THE UNITARY COMPLETION AND QR ITERATIONS FOR A CLASS OF STRUCTURED MATRICES

D. A. BINI, Y. EIDELMAN, L. GEMIGNANI, AND I. GOHBERG

ABSTRACT. We consider the problem of completion of a matrix with a specified lower triangular part to a unitary matrix. In this paper we obtain the necessary and sufficient conditions of existence of a unitary completion without any additional constraints and give a general formula for this completion. The paper is mainly focused on matrices with the specified lower triangular part of a special form. For such a specified part the unitary completion is a structured matrix, and we derive in this paper the formulas for its structure. Next we apply the unitary completion method to the solution of the eigenvalue problem for a class of structured matrices via structured QR iterations.

1. INTRODUCTION

In this paper we consider the problem of completing a given lower triangular part $U_L = \{u_{ij}, i \geq j\}$ to a unitary matrix. The problem of completing a given lower triangular part U_L of a block matrix to a unitary matrix U was stated and studied in the paper [4] in the assumption that the completion U admits LU and UL factorizations. In this paper we obtain the necessary and sufficient condition for the existence of a unitary completion without any additional constraints and give a general formula for this completion. The paper is mainly focused on a class of structured matrices. More precisely, we consider a partially specified matrix $U = \{u_{ij}\}_{i,j=1}^N$ with the specified lower triangular part $U_L = \{u_{ij}, i \geq j\}$ of the form

$$U_L(i+1,i) = \beta_i, \ i = 1, \ldots, N-1; \quad U_L(i,i) = d_i, \ i = 1, \ldots, N;$$
$$U_L(i,j) = p(i)q(j), \quad 1 \leq j \leq i-2, \ 3 \leq i \leq N;$$

with some $\beta_i, d_i, p(i), q(i) \in \mathbb{C}$. For such a specified part the unitary completion is a structured matrix, and we derive in this paper the formulas for its structure.

Next we apply the unitary completion method to the solution of the eigenvalue problem for a class of structured matrices via structured QR iterations. In particular, we solve the eigenvalue problem for the class $\mathcal{H}_N$ of $N \times N$ upper Hessenberg matrices A which may be represented in the form $A = U - pq^T$, where U is a unitary matrix, p and q are vectors and q^T denotes the transpose of q. This class includes both *companion* and *fellow* matrices. Eigenvalue problems with these kinds

of matrices frequently arise in signal processing [3]. An efficient QR eigenvalue algorithm for such matrices was devised in our previous paper [1]. The algorithm achieves a substantial reduction in computational complexity by working with a structured representation of A by means of $O(N)$ parameters instead of with the entire matrix. A set of rules is provided which allow one to compute the parametric description of the new iterate $A^{(1)}$ starting from the one of $A = A^{(0)}$ at a linear cost. The combination of the structural properties of A with this $O(N)$ updating procedure is the core of the fast adaptation of the QR algorithm in [1]. The algorithm presented in this paper has a common point with the algorithm from [1] in the QR factorization step of the method, whereas the RQ step is carried out in a completely different way. The procedure given here is essentially based on the unitary completion method and decreases the arithmetic cost with respect to the corresponding computation in [1].

The paper contains seven sections. The first section is the Introduction. The second section contains some auxiliary relations. In Section 3 we solve the general unitary completion problem. In Section 4 we state the structured unitary completion problem and derive necessary and sufficient conditions for the existence and uniqueness of the unitary completion in terms of the structure of the specified lower triangular part. In Section 5 we derive explicit formulas for the structure of the strictly upper triangular part of the unitary completion. In Section 6 we apply the unitary completion method to the solution of the eigenvalue problem for the matrices $A \in \mathcal{H}_N$. In Section 7 we present results of numerical experiments.

For the indication of submatrices we use MATLAB style, i.e., for a matrix A, $A(i:j, p:k)$ selects rows i to j of columns p to k, and a colon without an index range selects all of the rows or columns ($A(:, p:k)$ or $A(i:j,:)$). The symbol $\|\cdot\|$ denotes the Euclidean norm of a vector or of a matrix.

2. The auxiliary relations

This section contains properties of some matrices partitioned in a special form. The relations presented here are used frequently in the proofs of the results of the paper.

At first we consider some relations for positive semidefinite matrices.

Lemma 2.1. *Let*

$$A_0 = \begin{pmatrix} A & f \\ f^* & d \end{pmatrix},$$

where A is a square matrix, f is a vector-column, and d is a number. Then:

(1) *If the matrix A_0 is positive semidefinite, then $f \in \mathrm{Im}(A)$, and for any ξ such that $A\xi = f$ the relation $d - f^*\xi \geq 0$ holds. Moreover, if the matrix A_0 is singular and $\det A \neq 0$, then $d - f^*\xi = 0$.*

(2) *If the matrix A is positive definite and $d - f^*A^{-1}f = 0$, then the matrix A_0 is positive semidefinite and singular.*

Proof. Since the matrix A_0 is positive semidefinite, then there exists a matrix K such that $A_0 = K^*K$. Let k be the last column of K, i.e., $K = \begin{bmatrix} K' & k \end{bmatrix}$ for some submatrix K'. We have

$$\begin{pmatrix} A & f \\ f^* & d \end{pmatrix} = \begin{bmatrix} (K')^* \\ k^* \end{bmatrix} \begin{bmatrix} K' & k \end{bmatrix}.$$

The matrix A_0 is positive semidefinite and, therefore, its submatrix A is Hermitian. Let us prove that $f \perp \text{Ker}(A)$, which implies $f \in \text{Im}(A)$. Indeed, for any $x \in \text{Ker}(A)$ we have $x^* A x = x^*(K')^* K' x = \|K' x\| = 0$ and, therefore, $K' x = 0$. Whence $f^* x = k^* K' x = 0$.

Next let ξ be a solution of the equation $A\xi = f$. We use the factorization

$$(2.1) \qquad \begin{pmatrix} A & f \\ f^* & d \end{pmatrix} = \begin{pmatrix} I & 0 \\ \xi^* & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & d - f^*\xi \end{pmatrix} \begin{pmatrix} I & \xi \\ 0 & 1 \end{pmatrix}.$$

Since the matrix A_0 is positive semidefinite this implies that the matrix

$$(2.2) \qquad \tilde{A} = \begin{pmatrix} A & 0 \\ 0 & d - f^*\xi \end{pmatrix}$$

is positive semidefinite and, hence, the entry $d - f^*\xi$ is nonnegative. If the matrix A_0 is singular, then $\tilde{A}$ is also singular and, moreover, if the matrix A is nonsingular, then we get $d - f^*\xi = 0$. Finally from (2.1) it follows that, if the matrix A is positive definite and $d - f^* A^{-1} f = 0$, then the matrix $\tilde{A}$ is positive semidefinite and singular and, hence, by using (2.2) we conclude that the matrix A_0 is positive semidefinite and singular. $\qquad \square$

Next we consider the conditions in which a matrix partitioned in a special form has the unit norm.

Theorem 2.2. *Let Δ be a matrix partitioned in the form*

$$\Delta = \begin{bmatrix} g & d \\ B & f \end{bmatrix},$$

where f is a vector column, g is a vector row and d is a number. Assume that the matrix $\Delta' = \begin{bmatrix} g \\ B \end{bmatrix}$ satisfies the condition $\|\Delta'\| < 1$, and set

$$(2.3) \qquad I - (\Delta')^* \Delta' = V D^2 V^*,$$

where V is a unitary matrix and D is a real diagonal invertible matrix.
The conditions $\|\Delta\| = 1$ and $|d + a| = \rho$, where

$$(2.4) \qquad a = \frac{\tilde{g}^* \tilde{f}}{1 + \|\tilde{g}\|^2}, \quad \rho = \left(\frac{1 - \|f\|^2 - \|\tilde{f}\|^2}{1 + \|\tilde{g}\|^2} + |a|^2 \right)^{1/2},$$

$$\tilde{g} = D^{-1} V^* g^*, \quad \tilde{f} = D^{-1} V^* B^* f,$$

are equivalent.

Proof. The condition $\|\Delta\| = 1$ holds if and only if the matrix $I - \Delta^* \Delta$ is positive semidefinite and singular.

Set $f' = \begin{bmatrix} d \\ f \end{bmatrix}$. We have $\Delta = \begin{bmatrix} \Delta' & f' \end{bmatrix}$ and therefore

$$I - \Delta^* \Delta = I - \begin{bmatrix} (\Delta')^* \\ (f')^* \end{bmatrix} \begin{bmatrix} \Delta' & f' \end{bmatrix} = \begin{bmatrix} I - (\Delta')^* \Delta' & -(\Delta')^* f' \\ -(f')^* \Delta' & 1 - (f')^* f' \end{bmatrix},$$

where the matrix $I - (\Delta')^* \Delta'$ is positive definite. Hence, by Lemma 2.1 the matrix $I - \Delta^* \Delta$ is positive semidefinite and singular if and only if the equality

$$1 - (f')^* \Delta' (I - (\Delta')^* \Delta')^{-1} (\Delta')^* f' - (f')^* f = 0$$

holds. Using (2.3) we rewrite this equality in the form

$$\|f'\|^2 + \|D^{-1}V^*(\Delta')^*f'\|^2 = 1. \tag{2.5}$$

By using the representations $f' = \begin{bmatrix} d \\ f \end{bmatrix}$, $\Delta' = \begin{bmatrix} g \\ B \end{bmatrix}$, one can rewrite condition (2.5) in the form

$$|d|^2 + \|f\|^2 + \|D^{-1}V^*g^*d + D^{-1}V^*B^*f\|^2 = 1,$$

i.e.,

$$|d|^2 + \|\tilde{g}d + \tilde{f}\|^2 = 1 - \|f\|^2. \tag{2.6}$$

Straightforward computations show that

$$|d|^2 + \|d\tilde{g} + \tilde{f}\|^2 = (1 + \|\tilde{g}\|^2)(|d + a|^2 - |a|^2) + \|\tilde{f}\|^2 \tag{2.7}$$

with a defined by (2.4). From (2.7) and (2.6) we obtain

$$(1 + \|\tilde{g}\|^2)(|d + a|^2 - |a|^2) + \|\tilde{f}\|^2 = 1 - \|f\|^2,$$

which is equivalent to the condition $|d + a| = \rho$.   □

3. The general unitary completion problem

Let $U = \{u_{ij}\}_{i,j=1}^N$ be a partially specified matrix with the specified lower triangular part $U_L = \{u_{ij}, i \geq j\}$. In this section we consider the problem of completing a given lower triangular part U_L to a unitary matrix U. Throughout the paper we set up the following notations for denoting certain submatrices of the specified part:

$$\begin{aligned} U_j &= U_L(j : N, 1 : j), \quad j = 1, \ldots, N, \\ U_j' &= U_L(j + 1 : N, 1 : j), \quad j = 1, \ldots, N - 1, \\ f_j &= U_L(j : N, j), \quad j = 1, \ldots, N. \end{aligned}$$

We also use the notations $\hat{U}_j = U(1 : j, 1 : j)$, $j = 1, \ldots, N$, for the principal leading submatrices of the completed matrix U and the notations $x_j = U(1 : j - 1, j)$, $j = 2, \ldots, N$, for certain $j-1$-dimensional columns in the strictly upper triangular part of U.

The problem of completing a given lower triangular part U_L of a block matrix to a unitary matrix U was stated and studied in the paper [4] under the assumption that the completion U admits LU and UL factorizations. Differently, in this section we obtain the necessary and sufficient condition for the existence of a unitary completion without any additional constraints and give a general formula for this completion.

