Fast QR factorization of Cauchy-like matrices

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Report TW 469, September 2006

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AMS(MOS) Classification : Primary : 65F30, Secondary : 65F18.

Fast QR Factorization of Cauchy-like Matrices

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Abstract

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[1] Supported by MIUR under project 2004015437.

[2] The research was partially supported by the Research Council K.U.Leuven, project OT/05/40 (Large rank structured matrix computations), Center of Excellence: Optimization in Engineering, by the Fund for Scientific Research–Flanders (Belgium), G.0455.0 (RHPH: Riemann-Hilbert problems, random matrices and Padé-Hermite approximation), G.0423.05 (RAM: Rational modeling: optimal conditioning and stable algorithms), and by the Belgian Programme on Interuniversity Poles of Attraction, initiated by the Belgian State, Prime Minister's Office for Science, Technology and Culture, project IUAP V-22 (Dynamical Systems and Control: Computation, Identification & Modeling). The scientific responsibility rests with the authors.

1 Introduction

This paper is motivated by the search for efficient algorithms to compute a rank-revealing factorization of a displacement structured matrix $A \in \mathbb{C}^{n\times n}$. The design of efficient algorithms for computing the singular value decomposition (SVD) is a challenging problem. In the past years a number of different methods have been developed to alleviate the computational burden of the SVD, yet retaining its numerical robustness. Among these, it is worth mentioning the *orthogonal-triangular decompositions* of the form $A = UTV$, where U and V are unitary whereas T is upper triangular (see [10,16] and the references therein). These decompositions are useful in the solution of least squares problems and to provide an initial approximation which can be refined by some iterative scheme approaching a rank-revealing factorization of A.

It is well known that a *Toeplitz-like* and a *Hankel-like* matrix can be reduced into a *Cauchy-like* form $C = \left(\frac{\boldsymbol{g}_i{}^T\boldsymbol{h}_j}{d_i^{(1)}-d_j^{(2)}}\right)$, $(\boldsymbol{g}_i, \boldsymbol{h}_j \in \mathbb{C}^p)$, using the FFT or other trigonometric unitary transformations. The elements $d_j^{(i)}$ are generally referred to as *interpolation nodes*, *nodes* for short, whereas the row-vectors $\boldsymbol{g}_i$ and the column-vectors $\boldsymbol{h}_j$ are the *generators* of C. Depending on the displacement operator employed in this reduction we find that the nodes of the matrix C lye either on the real axis $\mathbb{R}$ or on the unit circle $\mathbb{T}$ in the complex plane.

The use of the transformation of displacement structured matrices to generalized Cauchy matrices was first suggested in [17] and then systematically applied in [14] to obtain fast and stable linear solvers which incorporate pivoting strategies. The same approach can ideally be pursued for computing orthogonal-triangular decompositions of Toeplitz-like and Hankel-like matrices. Since C is unitarily similar to A, then the QR factorization of C gives a UTV decomposition of A. The overall cost of the resulting method is dominated by the cost of computing the QR factorization of a Cauchy-like matrix C with nodes on the real axis or on the unit circle.

In this paper we present two fast $O(n^2)$ numerical methods for the QR factorization of such a matrix C based on the reduction of this computation to solving an inverse eigenvalue problem for an associated *quasiseparable* matrix $H \in \mathbb{C}^{n\times n}$. Roughly speaking, a matrix $H \in \mathbb{C}^{n\times n}$ is quasiseparable (of order r) if all its submatrices which do not contain the diagonal have small rank (less than or equal to r).

More precisely, it is shown that the rows of the Q-factor of C are the eigenvectors of a quasiseparable matrix H of order r, with r less than or equal to the displacement rank of A, partially determined by some given spectral data. The computation of Q can thus be reduced to reconstructing the whole matrix

H with a prescribed quasiseparable structure from some partial information about its eigensystem. Once H is found, the upper triangular factor R can be determined column-by-column by solving n quasiseparable linear systems of the form $H - \alpha I_n$ for a suitable α. Software is available to solve each system at the cost of $O(n)$ flops in a backward stable way.

