  $Q$ , and  $\tilde{Q}$  define QR factorizations of  $K := (A - \kappa A^\star)^{-\star} (A - \kappa A^\star)$ . Indeed,

$$\begin{aligned} \tilde{Q}K &= \tilde{Q}_2^\star \tilde{Q}_1^\star (A - \kappa A^\star)^{-\star} \tilde{Q}_1 \tilde{Q}_1^\star (A - \kappa A^\star) \\ &= (\tilde{Q}_2^\star \tilde{Q}_1^\star (A - \kappa A^\star) \tilde{Q}_1^{\star\star})^{-\star} \tilde{Q}_1^\star (A - \kappa A^\star) \\ &= (\tilde{Q}_2^\star (A_1 - \kappa A_1^\star))^{-\star} \tilde{Q}_1^\star (A - \kappa A^\star) \\ &= \tilde{R}_2^{-\star} \tilde{R}_1 = \begin{array}{|c} \nabla \\ \hline \end{array} \cdot \begin{array}{|c} \triangle \\ \hline \end{array} = \begin{array}{|c} \nabla \\ \hline \end{array}. \end{aligned}$$

On the other hand, noting that  $\kappa = \frac{a_{1n}}{a_{n1}} = \frac{b_{nn}}{c_{nn}} = \mu$  and  $\kappa = \frac{a_{1n}}{a_{n1}} = \frac{c_{11}^\star}{b_{11}^\star} = \frac{1}{\theta^\star}$ , we have

$$\begin{aligned} QK &= Z_2 Z_1 (A - \kappa A^\star)^{-\star} (A - \kappa A^\star) \\ &= ((A^\star - \frac{1}{\theta^\star} A) Z_1^\star Z_2^\star)^{-1} F Q_1 Q_1^\star F (A - \mu A^\star) \\ &= (Q_1^\star (C - \frac{1}{\theta^\star} B) Z_1^\star Z_2^\star)^{-1} Q_1^\star (B - \mu C) \\ &= \frac{1}{\theta^\star} ((\theta^\star C_1 - B_1) Z_2^\star)^{-1} Q_1^\star (B - \mu C) \\ &= -\frac{1}{\theta^\star} R_2^{-1} R_1 = \begin{array}{|c} \nabla \\ \hline \end{array} \cdot \begin{array}{|c} \nabla \\ \hline \end{array} = \begin{array}{|c} \nabla \\ \hline \end{array}. \end{aligned}$$

Since the QR factorization of the non-singular matrix  $K$  is unique up to a unitary diagonal factor, there exists a unitary and diagonal  $D$  such that  $\tilde{Q} = DQ$ . Thus,  $S = \tilde{Q} A^{-\star} A \tilde{Q}^\star = DQA^{-\star}AQ^\star D^\star = DTD^\star$ .  $\square$

**3.1. Multiple shifts.** In order to get even faster convergence, it is natural to employ multiple shifts in a single iteration. If one tries two shifts an obvious shift function to use is

$$f(\lambda) = \frac{\lambda - \kappa_1}{1 - \kappa_1^\star \lambda} \cdot \frac{\lambda - \kappa_2}{1 - \kappa_2^\star \lambda}.$$

However, it is not clear how a shifted pencil  $(\tilde{A}, \tilde{A}^\star)$  can be constructed from  $A$  such that an eigenpair  $(\lambda, x)$  of  $(A, A^\star)$  corresponds to an eigenpair  $(f(\lambda), x)$  of  $(\tilde{A}, \tilde{A}^\star)$ . We will come back to this problem later, see Algorithm 4 below.

The situation is different with three shifts! By direct calculation (analogous to the proof of Lemma 9) it is easy to verify that if  $(\lambda, x)$  is an eigenpair of  $(A, A^\star)$ , then

$$\underbrace{(A - \kappa_3 A^\star)(A - \kappa_2 A^\star)^{-\star}(A - \kappa_1 A^\star)}_{\tilde{A}} x = \tilde{\lambda} \underbrace{(A^\star - \kappa_1^\star A)(A^\star - \kappa_2^\star A)^{-\star}(A^\star - \kappa_3^\star A)}_{\tilde{A}^\star} x$$

with

$$\tilde{\lambda} = f(\lambda) = \frac{\lambda - \kappa_1}{1 - \kappa_1^\star \lambda} \cdot \frac{\lambda - \kappa_2}{1 - \kappa_2^\star \lambda} \cdot \frac{\lambda - \kappa_3}{1 - \kappa_3^\star \lambda}.$$

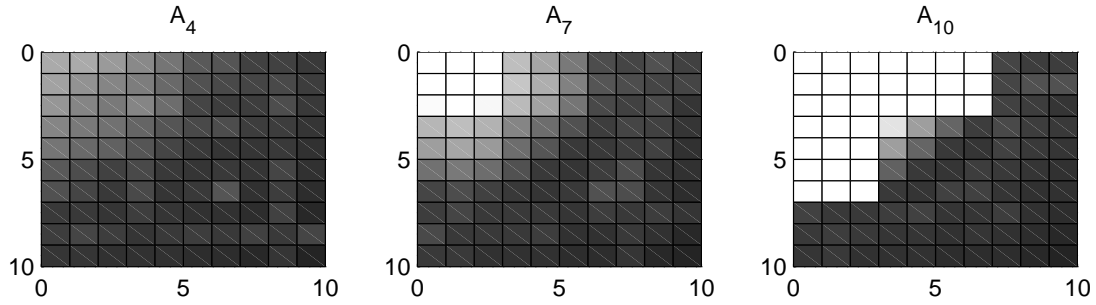


FIG. 3.2. Convergence history of the palindromic QR iteration using 3 shifts

More generally, for any odd number of shifts,  $k$ , the shifted matrix is given by

$$\tilde{A} = (A - \kappa_k A^*)(A - \kappa_{k-1} A^*)^{-*} (A - \kappa_{k-2} A^*) \cdots (A - \kappa_2 A^*)^{-*} (A - \kappa_1 A^*). \quad (3.5)$$

This corresponds to the eigenvalue transformation

$$\tilde{\lambda} = f(\lambda) = \prod_{i=1}^k \frac{\lambda - \kappa_i}{1 - \kappa_i^* \lambda},$$

i.e., all eigenvalues near one of the shifts get mapped approximately to 0. Hence, one palindromic QR step applied to the shifted pencil will drive convergence towards the (typically  $k$ ) eigenvalues near  $\kappa_1, \dots, \kappa_k$  and the multi-shift algorithm can be expected to converge to a block skew triangular form (2.9) with  $p = k$ , so that the problem can be deflated.

A *multi shift palindromic QR step* is very similar to the single-shift variant, except for the formation of the shifted matrix  $\tilde{A}$ .

ALGORITHM 3. Multi shift palindromic QR step (odd  $k$ )

- 1: choose  $\kappa_1, \dots, \kappa_k$
- 2:  $\tilde{A} \leftarrow (A - \kappa_k A^*)(A - \kappa_{k-1} A^*)^{-*} \cdots (A - \kappa_1 A^*)$
- 3:  $\tilde{A} \rightarrow QR$  with  $R = \begin{array}{c} \diagup \\ \square \end{array}$
- 4:  $A_1 \leftarrow Q^* A Q^{**}$

The the shifts,  $\kappa_1, \dots, \kappa_k$ , can chosen similarly than in the single-shift case. Partition  $A$  as

$$A = \begin{array}{ccc} & k & n-2k & k \\ k & \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} & & \end{array}$$

and use the eigenvalues of the pencil  $(A_{13}, A_{31}^*)$  as shifts. This will give good approximations to eigenvalues of  $(A, A^*)$  if  $A_{11}$ ,  $A_{12}$ , and  $A_{21}$  are small in norm.

EXAMPLE 3. We have applied Algorithm 3 for  $k = 3$  to the matrix from Example 1 and plotted the results in Figure 3.2. After 10 iterations a block of 3 eigenvalue pairs converged.  $\square$  The following results relate the single-shift and the multi-shift palindromic QR algorithms. The results will be used in a later section. The first lemma states that one multi-shift palindromic QR step with the shifts  $\kappa_1, \dots, \kappa_k$  is equivalent to  $k$  single-shift steps with the same shifts.

LEMMA 11. Let  $A \in \mathbb{C}^{n,n}$  such that  $(A, A^*)$  is a regular pencil. Let  $\kappa_1, \dots, \kappa_k$  be an odd number of complex numbers, that are not exact eigenvalues of  $(A, A^*)$  and that satisfy  $\kappa_i^* \kappa_i \neq 1$ . Let  $A_k$  be the result of  $k$  steps of the single-shift palindromic QR iteration (Algorithm 2) applied to  $A$  using the shifts  $\kappa_1, \dots, \kappa_k$ . Further, define  $A_+$  as the result of one multi-shift palindromic QR step (Algorithm 3) applied to  $A$ , using the shifts  $\kappa_1, \dots, \kappa_k$ .

Then there exists a unitary diagonal matrix  $D$  such that  $A_+ = D^* A_k D$ .