Theorem 3.1. *Let* $U = \{u_{ij}\}_{i,j=1}^N$ *be a partially specified matrix with a specified lower triangular part* $U_L = \{u_{ij}, i \geq j\}$. *The specified part* U_L *has a unitary completion* U *if and only if*

$$\|U_j\| = 1, \quad j = 1, \ldots, N. \tag{3.1}$$

Moreover the unspecified entries of this completion are determined consecutively by the relations

$$x_j = x_j^{(1)} + x_j^{(2)}, \quad j = 2, \ldots, N, \tag{3.2}$$

where

$$(3.3) \qquad\qquad x_j^{(1)} = \hat{U}_{j-1}\xi_j,$$

the vector ξ_j is a solution of the equation

$$(3.4) \qquad\qquad (I - (U_{j-1}')^* U_{j-1}')\xi_j = -(U_{j-1}')^* f_j,$$

and the vector $x_j^{(2)}$ is an arbitrary solution of the equation

$$(3.5) \qquad\qquad \hat{U}_{j-1}^* x_j^{(2)} = 0$$

satisfying the condition

$$(3.6) \qquad\qquad (x_j^{(2)})^* x_j^{(2)} = 1 - f_j^* f_j - (x_j^{(1)})^* x_j^{(1)}.$$

The element $x_j^{(1)}$ is defined uniquely, i.e., does not depend on the choice of solution ξ_j of equation (3.4). If condition (3.1) holds and additionally

$$(3.7) \qquad\qquad \|U_j'\| < 1, \quad j = 1, \ldots, N-1,$$

then the matrices $\hat{U}_j$ are nonsingular, the unitary completion U is unique and the unspecified entries of U are determined consecutively by the relations

$$(3.8) \qquad x_j = -\hat{U}_{j-1}(I - (U_{j-1}')^* U_{j-1}')^{-1}(U_{j-1}')^* f_j, \quad j = 2, \ldots, N.$$

Proof. First we prove the sufficiency. Assume that the condition of the theorem holds. This in particular means that the first column $U(:,1) = U_1 = U_L(1:N,1)$ has the unit norm. Then for $j = 2, \ldots, N$ we subsequently determine the columns $U(:,j)$ of the completion U in such a way that these columns will be orthonormal. Suppose that for some j, $1 < j < N$, the first $j-1$ columns, i.e., the submatrix $U(:,1:j-1)$, have been just constructed. We show that one can determine the vector-column x_j of size $j-1$ in such a way that $\begin{pmatrix} x_j \\ f_j \end{pmatrix}$ is orthogonal to the columns $U(:,k)$, $k = 1, \ldots, j-1$, and has the unit norm. Then we set

$$U(:,j) = \begin{pmatrix} x_j \\ f_j \end{pmatrix}.$$

By using the representation

$$(3.9) \qquad\qquad U(:,1:j-1) = \begin{bmatrix} \hat{U}_{j-1} \\ U_{j-1}' \end{bmatrix}$$

we obtain that the vector x_j is defined by the relations

$$(3.10) \qquad\qquad \hat{U}_{j-1}^* x_j + (U_{j-1}')^* f_j = 0,$$

$$(3.11) \qquad\qquad x_j^* x_j + f_j^* f_j = 1.$$

We prove that the system of equations (3.10), (3.11) has a solution which is given by the relations (3.2)-(3.6).

Since the columns of the matrix $U(:,1:j-1)$ are orthonormal, by using the representation (3.9) we obtain the equality

$$(3.12) \qquad\qquad \hat{U}_{j-1}^* \hat{U}_{j-1} = I - (U_{j-1}')^* U_{j-1}'.$$

Next condition (3.1) implies that the matrix $I - U_j^* U_j$ is positive semidefinite and singular. By using the representation

$$U_j = \begin{bmatrix} U_{j-1}' & f_j \end{bmatrix}$$

we obtain

$$(3.13) \qquad I - U_j^* U_j = \begin{bmatrix} I - (U'_{j-1})^* U'_{j-1} & -(U'_{j-1})^* f_j \\ -f_j^* U'_{j-1} & 1 - f_j^* f_j \end{bmatrix}.$$

By applying the first part of Lemma 2.1 to the matrix $I - U_j^* U_j$ we conclude that equation (3.4) has a solution. Moreover, one can easily check that the formula (3.3) yields a solution of equation (3.10). In fact, from (3.12) we obtain

$$\hat{U}_{j-1}^* x_j^{(1)} = \hat{U}_{j-1}^* \hat{U}_{j-1} \xi_j = (I - (U'_{j-1})^* U'_{j-1}) \xi_j = -(U'_{j-1})^* f_j.$$

Furthermore, the vector $x_j^{(1)}$ does not depend on the choice of the solution ξ_j of equation (3.4). Indeed, for any ξ such that $(I - (U'_{j-1})^* U'_{j-1}) \xi = 0$ by using (3.12) we obtain that $\hat{U}_{j-1} \xi = 0$. Thus (3.10) has a solution $x_j^{(1)}$ and, moreover, any solution of equation (3.10) has the form $x_j = x_j^{(1)} + x_j^{(2)}$, where $x_j^{(2)}$ is an arbitrary solution of equation $\hat{U}_{j-1}^* x_j^{(2)} = 0$.

In order to satisfy equation (3.11) one should determine the vector $x_j^{(2)} \in \mathrm{Ker}(\hat{U}_{j-1}^*)$ such that the relation (3.6) holds. The latter is possible if and only if the right-hand part of the equality (3.6) is nonnegative and in the case $\mathrm{Ker}(\hat{U}_{j-1}^*) = \{0\}$ is vanishing. Notice that one can write the right-hand part of the equality (3.6) in the form

$$\begin{aligned} 1 - f_j^* f_j - (x_j^{(1)})^* x_j^{(1)} &= 1 - f_j^* f_j - \xi_j^* \hat{U}_{j-1}^* \hat{U}_{j-1} \xi_j \\ &= 1 - f_j^* f_j - [(I - (U'_{j-1})^* U'_{j-1}) \xi_j]^* \xi_j \\ &= 1 - f_j^* f_j + f_j^* U'_{j-1} \xi_j, \end{aligned}$$

where ξ_j is a solution of equation (3.4). By applying the first part of Lemma 2.1 to the matrix $I - U_j^* U_j$ represented in the form (3.13) we obtain the inequality

$$1 - f_j^* f_j + f_j^* U'_{j-1} \xi_j \geq 0.$$

Finally, in the case $\mathrm{Ker}(\hat{U}_{j-1}^*) = \{0\}$, by using the equality (3.12) we have

$$\mathrm{Ker}(I - (U'_{j-1})^* U'_{j-1}) = \{0\}.$$

Hence, by Lemma 2.1 we obtain $1 - f_j^* f_j + f_j^* U'_{j-1} \xi_j = 0$.

Now we prove the necessity. Let U be a unitary completion of the lower triangular part U_L. For $j = 1$ we have $U_1 = U(:,1)$ and, hence, $U_1^* U_1 = 1$. For $j = 2, \ldots, N$ we use the representations

$$U_j = \begin{bmatrix} U'_{j-1} & f_j \end{bmatrix}, \quad U(:,1:j) = \begin{bmatrix} \hat{U}_{j-1} & x_j \\ U'_{j-1} & f_j \end{bmatrix}.$$

The orthonormality of the columns of the matrix $U(:,1:j)$ implies that

$$\begin{aligned} \hat{U}_{j-1}^* x_j + (U'_{j-1})^* f_j &= 0, \\ x_j^* x_j + f_j^* f_j &= 1, \qquad\qquad j = 2, \ldots, N. \\ \hat{U}_{j-1}^* \hat{U}_{j-1} + (U'_{j-1})^* U'_{j-1} &= I. \end{aligned}$$

One can write these equalities in the form

$$\begin{aligned} -(U'_{j-1})^* f_j &= \hat{U}_{j-1}^* x_j, \quad -f_j^* U'_{j-1} = x_j^* \hat{U}_{j-1}, \\ I - (U'_{j-1})^* U'_{j-1} &= \hat{U}_{j-1}^* \hat{U}_{j-1}, \quad 1 - f_j^* f_j = x_j^* x_j, \end{aligned}$$

i.e.,

$$\left[\begin{array}{cc} I - (U'_{j-1})^* U'_{j-1} & -(U'_{j-1})^* f_j \\ -f_j^* U'_{j-1} & 1 - f_j^* f_j \end{array} \right] = \left[\begin{array}{c} \hat{U}_{j-1}^* \\ x_j^* \end{array} \right] \left[\begin{array}{cc} \hat{U}_{j-1} & x_j \end{array} \right], \quad j = 2, \ldots, N.$$

This implies $I_j - U_j^* U_j = K_j^* K_j$, $j = 2, \ldots, N$, where $K_j = \left[\begin{array}{cc} \hat{U}_{j-1} & x_j \end{array} \right]$. Hence, it follows that $\|U_j\| \leq 1$. Moreover, since the matrix K_j has size $(j-1) \times j$, the matrix $K_j^* K_j$ turns out to be singular. Whence $\|U_j\| = 1$.

Finally we check that if the conditions (3.7) hold, then the unitary completion U is unique and the formulas (3.8) also hold. The conditions (3.7) imply that the matrices $I - (U'_{j-1})^* U'_{j-1}$, $j = 2, \ldots, N$, are invertible. Moreover, by using the formulas (3.2)-(3.5) we obtain that the unspecified entries of the unitary completion are determined by the relations

$$x_j = -\hat{U}_{j-1}(I - (U'_{j-1})^* U'_{j-1})^{-1}(U'_{j-1})^* f_j + x_j^{(2)}, \quad j = 2, \ldots, N,$$

where $x_j^{(2)} \in \mathrm{Ker}(\hat{U}_{j-1}^*)$. But the equality (3.12) implies that $\mathrm{Ker}(\hat{U}_{j-1}^*) = \{0\}$ and, therefore, $x_j^{(2)} = 0$. Hence, we conclude that the unitary completion U is unique and the relations (3.8) hold.   □

From the equalities (3.12) it follows that the uniqueness conditions (3.7) imply the strong regularity of the completion U. The conditions (3.7) look like the ones in [4]. However, here instead of the factorized form we use the element-wise representations (3.8), which turn out to be more appropriate for the solution of the structured completion problem addressed in the next section.

In conclusion we give a simple example showing that the unitary completion can not be unique. Consider the matrix $C = (c_{i,j})$ such that $c_{i+1,i} = 1$, $i = 1, \ldots, n-1$, $c_{1,N} = z$ and $c_{i,j} = 0$ elsewhere. For any choice of z with $|z| = 1$ this matrix may be treated as a unitary completion of its specified lower triangular part.

4. The structured unitary completion

Now we consider a partially specified matrix $U = \{u_{ij}\}_{i,j=1}^N$ with the specified lower triangular part $U_L = \{u_{ij}, i \geq j\}$ of the form

(4.1) $U_L(i+1, i) = \beta_i$, $i = 1, \ldots, N-1$; $U_L(i, i) = d_i$, $i = 1, \ldots, N$;

(4.2) $U_L(i, j) = p(i)q(j)$, $1 \leq j \leq i-2$, $3 \leq i \leq N$,

with some $\beta_i, d_i, p(i), q(i) \in \mathbb{C}$. For notational convenience we also define the values $q(-1), q(0), q(N-1), q(N), \beta_0, \beta_N, p(1), p(2), p(N+1), p(N+2)$ assuming them to be zeros.