At the core of our QR algorithm there are two alternative fast methods for the solution of the inverse eigenvalue problem, each of them requiring $O(n^2)$ flops and $O(n)$ memory space. The first method is a straightforward generalization of the procedure outlined in [19] for the case $r = 1$. The method makes use of a representation of H of the form $H = D + \text{tril}(X^H \cdot Y, -1) + \text{triu}(Z^H \cdot W, 1)$ for suitable $X, Y, Z, W \in \mathbb{C}^{r\times n}$ and a diagonal matrix D. Generally speaking, this means that the strictly lower triangular part of H coincides with the strictly lower triangular part of a rank-r matrix and the same property holds for the strictly upper triangular part. It is well known [21] that there are order-r quasiseparable matrices which do not admit such a representation in terms of rank-r matrices and, therefore, from a numerical standpoint the employed parametrization can potentially break down and/or to be very poorly conditioned. Similar issues have been recently addressed in several papers [3,9,20,2] concerning the design of fast adaptations of the QR (QL) iteration for eigenvalue computation of quasiseparable matrices.

The second method circumvents the numerical difficulty by taking a different look at the recursive process of reconstructing the matrix H. The basic idea, suggested by some results in [18,1], is to formulate the reverse process as a sequence of QL iterations with ultimate shifts. Each QL iteration can again be reversed by yielding a shifted LQ step. In this way it is shown that the original reconstruction process can be thought of as a sequence of shifted LQ steps with prescribed shifts. The LQ formulation is easier to implement in a numerically robust way than the first method. In fact the resulting algorithm can be simply constructed from a small set of building blocks for matrix manipulations with quasiseparable structures, including matrix multiplication, QR factorization and Schur-like decompositions of unitary quasiseparable matrices. Highly accurate and efficient implementations of these blocks are available (see [8,7,5,6] and the references given therein).

The paper is organized as follows. In sect. 2 we recall some basic facts concerning the properties of the QR factorization of a Cauchy-like matrix C as well as its relationships with the solution of an inverse eigenvalue problem for a certain quasiseparable matrix H. In sect. 3 we extend the procedure described in [19] for the fast solution of the inverse eigenvalue problem under some additional mild assumptions on C. In sect. 4 we establish the QL formulation and present a fast LQ-based algorithm to solve the inverse eigenvalue problem without any additional requirement. Finally, the conclusion and a discussion are the subjects of Sect. 5.

2 Preliminaries and Basic Reductions

In this section we exploits some well-known properties of displacement and rank structured matrices by showing that the QR factorization of a Cauchy-like matrix C with nodes on the real axis or on the unit circle can be computed by solving an inverse eigenvalue problem for a quasiseparable matrix $H \in \mathbb{C}^{n\times n}$ with some prescribed spectral data.

Given a set of pairwise distinct points $\{d_j^{(i)}\}$, $1 \le j \le n$, $i = 1, 2$, and two matrices $G \in \mathbb{C}^{n\times p}$, $G^T = [\boldsymbol{g}_1|\dots|\boldsymbol{g}_n]$, and $H \in \mathbb{C}^{p\times n}$, $H = [\boldsymbol{h}_1|\dots|\boldsymbol{h}_n]$, the Cauchy-like matrix $C \in \mathbb{C}^{n\times n}$ with nodes $\{d_j^{(i)}\}$ and generators $\boldsymbol{g}_i, \boldsymbol{h}_i \in \mathbb{C}^p$, $1 \le i \le n$, is defined by

$$C = \left(\frac{\boldsymbol{g}_i{}^T \boldsymbol{h}_j}{d_i^{(1)} - d_j^{(2)}} \right)_{1\le i\le n, 1\le j\le n} \tag{1}$$