*Proof.* The imposed requirements on the shifts assure the existence of the inverses used below. Applying  $k$  single-shift steps to  $A$  amounts to

$$\begin{aligned} A_{i-1} - \kappa_i A_{i-1}^{\star} &=: Q_i R_i, \text{ with } R_i = \begin{array}{|c} \diagup \\ \hline \end{array}, \\ A_i &:= Q_i^* A_{i-1} Q_i^{*\star}, i = 1, \dots, k, \end{aligned}$$

with  $A_0 = A$ . Define  $V_i := Q_1 \cdots Q_i$  and note that  $V_i^*(A - \kappa_i A^{\star})V_{i-1}^{*\star} = R_i$  and  $V_k^* A V_k^{*\star} = A_k$ . Further, set

$$R := R_k R_{k-1}^{-\star} R_{k-2} \cdots R_2^{-\star} R_1 = \begin{array}{|c} \diagup \\ \hline \end{array} \cdot \begin{array}{|c} \diagdown \\ \hline \end{array} \cdot \begin{array}{|c} \diagup \\ \hline \end{array} \cdots \begin{array}{|c} \diagdown \\ \hline \end{array} \cdot \begin{array}{|c} \diagup \\ \hline \end{array} = \begin{array}{|c} \diagup \\ \hline \end{array}.$$

Then  $V_k R$  is a skew QR factorization of  $\tilde{A}$  (as defined in (3.5)), since

$$\begin{aligned} V_k R &= V_k R_k R_{k-1}^{-\star} R_{k-2} \cdots R_2^{-\star} R_1 \\ &= (V_k R_k V_{k-1}^{\star})(V_{k-1} R_{k-1} V_{k-2}^{\star})^{-\star} \cdots (V_2 R_2 V_1^{\star})^{-\star} (V_1 R_1) \\ &= (A - \kappa_k A^{\star})(A - \kappa_{k-1} A^{\star})^{-\star} (A - \kappa_{k-2} A^{\star}) \cdots (A - \kappa_2 A^{\star})^{-\star} (A - \kappa_1 A^{\star}) \\ &= \tilde{A}. \end{aligned}$$

Hence, an application of the multi-shift palindromic QR step using this skew QR factorization yields  $A_+ = V_k^* A V_k^{*\star} = A_k$ . The result follows, since skew QR factorizations of nonsingular matrices are unique up to a unitary diagonal factor.  $\square$

From the proof, it is easy to derive the following implicit variant of Algorithm 3 that does not involve inverted matrices.

ALGORITHM 4. Multi-shift palindromic QR step (general  $k$ )

- 1: choose  $\kappa_1, \dots, \kappa_k$
- 2: for  $i = 1, \dots, k$  do  $(A - \kappa_i A^{\star})Q_{i-1}^{*\star} \rightarrow Q_i R_i$  with  $R_i = \begin{array}{|c} \diagup \\ \hline \end{array}$ ,  $Q_0 = I$
- 3:  $A_1 \leftarrow Q_k^* A Q_k^{*\star}$

Note, that this variant is not restricted to odd  $k$ . For even  $k$ , the shifted matrix is given by

$$\tilde{A} = (A - \kappa_k A^{\star})^{-\star} (A - \kappa_{k-1} A^{\star}) \cdots (A - \kappa_2 A^{\star})^{-\star} (A - \kappa_1 A^{\star}). \quad (3.6)$$

In the even case, however, if  $x$  is an eigenvector of  $(A, A^{\star})$  it does *not* mean that  $x$  is also eigenvector of  $(\tilde{A}, \tilde{A}^{\star})$ . Therefore, the original and the shifted pencils are not related as strongly as in the case of an odd number of shifts. From here on,  $k$  is no longer restricted to be odd. The next lemma is about the order of the steps.

LEMMA 12. *Let  $A \in \mathbb{C}^{n,n}$  be non-singular and  $k \in \mathbb{N}$ . Further, suppose that none of the shifts  $\kappa_1, \dots, \kappa_k$  is an exact eigenvalue of  $(A, A^{\star})$ . Then  $\tilde{A}$  as of (3.5) or (3.6) is independent of the orders of the odd numbered shifts  $(\kappa_1, \kappa_3, \kappa_5, \dots)$  and the even numbered shifts  $(\kappa_2, \kappa_4, \kappa_6, \dots)$ .*

*Proof.* The assumptions imply that every inverse used in the following exists. The shifted matrix  $\tilde{A}$  can be written as a product of  $k$  matrices as follows,

$$\tilde{A} = \cdots \underbrace{(A - \kappa_4 A^{\star})^{-\star}}_{B_4} \underbrace{(A - \kappa_3 A^{\star})}_{B_3} \underbrace{(A - \kappa_2 A^{\star})^{-\star}}_{B_2} \underbrace{(A - \kappa_1 A^{\star})}_{B_1}.$$

It is enough to show that exchanging  $\kappa_i$  with  $\kappa_{i+2}$  does not change  $\tilde{A}$  as then any order within the sets of shifts with even/odd indices can be reached. Since exchanging  $\kappa_i$  with  $\kappa_{i+2}$  leaves the first  $(k - i - 2)$  factors and the last  $(i - 1)$  ones unchanged, it suffices to prove that

$$B_{i+2} B_{i+1} B_i = B_i B_{i+1} B_{i+2}. \quad (3.7)$$

Assume that  $i$  is odd. Then,

$$\begin{aligned} B_{i+2} B_{i+1} B_i &= A B_{i+1} A - \kappa_{i+2} A^{\star} B_{i+1} A - \kappa_i A B_{i+1} A^{\star} + \kappa_{i+2} \kappa_i A^{\star} B_{i+1} A^{\star}, \\ B_i B_{i+1} B_{i+2} &= A B_{i+1} A - \kappa_{i+2} A B_{i+1} A^{\star} - \kappa_i A^{\star} B_{i+1} A + \kappa_{i+2} \kappa_i A^{\star} B_{i+1} A^{\star}. \end{aligned}$$

So, (3.7) holds if and only if  $AB_{i+1}A^\star = A^\star B_{i+1}A$ . This is indeed the case since

$$\begin{aligned}
AB_{i+1}A^\star &= A(A - \kappa_{i+1}A^\star)^{-\star}A^\star \\
&= (A^{-\star}(A - \kappa_{i+1}A^\star)A^{-1})^{-\star} \\
&= (A^{-\star}AA^{-1} - \kappa_{i+1}A^{-\star}A^\star A^{-1})^{-\star} \\
&= (A^{-1}AA^{-\star} - \kappa_{i+1}A^{-1}A^\star A^{-\star})^{-\star} \\
&= (A^{-1}(A - \kappa_{i+1}A^\star)A^{-\star})^{-\star} \\
&= A^\star(A - \kappa_{i+1}A^\star)^{-\star}A = A^\star B_{i+1}A.
\end{aligned}$$

If  $i$  is even we prove  $(B_{i+2}B_{i+1}B_i)^{-\star} = (B_iB_{i+1}B_{i+2})^{-\star}$  instead. The proof is the same.  $\square$

This lemma can be used to construct a method for real matrices. If  $A$  is real and both, the even numbered shifts and the odd numbered shifts, are closed under complex conjugation, then  $\tilde{A}$  is real as well and with it also the next iterate  $A_1$ . We show this for  $k = 4$ . The general case follows analogously. So, let  $\kappa_1, \dots, \kappa_4$  be four complex shifts with  $\kappa_3 = \overline{\kappa_1}$  and  $\kappa_4 = \overline{\kappa_2}$ . We have for  $\tilde{A}$

$$\begin{aligned}
\tilde{A} &= \overline{(A - \overline{\kappa_2}A^T)^{-T}(A - \overline{\kappa_1}A^T)(A - \kappa_2A^T)^{-T}(A - \kappa_1A^T)} \\
&= (A - \kappa_2A^T)^{-T}(A - \kappa_1A^T)(A - \overline{\kappa_2}A^T)^{-T}(A - \overline{\kappa_1}A^T) \\
&\stackrel{(\text{Lemma 12})}{=} (A - \overline{\kappa_2}A^T)^{-T}(A - \overline{\kappa_1}A^T)(A - \kappa_2A^T)^{-T}(A - \kappa_1A^T) = \tilde{A}.
\end{aligned}$$

To summarize, as expected, shifting greatly reduces the number of necessary iterations of the palindromic QR algorithm. Based on our observations with single shifts it takes on average 6 to 8 iterations for a reciprocal eigenvalue pair to converge. Thus, on average  $\mathcal{O}(n)$  iterations seem to be enough to get all the eigenvalues.

**4. Skew Hessenberg matrices.** The dominating operation in a palindromic QR step is the skew QR factorization which takes  $\mathcal{O}(n^3)$  floating point operations. This makes the whole iteration an expensive  $\mathcal{O}(n^4)$  process. The standard QR algorithm has the same problem, but for Hessenberg matrices the cost is reduced by one order of magnitude. In this section we introduce Hessenberg-like matrices that play an analogous role for the palindromic QR algorithm.

**DEFINITION 13.** A square matrix  $A \in \mathbb{C}^{n,n}$  is called skew Hessenberg, if  $a_{ij} = 0$  whenever  $i + j < n$ . Such a matrix is depicted by  $A = \begin{array}{c} \diagdown \\ \square \\ \diagup \end{array}$ .

A skew QR factorization of a skew Hessenberg matrix can be achieved by a series of  $n - 1$  Givens rotations and can thus be computed in  $\mathcal{O}(n^2)$  operations. Therefore, if the result of a palindromic QR step applied to a skew Hessenberg matrix is again skew Hessenberg, then the whole algorithm will be one order of magnitude faster than for general matrices. The following result states that although this is *not* the case, an equally attractive statement holds.