By means of the elements $p(i)$ and $q(j)$ of the structure (4.2) we define the numbers

(4.3) $\alpha_k = \sum_{j=1}^k |q(j)|^2$, $k = 1, \ldots, N-2$,

(4.4) $z_k = \sum_{j=k}^N |p(j)|^2$, $k = N, \ldots, 3$,

and the vector-columns and the vector-rows
(4.5)
$$p_i = \begin{pmatrix} p(i) \\ \vdots \\ p(N) \end{pmatrix}, \ i = 3, \ldots, N, \quad q_j = \begin{pmatrix} q(1) & \cdots & q(j) \end{pmatrix}, \ j = 1, \ldots, N-2.$$

Obviously, we have

(4.6)
$$p_N = p(N), \ p_i = \begin{pmatrix} p(i) \\ p_{i+1} \end{pmatrix}, \ i = 3, \ldots, N-1,$$

$$q_1 = q(1), \ q_j = \begin{pmatrix} q_{j-1} & q(j) \end{pmatrix}, \ j = 1, \ldots, N-2.$$

We also set $q_{-1} = q_0 = 0$, $p_{N+1} = p_{N+2} = 0$, $\alpha_{-1} = \alpha_0 = z_{N+1} = z_{N+2} = 0$. It is clear that $\|q_k\| = \sqrt{\alpha_k}$, $\|p_k\| = \sqrt{z_k}$. Furthermore, we introduce the unit vectors $q_j^{(0)}$ and $p_j^{(0)}$ such that

(4.7)
$$q_j = \sqrt{\alpha_j} q_j^{(0)}, \quad p_j = \sqrt{z_j} p_j^{(0)}.$$

In the case under consideration the condition of Theorem 3.1 may be expressed via the corresponding properties of certain 3×3 matrices formed by the elements of the structure (4.1)-(4.4).

Theorem 4.1. *Let $U = \{u_{ij}\}_{i,j=1}^N$ be a partially specified matrix with a specified lower triangular part $U_L = \{u_{ij}, i \geq j\}$ of the form (4.1), (4.2). Set*

(4.8) $\Delta_j = \begin{pmatrix} p(j)\sqrt{\alpha_{j-2}} & \beta_{j-1} & d_j \\ p(j+1)\sqrt{\alpha_{j-2}} & p(j+1)q(j-1) & \beta_j \\ \sqrt{z_{j+2}}\sqrt{\alpha_{j-2}} & \sqrt{z_{j+2}}q(j-1) & \sqrt{z_{j+2}}q(j) \end{pmatrix}, \quad j = 1, \ldots, N.$

The specified part U_L has a unitary completion U if and only if

(4.9) $$\|\Delta_j\| = 1, \quad j = 1, \ldots, N.$$

If the condition (4.9) holds and additionally the matrices

(4.10) $A_j = \begin{pmatrix} p(j+1)\sqrt{\alpha_{j-1}} & \beta_j \\ \sqrt{z_{j+2}}\sqrt{\alpha_{j-1}} & \sqrt{z_{j+2}}q(j) \end{pmatrix}, \quad j = 1, \ldots, N-1,$

satisfy the condition

(4.11) $$\|A_j\| < 1, \quad j = 1, \ldots, N-1,$$

then the unitary completion U is unique.

Proof. Set

$$L_1 = \begin{bmatrix} 0 & 0 & U_1 \end{bmatrix}, \ L_2 = \begin{bmatrix} 0 & U_2 \end{bmatrix},$$
$$L_j = U_j, \quad j = 3, \ldots, N-2,$$

$$L_{N-1} = \begin{bmatrix} U_{N-1} \\ 0 \end{bmatrix}, \ L_N = \begin{bmatrix} U_N \\ 0 \\ 0 \end{bmatrix},$$

where zeros mean zero columns and zero rows of the corresponding sizes. The relations (4.1), (4.2) and (4.5) imply

$$L_j = \begin{pmatrix} p(j)q_{j-2} & \beta_{j-1} & d_j \\ p(j+1)q_{j-2} & p(j+1)q(j-1) & \beta_j \\ p_{j+2}q_{j-2} & p_{j+2}q(j-1) & p_{j+2}q(j) \end{pmatrix}, \quad j = 1, \ldots, N.$$

Obviously we have $\|U_j\| = \|L_j\|$, $j = 1, \ldots, N$, and, hence, by Theorem 3.1 the specified part U_L has a unitary completion if and only if $\|L_j\| = 1$, $j = 1, \ldots, N$. One can easily check that $L_j = P_j \cdot \Delta_j \cdot Q_j$, $j = 1, \ldots, N$, where

$$Q_j = \begin{pmatrix} q_{j-2}^{(0)} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad P_j = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & p_{j+2}^{(0)} \end{pmatrix}$$

and the matrices Δ_j and the unit vectors $q_{j-2}^{(0)}, p_{j+2}^{(0)}$ are defined as in (4.8) and in (4.7), respectively. Since the operators P_j and Q_j^* are isometries we conclude that $\|L_j\| = \|\Delta_j\|$, $j = 1, \ldots, N$. Hence it follows that the specified part U_L has a unitary completion U if and only if the condition (4.9) holds.

Now we prove the uniqueness of the completion. Similarly as above we set

$$(4.12) \quad L_1' = \begin{bmatrix} 0 & U_1' \end{bmatrix}, \quad L_j' = U_j', \quad j = 2, \ldots, N - 2; \quad L_{N-1}' = \begin{bmatrix} U_{N-1}' \\ 0 \end{bmatrix},$$

where zeros mean zero columns and zero rows of the corresponding sizes. By virtue of (4.1), (4.2) and (4.5) we obtain

$$(4.13) \qquad L_j' = \begin{pmatrix} p(j+1)q_{j-1} & \beta_j \\ p_{j+2}q_{j-1} & p_{j+2}q(j) \end{pmatrix}, \quad j = 1, \ldots, N - 1.$$

Again we find $\|U_j'\| = \|L_j'\|$, $j = 1, \ldots, N - 1$, and, hence, the condition (3.7) is equivalent to the condition $\|L_j'\| < 1$, $j = 1, \ldots, N - 1$. One can easily check that

$$(4.14) \qquad\qquad L_j' = P_j' \cdot A_j \cdot Q_j', \quad j = 1, \ldots, N - 1,$$

where

$$Q_j' = \begin{pmatrix} q_{j-1}^{(0)} & 0 \\ 0 & 1 \end{pmatrix}, \quad P_j' = \begin{pmatrix} 1 & 0 \\ 0 & p_{j+2}^{(0)} \end{pmatrix}$$

and the matrices A_j and the unit vectors $q_{j-1}^{(0)}, p_{j+2}^{(0)}$ are defined as in (4.10) and in (4.7), respectively. Since the operators P_j' and $(Q')_j^*$ are isometries we conclude that $\|L_j'\| = \|A_j\|$, $j = 1, \ldots, N - 1$, which completes the proof. $\qquad\square$

Remark 4.2. Under the hypotheses of Theorem 4.1 the unitary matrix U with a specified lower triangular part $U_L = \{u_{ij}, i \geq j\}$ of the form (4.1), (4.2) is completely defined via the parameters d_i, $i = 1, \ldots, N$, β_i, $i = 1, \ldots, N - 1$, $p(i)$, $i = 3, \ldots, N - 1$ and $q(i)$, $i = 1, \ldots, N - 2$.

In the next theorem we reformulate the necessary and sufficient conditions for the existence of a unitary completion of the specified part U_L under the assumption that all the parameters of the structure (4.1), (4.2) are fixed except the diagonal entries d_j. In this theorem we assume that the conditions (4.10) and (4.11) hold and therefore, this completion will be unique automatically.

Theorem 4.3. *Let $U = \{u_{ij}\}_{i,j=1}^N$ be a partially specified matrix with a specified lower triangular part $U_L = \{u_{ij}, i \geq j\}$ of the form (4.1), (4.2), let the conditions (4.10), (4.11) hold and let*

$$(4.15) \qquad\qquad I - A_j^* A_j = V_j D_j^2 V_j^*, \quad j = 1, \ldots, N - 1,$$

where V_j are unitary and D_j are real diagonal invertible matrices.

Then the specified part U_L has a unique unitary completion if and only if

$$(4.16) \qquad\qquad |d_j + a_j| = \rho_j, \quad j = 1, \ldots, N,$$

where

(4.17)

$$a_j = \frac{\tilde{g}_j^* \tilde{f}_j}{1 + \|\tilde{g}_j\|^2}, \quad \rho_j = \left(\frac{1 - |\beta_j|^2 - z_{j+2}|q(j)|^2 - \|\tilde{f}_j\|^2}{1 + \|\tilde{g}_j\|^2} + |a_j|^2 \right)^{1/2}, \quad j = 1, \ldots, N,$$

(4.18)

$$\tilde{f}_1 = \tilde{g}_1 = 0; \quad \tilde{g}_j = D_{j-1}^{-1} V_{j-1}^* \begin{pmatrix} \sqrt{\alpha_{j-2}} p^*(j) \\ \beta_{j-1}^* \end{pmatrix}, \quad \tilde{f}_j = D_{j-1}^{-1} V_{j-1}^* \begin{pmatrix} \sqrt{\alpha_{j-2}} \\ q^*(j-1) \end{pmatrix} \beta_j',$$

(4.19)

$$\beta_j' = p^*(j+1)\beta_j + z_{j+2}q(j), \quad j = 2, \ldots, N.$$

Proof. By Theorem 4.1 we should prove the equivalence of the conditions (4.9), involving the matrices Δ_j, $j = 1, \ldots, N$, defined in (4.8), and the conditions (4.16). We use the representations

$$\Delta_j = \begin{bmatrix} g_{j-1} & d_j \\ B_{j-1} & f_j \end{bmatrix}, \quad j = 1, \ldots, N,$$

where

$$g_{j-1} = \begin{pmatrix} p(j)\sqrt{\alpha_{j-2}} & \beta_{j-1} \end{pmatrix}, \quad f_j = \begin{pmatrix} \beta_j \\ \sqrt{z_{j+2}}q(j) \end{pmatrix},$$

$$B_{j-1} = \begin{pmatrix} p(j+1)\sqrt{\alpha_{j-2}} & p(j+1)q(j-1) \\ \sqrt{z_{j+2}}\sqrt{\alpha_{j-2}} & \sqrt{z_{j+2}}q(j-1) \end{pmatrix}.$$

For $j = 1$ we have $g_0 = 0$, $B_0 = 0$ and, hence, the condition $\|\Delta_1\| = 1$ holds if and only if $\|f_1\|^2 + |d_1|^2 = 1$, i.e., $|d_1|^2 = 1 - |\beta_1|^2 - z_3|q(1)|^2$.