The generators of a Cauchy-like matrix C are not uniquely determined in the sense that the matrix $G\cdot H$ can virtually admit several different decompositions of the form $G\cdot H = G'\cdot H'$, where $G'^T, H' \in \mathbb{C}^{s\times n}$ for a certain s. However, if C has a full-rank pair of generators (G, H), that is, $\text{rank}(G) = \text{rank}(H) = p$, then any pair of generators (G', H') of C satisfies the same property $\text{rank}(G') = \text{rank}(H') = p$ and, moreover, if the number of columns of G' (the number of rows of H') is p, then $G' = GB$ and $H' = B^{-1}H$ for a suitable invertible matrix $B \in \mathbb{C}^{p\times p}$.

Cauchy-like matrices frequently arise in functional approximation problems concerning rational functions [11], [19]. The transformation of displacement structured matrix A to a generalized Cauchy matrix C was also systematically investigated with the aim of developing fast and stable linear solvers which incorporate pivoting strategies [14].

This latter application is particularly meaningful for us since the same approach can be exploited for the efficient computation of the UTV decomposition of A provided that we have a fast algorithm for the QR factorization of C. Depending on the displacement operator employed in the transformation from A to C we find that the nodes of C may lye on the real axis or on the unit circle in the complex plane . Hence, throughout this paper it is always assumed that $\{d_j^{(i)}\} \subset \mathbb{R}$ or $\{d_j^{(i)}\} \subset \mathbb{T}$, $\mathbb{T} = \{z \in \mathbb{C} \ : \ |z| = 1\}$.

The matrix C in (1) satisfies the displacement equation

$$D_1 \cdot C - C \cdot D_2 = G \cdot H, \tag{2}$$

where $D_1 = \text{diag}[d_1^{(1)}, \dots, d_n^{(1)}]$ and $D_2 = \text{diag}[d_1^{(2)}, \dots, d_n^{(2)}]$ are diagonal matrices. In addition, these matrices are Hermitian for real nodes and unitary for nodes of modulus 1. By substituting the QR factorization of C, $C = QR$, into the equation (2), we obtain that

$$D_1 \cdot QR - QR \cdot D_2 = G \cdot H, \quad G \in \mathbb{C}^{n\times p}, H \in \mathbb{C}^{p\times n},$$

which yields

$$M = Q^H D_1 Q = RD_2R^{-1} + (Q^H G) \cdot (HR^{-1}), \tag{3}$$

whenever C is invertible.

We next look at the structure of the matrix M into more detail. Since RD_2R^{-1} is upper triangular with diagonal elements equal to the diagonal elements of D_2 and $(Q^H G) \cdot (HR^{-1})$ has rank at most p, then M turns out to be lower quasiseparable of order p.

A matrix $B \in \mathbb{C}^{n\times n}$ is called order (n_L, n_U)-*quasiseparable* [7] if

$$n_L \geq \max_{1\leq k\leq n-1} \mathrm{rank} B[k+1\colon n, 1\colon k], \quad n_U \geq \max_{1\leq k\leq n-1} \mathrm{rank} B[1\colon k, k+1\colon n], \tag{4}$$

where $B[i\colon j, k\colon l]$ is the submatrix of B with entries having row and column indices in the ranges i through j and k through l, respectively [3]. In case $n_U = n_L = p$ one refers to A as an order-p-quasiseparable matrix.

A more complete description of the quasiseparable structure of M is achieved by taking into account the localization of the interpolation nodes. For the case of real nodes, since D_1, and a fortiori M, is Hermitian, it immediately follows that $M = D_2 + S$ and S is Hermitian quasiseparable of order p. In the unit circle case the matrix D_1, and a fortiori M, is unitary. By virtue of the following result [12], also in this case the matrix M can be split as $M = D_2 + S$ where S is quasiseparable of order p.

Theorem 2.1 *Let $F \in \mathbb{C}^{n\times n}$ be a unitary matrix with a quasiseparable structure of order r in its strictly lower triangular part. Then F is an order-r-quasiseparable matrix.*

The conclusion is summarized in the next theorem where the additional assumption $|\det A| = |\det C| \neq 0$ is removed.