**THEOREM 14.** Let  $A \in \mathbb{C}^{n,n}$  be non-singular. Further, suppose that none of the values  $\kappa_1, \dots, \kappa_k$  with  $\kappa_i^\star \kappa_i \neq 1$  is an exact eigenvalue of  $(A, A^\star)$ . Let  $A_2$  be the result of two multi-shift palindromic QR steps, the first using the shifts  $\kappa_1, \dots, \kappa_k$ , the second using the shifts  $\kappa_k, \dots, \kappa_1$ . Then there is an upper triangular matrix  $R$  with  $A_2 = R^\star AR$ .

In particular, if  $A$  is skew Hessenberg then so is  $A_2$ .

*Proof.* Case 1 (unshifted, i.e.,  $k = 1, \kappa_1 = 0$ ): Applying two palindromic QR steps to  $A$  yields

$$\begin{aligned}
A &= Q_1 R_1, \text{ with } R_1 = \begin{array}{c} \diagdown \\ \square \\ \diagup \end{array}, & A_1 &= R_1 Q_1^{\star\star}, \\
A_1 &= Q_2 R_2, \text{ with } R_2 = \begin{array}{c} \diagdown \\ \square \\ \diagup \end{array}, & A_2 &= R_2 Q_2^{\star\star}.
\end{aligned} \tag{4.1}$$

From (4.1) we have  $A^{-\star} = Q_1^{\star\star} R_1^{-\star}$ , thus  $A_1 = R_1 A^{-\star} R_1^\star$ . Analogously,

$$A_2 = R_2 A_1^{-\star} R_2^\star = R_2 R_1^{-\star} A R_1^{-1} R_2^\star = R^\star A R,$$

where  $R := R_1^{-1} R_2^\star = \begin{array}{c} \diagup \\ \square \\ \diagdown \end{array} \cdot \begin{array}{c} \diagdown \\ \square \\ \diagup \end{array} = \begin{array}{c} \square \\ \diagdown \\ \diagup \end{array}$  is upper triangular.

Case 2 (single shift, i.e.,  $k = 1$ ,  $\kappa_1 \neq 0$ ): The procedure of two single-shift palindromic QR steps with the same shift  $\kappa_1$  is described as follows:

- 1: shift with  $\kappa_1$ ,
- 2: apply unshifted palindromic QR step,
- 3: unshift with  $\kappa_1$ ,
- 4: shift with  $\kappa_1$ ,
- 5: apply unshifted palindromic QR step,
- 6: unshift with  $\kappa_1$ .

Steps 3 and 4 cancel each other. Hence, the two unshifted palindromic QR steps are carried out successively. Thus, as in case 1, there is an upper triangular  $R$  such that  $A_2$  can be written as

$$\begin{aligned} A_2 &= \frac{1}{1 - \kappa_1^* \kappa_1} (\tilde{A}_2 + \kappa_1 \tilde{A}_2^*) = \frac{1}{1 - \kappa_1^* \kappa_1} (R^* \tilde{A} R + \kappa_1 (R^* \tilde{A} R)^*) \\ &= \frac{1}{1 - \kappa^* \kappa} (R^* (A - \kappa A^*) R + \kappa R^* (A - \kappa A^*)^* R) \\ &= R^* A R. \end{aligned}$$

Case 3 (multi-shift, i.e.,  $k > 1$ ): By Lemma 11, performing two steps of the multi-shift palindromic QR iteration, one with the shifts  $\kappa_1, \dots, \kappa_k$ , the second one with the shifts  $\kappa_k, \dots, \kappa_1$ , equals carrying out one step with the  $2k - 1$  shifts

$$\kappa_1, \dots, \kappa_k, \kappa_k, \kappa_{k-1}, \dots, \kappa_2 \quad (4.2)$$

followed by a single-shift step with shift  $\kappa_1$ . Within the sequence (4.2), the set of shifts with odd index consists of all shifts  $\kappa_1, \dots, \kappa_k$ , while the set of shifts with even index consists of  $\kappa_2, \kappa_3, \dots, \kappa_k$ . Hence, by Lemma 12, both sets can be reordered to change the sequence (4.2) into  $\kappa_k, \kappa_k, \kappa_{k-1}, \kappa_{k-1}, \dots, \kappa_2, \kappa_2, \kappa_1$ . A palindromic QR step with these shifts followed by a single-shift step using  $\kappa_1$  is, by Lemma 11, equivalent to two single-shift steps with  $\kappa_k$  followed by two single-shift steps with  $\kappa_{k-1}$ , and so on. Hence, by case 2, there are upper triangular matrices  $R_k, \dots, R_1$ , such that  $A_2$  can be written as  $A_2 = R_1^* (R_2^* \cdots (R_k^* A R_k) \cdots R_2) R_1 = R^* A R$ , where  $R = R_k \cdots R_2 R_1$  is upper triangular.

Finally, if  $A$  is skew Hessenberg, then so is  $A_2 = R^* A R = \begin{smallmatrix} \diagdown & & \\ & \diagup & \\ & & \diagdown \end{smallmatrix} = \begin{smallmatrix} \diagup & & \\ & \diagdown & \\ & & \diagup \end{smallmatrix}$ .  $\square$

REMARK 15. It is not surprising and easy to show that the first iterate  $A_1$  has some structure, as well. It belongs to the set of matrices that, in the spirit of [8], could be called skew generalized Hessenberg matrices. Such a matrix fulfills  $\text{rank}(A(1:i+1, 1:n-i)) = 1$  for  $i = 1, \dots, n-2$ .  $\square$

We have motivated our interest in skew Hessenberg matrices with the fact that they can be factored in  $\mathcal{O}(n^2)$  flops. But Theorem 14 tells that only every second iterate is again a skew Hessenberg matrix. Thus, in every other palindromic QR step still a full matrix has to be factored. Fortunately, the computations of two consecutive steps can be reordered to be carried out in  $\mathcal{O}(n^2)$  flops.

ALGORITHM 5. Unshifted palindromic QR double step for skew Hessenberg matrices

- 1: **for**  $i = 1, \dots, n-1$  **do**
- 2:  $A \leftarrow G_i^* A$  where  $G_i$  is a Givens rotation such that  $G_i^* A(n-i:n-i+1, i) = \begin{bmatrix} 0 \\ * \end{bmatrix}$
- 3: **end for**
- 4: **for**  $i = 1, \dots, n-1$  **do**
- 5:  $A \leftarrow A G_i$
- 6:  $A \leftarrow \tilde{G}_i^* A$  where  $\tilde{G}_i$  is a Givens rotation such that  $\tilde{G}_i^* A(i:i+1, n-i) = \begin{bmatrix} 0 \\ * \end{bmatrix}$
- 7: **end for**
- 8: **for**  $i = 1, \dots, n-1$  **do**
- 9:  $A \leftarrow A \tilde{G}_i$
- 10: **end for**

EXAMPLE 4. For  $n = 3$  Algorithm 5 proceeds as follows. The first for-loop computes

$$A = \begin{bmatrix} x & x \\ x & x & x \\ x & x & x \end{bmatrix}, G_1^* A = \begin{bmatrix} x & x \\ 0 & x & x \\ x & x & x \end{bmatrix}, G_2^* G_1^* A = \begin{bmatrix} 0 & x \\ x & x \\ x & x & x \end{bmatrix} = R_1.$$

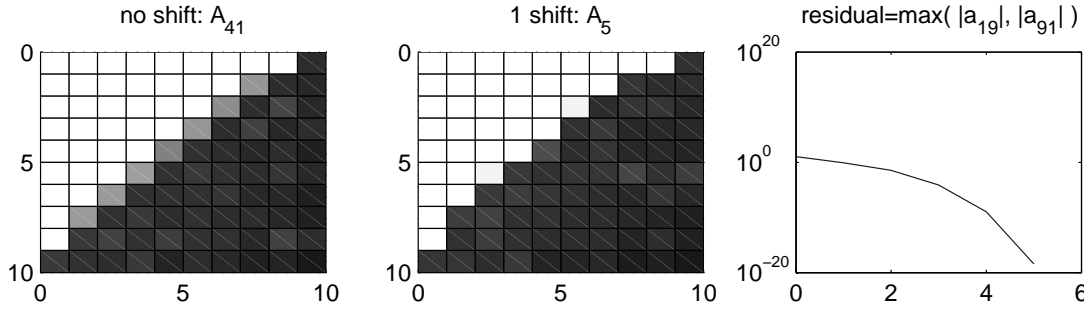


FIG. 4.1. The unshifted algorithm needs 41 double steps until the first eigenvalue pair has converged. When using single shifting this number decreases to 5 and the third graph indicates quadratic convergence.