For $j = 2, \ldots, N$ we show that

(4.20)

$$(\Delta_{j-1}')^* \Delta_{j-1}' = A_{j-1}^* A_{j-1}, \quad j = 2, \ldots, N.$$

Set

(4.21)

$$\Gamma_k = \begin{pmatrix} p(k+1) & \beta_k \\ 1 & q(k) \end{pmatrix},$$

$$\Lambda_k = \begin{pmatrix} \sqrt{\alpha_{k-1}} & 0 \\ 0 & 1 \end{pmatrix}, \quad k = 1, \ldots, N-1.$$

$$Z_k = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{z_{k+2}} \end{pmatrix},$$

By direct computations it is verified that $A_k = Z_k \Gamma_k \Lambda_k$, $k = 1, \ldots, N-1$. Furthermore, we have

(4.22)

$$\Delta_{j-1}' = Z_j' \Gamma_{j-1} \Lambda_{j-1},$$

where

(4.23)

$$Z_j' = \begin{pmatrix} 1 & 0 \\ 0 & p(j+1) \\ 0 & \sqrt{z_{j+2}} \end{pmatrix}.$$

By using the equality $(Z_j')^* Z_j' = Z_{j-1}^* Z_{j-1}$ we obtain (4.20). Furthermore using (4.15) we obtain

(4.24)

$$I - (\Delta_{j-1}')^* \Delta_{j-1}' = V_{j-1} D_{j-1}^2 V_{j-1}^*.$$

Moreover, it is easily verified that

$$B_{j-1}^* f_j = \begin{pmatrix} \sqrt{\alpha_{j-2}} \\ q(j-1)^* \end{pmatrix} \beta_j',$$

where β_j' is given by the formula (4.19). Thus, by applying Theorem 2.2, we conclude that for $j = 2, \ldots, N$ the corresponding equalities in the conditions (4.9) and (4.16) are equivalent. $\square$

5. The generators

Let $U = \{u_{ij}\}_{i,j=1}^N$ be a unitary matrix whose entries below the first subdiagonal have the form (4.2), i.e., $U(i,j) = p(i)q(j)$, $1 \le j \le i-2$, $3 \le i \le N$. Hence, it follows that $\text{rank} U(k+1 : N, 1 : k) \le 2$, $k = 1, \ldots, N-1$. Since the matrix U is unitary, Corollary 2.2 from [6] implies that

$$\text{rank} U^{-1}(k+1 : N, 1 : k) = \text{rank} U(1 : k, k+1 : N) \le 2, \quad k = 1, \ldots, N-1.$$

Therefore, by Theorem 3.5 from [5] we find that the entries in the strictly upper triangular part of the matrix U have the form

$$(5.1) \qquad\qquad U(i,j) = v(i) b_{ij}^\times u(j), \quad 1 \le i < j \le N,$$

where $v(i)$, $i = 1, \ldots, N-1$, are two-dimensional rows, $u(j)$, $j = 2, \ldots, N$, are two-dimensional columns, $b_{ij}^\times = b(i+1) \cdots b(j-1)$ for $N \ge j > i+1 \ge 2$, $b_{k,k+1}^\times = I$ for $1 \le k \le N-1$ and $b(k)$, $k = 2, \ldots, N-1$, are 2×2 matrices. The elements $v(i), u(j), b(k)$ are called *upper generators* of the matrix U. Notice that the relations (5.1) may be written down column-by-column in the form

$$U(1 : j-1, j) = \tilde{W}_{j-1} u(j), \quad j = 2, \ldots, N,$$

where $\tilde{W}_{j-1}$ are $(j-1) \times 2$ matrices given by $\tilde{W}_{j-1} = \text{col}(v(i) b_{ij}^\times)_{i=1}^{j-1}$, $j = 2, \ldots, N$. One can easily check that the matrices $\tilde{W}_k$ satisfy the recursive relations:

$$(5.2) \qquad \tilde{W}_1 = v(1); \quad \tilde{W}_i = \begin{pmatrix} \tilde{W}_{i-1} b(i) \\ v(i) \end{pmatrix}, \quad i = 2, \ldots, N-1.$$

In the next theorem we derive explicit formulas for the upper generators of the unitary completion of a partially specified matrix with the specified lower triangular part of the form (4.1), (4.2).

Theorem 5.1. *Let* $U = \{u_{ij}\}_{i,j=1}^N$ *be a partially specified matrix with a specified lower triangular part* $U_L = \{u_{ij}, i \ge j\}$ *of the form*

$$(5.3) \qquad U_L(i+1,i) = \beta_i, \ i = 1, \ldots, N-1, \quad U_L(i,i) = d_i, \ i = 1, \ldots, N,$$

$$(5.4) \qquad\quad U_L(i,j) = p(i)q(j), \quad 1 \le j \le i-2, \ 3 \le i \le N,$$

and let condition (4.9) *of Theorem 4.1 hold. Set*

$$(5.5) \qquad \alpha_{-1} = \alpha_0 = 0, \quad \alpha_k = \sum_{j=1}^{k} |q(j)|^2, \ k = 1, \ldots, N-2,$$

$$(5.6) \qquad z_{N+2} = z_{N+1} = 0, \quad z_k = \sum_{j=k}^{N} |p(j)|^2, \ k = N, \ldots, 3,$$

$$(5.7) \quad \Gamma_k = \begin{pmatrix} p(k+1) & \beta_k \\ 1 & q(k) \end{pmatrix}, \ \Lambda_k = \begin{pmatrix} \sqrt{\alpha_{k-1}} & 0 \\ 0 & 1 \end{pmatrix}, \ Z_k = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{z_{k+2}} \end{pmatrix},$$

$$(5.8) \qquad A_k = Z_k \Gamma_k \Lambda_k, \quad k = 1, \ldots, N-1,$$

and assume that $\|A_j\| < 1$, $j = 1, \ldots, N-1$. *Also set*

$$(5.9) \qquad I - A_k^* A_k = V_k D_k^2 V_k^*, \quad k = 1, \ldots, N-1,$$

where V_k *is a unitary matrix and* D_k *is a real diagonal invertible matrix.*

   Then the specified part U_L *has the unique unitary completion* U *and the upper generators* $v(i)$, $i = 1, \ldots, N-1$, $u(j)$, $j = 2, \ldots, N$, $b(k)$, $k = 2, \ldots, N-1$, *of the matrix* U *are given by the formulas*

$$(5.10) \qquad v(i) = - \begin{bmatrix} p(i)\sqrt{\alpha_{i-2}}\alpha_i' + \beta_{i-1}\alpha_i'' & d_i \end{bmatrix} V_i D_i^{-1}, \quad i = 1, \ldots, N-1,$$

$$(5.11) \quad u(j) = D_{j-1}^{-1} V_{j-1}^* \Lambda_{j-1} \Gamma_{j-1}^* \begin{pmatrix} d_j \\ p(j+1)^* \beta_j + z_{j+2} q(j) \end{pmatrix}, \quad j = 2, \ldots, N,$$

$$(5.12) \qquad b(k) = \begin{bmatrix} D_{k-1} V_{k-1}^* q_k' & -u(k) \end{bmatrix} V_k D_k^{-1}, \quad k = 2, \ldots, N-1,$$

where
$$(5.13)$$
$$\alpha_i' = \begin{cases} \sqrt{\dfrac{\alpha_{i-2}}{\alpha_{i-1}}}, & \alpha_{i-1} \neq 0, \\ 0, & \alpha_{i-1} = 0, \end{cases} \quad \alpha_i'' = \begin{cases} \dfrac{q^*(i-1)}{\sqrt{\alpha_{i-1}}}, & \alpha_{i-1} \neq 0, \\ 1, & \alpha_{i-1} = 0, \end{cases} \quad q_i' = \begin{pmatrix} \alpha_i' \\ \alpha_i'' \end{pmatrix}.$$

Proof. Theorem 4.1 implies that the specified part U_L has the unique unitary completion U. Moreover, by the last part of Theorem 3.1, the unspecified entries of this completion are given by the relations

$$(5.14) \quad x_j := U(1 : j-1, j) = -\hat{U}_{j-1}(I - (U_{j-1}')^* U_{j-1}')^{-1}(U_{j-1}')^* f_j, \quad j = 2, \ldots, N,$$

where $U_j' = U_L(j+1 : N, 1 : j)$, $j = 1, \ldots, N-1$, and $f_j = U_L(j : N, j)$, $\hat{U}_j = U(1 : j, 1 : j)$, $j = 1, \ldots, N$.

   Set

$$(5.15) \qquad W_1 = \begin{bmatrix} 0 & \hat{U}_1 \end{bmatrix}, \quad W_j = \hat{U}_j, \ j = 2, \ldots, N-1,$$

$$w_j = f_j, \ j = 2, \ldots, N-1, \quad w_N = \begin{bmatrix} f_N \\ 0 \end{bmatrix},$$

and define the matrices L_j', $j = 1, \ldots, N-1$, via the relations (4.12). Clearly, we have

$$\hat{U}_{j-1}(I - (U_{j-1}')^* U_{j-1}')^{-1}(U_{j-1}')^* w_j$$
$$= W_{j-1}(I - (L_{j-1}')^* L_{j-1}')^{-1}(L_{j-1}')^* w_j, \quad j = 2, \ldots, N,$$

and, hence, the formula (5.14) gives

$$(5.16) \qquad x_j = -W_{j-1}(I - (L_{j-1}')^* L_{j-1}')^{-1}(L_{j-1}')^* w_j, \quad j = 2, \ldots, N.$$

Next set

(5.17)
$$Q_i' = \begin{pmatrix} q_{i-1}^{(0)} & 0 \\ 0 & 1 \end{pmatrix}, \quad i = 1, \ldots, N-1,$$

where

$$q_{i-1}^{(0)} = \begin{cases} \frac{1}{\sqrt{\alpha_{i-1}}} q_{i-1}, & \alpha_{i-1} \neq 0, \\ e_{i-1}^T, & \alpha_{i-1} = 0, \end{cases}$$

$e_0 = 1$ and e_i, $i = 1, \ldots, N-1$, is the i-th vector of the standard basis. By virtue of (4.14) we have

(5.18)
$$(L_{j-1}')^* L_{j-1}' = (Q_{j-1}')^* A_{j-1}^* A_{j-1} Q_{j-1}', \quad j = 2, \ldots, N,$$

and from (4.13) we obtain

(5.19)
$$(L_{j-1}')^* = (Q_{j-1}')^* \Lambda_{j-1} \Gamma_{j-1}^* \begin{pmatrix} 1 & 0 \\ 0 & p_{j+1}^* \end{pmatrix}, \quad j = 2, \ldots, N.$$

Consider the products

(5.20)
$$\hat{f}_j = \begin{pmatrix} 1 & 0 \\ 0 & p_{j+1}^* \end{pmatrix} w_j, \quad j = 2, \ldots, N.$$

By using the relations (4.1), (4.2) and (4.5) we obtain

$$w_j = \begin{pmatrix} d_j \\ \beta_j \\ p_{j+2} q(j) \end{pmatrix}, \ j = 2, \ldots, N-2, \quad w_{N-1} = \begin{pmatrix} d_{N-1} \\ \beta_{N-1} \end{pmatrix}, \quad w_N = \begin{pmatrix} d_N \\ 0 \end{pmatrix}$$

and, hence, from (4.6) and the initializations $\beta_N = z_{N+1} = z_{N+2} = 0$ we get

(5.21)
$$\hat{f}_j = \begin{pmatrix} d_j \\ p^*(j+1)\beta_j + z_{j+2} q(j) \end{pmatrix}, \quad j = 2, \ldots, N.$$

In this way, by combining together (5.16), (5.18), (5.19) and (5.20) we obtain
(5.22)
$$x_j = -W_{j-1}(I - (Q_{j-1}')^* A_{j-1}^* A_{j-1} Q_{j-1}')^{-1}(Q_{j-1}')^* \Lambda_{j-1} \Gamma_{j-1}^* \tilde{f}_j, \quad j = 2, \ldots, N,$$

where $\hat{f}_j$ are defined as in (5.21). Next consider the matrix

$$\Upsilon_j = (I - (Q_{j-1}')^* A_{j-1}^* A_{j-1} Q_{j-1}')^{-1}(Q_{j-1}')^*.$$

Recall that if V and B are matrices of appropriate sizes such that $I - VB$ is invertible, then the Sherman-Morrison-Woodbury formula [9] states that

(5.23)
$$(I - VB)^{-1} = I + V(I - BV)^{-1}B.$$

By taking $V = (Q_{j-1}')^*, B = A_{j-1}^* A_{j-1} Q_{j-1}'$ and using the fact that the columns of the matrix $(Q_{j-1}')^*$ are orthonormal we obtain

$$\Upsilon_j = [I + (Q_{j-1}')^*(I - A_{j-1}^* A_{j-1})^{-1} A_{j-1}^* A_{j-1} Q_{j-1}'](Q_{j-1}')^*$$
$$= (Q_{j-1}')^*[I + (I - A_{j-1}^* A_{j-1})^{-1} A_{j-1}^* A_{j-1}].$$

Now by the formula (5.23) applied with $V = I$ and $B = A_{j-1}^* A_{j-1}$ we get

$$\Upsilon_j = (Q_{j-1}')^*(I - A_{j-1}^* A_{j-1})^{-1}.$$

Substituting the latter expression in (5.22) and then using the decomposition (5.9) gives

$$x_j = -W_{j-1}(Q_{j-1}')^* V_{j-1} D_{j-1}^{-2} V_{j-1}^* \Lambda_{j-1} \Gamma_{j-1}^* \hat{f}_j, \quad j = 2, \ldots, N.$$

Hence, it follows that

(5.24)
$$x_j = \tilde{W}_{j-1} u(j), \quad j = 2, \ldots, N,$$

where

(5.25)
$$\tilde{W}_i = -W_i (Q'_i)^* V_i D_i^{-1}, \quad i = 1, \ldots, N-1,$$

and $u(j)$, $j = 2, \ldots, N$, are defined as in (5.11).