Theorem 2.2 *Let $C = \left(\frac{\boldsymbol{g}_i{}^T \boldsymbol{h}_j}{d_i^{(1)} - d_j^{(2)}}\right) \in \mathbb{C}^{n\times n}$, where $\boldsymbol{g}_i, \boldsymbol{h}_j \in \mathbb{C}^p$ and $D_1 = \mathrm{diag}[d_1^{(1)}, \dots, d_n^{(1)}]$ and $D_2 = \mathrm{diag}[d_1^{(2)}, \dots, d_n^{(2)}]$ are diagonal matrices with mutually distinct entries located on the unit circle $\mathbb{T}$ or on the real axis $\mathbb{R}$. Then*

[3] This is a Matlab-style notation. Matlab is a registered trademark of The MathWorks, Inc.

there exists a QR factorization of C, $C = QR$, such that

$$Q^H D_1 Q = M = D_2 + S, \tag{5}$$

where S is quasiseparable of order p.

PROOF. It remains only to prove the theorem in the case where C is singular. We make use of a continuity argument. Let $E \in \mathbb{R}^{n\times p}$ be a matrix with all its entries equal to 1. Moreover, denote by $C(t)$ the Cauchy-like matrix such that

$$D_1 C(t) - C(t)\cdot D_2 = (G + tE)\cdot (H + tE^T).$$

Observe that $\det(C(t))$ is a polynomial in the variable t of degree at most $2n$ which is not identically zero. It follows that $\det(C(t)) = 0$ has finitely ($\leq 2n$) many solutions. Consider a sequence $\{t_k\}$ approaching zero such that $\det(C(t_k)) = \det C_k \neq 0$ and let $C_k = Q_k R_k$, $k \geq 0$, be a QR factorization of C_k. Obviously $C_k \to C$. Further, since $\{Q_k\}$ is a bounded sequence from the Bolzano-Weierstrass theorem we get that $\{Q_k\}$ admits a subsequence $\{Q_{k_j}\}$ converging to a certain unitary matrix Q. Then the corresponding subsequence $\{R_{k_j}\}$ approaches the upper triangular matrix $R = Q^H C$. From (5) we obtain that

$$Q_{k_j}^H D_1 Q_{k_j} = M = D_2 + S_{k_j},$$

where S_{k_j} is quasiseparable of order p. Since the rank constrains (4) pass to the limit, we find that $Q^H D_1 Q - D_2$ is also quasiseparable of order p which completes the proof.

Some comments on this theorem are in order. Roughly speaking, the theorem says that the computation of a QR factorization of the Cauchy-like matrix C can be reduced to determining a matrix S and a unitary matrix Q satisfying (5) given in input some (partial) information about the structure and the eigensystem of the matrix $M = D_2 + S$. This task can also be regarded as a structured *inverse eigenvalue problem*, IEP for short, for the matrix M. If C is singular we know that its QR factorization is essentially unique. This means that in this case any QR factorization of C verifies (5). In the singular case the uniqueness property of Q is lost and we can find QR factorizations of C which do not satisfy (5). In the case $p = 1$ it is also possible to prove a sort of converse result by showing that the solution of the IEP (5) is also essentially unique [19]. The same proof does not work in the case $p > 1$ and conditions ensuring the uniqueness of the solution of the IEP (5) are much more difficult to find. In this case in order to guarantee that the computed matrix Q is the $Q-$factor of a certain QR factorization of C, that is, $Q^H \cdot C$ is upper triangular, we proceed in a substantially different way. Our approach is recursive in nature. The basic idea is to compute a matrix Q satisfying (5) given in input the QR factorization of a certain $(n-1)\times(n-1)$ submatrix of C. Since this construction is essentially unique, then we are able to show that the computed Q has the desired property.