The second for-loop computes

$$R_1 G_1 = \begin{bmatrix} x & x \\ x & x \\ x & x \end{bmatrix}, \tilde{G}_1^* R_1 G_1 = \begin{bmatrix} 0 & x \\ x & x \\ x & x \end{bmatrix}, \tilde{G}_1^* R_1 G_1 G_2 = \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix}, \tilde{G}_2^* \tilde{G}_1^* R_1 G_1 G_2 = \begin{bmatrix} 0 & x & x \\ x & x & x \\ x & x & x \end{bmatrix} = R_2.$$

Finally, the third for-loop computes

$$R_2 \tilde{G}_1 = \begin{bmatrix} x & x \\ x & x & x \\ x & x & x \end{bmatrix}, R_2 \tilde{G}_1 \tilde{G}_2 = \begin{bmatrix} x & x \\ x & x & x \\ x & x & x \end{bmatrix}.$$

The latter is the result which is in skew Hessenberg form.  $\square$

LEMMA 16. Let  $A \in \mathbb{C}^{n,n}$  be a nonsingular skew Hessenberg matrix. Let  $A_2$  be the result of two steps of Algorithm 1 and let  $A_+$  be the result of Algorithm 5. Then there exists a unitary diagonal matrix  $D$  such that  $A_2 = D^* A_+ D$ .

*Proof.* We need some intermediate results of Algorithm 5. Let  $R_1, R_2$  be the value of the matrix  $A$  at the end of the first and second respectively second for loop. Note that  $R_1$  and  $R_2$  are skew triangular. Set  $Q_1 = G_1 G_2 \cdots G_{n-1}$  and  $Q_2 = \tilde{G}_1 \tilde{G}_2 \cdots \tilde{G}_{n-1}$ . Note that  $R_1 = Q_1^* A$ , so  $Q_1^* R_1$  is a skew QR factorization of  $A$ . Note further that  $R_2 = Q_2^* R_1 Q_1$ , and thus  $Q_2^* R_2$  is a skew QR factorization of  $R_1 Q_1 =: A_1$ . Finally, we have  $A_+ = R_2 Q_2$ . The assertion follows, since skew QR factorizations of nonsingular matrices are unique up to a unitary diagonal factor.  $\square$

Employing shifts is now straightforward.

ALGORITHM 6. Single-shift palindromic QR double step for Hessenberg matrices

- 1: choose  $\kappa$
- 2:  $\tilde{A} \leftarrow A - \kappa A^*$
- 3: apply Algorithm 5 to  $\tilde{A}$  yielding  $\tilde{A}_1$
- 4:  $A_1 \leftarrow \frac{1}{1 - \kappa^* \kappa} (\tilde{A}_1 + \kappa \tilde{A}_1^*)$

As before, the last unshifting step can be carried out in an alternative way by applying the transformations  $G_i, \tilde{G}_i$  directly to  $A$ . As mentioned before, the latter approach is more stable. However, during the course of the step the matrix becomes fully populated and although  $A_1$  is a skew Hessenberg matrix in exact arithmetic, this may numerically not be the case. Developing an implicit version of Algorithm 6 is topic of a subsequent paper.

EXAMPLE 5. We applied Algorithms 5, and 6, to a skew Hessenberg matrix constructed as follows: let  $\tilde{A}$  be the 10-by-10 matrix from Example 1. We computed the unitary matrix  $Q$  that transforms  $\hat{A} = \tilde{A}(1:9, 1:9)$  to palindromic Schur form by the single-shift palindromic QR iteration. Then, with  $\tilde{Q} = Q \oplus 1$ ,  $A := \tilde{Q}^T \tilde{A} \tilde{Q}$  is a skew Hessenberg matrix. Since  $Q$  happened to be real also  $A$  is real.

Figure 4.1 shows plots of the matrix after convergence of the first eigenvalue pair.  $\square$

Summarizing, skew Hessenberg matrices are for the palindromic QR algorithm, what Hessenberg matrices are for the standard QR algorithm. For these matrices the iterations can be carried out one order of magnitude faster than for general matrices.

**5. On the reduction to skew Hessenberg form.** In this section we aim at developing a direct algorithm of complexity  $\mathcal{O}(n^3)$  that reduces a given matrix  $A$  with a unitary matrix  $Q \in \mathbb{C}^{n,n}$  to  $Q^\star A Q$  which has skew Hessenberg structure. Unfortunately, this task is related to an unsolved problem concerning Hamiltonian matrices. A matrix  $H \in \mathbb{R}^{2n,2n}$  is called *Hamiltonian* if  $JH = (JH)^T$ , where  $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$ . The Hamiltonian eigenvalue problem has attracted a lot of interest, see, e.g., [1, 2, 3, 4, 6, 14, 17, 18, 22] and the references therein. A structure preserving QR-like algorithm has been developed in [5], but the reduction to a Hessenberg-like form is missing.

Any Hamiltonian eigenvalue problem can be transformed into a palindromic eigenvalue problem as follows

$$Hx = \lambda x \quad \Leftrightarrow \quad JHx = \lambda Jx \quad \Leftrightarrow \quad (JH + J)x = \frac{\lambda + 1}{\lambda - 1}(JH - J)x \quad \Leftrightarrow \quad Ax = \mu A^T x$$

with  $A = JH + J$  and  $\mu = \frac{\lambda + 1}{\lambda - 1}$ . Thus it is not surprising that the palindromic eigenvalue problem inherits some of the complications arising in the Hamiltonian eigenvalue problem.

In the following, we will present our various approaches to the skew Hessenberg reduction, discuss why they fail and draw connections to the Hamiltonian case. Closing this section we discuss special situations in which the transformation is known.

The first approach is to determine a matrix of the form  $Q \oplus 1$  where  $Q$  is a matrix that skew triangularizes  $A_{1:n-1,1:n-1}$ , the leading principal submatrix of  $A$ . Indeed, if such a matrix exists, then

$$(Q \oplus 1)^\star A (Q \oplus 1) = \begin{matrix} n-1 & 1 \\ \begin{bmatrix} \triangle & \vdots \\ * \dots * & * \end{bmatrix} \\ 1 \end{matrix} = \begin{matrix} \triangle & \vdots \\ * \dots * & * \end{matrix}$$

A setting where this approach is successful are projection methods, usually used for large and sparse problems. In the  $k$ -th iteration of a projection method a palindromic eigenvalue problem has to be solved for a  $k$  by  $k$  matrix  $A_k$  that arises from the matrix  $A_{k-1}$  from the last iteration by adding a further row and column. Hence, the wanted matrix  $Q$  that skew triangularizes the leading principal submatrix of  $A_k$  is just the solution of the last iteration.

In the general setting however, the matrix  $Q$  is not available and its computation would require to solve a palindromic eigenvalue problem of size  $n-1$  which takes  $\mathcal{O}(n^4)$  flops without a reduction to skew Hessenberg form. Also a recursive approach would take  $\mathcal{O}(n^4)$  flops. So, this choice is not practical in general, but for  $\star = T$  it proves existence of a transformation to skew Hessenberg form (by Remark 4).

A different approach is based on the observation that the leading principal submatrix of a skew Hessenberg matrix of size  $\lfloor \frac{n}{2} \rfloor - 1$  is zero. Therefore, it is reasonable to generate a zero block in the upper left corner of  $A$ . We illustrate this with a 5-by-5 matrix:

$$A = \left[ \begin{array}{cc|ccc} * & * & * & * & * \\ * & * & * & * & * \\ \hline * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{array} \right] = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix},$$

where  $A$  is partitioned according to the lines. We begin by generating a zero in the top left corner by solving the 2 by 2 palindromic problem for  $A_{11}$ , i.e., by computing a 2-by-2 unitary matrix  $Q$  with  $Q^\star A_{11} Q = \begin{bmatrix} 0 & * \\ * & * \end{bmatrix}$  and applying a congruence with  $(Q \oplus I)$  to  $A$ . Again, in the  $\star = T$  case such  $Q$  always exists, while in the case  $\star = *$  we have to assume that it does. This results in

$$\tilde{A} = (Q \oplus I)^\star A (Q \oplus I) = \left[ \begin{array}{c|cccc} 0 & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{array} \right] = \begin{bmatrix} 0 & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{22} \end{bmatrix}.$$



We then introduce zeros in the first row and column. To this end, let  $H \in \mathbb{C}^{4,4}$  be a unitary matrix such that  $[\hat{A}_{21}, \hat{A}_{12}^\star]^\star H = \begin{bmatrix} 0 & 0 & 0 & * \\ 0 & 0 & * & * \end{bmatrix}$ . Then, applying a congruence with  $(1 \oplus H)$  to  $\hat{A}$  yields

$$\hat{A} = (1 \oplus H)^\star \tilde{A} (1 \oplus H) = \left[ \begin{array}{ccc|cc} 0 & 0 & 0 & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \\ \hline 0 & * & * & * & * \\ * & * & * & * & * \end{array} \right] = \begin{bmatrix} 0 & 0 & \hat{A}_{13} \\ 0 & \hat{A}_{22} & \hat{A}_{23} \\ \hat{A}_{31} & \hat{A}_{32} & \hat{A}_{33} \end{bmatrix}.$$

In order to preserve the zeros just generated, we restrict our further actions to the submatrix  $\hat{A}_{22}$  that arises from  $\hat{A}$  by deleting the last two and the first rows and columns. In this case,  $\hat{A}_{22}$  is a 2-by-2 matrix that can be skew triangularized by a unitary  $Q_2$  as  $Q_2^\star \hat{A}_{22} Q_2 = \begin{bmatrix} 0 & * \\ * & * \end{bmatrix}$ . A last congruence with  $(1 \oplus Q_2 \oplus I_2)$  finally gives

$$\check{A} \leftarrow (1 \oplus Q_2 \oplus I_2)^\star \hat{A} (1 \oplus Q_2 \oplus I_2) = \begin{bmatrix} 0 & 0 & 0 & * & * \\ 0 & 0 & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \\ * & * & * & * & * \end{bmatrix}.$$

which actually is in skew Hessenberg form.