It remains to show that the matrices $\tilde{W}_i$, $i = 1, \ldots, N-1$, satisfy the relations (5.2) with two-dimensional rows $v(i)$ and 2×2 matrices $b(i)$ defined as in (5.10) and (5.12). Without restriction we can suppose that $3 \le i \le N-1$. The proof for $i = 1$ and $i = 2$ follows as in the general case $3 \le i \le N-1$ by using the appropriate initializations. By virtue of (5.15) and (4.1)-(4.2) we have

(5.26)
$$W_i = \hat{U}_i = \begin{bmatrix} W_{i-1} & x_i \\ g_i & d_i \end{bmatrix}, \quad i = 3, \ldots, N-1,$$

where

(5.27)
$$g_i = \begin{bmatrix} p(i) q_{i-2} & \beta_{i-1} \end{bmatrix}.$$

Next we show that

(5.28)
$$(Q'_i)^* = \begin{pmatrix} (Q'_{i-1})^* q'_i & 0 \\ 0 & 1 \end{pmatrix}, \quad i = 3, \ldots, N-1.$$

By virtue of (5.17) one should check that

(5.29)
$$(q_{i-1}^{(0)})^* = \begin{pmatrix} (q_{i-2}^{(0)})^* & 0 \\ 0 & 1 \end{pmatrix} q'_i, \quad i = 3, \ldots, N-1.$$

In the case $\alpha_{i-1} \ne 0$, from the equalities

$$\sqrt{\alpha_{i-1}} (q_{i-1}^{(0)})^* = q_{i-1}^*, \quad \sqrt{\alpha_{i-2}} (q_{i-2}^{(0)})^* = q_{i-2}^*, \quad q_{i-1}^* = \begin{pmatrix} q_{i-2}^* \\ q^*(i-1) \end{pmatrix},$$

we obtain

$$\sqrt{\alpha_{i-1}} (q_{i-1}^{(0)})^* = \begin{pmatrix} \sqrt{\alpha_{i-2}} (q_{i-2}^{(0)})^* \\ q^*(i-1) \end{pmatrix} = \begin{pmatrix} (q_{i-2}^{(0)})^* & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{\alpha_{i-2}} \\ q^*(i-1) \end{pmatrix},$$

which, by virtue of (5.13), implies (5.29). If, otherwise, $\alpha_{i-1} = 0$, then $\alpha_{i-2} = 0$, too. Hence

$$(q_{i-1}^{(0)})^* = e_{i-1} = \begin{pmatrix} e_{i-2} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} (q_{i-2}^{(0)})^* & 0 \\ 0 & 1 \end{pmatrix} q'_i.$$

Thus, by using (5.26), (5.28) and (5.24) we obtain

$$-W_i (Q'_i)^* = - \begin{bmatrix} W_{i-1} & \tilde{W}_{i-1} u(i) \\ g_i & d_i \end{bmatrix} \begin{bmatrix} (Q'_{i-1})^* q'_i & 0 \\ 0 & 1 \end{bmatrix},$$

i.e.,

(5.30)
$$-W_i (Q'_i)^* = - \begin{bmatrix} W_{i-1} (Q'_{i-1})^* q'_i & \tilde{W}_{i-1} u(i) \\ g_i (Q'_{i-1})^* q'_i & d_i \end{bmatrix}.$$

Moreover, by using (5.25) we get

$$-W_{i-1} (Q'_{i-1})^* = -W_{i-1} (Q'_{i-1})^* V_{i-1} D_{i-1}^{-1} D_{i-1} V_{i-1}^* = \tilde{W}_{i-1} D_{i-1} V_{i-1}^*$$

and, therefore,

$$(5.31) \qquad \begin{aligned} -\left[\ W_{i-1}(Q'_{i-1})^*q'_i \quad \tilde{W}_{i-1}u(i)\ \right]V_iD_i^{-1} \\ = \tilde{W}_{i-1}\left[\ D_{i-1}V_{i-1}^*q'_i \quad -u(i)\ \right]V_iD_i^{-1} = \tilde{W}_{i-1}b(i). \end{aligned}$$

Furthermore, by virtue of (5.27), (5.17), (5.13) and the equality $q_{i-2}(q_{i-2}^{(0)})^* = \sqrt{\alpha_{i-2}}$ we obtain

$$g_i(Q'_{i-1})^*q'_i = \left[\ p(i)q_{i-2} \quad \beta_{i-1}\ \right]\left[\begin{matrix}(q_{i-2}^{(0)})^* & 0 \\ 0 & 1\end{matrix}\right]\left[\begin{matrix}\alpha'_i \\ \alpha''_i\end{matrix}\right] = p(i)\sqrt{\alpha_{i-2}}\alpha'_i + \beta_{i-1}\alpha''_i,$$

and, hence,

$$(5.32)$$
$$-\left[\ g_i(Q'_{i-1})^*q'_i \quad d_i\ \right]V_iD_i^{-1} = -\left[\ p(i)\sqrt{\alpha_{i-2}}\alpha'_i + \beta_{i-1}\alpha''_i \quad d_i\ \right]V_iD_i^{-1} = v(i).$$

Finally, by combining together (5.25), (5.30), (5.31) and (5.32) we obtain (5.2), with $v(i)$ and $b(i)$ given as in (5.10) and (5.12), respectively, which completes the proof. $\qquad\square$

6. THE QR ITERATION STEP

In this section we apply the unitary completion method to the efficient solution of the eigenvalue problem for a class of structured matrices via structured QR iterations. Exploiting the structure of the associated eigenvalue problems enables us to perform the QR iteration in linear time using a linear memory space. At the same time the novel algorithm is just a fast adaptation of the classical QR iteration and, therefore, it remains robust and converges as fast as the customary QR algorithm.

6.1. **The class $\mathcal{H}_N$.** We consider the class $\mathcal{H}_N$ of upper Hessenberg matrices $A \in \mathbb{C}^{N\times N}$ of the form

$$(6.1) \qquad\qquad A = U - pq^T,$$

where $U \in \mathbb{C}^{N\times N}$ is unitary and $p, q \in \mathbb{C}^N$. The vectors $p = (p(i))_{i=1}^N$, $q = (q(i))_{i=1}^N$ are called *the perturbation vectors* of the matrix A. This class includes three well-known subclasses of matrices: unitary Hessenberg matrices, companion matrices and fellow matrices.

Since the matrix A is upper Hessenberg the entries below the first subdiagonal of the matrix U have the form (4.2), i.e.,

$$U(i, j) = p(i)q(j), \quad 1 \le j \le i - 2, \ 3 \le i \le N.$$

Hence, the matrix U has upper generators $v(i)$, $i = 1, \ldots, N-1$, $u(j)$, $j = 2, \ldots, N$, and $b(k)$, $k = 2, \ldots, N-1$, given in accordance with the definition (5.1). Next set

$$U(i+1, i) = \beta_i, \ i = 1, \ldots, N-1, \quad U(i, i) = d_i, \ i = 1, \ldots, N.$$

Therefore, the matrix A is completely defined by the following parameters:
   (1) the subdiagonal entries $\beta_k = U(k+1, k)$, $k = 1, \ldots, N-1$, of the matrix U;
   (2) the diagonal entries $d_k = U(k, k)$, $k = 1, \ldots, N$, of the matrix U;
   (3) the upper generators $v(i)$, $i = 1, \ldots, N-1$, $u(j)$, $j = 2, \ldots, N$, $b(k)$, $k = 2, \ldots, N-1$, of the matrix U;
   (4) the perturbation vectors $p = (p(i))_{i=1}^N$, $q = (q(i))_{i=1}^N$.

These parameters are also called *the generating elements* of the matrix A.

Thus the entries of the matrix A are specified as follows:

(6.2)
$$\begin{aligned} A(i,i) &= d_i - p(i)q(i), & i &= 1,\ldots,N, \\ A(i+1,i) &= \beta_i - p(i+1)q(i), & i &= 1,\ldots,N-1, \\ A(i,j) &= 0, & i-j &> 1, \end{aligned}$$

(6.3) $A(i,j) = -p(i)q(j) + v(i)b_{ij}^\times u(j), \quad 1 \le i < j \le N.$

Let A be a matrix from the class $\mathcal{H}_N$. Consider one single step of the QR iteration for this matrix with the shift α:

$$\begin{cases} A - \alpha I = QR, \\ A^{(1)} = \alpha I + RQ, \end{cases}$$

where Q is a unitary matrix and R is an upper triangular matrix. Since A is upper Hessenberg, then the matrix Q may be taken in the upper Hessenberg form (see for instance [9]) and, therefore, the matrix $A^{(1)} = \alpha I + RQ$ is still upper Hessenberg. Moreover, the unitary factor Q can be represented by its Schur parametrization [7]

(6.4) $Q = \tilde{Q}_1 \tilde{Q}_2 \cdots \tilde{Q}_{N-1},$

where

(6.5) $\tilde{Q}_i = \begin{pmatrix} I_{i-1} & 0 & 0 \\ 0 & Q_i & 0 \\ 0 & 0 & I_{N-i-1} \end{pmatrix}, \quad Q_i = \begin{pmatrix} c_i & -s_i \\ \overline{s_i} & c_i \end{pmatrix}, \quad i = 1,\ldots,N-1,$

with c_i real, $c_i^2 + |s_i|^2 = 1$, $i = 1,\ldots,N-1$,. From $R = \tilde{Q}_{N-1}^* \cdots \tilde{Q}_1^*(A - \alpha I)$ it follows that the entries of R can also be specified in terms of a small set of generators:

(6.6) $R(i,i) = d_i', \quad i = 1,\ldots,N,$

(6.7) $R(i,i+1) = \gamma_i, \quad i = 1,\ldots,N-1,$

(6.8) $R(i,j) = \tilde{v}(i)b_{i+1,j}^\times u(j) - p^{(1)}(i)q(j), \quad 1 \le i < j-1 \le N-1,$

(6.9) $R(i,j) = 0, \quad i > j.$

Further, we have $A^{(1)} = Q^*AQ$ and, by virtue of (6.1),

(6.10) $A^{(1)} = Q^*UQ - (Q^*p) \cdot (q^T Q).$

Hence, $A^{(1)}$ is again a matrix from the class $\mathcal{H}_N$ and, therefore, our goal is to compute the decomposition (6.4), a complete set of generators of R as well as the generating elements of the new iterate $A^{(1)}$ in an efficient way.