3 The First Solution Method: A Generator-Based Approach

In this section we describe a recursive method for computing a QR factorization of a Cauchy-like matrix $C = QR$ based on the characterization of the unitary factor Q given in Theorem 2.2 as the solution of a suitable IEP. The method relies upon the following approach. Assume that a QR factorization of $C([n-k+1:n],[1:k]) = Q_k R_k$ is available, $1 < k < n$, then we may compute Q_{k+1} by solving the IEP problem (5) for the Cauchy-like matrix $C([n-k:n],[1:k+1])$. Once Q_{k+1} is determined, the upper triangular factor R_{k+1} such that $C([n-k:n],[1:k+1]) = Q_{k+1}R_{k+1}$ is a QR factorization of $C([n-k:n],[1:k+1])$ can be found at the additional cost of $O(k^2)$ flops [4,8] by solving $k+1$ linear systems with the order-p $(k+1)\times(k+1)$ quasiseparable matrix $Q_{k+1}^H D_1([n-k:n],[n-k:n])Q_{k+1}$ given in (5).

If $C([n-k:n],[1:k+1])$ is assumed invertible, then from (3) we obtain that the entries located in the strictly lower triangular part of the matrix $Q_{k+1}^H D_1([n-k:n],[n-k:n])Q_{k+1}$ can be completely specified by the row vectors of $Q_{k+1}^H G([n-k:n],[1:p])$ and the column vectors of $H([1:p],[1:n-1])R_{k+1}^{-1}$ which are called the *generators* of the (lower) quasiseparable structure of the matrix. The algorithm proposed in this section for the solution of the IEP problem exploits the properties of such a condensed representation for the entries of the quasiseparable matrices involved. This is because it is referred to as a *generator-based* algorithm. Since for a given quasiseparable matrix such a kind of representation can not exist [21], in theory the applicability of the algorithm is restricted to strongly nonsingular (w.r.t. the main antidiagonal) Cauchy-like matrices and in practice the algorithm may suffer from numerical drawbacks due to poorly conditioned computations (compare with Example 3.1 at the end of this section).

For the sake of notational simplicity set $k = n-1$ and let $\widehat{D}_1 = D_1([2:n],[2:n])$ and $\widehat{D}_2 = D_2([1:n-1],[1:n-1])$ be the trailing and the leading principal submatrix of D_1 and D_2, respectively. Also, let $Q_{n-1} = \widehat{Q}$ and $R_{n-1} = \widehat{R}$ be, respectively, the unitary and the upper triangular factor in the QR factorization of the Cauchy-like matrix $C([2:n],[1:n-1]) = \widehat{C}$. The matrix $\widehat{Q} \in \mathbb{C}^{(n-1)\times(n-1)}$ satisfies

$$\widehat{Q}^H \widehat{D}_1 \widehat{Q} = \widehat{D}_2 + \widehat{S}, \quad \mathrm{tril}(\widehat{S},0) = \mathrm{tril}(\widehat{Q}^H \widehat{G} \cdot \widehat{H}\widehat{R}^{-1}) = \mathrm{tril}(\widehat{X}^H \cdot \widehat{Y},0), \quad (6)$$

where $\widehat{G} = G([2:n],[1:p])$, $\widehat{H} = G([1:p],[1:n-1])$, $\widehat{X} = [\hat{\boldsymbol{x}}_1|\ldots|\hat{\boldsymbol{x}}_{n-1}] \in \mathbb{C}^{p\times(n-1)}$ and $\widehat{Y} = \left[\hat{\boldsymbol{y}}_1|\ldots|\hat{\boldsymbol{y}}_{n-1}\right] \in \mathbb{C}^{p\times(n-1)}$. Here we adopt the Matlab notation $\mathrm{tril}(B,p) = (t_{i,j})$ to denote the lower triangular portion of $B = (b_{i,j}) \in \mathbb{C}^{n\times n}$ such that $t_{i,j} = b_{i,j}$ for $j - i \leq p$, and $t_{i,j} = 0$ elsewhere. Analogously, the $n \times n$ matrix $T = \mathrm{triu}(B,p)$ is formed by the upper triangular portion of B such that $t_{i,j} = b_{i,j}$ for $j - i \geq p$, and $t_{i,j} = 0$ elsewhere.