Generalizing this procedure to larger dimensions yields the following algorithm.

ALGORITHM 7.

- 1: **if**  $n \leq 1$  **then return**
- 2: compute  $Q \in \mathbb{C}^{2,2}$  unitary, such that  $Q^\star A_{1:2,1:2} Q = \begin{bmatrix} 0 & * \\ * & * \end{bmatrix}$
- 3: **if** such  $Q$  does not exist **then**
- 4:   signal break down, stop
- 5: **end if**
- 6: set  $A \leftarrow (Q \oplus I_{n-2})^\star A (Q \oplus I_{n-2})$
- 7: **if**  $n = 2$  **then return**
- 8: compute  $H \in \mathbb{C}^{n-1, n-1}$  unitary, such that  $H^\star A_{2:n,1} = \alpha e_{n-1}$
- 9: set  $A \leftarrow (1 \oplus H)^\star A (1 \oplus H)$
- 10: compute  $G \in \mathbb{C}^{n-2, n-2}$  unitary, such that  $A_{1,2:n-1} G = \beta e_{n-2}^T$
- 11: set  $A \leftarrow (1 \oplus G \oplus 1)^\star A (1 \oplus G \oplus 1)$
- 12: apply this algorithm to  $A_{2:n-2, 2:n-2}$

Note that the breakdown can only happen in the  $\star = *$  case (see Remark 4).

The result of this algorithm can be postprocessed to get the following condensed form.

LEMMA 17. *Let  $A \in \mathbb{C}^{n,n}$ . Define  $k = \lfloor \frac{n+1}{3} \rfloor$ . If  $\star = *$  assume that  $A$  is such that Algorithm 7 does not break down. Then a unitary matrix  $Q$  can be computed by a direct reduction process of complexity  $\mathcal{O}(n^3)$  such that*

$$Q^\star A Q = \begin{matrix} & & k & & k \\ & & \left[ \begin{array}{ccc} 0 & A_{12} & \square \\ 0 & \square & \square \\ \triangle & \square & \square \end{array} \right] & & \\ k & & & & \end{matrix}, \quad (5.1)$$

where  $A_{12}$  is of one of the following shapes

$$k \begin{bmatrix} 1 & k \\ 0 & \triangle \end{bmatrix}, \quad k \begin{bmatrix} k \\ \triangle \end{bmatrix}, \quad k-1 \begin{bmatrix} k-1 \\ 0 \\ \triangle \end{bmatrix},$$

depending on whether  $n - 3k$  equals 1, 0, or  $-1$ .

*Proof.* If Algorithm 7 does not break down, then it yields a matrix of form

$$A = \begin{matrix} & k & n-k \\ k & \begin{bmatrix} 0 & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \\ n-k & \end{matrix}$$

where  $k = \lfloor \frac{n+1}{3} \rfloor$ . Let  $Q$  be a unitary matrix such that

$$Q^* A_{21} = \begin{matrix} & k \\ n-2k & \begin{bmatrix} 0 \\ \tilde{A}_{31} \end{bmatrix} \end{matrix}, \text{ with } \tilde{A}_{31} = \begin{matrix} \diagup \\ \square \end{matrix}.$$

Then a congruence with  $I_k \oplus Q$  results in

$$\tilde{A} = (I_k \oplus Q)^* A (I_k \oplus Q) = \begin{matrix} & k & n-2k & k \\ k & \begin{bmatrix} 0 & \tilde{A}_{12} & \tilde{A}_{13} \\ 0 & \tilde{A}_{22} & \tilde{A}_{23} \\ \tilde{A}_{31} & \tilde{A}_{21} & \tilde{A}_{22} \end{bmatrix} \\ n-2k & & & \\ k & & & \end{matrix}.$$

Next, the block  $\tilde{A}_{12}$  will be skew triangularized. This block is of dimension  $k$ -by- $(n-2k)$ . The transformation depends on whether  $k \leq n-2k$  or not.

Case 1: Assume  $k \leq n-2k$ . Then let  $Q$  be a unitary matrix such that

$$\tilde{A}_{12} Q = \begin{matrix} & n-3k & k \\ k & \begin{bmatrix} 0 & \diagup \\ \square & \end{bmatrix} \end{matrix}.$$

A congruence with  $(I_k \oplus Q \oplus I_k)$  yields form (5.1).

Case 2: If, on the other hand,  $k > n-2k$ , then define unitary matrices  $Q, Z$  such that

$$Q^* \tilde{A}_{12} = \begin{matrix} & k-1 \\ 1 & \begin{bmatrix} 0 \\ \diagup \\ \square \end{bmatrix} \end{matrix}, Z^* \tilde{A}_{31} Q = \begin{matrix} \diagup \\ \square \end{matrix}$$

and apply a congruence with  $(Q \oplus I_{n-2k} \oplus Z)$  to get form (5.1).  $\square$

It turns out, that Algorithm 7 yields skew Hessenberg structure only for matrices of size  $n$  up to 5. For  $n \geq 6$ , the result can still be described as 'skew triangular with  $k$  additional skew diagonals', but here  $k \approx \frac{n}{3}$  instead of just one (what would correspond to skew Hessenberg form). The form (5.1) is invariant under double steps of the palindromic QR iteration, see Theorem 14. Also, the skew QR factorization of a matrix of form (5.1) needs much less work than for a general matrix, but still requires  $\mathcal{O}(n^3)$  flops. So, the palindromic QR iteration still has a complexity of  $\mathcal{O}(n^4)$ .

In the next section, we introduce another condensed form and give a reason why the transformation to skew Hessenberg form is so difficult to obtain for general matrices.

**5.1. The palindromic PVL form.** In this section we only consider the case  $\star = T$ , because the methods require the diagonal of  $A - A^*$  to be zero, which is not guaranteed for  $\star = *$ . Also, we restrict  $n$  to be even. Comments on the case when  $n$  is odd are made at the end of this section.

The procedure that leads to the condensed form (5.1) was motivated by the aim to generate a large zero block in the top left corner of the matrix  $A$ . In this section we relax this condition and admit nonzero diagonal entries in the condensed form. This leads to the following definition.

DEFINITION 18. *A matrix  $A \in \mathbb{C}^{n,n}$  is said to be in palindromic PVL form if it can be written as a sum  $A = D + H + T$  where  $D$  is diagonal,  $H$  is symmetric and in skew Hessenberg form, and  $T$  is skew symmetric and skew triangular, i.e., if*

$$A + A^T = \begin{matrix} \diagdown \\ \square \end{matrix} + \begin{matrix} \diagup \\ \square \end{matrix} \text{ and } A - A^T = \begin{matrix} \diagup \\ \square \end{matrix}.$$

The name 'PVL form' stems from an analogous condensed form for Hamiltonian matrices that was introduced by Paige and van Loan [18]. We now want to study the transformation of a general matrix to PVL form.

**THEOREM 19.** *Let  $A \in \mathbb{C}^{n,n}$  where  $n$  is even. Then there exist a unitary matrix  $Q \in \mathbb{C}^{n,n}$  that is computable by a direct algorithm of complexity  $\mathcal{O}(n^3)$  such that  $Q^T A Q$  is in palindromic PVL form.*

*Proof.* We will prove in a constructive way that for any symmetric/skew symmetric pair of matrices  $M = M^T, N = -N^T$ , there is a unitary  $Q$  such that  $Q^T N Q = \begin{smallmatrix} \triangle \\ \square \end{smallmatrix}$  and  $Q^T M Q$  is in palindromic PVL form. If  $M$  and  $N$  are chosen as symmetric and skew symmetric parts of  $A$ , then  $Q^T A Q = Q^T M Q + Q^T N Q$  is also in palindromic PVL form.

As a first step, we compute a unitary  $Q$  such that  $Q^T N Q = \begin{smallmatrix} \triangle \\ \square \end{smallmatrix}$ . Such a  $Q$  always exists and may be computed, e.g., by a series of Householder transformations in  $\mathcal{O}(n^3)$  flops, see the skew  $QRQ^T$  factorization in [21]. Applying this  $Q$  yields new matrices  $M$  and  $N$ :  $M \leftarrow Q^T M Q = \begin{smallmatrix} \square \\ \square \end{smallmatrix}, N \leftarrow Q^T N Q = \begin{smallmatrix} \triangle \\ \square \end{smallmatrix}$ . We now transform  $M$  to 'skew Hessenberg plus diagonal' form while keeping  $N$  in skew triangular form.

Let  $k = \frac{n}{2}$  for the entire proof. First annihilate the  $(2, 1)$  element of  $M$  by a rotation in the  $(2, 3)$  plane applied as congruence. This also zeros out  $m_{12}$  and introduces non zero elements in  $N$  at position  $(2, n - 2)$  and  $(n - 2, 2)$ . These new elements are being zeroed again by a congruence rotation in the  $(n - 2, n - 1)$  plane which restores the skew triangular form of  $N$ , but leaves invariant the zero pattern of  $M$ . This can be repeated for the entries  $(3, 1), (4, 1), \dots, (k - 1, 1)$ .