6.2. The QR factorization. Let us start by considering the QR factorization of the matrix A from the class $\mathcal{H}_N$. An algorithm for computing the decomposition (6.4) together with a condensed representation for the factor R was derived in our previous paper [1]. For the sake of completeness, the algorithm is summarized below and a (different) proof of its correctness is also given.

Theorem 6.1. *Let A be a matrix from the class $\mathcal{H}_N$ with generating elements d_k, $k = 1,\ldots,N$, β_k, $v(k)$, $k = 1,\ldots,N-1$, $u(k)$, $k = 2,\ldots,n$, $b(k)$, $k = 2,\ldots,N-1$, and $p = (p(i))_{i=1}^N$, $q = (q(i))_{i=1}^N$. Then the elements c_i, s_i, $i = 1, N-1$, and d_i', $i = 1,\ldots,N$, γ_i, $\tilde{v}(i)$, $i = 1,\ldots,N-1$, $p^{(1)}(i)$, $i = 1,\ldots,N$, which define the unitary factor Q in (6.4)-(6.5) and the upper triangular factor R in (6.6)-(6.8), respectively, are generated by the following algorithm:*

(1) *Initialize* $p'(1) = p(1)$, $v'(1) = v(1)$, $\varepsilon_1 = d_1 - \alpha - p(1)q(1)$, $v(N) = 0_{1 \times 2}$, $b(N) = 0_{2 \times 2}$.

(2) *For* $i = 1, \ldots, N - 1$ *do:*

   (a) *Find the complex Givens rotation matrix* Q_i *such that*

$$(6.11) \qquad Q_i^* \begin{pmatrix} \varepsilon_i \\ \beta_i - p(i+1)q(i) \end{pmatrix} = \begin{pmatrix} d_i' \\ 0 \end{pmatrix}.$$

   (b) *Compute*

$$(6.12) \qquad \rho_i = v'(i)u(i+1) - p'(i)q(i+1), \quad \rho_i' = d_{i+1} - \alpha - p(i+1)q(i+1),$$

$$(6.13) \qquad \begin{pmatrix} \gamma_i & p^{(1)}(i) & \tilde{v}(i) \\ \varepsilon_{i+1} & p'(i+1) & v'(i+1) \end{pmatrix} = Q_i^* \begin{pmatrix} \rho_i & p'(i) & v'(i)b(i+1) \\ \rho_i' & p(i+1) & v(i+1) \end{pmatrix}.$$

   (c) *Set* $d_N' = \varepsilon_N$, $p^{(1)}(N) = p'(N)$.

Proof. We set $A_\alpha = A - \alpha I$ and, moreover,

$$A_k = \tilde{Q}_k^* \cdots \tilde{Q}_1^* A_\alpha, \ k = 1, \ldots, N-1, \quad A_{N-1} = Q^* A_\alpha := R,$$

where the unitary matrices $\tilde{Q}_k$, $k = 1, \ldots, N-1$, are defined by the conditions of the theorem. One should check that the matrix R satisfies the relations (6.6)-(6.9). The multiplication by the matrix $\tilde{Q}_1^*$ changes only the first two rows of the matrix A_α, the multiplication by $\tilde{Q}_2^*$ affects only the second and the third row of the matrix A_1 and so on. Hence, we have

$$A_k = \begin{pmatrix} R(1:k,:) \\ y_{k+1} \\ A_\alpha(k+2:N,:) \end{pmatrix}, \ k = 1, \ldots, N-2, \quad R = A_{N-1} = \begin{pmatrix} R(1:N-1,:) \\ y_N \end{pmatrix},$$

where the rows $R(i,:)$ and y_i, $i = 1, \ldots, N$, are defined recursively via the following relations:

$$y_1 = A_\alpha(1,:),$$

$$(6.14) \qquad \begin{pmatrix} R(k,:) \\ y_{k+1} \end{pmatrix} = Q_k^* \begin{pmatrix} y_k \\ A_\alpha(k+1,:) \end{pmatrix}, \quad k = 1, \ldots, N-1,$$

$$R(N,:) = y_N.$$

Let us introduce the $2 \times i$ matrices H_i and i-dimensional rows q_i defined in terms of the generating elements $q(k)$, $u(k)$, $b(k)$ by

$$(6.15) \qquad H_i = \mathrm{row}(b_{i-1,k}^\times u(k))_{k=i}^N, \quad q_i = [q(i), \ldots, q(N)], \quad i = 2, \ldots, N.$$

It is clear that

$$(6.16) \qquad \begin{matrix} H_i = \begin{bmatrix} u(i) & b(i)H_{i+1} \end{bmatrix}, \ q_i = \begin{bmatrix} q(i) & q_{i+1} \end{bmatrix}, \quad i = 2, \ldots, N-1, \\ H_N = u(N), \ q_N = q(N). \end{matrix}$$

From the relations (6.2) and (6.3) it follows that

$$(6.17) \qquad A_\alpha(1,:) = \begin{pmatrix} d_1 - \alpha & v(1)H_2 \end{pmatrix} - p(1)q_1,$$

$$(6.18) \qquad \begin{matrix} A_\alpha(i,:) = \begin{pmatrix} 0_{1 \times (i-2)} & \beta_{i-1} & d_i - \alpha & v(i)H_{i+1} \end{pmatrix} \\ - \begin{pmatrix} 0_{1 \times (i-2)} & p(i)q_{i-1} \end{pmatrix}, \quad i = 2, \ldots, N-1, \end{matrix}$$

$$(6.19) \quad A_\alpha(N,:) = \begin{pmatrix} 0_{1 \times (N-2)} & \beta_{N-1} - p(N)q(N-1) & d_N - \alpha - p(N)q(N) \end{pmatrix}.$$

Now we prove by induction that
(6.20)
$$y_k = \left(\begin{array}{ccc} 0_{1\times(k-1)} & \varepsilon_k & v'(k)H_{k+1} \end{array} \right) - \left(\begin{array}{cc} 0_{1\times k} & p'(k)q_{k+1} \end{array} \right), \quad k = 1, \ldots, N-1,$$

and, moreover, that

(6.21)
$$R(k,:) = \left(\begin{array}{cccc} 0_{1\times(k-1)} & d'_k & \gamma_k & \tilde{v}(k)H_{k+2} \end{array} \right) \\ - \left(\begin{array}{cc} 0_{1\times k} & p^{(1)}(k)q_{k+1} \end{array} \right), \quad k = 1, \ldots, N-2.$$

For $k = 1$ the relation (6.20) follows from the formula (6.17) and the equalities $y_1 = A_\alpha(1,:)$ and $p'(1) = p(1)$, $v'(1) = v(1)$, $\varepsilon_1 = d_1 - \alpha$. Assume that (6.20) is valid for some k with $1 \le k \le N-2$. By using the recursive relations (6.16), the relation (6.20) may be given in the form

(6.22) $y_k = \left(\begin{array}{cccc} 0_{1\times(k-1)} & \varepsilon_k & \rho_k & v'(k)b(k+1)H_{k+2} \end{array} \right) - \left(\begin{array}{cc} 0_{1\times(k+1)} & p'(k)q_{k+2} \end{array} \right)$

and moreover from (6.18) we obtain

(6.23)
$$A_\alpha(k+1,:) = \left(\begin{array}{cccc} 0_{1\times(k-1)} & \beta_k - p(k+1)q(k) & \rho'_k & v(k+1)H_{k+2} \end{array} \right) \\ - \left(\begin{array}{cc} 0_{1\times(k+1)} & p(k+1)q_{k+2} \end{array} \right),$$

with ρ_k, ρ'_k defined in (6.12). By substituting (6.22) and (6.23) in (6.14) and using (6.11), (6.13) we conclude that

$$y_{k+1} = \left(\begin{array}{ccc} 0_{1\times k} & \varepsilon_{k+1} & v'(k+1)H_{k+2} \end{array} \right) - \left(\begin{array}{cc} 0_{1\times(k+1)} & p'(k+1)q_{k+2} \end{array} \right)$$

and, moreover, the relation (6.21) holds.

From (6.21) using (6.15) we obtain the relations (6.6)-(6.9) for $i = 1, \ldots, N-2$. Next by using (6.14) and (6.20) with $k = N-1$ together with the equalities $y_N = R(N,:)$, $H_N = u(N)$, $q_N = q(N)$ and (6.2) we get

$$\left(\begin{array}{c} R(N-1,:) \\ R(N,:) \end{array} \right) = Q^*_{N-1} \left(\begin{array}{ccc} 0_{1\times(N-2)} & \varepsilon_{N-1} & \rho_{N-1} \\ 0_{1\times(N-2)} & \beta_{N-1} - p(N)q(N-1) & \rho'_{N-1} \end{array} \right).$$

Thus, from (6.11) and (6.13) with $i = N-1$ we get

$$R(N-1,:) = \left(\begin{array}{ccc} 0_{1\times(N-2)} & d'_{N-1} & \gamma_{N-1} \end{array} \right), \quad R(N,:) = \left(\begin{array}{cc} 0_{1\times(N-1)} & d'_N \end{array} \right),$$

which implies (6.6), (6.7) and (6.9) for $i = N-1, N$.   □

Remark 6.2. It is immediately seen that the elements $p^{(1)}(i)$, $i = 1, \ldots, N$, computed by the previous algorithm are determined via recursive relations as follows:

$$p'(1) = p(1), \quad \left(\begin{array}{c} p^{(1)}(i) \\ p'(i+1) \end{array} \right) = Q^*_i \left(\begin{array}{c} p'(i) \\ p(i+1) \end{array} \right), \quad i = 1, \ldots, N-1, \quad p^{(1)}(N) = p'(N),$$

which, by virtue of (6.4) and (6.5), imply $p^{(1)} = \text{col}(p_i^{(1)})_{i=1}^{N} = Q^*p$. In this way, by using the formula (6.10), we may conclude that $p^{(1)}$ is the corresponding perturbation vector of the matrix $A^{(1)}$.

6.3. **The RQ step via unitary completion.** Once the QR factorization of $A - \alpha I$ has been computed, at the second stage of the QR iteration the unitary factor Q and the upper triangular factor R are multiplied back together in the reverse order to produce $A^{(1)} = RQ + \alpha I$. In this section we describe how this computation can be carried out in terms of generating elements. In particular, we determine the generating elements of the new iterate $A^{(1)} = RQ + \alpha I$ by means of the parameters defining the structure of the matrices Q and R obtained at the previous stage.