Now let us consider the extension $C \in \mathbb{C}^{n\times n}$ of $\widehat{C}$,

$$C = \left[\begin{array}{ccc|c} \frac{\boldsymbol{g}_1^H \boldsymbol{h}_1}{d_1^{(1)} - d_1^{(2)}} & \cdots & \frac{\boldsymbol{g}_1^H \boldsymbol{h}_{n-1}}{d_1^{(1)} - d_{n-1}^{(2)}} & \frac{\boldsymbol{g}_1^H \boldsymbol{h}_n}{d_1^{(1)} - d_n^{(2)}} \\ \hline & & & \vdots \\ & \widehat{C} & & \frac{\boldsymbol{g}_n^H \boldsymbol{h}_n}{d_n^{(1)} - d_n^{(2)}} \end{array}\right].$$

Observe that

$$P = \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q}^H \end{array}\right] C = \left[\begin{array}{ccc|c} \frac{\boldsymbol{g}_1^H \boldsymbol{h}_1}{d_1^{(1)} - d_1^{(2)}} & \cdots & \frac{\boldsymbol{g}_1^H \boldsymbol{h}_{n-1}}{d_1^{(1)} - d_{n-1}^{(2)}} & \frac{\boldsymbol{g}_1^H \boldsymbol{h}_n}{d_1^{(1)} - d_n^{(2)}} \\ \hline & & & \rho_1 \\ & \widehat{R} & & \vdots \\ & & & \rho_{n-1} \end{array}\right], \tag{7}$$

is upper Hessenberg. Whence, we can find $n-1$ unitary matrices $\mathcal{G}_j = I_{j-1} \oplus G_j \oplus I_{n-j-1}$, $1 \leq j \leq n-1$, where G_j is of the form

$$G_j = \begin{bmatrix} 1 & \alpha_j \\ -\bar{\alpha}_j & 1 \end{bmatrix} /(1 + |\alpha_j|^2) \quad \text{or} \quad G_j = \begin{bmatrix} \alpha_j & 1 \\ -1 & \bar{\alpha}_j \end{bmatrix} /(1 + |\alpha_j|^2), \quad |\alpha_j| \leq 1,$$

such that

$$\mathcal{G}_{n-1} \cdots \mathcal{G}_1 \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q}^H \end{array}\right] C = \mathcal{G}_{n-1} \cdots \mathcal{G}_1 P = R \tag{8}$$

yields a QR factorization of the extended Cauchy-like matrix C.

Set $Q_n^H = Q^H = \mathcal{G}_{n-1} \cdots \mathcal{G}_1 \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q}^H \end{array}\right]$. From (3), we have

$$Q^H D_1 Q = D_2 + S, \quad \mathrm{tril}(S,0) = \mathrm{tril}(X^H \cdot Y, 0), \tag{9}$$

where $X = [\boldsymbol{x}_1|\ldots|\boldsymbol{x}_n] \in \mathbb{C}^{p\times n}$ and $Y = [\boldsymbol{y}_1|\ldots|\boldsymbol{y}_n] \in \mathbb{C}^{p\times n}$. We can rewrite (9) as follows

$$\mathcal{G}_{n-1} \cdots \mathcal{G}_1 \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q}^H \end{array}\right] \left[\begin{array}{c|c} d_1^{(1)} & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{D}_1 \end{array}\right] \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q} \end{array}\right] \mathcal{G}_1^H \cdots \mathcal{G}_{n-1}^H = \left[\begin{array}{c|c} \widehat{D}_2 & \mathbf{0} \\ \hline \mathbf{0}^H & \widehat{d}_n^{(2)} \end{array}\right] + S.$$