We next zero out element  $(k, 1)$  of  $M$ . This is done with a congruence rotation in the  $(k, k + 1)$  plane. This rotation also zeroes out the element  $(1, k)$  of  $M$ , but leaves  $N$  skew triangular, because 2-by-2 skew symmetric matrices can only have one zero pattern namely  $\begin{bmatrix} 0 & * \\ * & 0 \end{bmatrix}$ .

We continue by eliminating the element  $(k + 1, 1)$  of  $M$  by a congruence rotation in the  $(k + 1, k + 2)$  plane. This congruence rotation also eliminates  $m_{1,k+1}$ , but introduces non zero entries in  $N$  at positions  $(k + 1, k - 1)$  and  $(k - 1, k + 1)$ . These can be zeroed out again by a further congruence rotation in the  $(k - 1, k)$  plane leaving invariant the zero pattern of  $M$ . This can be repeated for the entries  $(k + 2, 1), (k + 3, 1), \dots, (n - 2, 1)$ .

At this point, all necessary zeros in the first row and column of  $M$  have been generated. This required roughly  $2n$  rotations taking  $\mathcal{O}(n^2)$  flops to be applied.

Note, that the last row and column of  $M$  and  $N$  were not altered during the described procedure. Thus, the zeros in the first row and column of  $M$  are preserved when the procedure is applied recursively to the submatrices that arise from  $M$  and  $N$  by deleting the first and last rows and columns. This yields a palindromic PVL form for  $M$ , thus for  $A$  in  $\mathcal{O}(n^3)$  flops. This finishes the proof.  $\square$

In terms of additional non-zeros the palindromic PVL form is much closer to skew Hessenberg form than the condensed form (5.1). However, it is in general *not* invariant under palindromic QR steps. The palindromic PVL form is invariant only if the diagonal elements  $a_{11}, a_{22}, \dots, a_{\frac{n}{2}-1, \frac{n}{2}-1}$  are zero, i.e., if the palindromic PVL form reduces to skew Hessenberg form.

Thus, the reduction to palindromic PVL form is not suited as a preliminary step for the palindromic QR iteration, unless it yields a skew Hessenberg matrix. The remainder of this section analyses when a palindromic PVL form actually is skew Hessenberg. We start with the following uniqueness result which is similar to the implicit Q theorem and states that a palindromic PVL form is fixed, once the first or last column of  $Q$  is known.

**THEOREM 20.** *Let  $A \in \mathbb{C}^{n,n}$  where  $n$  is even such that  $A - A^T$  is non-singular. Let  $Q_1, Q_2 \in \mathbb{C}^{n,n}$  be two unitary matrices with  $Q_1 e_1 = Q_2 e_1$  or  $Q_1 e_n = Q_2 e_n$ . Further, let  $P_1, P_2 \in \mathbb{C}^{n,n}$  be two matrices in palindromic PVL form such that the skew diagonal entries of  $P_i - P_i^T$  and the skew super diagonal entries of  $P_i + P_i^T$  are real, positive, and non-zero, and  $Q_i^T A Q_i = P_i$  for  $i = 1, 2$ .*

*Then  $Q_1 = Q_2$  and  $P_1 = P_2$ .*

*Proof.* Let  $M = \frac{1}{2}(A + A^T), N = \frac{1}{2}(A - A^T)$  be the symmetric and skew symmetric parts of  $A$  respectively. Analogously, let  $K = \frac{1}{2}(P_1 + P_1^T), L = 2(P_1 - P_1^T)^{-1}$ . Then  $A = M + N$  and

$P_1 = K + L^{-1}$ . Further, let  $Q_1 = [q_1, q_2, \dots, q_n]$ . We will prove that given  $q_1$  or  $q_n$  then  $K, L$  and the remaining columns of  $Q$  are fixed.

Consider the relation  $x = \alpha y$  for a given non-zero vector  $x$ , an unknown normalized vector  $y$  and a unknown scalar  $\alpha$ . It follows that  $|\alpha| = \|\alpha y\| = \|x\|$  and  $y = \frac{1}{\alpha}x$ . So,  $\alpha$  can be freely chosen on the circle of radius  $\|x\|$ . But if  $\alpha$  is restricted to be real and positive, then the solution is unique. Similar relations will arise involving the skew diagonal entries of  $P_1 - P_1^T$  and the skew super diagonal entries of  $P_1 + P_1^T$ . Thus, they must be restricted to be real, positive, and non-zero in order to have uniqueness.

We have

$$\begin{aligned} Q_1^T M Q_1 &= K, \\ Q_1^T N Q_1 &= L^{-1}, \end{aligned}$$

hence

$$M Q_1 = \bar{Q}_1 K, \quad (5.2)$$

$$N^{-1} \bar{Q}_1 = Q_1 L. \quad (5.3)$$

Multiplying (5.3) from the right by  $e_n$  gives (note, that  $L$  is upper skew triangular)

$$N^{-1} \bar{q}_n = q_1 l_{1,n}$$

If  $q_n$  is given then this relation yields  $l_{1,n} = \|N^{-1} \bar{q}_n\|$  and  $q_1 = \frac{1}{l_{1,n}} N^{-1} \bar{q}_n$ . If, on the other hand,  $q_1$  is given, the relation yields  $l_{1,n}^{-1} = \|N q_1\|$  and  $q_n = \overline{l_{1,n} N q_1}$ . In both cases, at this point  $q_1, q_n, l_{1,n}$ , and  $l_{n,1} = -l_{1,n}$  are known.

Multiplying (5.2) from the right by  $e_1$  yields (as  $K$  is in PVL form)

$$M q_1 = \bar{q}_1 k_{1,1} + \bar{q}_{n-1} k_{n-1,1} + \bar{q}_n k_{n,1}.$$

From this relation we can read off the following elements:

$$\begin{aligned} k_{1,1} &= q_1^T M q_1, \\ k_{n,1} &= q_n^T M q_1, \\ k_{n-1,1} &= \|M q_1 - \bar{q}_1 k_{1,1} - \bar{q}_n k_{n,1}\|, \end{aligned}$$

and

$$q_{n-1} = \frac{1}{k_{n-1,1}} (M q_1 - \bar{q}_1 k_{1,1} - \bar{q}_n k_{n,1}).$$

Thus, at this point we know  $q_1, q_{n-1}, q_n$  as well as the first row and column of  $K$  and the last row and column of  $L$ .

The rest follows by induction. Assume that the first  $i-1$  and the last  $i$  columns of  $Q_1$  as well as the first  $i-1$  rows and columns of  $K$  and the last  $i-1$  rows and columns of  $L$  are known. Multiplying (5.3) from the right by  $e_{n+1-i}$  gives

$$N^{-1} \bar{q}_{n+1-i} = \sum_{j=1}^i q_j l_{j,n+1-i}. \quad (5.4)$$

The vector  $q_i$  is the only unknown vector in this relation. We get

$$\begin{aligned} l_{j,n+1-i} &= q_j^* N^{-1} \bar{q}_{n+1-i}, \quad j = 1, \dots, i-1, \\ l_{i,n+1-i} &= \|N^{-1} \bar{q}_{n+1-i} - \sum_{j=1}^{i-1} q_j l_{j,n+1-i}\|, \end{aligned}$$

$$q_i = \frac{1}{l_{i,n+1-i}} \left( N^{-1} \bar{q}_{n+1-i} - \sum_{j=1}^{i-1} q_j l_{j,n+1-i} \right).$$

At this point, also  $q_i$  and the  $(n + 1 - i)$ st row and column of  $L$  are known.

Next, we multiply (5.2) from the right by  $e_i$ , yielding

$$Mq_i = \bar{q}_i k_{i,i} + \sum_{j=n-i}^n \bar{q}_j k_{j,i}. \quad (5.5)$$

From this equation we get for  $q_{n-i}$  and the  $i$ th column of  $K$

$$\begin{aligned} k_{j,i} &= q_j^T Mq_i, \quad j = i \text{ and } j = n - i + 1, n - i + 2, \dots, n, \\ k_{n-i,i} &= \|Mq_i - \bar{q}_i k_{i,i} - \sum_{j=n+1-i}^n \bar{q}_j k_{j,i}\|, \\ q_{n-i} &= \frac{1}{k_{n-i,i}} \left( Mq_i - \bar{q}_i k_{i,i} - \sum_{j=n+1-i}^n \bar{q}_j k_{j,i} \right). \end{aligned}$$

Carrying out this procedure for  $i = 2, \dots, \frac{n}{2}$  fixes  $Q_1$  and thus also  $P_1, K$ , and  $L$ .  $\square$

So, a palindromic PVL form  $P = Q^T A Q$  is determined by  $A$  and the first (as well as the last) column of  $Q$ . This changes our question of 'when is a palindromic PVL form a skew Hessenberg matrix?' to 'what conditions should  $q_1$  fulfill so that the resulting palindromic PVL form is in skew Hessenberg form?'. For example, in order for  $p_{1,1}$  to be zero,  $q_1$  has to satisfy  $p_{1,1} = q_1^T A q_1 = 0$ . The following theorem is a generalization of a result in [1] for Hamiltonian matrices.