Since R is upper triangular and Q is upper Hessenberg, we have

$$A^{(1)}(i,i) = R(i,i)Q(i,i) + R(i,i+1)Q(i+1,i) + \alpha, \ i = 1,\ldots,N-1,$$
$$A^{(1)}(N,N) = R(N,N)Q(N,N) + \alpha,$$
$$A^{(1)}(i+1,i) = R(i+1,i+1)Q(i+1,i), \quad i = 1,\ldots,N-1.$$

From (6.4), (6.5) one can easily see that

$$Q(i,i) = c_{i-1}c_i, \ i = 1,\ldots,N, \quad Q(i+1,i) = \overline{s_i}, \ i = 1,\ldots,N-1.$$

Hence, by using the formulas (6.6), (6.7) we obtain

(6.24)
$$A^{(1)}(i,i) = d'_i c_{i-1}c_i + \gamma_i \overline{s}_i + \alpha, \ i = 1,\ldots,N-1, \quad A^{(1)}(N,N) = d'_N c_{N-1}c_N + \alpha,$$

(6.25)
$$A^{(1)}(i+1,i) = d'_{i+1}\overline{s}_i, \quad i = 1,\ldots,N-1.$$

From (6.10) one deduces that the second perturbation vector $q^{(1)} = (q^{(1)}(i))_{i=1}^N$ of the matrix $A^{(1)}$ has the form $q^{(1)} = Q^T q$; moreover, by using (6.4) we have

$$q^{(1)} = \tilde{Q}_{N-1}^T \cdots \tilde{Q}_1^T q.$$

Due to (6.5) the perturbation vector $q^{(1)}$ can be computed as follows:
(6.26)
$$q'(1) = q(1), \ \begin{pmatrix} q^{(1)}(i) \\ q'(i+1) \end{pmatrix} = Q_i^T \begin{pmatrix} q'(i) \\ q(i+1) \end{pmatrix}, \ i = 1,\ldots,N-1, \ q^{(1)}(N) = q'(N).$$

Now let us consider the unitary matrix $U^{(1)} = A^{(1)} + p^{(1)}(q^{(1)})^T$. Using (6.24), (6.25) we obtain the formulas

$$d_i^{(1)} := U^{(1)}(i,i) = d'_i c_{i-1}c_i + \gamma_i \overline{s}_i + \alpha + p^{(1)}(i)q^{(1)}(i), \ i = 1,\ldots,N-1,$$

(6.27)
$$d_i^{(1)} := U^{(1)}(N,N) = d'_N c_{N-1}c_N + \alpha + p^{(1)}(N)q^{(1)}(N),$$

(6.28)
$$\beta_i^{(1)} := U^{(1)}(i+1,i) = d'_{i+1}\overline{s}_i + p^{(1)}(i+1)q^{(1)}(i), \quad i = 1,\ldots,N-1.$$

Furthermore, the entries of $U^{(1)}$ below the subdiagonal have the form

$$U^{(1)}(i,j) = p^{(1)}(i)q^{(1)}(j), \quad 1 \le j \le i-2, \ 3 \le i \le N.$$

By Theorem 4.3 the data $d_i^{(1)}$, $\beta_i^{(1)}$, $p^{(1)}(i)$, $q^{(1)}(i)$ have to satisfy the conditions (4.16)-(4.19). However, because of rounding errors, a progressive violation of the conditions (4.16)-(4.19) may take place during the iterative process, and this leads to a deterioration for the matrix $U^{(1)}$ to be unitary. To overcome this drawback we replace the diagonal entries $d_i^{(1)}$ with suitably corrected values $\hat{d}_i^{(1)}$ leaving unchanged the other elements $\beta_i^{(1)}$, $p^{(1)}(i)$, $q^{(1)}(i)$ of the structure of the lower triangular part of the matrix $U^{(1)}$. By Theorem 4.3 in this case the corrected values $(\hat{d}_U)_i$ have to be chosen so that the relations

(6.29)
$$|\hat{d}_i^{(1)} + a_i| = \rho_i, \quad i = 1,\ldots,N,$$

hold. Here the values ρ_i, a_i are defined via the elements $\beta_i^{(1)}$, $p^{(1)}(i)$, $q^{(1)}(i)$ by the formulas (4.17)-(4.19). Thus for every $i = 1,\ldots,N$ we choose the value $\hat{d}_i^{(1)}$ such

that equation (6.29) is valid and the value $|\hat{d}_i^{(1)} - d_i^{(1)}|$ is minimal. One can easily check that the desired values $\hat{d}_i^{(1)}$ are given by the formulas

$$(6.30) \qquad \hat{d}_i^{(1)} = \rho_i \frac{d_i^{(1)} + a_i}{|d_i^{(1)} + a_i|} - a_i, \quad i = 1, \ldots, N.$$

Notice that if the elements $\beta_i^{(1)}$, $p^{(1)}(i)$, $q^{(1)}(i)$ are fixed, then the corrected values $\hat{d}_i^{(1)}$ are uniquely defined. If the computations were made without rounding errors, then the values $d_i^{(1)}$ and $\hat{d}_i^{(1)}$ would coincide and the the matrix $U^{(1)}$ is unitary. Replacing $d_i^{(1)}$ with $\hat{d}_i^{(1)}$ by Theorem 4.3 we obtain a new matrix $\hat{U}^{(1)}$ which is unitary, and hence the new step of the algorithm will continue starting with the unitary matrix.

Now we are in a position to compute the upper generators of the unitary matrix $U^{(1)}$ by the formulas (5.10)-(5.13) in Theorem 5.1.

6.4. **The full description of the algorithm and its complexity.** The procedure presented below finds the generating elements of the matrix $A^{(1)}$ given in input the generating elements of $A = A^{(0)}$.

Algorithm 6.3.   – **Structured QR Iteration:**

   1: Using the algorithm of Theorem 6.1 and the formulas (6.26)-(6.27) compute the perturbation vectors $p^{(1)}, q^{(1)}$ of the matrix $A^{(1)}$ and the diagonal entries $d_k^{(1)}$, $k = 1, \ldots, N$, and the subdiagonal entries $\beta_k^{(1)}$, $k = 1, \ldots, N-1$, of the matrix $U^{(1)}$.

   2.1: Using the values $p^{(1)}(i), q^{(1)}(i)$ compute the auxiliary variables α_k, $k = -1, \ldots, N-2$, z_k, $k = 3, \ldots, N+2$, by the formulas (5.5), (5.6)

   2.2: For $k = 1, \ldots, N-1$ using the values $p^{(1)}(k), q^{(1)}(k), \beta_k, \alpha_k, z_k$ compute the matrices $\Gamma_k, \Lambda_k, Z_k, A_k$ by the formulas (5.7), (5.8) and determine the unitary matrices V_k and the real diagonal matrices D_k such that $I - A_k^* A_k = V_k D_k^2 V_k^*$.

   2.3: For $k = 1, \ldots, N$ using the formulas (4.18), (4.19), (4.17) compute the values a_k, ρ_k.

   Thus we have obtained the preliminary data to compute the upper generators of the matrix $U^{(1)}$.

   3: Using the formulas (6.30) compute the corrected values $\hat{d}_i^{(1)}$ of the diagonal entries of the matrix $U^{(1)}$. Thus we have performed the correction of the diagonal entries of the matrix $U^{(1)}$ in order to preserve the property of this matrix of being unitary.

   4: Using the formulas (5.13), (5.10)-(5.12) compute upper generators of the matrix $U^{(1)}$.

Straightforward computations show that the total complexity of Algorithm 6.3 is about $(97 + \rho + 3s + \sigma)N$ flops, i.e., arithmetic operations of the form $a \pm bc$. Here the parameters ρ and s denote the complexity of the computation of the complex Givens rotation and of the square root of a positive number. Moreover, σ yields the complexity of computing the decomposition $\hat{A} = VD^2V^*$, where $\hat{A}$ is a 2×2 positive definite matrix, V is unitary and D is diagonal.

7. Numerical experiments

The purpose of this section is to show that the algorithms for the structured unitary completion problem presented above can be used as building blocks in the design of a numerically robust and computationally efficient QR-based eigenvalue algorithm for input matrices $A \in \mathcal{H}_N$. Very recently, a fast adaptation of the QR eigenvalue algorithm for such matrices has been devised in [1]. Some other fast QR methods have been announced in the talks by J. Demmel at the late Householder Symposium XVI and by M. Gu at the late Sixteenth IWOTA Conference. The cost per step of the algorithm in [1] is about twice that of the QR iteration described in Sect. 6.4. These two algorithms only differ by the way used to carry out the RQ step where the factors $Q^{(k)}$ and $R^{(k)}$ are multiplied back together in the reverse order to produce $A^{(k+1)}$. Our initial rough implementation of the algorithm in [1] starts being faster than the highly tuned LAPACK QR eigensolver employed in MATLAB for N between 300 and 400, and becomes definitely faster for larger N. Thus, although theoretically the complexity of the algorithm in [1] is within the optimal liner bound, in practice it seems that more work needs to be done to make the algorithm competitive for moderate values of the size of the input matrix.

Computational savings can be obtained by using the techniques described in [2] but, unfortunately, this turns out in a numerically unstable algorithm. Here we pursue a different approach to perform the RQ step based on the combination of both the procedure in Sect. 6.4 and the one in [1]. The latter behaved stably on all the examples we have tried so far, while the former is faster but its accuracy can deteriorate if matrices D_k with small diagonal entries are encountered in the iterative process. These considerations, therefore, motivate the following strategy: The RQ step for the matrix $A^{(k)}$, generated at the k-th iteration of the QR eigenvalue algorithm applied to the input matrix $A = A^{(0)} \in \mathcal{H}_N$, is carried out in two different ways depending on the magnitude of the entries of the matrices D_k computed in step 2.4 of the algorithm in Sect. 6.4. In particular, given a fixed prescribed tolerance tol, the proposed composite method executes the RQ step as specified in Sect. 6.4 if all the diagonal entries of the matrices D_k are greater than tol; otherwise, the RQ step is performed as stated in the algorithm in [1]. If p denotes the relative frequency of calls to the algorithm in [1], we find that the resulting algorithm has a cost per step of about $200 \cdot p + 100 \cdot (1 - p)$. The algorithm has been implemented in MATLAB, and numerical experiments have been performed to get indications about the behavior of p and errors as functions of tol.

The main program incorporates the following shifting strategy suggested in [12, p. 549]. At the beginning the shift parameter α is equal to zero. If $A^{(s)} = (a_{i,j}^{(s)}) \in \mathbb{C}^{N \times N}$ satisfies

$$(7.1) \qquad |a_{N,N}^{(s-1)} - a_{N,N}^{(s)}| \le 0.3 \cdot |a_{N,N}^{(s-1)}|,$$

then we apply nonzero shifts by setting $\alpha_k = a_{N,N}^{(k)}$, $k = s, s + 1, \ldots$. This is called the *Rayleigh quotient shifting strategy* because $a_{N,N}^{(k)}$ can be viewed as a Rayleigh quotient [11]. We say that $a_{N,N}^{(k)}$ provides a numerical approximation of an eigenvalue λ of $A = A^{(0)}$ whenever

$$|\beta_N^{(k)}| \le eps \, (|a_{N,N}^{(k)}| + |a_{N-1,N-1}^{(k)}|),$$

where eps is the machine precision, i.e., $eps \simeq 2.2 \cdot 10^{-16}$. If this condition is fulfilled, then we set $\lambda = a_{N,N}^{(k)}$ and deflate the matrix. It is worth noting that the strategy is not tailored for real matrices with possible complex eigenvalues. In this case the use of a different shift strategy (the Wilkinson shift rather than the Rayleigh quotient shift) or, alternatively, the application of an initial random complex shift of the input matrix generally allows one to find all the eigenvalues using complex arithmetic. Differently, we can avoid complex numbers by implementing a structured adaptation of the double-step QR method. The customary approach is based on the double-step version of the *implicit* QR algorithm [11]. Here we only remark that the results presented in this paper on the unitary completion problem can also be used in the framework of implicit QR methods to provide fast adaptations for dealing with unitary+low-rank structures. These generalizations and extensions will be described elsewhere.

After nonzero shifting has begun, we check for the convergence of the last diagonal entry of the currently computed iterate A_k. If convergence fails to occur after 15 iterations, then at the 16-th iteration we set $\alpha_k = 1.5 \, (|a_{N,N}^{(k)}| + |\beta_N^{(k)}|)$ and continue with non-zero shifting. If $a_{N,N}^{(k)}$ does not converge in the next 15 iterations, then the program reports failure. In our experience such failure has never been encountered.