**THEOREM 21.** *Let  $A \in \mathbb{C}^{n,n}$ , with  $n$  even, be such that  $A - A^T$  is non-singular. Let  $Q \in \mathbb{C}^{n,n}$  be a unitary matrix such that  $Q^T A Q = P$  is in palindromic PVL form with unreduced super skew diagonal, i.e.,  $p_{i,n-i} \neq 0, i = 1, \dots, n - 1$ . Let  $q_1 = Q e_1$  be the first column of  $Q$ .*

*Then  $P$  is in skew Hessenberg form if and only if  $q_1$  satisfies the following conditions:*

$$q_1^T ((N^{-1} M)^i)^T M (N^{-1} M)^i q_1 = 0, \quad i = 0, \dots, \frac{n}{2} - 2, \quad (5.6)$$

where  $M = \frac{1}{2}(A + A^T)$ ,  $N = \frac{1}{2}(A - A^T)$ .

*Proof.* Set  $K := \frac{1}{2}(P + P^T) = Q^T M Q$ ,  $L := \frac{1}{2}(P - P^T) = Q^T N Q$ . Note that  $L$  is skew triangular with unreduced skew diagonal, i.e.,  $l_{i,n+1-i} \neq 0$  for  $i = 1, \dots, n$ , since  $N$  is non-singular. Further note that  $K$  is in palindromic PVL form with unreduced super skew diagonal, i.e.  $k_{i,n-i} \neq 0$  for  $i = 1, \dots, n - 1$ , since  $P$  has that property. Moreover,  $P$  is in skew Hessenberg form if and only if  $k_{i,i} = 0$  for  $i = 1, \dots, \frac{n}{2} - 1$ .

We will prove the following: if for some  $r \in \{1, \dots, \frac{n}{2} - 2\}$  we have that  $k_{1,1} = k_{2,2} = \dots = k_{r,r} = 0$ , then for all  $s = 0, \dots, r$ :

$$k_{r+1,r+1} = 0 \iff q_{r+1-s}^T ((N^{-1} M)^s)^T M (N^{-1} M)^s q_{r+1-s} = 0. \quad (5.7)$$

The assertion (5.6) follows from (5.7) by induction over  $r$ , in each step setting  $s = r$ .

So, assume  $r \in \{1, \dots, \frac{n}{2} - 2\}$  and  $k_{1,1} = k_{2,2} = \dots = k_{r,r} = 0$ . We will need the following product,  $K_s := ((L^{-1} K)^s)^T K (L^{-1} K)^s$ . Note that, because of the structure of  $L$  and  $K$ , the matrix  $K_s$  has the pattern

$$K_s = \begin{matrix} & & r-s \\ & & \boxed{\phantom{0}} \\ r-s+1 & \begin{bmatrix} 0 & \boxed{\phantom{0}} \\ \boxed{\phantom{0}} & \boxed{\phantom{0}} \end{bmatrix} \end{matrix}, \quad (5.8)$$

i.e., the matrix  $K_s$  consists of a zero block in the top left corner of size  $(r - s + 1) \times (r - s)$ . This can be seen by considering the action of the matrix  $L^{-1} K$  on the unit vectors  $e_i$  and noting that  $K_s e_i = \pm K (L^{-1} K)^{2s} e_i$ , where the sign depends on  $s$ . This also shows that, actually,  $K_s$  consists of many more zeros, but we will only use those claimed in (5.8). Multiplication with an upper

skew triangular matrix will not destroy the zero entries, but only move them to the bottom/right. Thus,

$$L^{-T}K_s = \begin{matrix} & r-s \\ & \left[ \begin{array}{cc} \square & \square \\ 0 & \square \end{array} \right] \\ r-s+1 & \end{matrix}, \quad L^{-T}K_sL^{-1} = \begin{matrix} & r-s \\ & \left[ \begin{array}{cc} \square & \square \\ \square & 0 \end{array} \right] \\ r-s+1 & \end{matrix}. \quad (5.9)$$

Moreover, multiplication with  $K$  just slightly reduces the zero block:

$$L^{-T}K_sL^{-1}K = \begin{matrix} & r-s \\ & \left[ \begin{array}{cc} \square & \square \\ 0 & \square \end{array} \right] \\ r-s & \end{matrix}. \quad (5.10)$$

The statement (5.7) is proved by induction over  $s$ . Clearly, it holds for  $s = 0$ , as  $k_{r+1,r+1} = q_{r+1}^T M q_{r+1}$ .

Now, we prove the step " $s \Rightarrow s+1$ ", i.e.,

$$q_{r+1-s}^T M_s q_{r+1-s} = 0 \iff q_{r-s}^T M_{s+1} q_{r-s} = 0, \text{ for } s = 0, \dots, r-1, \quad (5.11)$$

where  $M_s := ((N^{-1}M)^s)^T M (N^{-1}M)^s$ . By equation (5.4) with  $i = r+1-s$ , the vector  $q_{r+1-s}$  can be written as

$$q_{r+1-s} = \frac{1}{l_{r+1-s,n-r+s}} (N^{-1} \bar{q}_{n-r+s} - \sum_{j=1}^{r-s} l_{j,n-r+s} q_j).$$

Here,  $l_{r+1-s,n-r+s} \neq 0$ , since it is on the skew diagonal of  $L$ .

Inserting this into the term  $q_{r+1-s}^T M_s q_{r+1-s}$  yields

$$\begin{aligned} q_{r+1-s}^T M_s q_{r+1-s} &= \frac{1}{l_{r+1-s,n-r+s}^2} \left( q_{n-r+s}^* N^{-T} M_s N^{-1} \bar{q}_{n-r+s} \right. \\ &\quad \left. - 2 \sum_{j=1}^{r-s} l_{j,n-r+s} (q_{n-r+s}^* N^{-T} M_s q_j) \right. \\ &\quad \left. + \sum_{i,j=1}^{r-s} l_{i,n-r+s} l_{j,n-r+s} (q_i^T M_s q_j) \right). \end{aligned} \quad (5.12)$$

In this sum only the first term is non-zero, because for  $j = 1, \dots, r-s$  we have

$$q_{n-r+s}^* N^{-T} M_s q_j = e_{n-r+s}^T Q^* N^{-T} M_s Q e_j = e_{n-r+s}^T L^{-T} K_s e_j \stackrel{(5.9)}{=} 0,$$

and for  $i, j = 1, \dots, r-s$

$$q_i^T M_s q_j = e_i^T Q^T M_s Q e_j = e_i^T K_s e_j \stackrel{(5.8)}{=} 0.$$

Thus, equation (5.12) reduces to

$$q_{r+1-s}^T M_s q_{r+1-s} = \frac{1}{l_{r+1-s,n-r+s}^2} q_{n-r+s}^* N^{-T} M_s N^{-1} \bar{q}_{n-r+s}. \quad (5.13)$$

The vector  $\bar{q}_{n-r+s}$  can, by equation (5.5) with  $i = r-s$ , be written as (note, that  $k_{r-s,r-s} = 0$ )

$$\bar{q}_{n-r+s} = \frac{1}{k_{n-r+s,r-s}} (M q_{r-s} - \sum_{j=n-r+1+s}^n k_{j,r-s} \bar{q}_j).$$

Here,  $k_{n-r+s, r-s} \neq 0$ , as it is on the super skew diagonal of  $K$ .

Inserting this into the term  $q_{n-r+s}^* N^{-T} M_s N^{-1} \bar{q}_{n-r+s}$  gives

$$\begin{aligned} q_{n-r+s}^* N^{-T} M_s N^{-1} \bar{q}_{n-r+s} &= \frac{1}{k_{n-r+s, r-s}^2} \left( q_{r-s}^T M N^{-T} M_s N^{-1} M q_{r-s} \right. \\ &\quad - 2 \sum_{j=n+1-r+s}^n k_{j, r-s} (q_j^* N^{-T} M_s N^{-1} M q_{r-s}) \\ &\quad \left. + \sum_{i, j=n+1-r+s}^n k_{i, r-s} k_{j, r-s} (q_i^* N^{-T} M_s N^{-1} \bar{q}_j) \right). \end{aligned} \quad (5.14)$$

Also here, only the first summand is non-zero. Indeed, for  $j = n + 1 - r + s, \dots, n$

$$q_j^* N^{-T} M_s N^{-1} M q_{r-s} = e_j^T Q^* N^{-T} M_s N^{-1} M Q e_{r-s} = e_j^T L^{-T} K_s L^{-1} K e_{r-s} \stackrel{(5.10)}{=} 0,$$

and for  $i, j = n + 1 - r + s, \dots, n$

$$q_i^* N^{-T} M_s N^{-1} \bar{q}_j = e_i^T Q^* N^{-T} M_s N^{-1} \bar{Q} e_j = e_i^T L^{-T} K_s L^{-1} e_j \stackrel{(5.9)}{=} 0.$$

Hence, equation (5.14) reduces to

$$q_{n-r+s}^* N^{-T} M_s N^{-1} \bar{q}_{n-r+s} = \frac{1}{k_{r-s, n-r+s}^2} q_{r-s}^T M N^{-T} M_s N^{-1} M q_{r-s}. \quad (5.15)$$

Equations (5.13) and (5.15) together yield

$$q_{r+1-s}^T M_s q_{r+1-s} = c \cdot q_{r-s}^T M N^{-T} M_s N^{-1} M q_{r-s} = c \cdot q_{r-s}^T M_{s+1} q_{r-s},$$

where  $c = \frac{1}{k_{r-s, n-r+s}^2 l_{r+1-s, n-r+s}^2} \neq 0$  which is equivalent to (5.11). Thus (5.7) follows and the proof is complete.  $\square$

We have proved that in order for  $Q^T A Q$  to be in skew Hessenberg form, the first column of  $Q$  has to fulfill the  $\frac{n}{2} - 1$  conditions (5.6). This is in sharp contrast to the standard eigenvalue problem. There, a unitary matrix  $Q$  with arbitrary first column can be found such that  $Q^* A Q$  is in standard Hessenberg form. This suggests, that the skew Hessenberg reduction is not possible without solving the (nonlinear) constraints (5.6). For the Hamiltonian eigenvalue problem this is known as "Van Loan's curse", see [3, 18].