We tested fellow [3] and companion matrices $A \in \mathcal{H}_N$ with random entries generated by the internal MATLAB function *rand*. Specifically, the input matrices are constructed as follows:

(1) Fellow matrices: $A = U + pq^T$, where U is unitary Hessenberg with *Schur parameters* $a_0 = 1$, $a_j = \text{rand} \cdot e^{\mathrm{i}2\pi \cdot \text{rand}}$, $1 \leq j \leq N-1$, $a_N = e^{\mathrm{i}2\pi \cdot \text{rand}}$ and *complementary parameters* $b_j = \sqrt{1 - |a_j|^2}$, $1 \leq j \leq N-1$; moreover, $q = e_N$ and $p = [p(1), \ldots, p(N)]$ with $p(j) = \text{rand} + \mathrm{i} \, \text{rand}$, $1 \leq j \leq N$.
(2) Companion matrices: $A = C + pq^T$, where $C = (c_{i,j})$, $c_{i,j} = 1$ for $i - j = 1$ mod N, $c_{i,j} = 0$ otherwise, is the generator of the *circulant* matrix algebra, and p and q are as above.

A computable worst-case estimate for the maximum error expected in the computation of the eigenvalues of A by using the shifted QR eigenvalue algorithm without balancing is $eps \, \max(\texttt{condeig}(A)) \cdot \| A \|$, where $\texttt{condeig}(A)$ is the vector of condition numbers for the eigenvalues of A. Roughly speaking, this means that $(rcond)^{-1} = \max(\texttt{condeig}(A)) \cdot \| A \|$ is such that the base 10 logarithm of $(rcond)^{-1}$ provides an estimate of the number of digits of accuracy which can be lost during the computation in the customary QR process (see for instance [12]). In our program the quantity $rcond$ is computed by using the internal MATLAB function *condeig* and returned as output. To compare the accuracy of our method and the QR eigensolver in MATLAB we measure the distance between the set of the computed eigenvalues and the set of the eigenvalues returned by the function $\texttt{eig}$ with the same input data. Let $\lambda(A)$ be the set of eigenvalues computed by the MATLAB function $\texttt{eig}$. Let $\tilde{\lambda}(A)$ denote the set of eigenvalues computed by our algorithm, and define the distance between the sets $\lambda(A)$ and $\tilde{\lambda}(A)$ by

$$\text{dist}(\lambda(A), \tilde{\lambda}(A)) = \max\{\max_{\tilde{\lambda} \in \tilde{\lambda}(A)} \delta(\tilde{\lambda}, \lambda(A)), \max_{\lambda \in \lambda(A)} \delta(\lambda, \tilde{\lambda}(A))\},$$

where $\delta(\lambda, \tilde{\lambda}(A)) = \min_{\tilde{\lambda} \in \tilde{\lambda}(A)} |\lambda - \tilde{\lambda}|$. We refer to this distance as the *error* in the eigenvalues computed by our algorithm. Therefore, we tacitly assume that the MATLAB function `eig` computes the eigenvalues exactly.

Figures 1, 2, 3 and 4 show the results of our numerical experiments. Specifically, Figures 1 and 2 cover our tests with fellow matrices of order $N(n) = 2^{1+n}$, $1 \leq n \leq 9$, for *tol*=0.1 and for *tol*=0.001, respectively. Analogously, Figures 3 and 4 cover our tests with companion matrices of order $N(n) = 2^{1+n}$, $1 \leq n \leq 9$, for *tol*=0.1 and for *tol*=0.001, respectively. For each size of the matrix we carried out 100 numerical experiments and report the average values. Each figure is subdivided into two graphs: The first plot reports the *error* and the value of *rcond*; the second plot indicates the relative frequencies of calls to the algorithm in [1] (circle).

The tests reported in Figures 2 and 4 illustrate the numerical behavior of the algorithm stated in the previous section. The potential occurrence of matrices D_k with small diagonal entries leads to an acceptable deterioration of the final accuracy of the computed results without producing any apparently relevant phenomenon of error amplification. In particular, experimental considerations lead to the following useful rule of thumb. If the diagonal entries of the matrices D_k are greater than 10^{-k}, then the final *error* is bounded from above by $(rcond)^{-1} \cdot 10^k$. In other words, in the worst-case situation we can lose k digits more than the number predicted by the conditioning estimates. A few steps of some iterative refinement method would be sufficient to recover the full accuracy of the eigenvalues.

The test reported in Figures 1 and 3 provide support for the composite strategy. Since here we use a very tight condition on the diagonal entries of the matrices D_k (*tol*=0.1), the method results are as accurate as the customary QR iteration. Furthermore, for moderate values of N, say $128 \leq N \leq 512$, the relative frequency p is about thirty percent. Therefore, the cost per step of the composite method is about $130 \, N$ with a significant acceleration with respect to the algorithm in [1]. Finally, it is worth observing that our composite method applied to an input
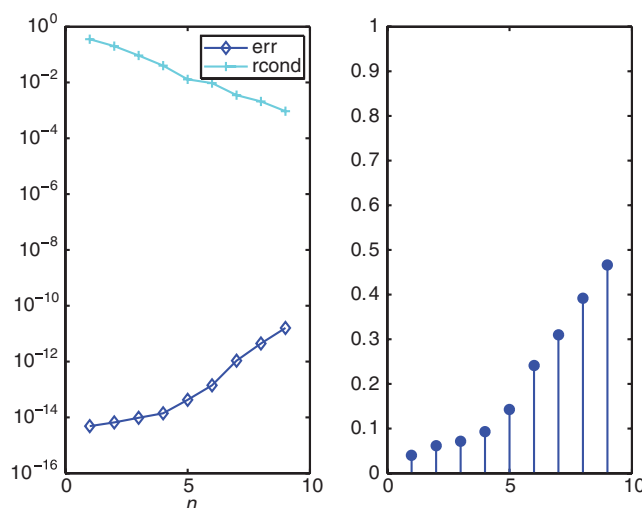

FIGURE 1. Fellow matrices of kind 1). Errors and relative frequencies for *tol*=0.1.

companion matrix $A = A^{(0)}$ always employs the algorithm in [1] at the very first iteration until we start with the nonzero shifting strategy. This explains the values for the relative frequencies in Figure 4 and also suggests that nonzero shifting could be used right from the start to further reduce the number of calls to the most expensive algorithm. Figure 5 reports the results obtained with this variant.
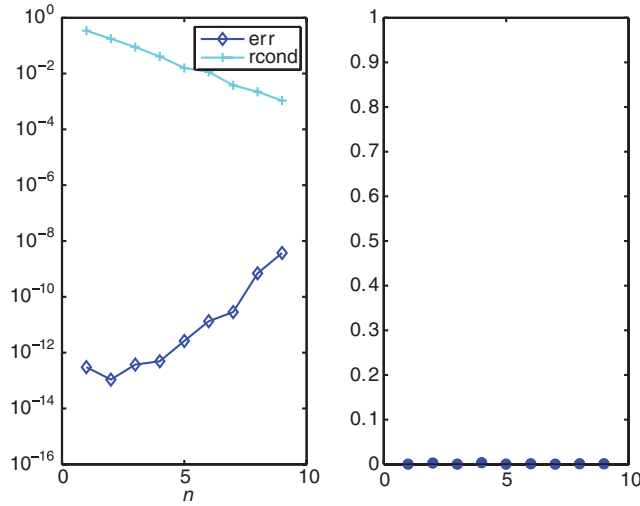

FIGURE 2. Fellow matrices of kind 1). Errors and relative frequencies for tol=0.001.
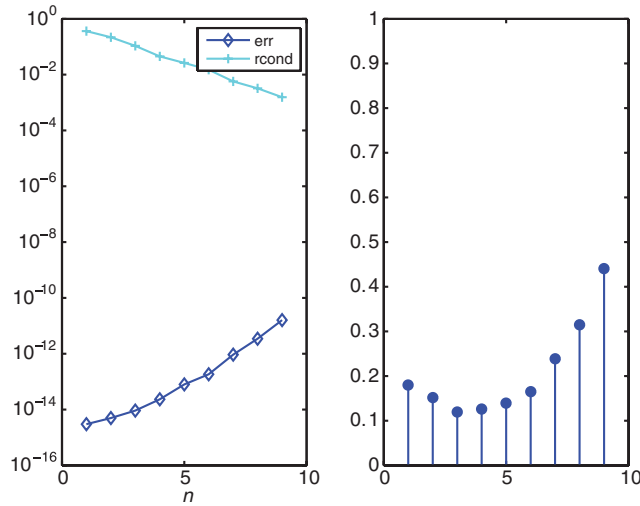
FIGURE 3. Companion matrices of kind 2). Errors and relative frequencies for tol=0.1.
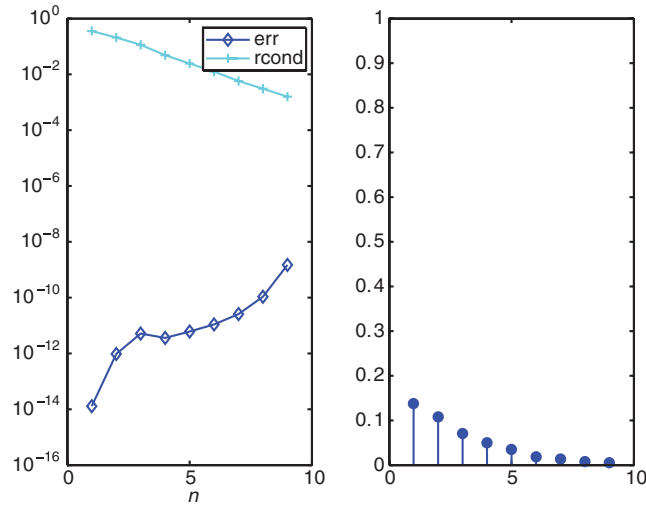
FIGURE 4. Companion matrices of kind 2). Errors and relative frequencies for tol=0.001.
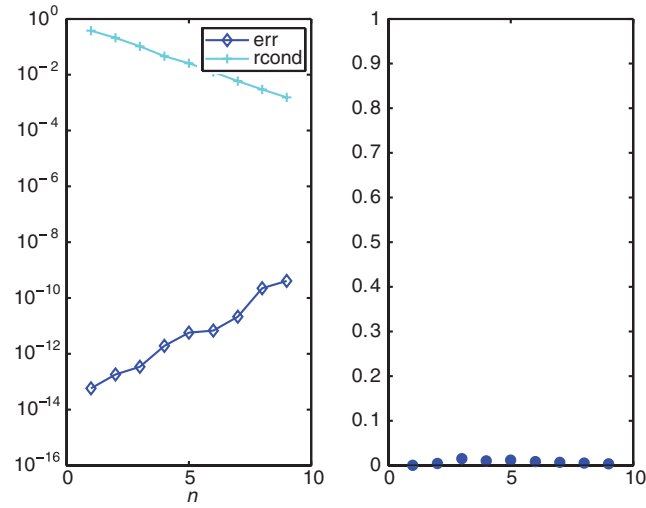

FIGURE 5. Companion matrices of kind 2). Errors and relative frequencies for tol=0.001 generated by the variant employing non-zero shifting right from the start.

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Dipartimento di Matematica, Università di Pisa, Largo Bruno Pontecorvo 5, 56127 Pisa, Italy
    E-mail address: bini@dm.unipi.it

School of Mathematical Sciences, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel-Aviv University, Ramat-Aviv 69978, Israel
    E-mail address: eideyu@post.tau.ac.il

Dipartimento di Matematica, Università di Pisa, Largo Bruno Pontecorvo 5, 56127 Pisa, Italy
    E-mail address: gemignan@dm.unipi.it

School of Mathematical Sciences, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel-Aviv University, Ramat-Aviv 69978, Israel
    E-mail address: gohberg@post.tau.ac.il