**REMARK 22.** In the case of odd dimension  $n$ , the skew symmetric part of  $A$ ,  $N = \frac{1}{2}(A - A^T)$  is singular, as every skew symmetric matrix of odd dimension is singular. Assuming that  $N$  is of rank  $n - 1$ , one can find a unitary  $Q$  such that  $P := Q^T A Q$  is of PVL-like form, such that  $P$  can be written as sum of a skew triangular and a diagonal matrix,  $P = \begin{array}{c} \triangleleft + \\ \searrow \end{array}$ , and  $P - P^T$  is of the form

$$P - P^T = \begin{array}{cc} & 1 & n-1 \\ & 0 & 0 \\ n-1 & 0 & \triangleleft \end{array}.$$

Here, the first column of  $Q$  is fixed as a vector that forms a basis of the nullspace of  $N$ . As before, the remaining columns follow from the first one. Thus the whole matrix  $Q$  is fixed.  $\square$

Summarizing, the chances to find a matrix  $Q$  that transforms  $A$  to skew Hessenberg form are limited. However, there are situations, in which this transformation is possible. Such are presented next.

**5.2. Skew Hessenberg reduction for SISO systems.** Here, and in the following section, we want to discuss how to reduce specially structured matrices to skew Hessenberg form. Note, that we no longer restrict to the T–case, but allow \*-palindromic pencils again.

Here, we assume that the matrix  $A$  is of the following structure,

$$P^*AP = \begin{matrix} & m & 1 & m \\ m & \begin{bmatrix} 0 & 0 & E \\ b^* & r & 0 \\ G & 0 & K \end{bmatrix} \\ & m & & \end{matrix}.$$

for some  $E, G, K \in \mathbb{C}^{m,m}, b \in \mathbb{C}^m, r \in \mathbb{C}$ . This structure arises, e.g., in optimal control problems for single input, single output (SISO) systems, see [5, 17].

We will describe how to transform  $A$  to skew Hessenberg form by a unitary congruence transformation. As a first step,  $b^*$  will be reduced. For this let  $\tilde{U}_1$  be a unitary matrix such that  $b^*\tilde{U}_1 = \alpha e_m^T$ , where  $\alpha$  is a constant. Defining  $U_1 := \text{diag}(\tilde{U}_1, I_{m+1})$  yields

$$\tilde{A} := U_1^*P^*APU_1 = \begin{matrix} & m & 1 & m \\ m & \begin{bmatrix} 0 & 0 & \tilde{E} \\ \alpha e_m^T & r & 0 \\ \tilde{G} & 0 & K \end{bmatrix} \\ & m & & \end{matrix},$$

with  $\tilde{E} = U_1^*E$  and  $\tilde{G} = GU_1$ .

We proceed with the reduction to skew Hessenberg, skew triangular form of  $\tilde{G}, \tilde{E}$ . Let  $Q, Z$  be two unitary matrices such that  $Q(F\tilde{G}^*, F\tilde{E})Z = (H, R) = \left( \begin{smallmatrix} \diagdown \\ \diagup \end{smallmatrix}, \begin{smallmatrix} \diagdown \\ \diagup \end{smallmatrix} \right)$  and  $Qe_1 = e_1$ . These can be obtained by the standard reduction to Hessenberg, triangular form for matrix pencils [9]. Define  $U_2 := \text{diag}(FQ^*F, 1, Z)$ , then

$$\hat{A} := U_2^*\tilde{A}U_2 = \begin{matrix} & m & 1 & m \\ m & \begin{bmatrix} 0 & 0 & \hat{E} \\ \hat{b} & r & 0 \\ \hat{G} & 0 & \hat{K} \end{bmatrix} \\ & m & & \end{matrix}, \text{ with } \begin{cases} \hat{E} &= FQF\tilde{E}Z = FR = \begin{smallmatrix} \diagdown \\ \diagup \end{smallmatrix}, \\ \hat{b} &= \alpha e_m^T FQ^*F = \alpha e_1^T Q^*F = \alpha e_m^T, \\ \hat{G} &= Z^*\tilde{G}FQ^*F = H^*F = \begin{smallmatrix} \diagdown \\ \diagup \end{smallmatrix}, \\ \hat{K} &= Z^*KZ. \end{cases}$$

Hence,  $\hat{A}$  is in skew Hessenberg form.

**5.3. Skew-Hessenberg reduction after symmetric rank–one updates.** Assume, that  $A \in \mathbb{C}^{n,n}$  is a symmetric rank one perturbation of a skew triangular matrix, i.e., there are a skew triangular matrix  $B = \begin{smallmatrix} \diagdown \\ \diagup \end{smallmatrix}$  and a vector  $b \in \mathbb{C}^n$  such that  $A = B + bb^*$ . We will show how to transform  $A$  to skew-Hessenberg form.

Set  $k = \lfloor \frac{n}{2} \rfloor - 1$  and let  $U = U_{1,2}U_{2,3} \cdots U_{k,k+1}$  be a product of Givens rotations, where  $U_{i,i+1}$  is a Givens rotation in the  $(i, i+1)$  plane, such that  $U^*b$  vanishes in the first  $k$  positions.

If  $n$  is even, then  $k = \frac{n}{2} - 1$  and

$$\begin{aligned} U^*AU &= U^*BU + U^*b(U^*b)^* \\ &= \frac{\frac{n}{2}}{\frac{n}{2}} \begin{bmatrix} 0 & \begin{smallmatrix} \diagdown \\ \diagup \end{smallmatrix} \\ \begin{smallmatrix} \diagdown \\ \diagup \end{smallmatrix} & \square \end{bmatrix} + \frac{\frac{n}{2}-1}{\frac{n}{2}+1} \begin{bmatrix} \frac{n}{2}-1 & \frac{n}{2}+1 \\ 0 & 0 \\ 0 & \square \end{bmatrix} = \begin{smallmatrix} \diagdown \\ \diagup \end{smallmatrix} \end{aligned}$$

is in skew Hessenberg form.



Similarly, if  $n$  is odd, then  $k = \frac{n-3}{2}$  and

$$U^*AU = U^*BU + U^*b(U^*b)^*$$

$$= 1 \begin{matrix} \frac{n-1}{2} \\ \frac{n-1}{2} \end{matrix} \begin{bmatrix} \frac{n-1}{2} & 1 & \frac{n-1}{2} \\ 0 & 0 & \begin{matrix} \diagup \\ \diagdown \end{matrix} \\ 0 & * & * \cdots * \\ \begin{matrix} \diagup \\ \diagdown \end{matrix} & \vdots & \square \end{bmatrix} + \begin{matrix} \frac{n-3}{2} \\ \frac{n+3}{2} \end{matrix} \begin{bmatrix} \frac{n-3}{2} & \frac{n+3}{2} \\ 0 & 0 \\ 0 & \square \end{bmatrix} = \begin{bmatrix} & & & & * & * \\ & & & & \vdots & * \\ & & & \ddots & & * \\ & & * & * & & * \\ & & * & * & & * \\ & \ddots & & & & \vdots \\ * & & & & & * \\ * & \cdots & * & * & \cdots & * \end{bmatrix}.$$

Finally, solving the  $2 \times 2$  problem in the  $(\frac{n-1}{2}, \frac{n+1}{2})$  plane (for  $\star = *$  we have to assume that a solution exists) results in skew Hessenberg form.

**6. Conclusion.** We discussed structure preserving algorithms for the palindromic eigenvalue problem  $Ax = \lambda A^*x$ . The development was oriented at the standard QR algorithm. First, we presented palindromic versions of the Schur form and the basic QR iteration. Then we adapted techniques that helped to speed up the standard QR algorithm like deflation, shifting and exploiting the invariance of Hessenberg-like matrices.

Let us summarize the practically relevant results of this paper. For general complex and real matrices, the single-shift palindromic QR iteration, Algorithm 2 can be used. Although this is a method of complexity  $\mathcal{O}(n^4)$ , it is still of practical use: in [16] the palindromic eigenvalue problem is treated by a combination of several methods. Roughly speaking, the eigenvalues far from the unit circle are deflated first with an unstructured method. Then, the remaining problem which contains the 'close to exceptional' eigenvalues is solved by our palindromic QR algorithm. This remaining problem is often of such small dimension that the complexity of the used method is less important.

For skew Hessenberg matrices an explicit single-shift algorithm of complexity  $\mathcal{O}(n^3)$  was provided. At this point we refer the reader to a forthcoming paper that will develop an implicit version being capable of incorporating multiple shifts and staying in real arithmetic for real problems.

In the last part we have discussed the problem of reducing a full matrix to skew Hessenberg form. We have shown several connections to the Hamiltonian eigenvalue problem, and like in the latter problem, a satisfying algorithm remains unknown. Filling this gap will be the hardest part of work in the development of efficient, structure preserving methods for the palindromic eigenvalue problem.

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