Using $\widehat{Q}^H \widehat{D}_1 \widehat{Q} = \widehat{D}_2 + \widehat{S}$, we get

$$\mathcal{G}_{n-1} \cdots \mathcal{G}_1 \left[\begin{array}{c|c} d_1^{(1)} & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{D}_2 + \widehat{S} \end{array}\right] \mathcal{G}_1^H \cdots \mathcal{G}_{n-1}^H = \left[\begin{array}{c|c} \widehat{D}_2 & \mathbf{0} \\ \hline \mathbf{0}^H & \widehat{d}_n^{(2)} \end{array}\right] + S. \tag{10}$$

Relation (10) provides the basis for the recursive construction of the matrix Q given the partial solution $\widehat{Q}$ of the smaller IEP problem. A set of generators of C is given by

$$G = [\boldsymbol{g}_1 | \hat{\boldsymbol{g}}_2 | \ldots | \hat{\boldsymbol{g}}_n]^H = \left[\boldsymbol{g}_1 | \widehat{G}\right]^H \in \mathbb{C}^{n \times p},$$

and

$$H = [\boldsymbol{h}_1 | \ldots | \boldsymbol{h}_{n-1} | \boldsymbol{h}_n] = \left[\widehat{H} | \boldsymbol{h}_n\right] \in \mathbb{C}^{p \times n}.$$

Due to the remark after (1) we know that G and H are uniquely determined up to multiplication by a small $p \times p$ matrix B and its inverse, respectively. There follows that the same property also holds for the generators X and Y of the (lower) quasiseparable structure of S. For the sake of simplicity we can take $B = I_p$. ¿From (3), we know that a possible choice for X^H in (9) is $X^H = Q^H G$. Hence, we find

$$G^H = \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q} \end{array}\right] \left[\boldsymbol{g}_1 | \widehat{X}\right]^H = \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q} \end{array}\right] \mathcal{G}_1^H \cdots \mathcal{G}_{n-1}^H X^H$$

which implies

$$X^H = \mathcal{G}_{n-1} \cdots \mathcal{G}_1 \left[\boldsymbol{g}_1 | \widehat{X}\right]^H. \tag{11}$$

Similarly, we can obtain recursive relations for the elements of H. We have with P defined by (7) and $HR^{-1} = Y$ from (3) that

$$\left[\mathbf{0} | \widehat{Y}\right] P = \left[\mathbf{0} | \widehat{Y}\right] \left[\begin{array}{ccc|c} \frac{\boldsymbol{g}_1^H \boldsymbol{h}_1}{d_1^{(1)} - d_1^{(2)}} & \cdots & \frac{\boldsymbol{g}_1^H \boldsymbol{h}_{n-1}}{d_1^{(1)} - d_{n-1}^{(2)}} & \frac{\boldsymbol{g}_1^H \boldsymbol{h}_n}{d_1^{(1)} - d_n^{(2)}} \\ \hline & & & \rho_1 \\ & \widehat{R} & & \vdots \\ & & & \rho_{n-1} \end{array}\right] = \left[\widehat{H} | \boldsymbol{\eta}\right],$$

for a suitable $\boldsymbol{\eta} \in \mathbb{C}^p$. Moreover, we find that

$$\widetilde{H} = \left[\widehat{H} | \boldsymbol{\eta}\right] = \left[\boldsymbol{y}_1 | \ldots | \boldsymbol{y}_{n-1} | \boldsymbol{\zeta}\right] R$$

for a suitable $\boldsymbol{\zeta} \in \mathbb{C}^p$. From (8), it follows that

$$\widetilde{H} = \left[\boldsymbol{y}_1 | \ldots | \boldsymbol{y}_{n-1} | \boldsymbol{\zeta}\right] \mathcal{G}_{n-1} \cdots \mathcal{G}_1 P$$

which gives

$$\left[\mathbf{0}|\widehat{Y}\right] P = \left[\boldsymbol{y}_1|\ldots|\boldsymbol{y}_{n-1}|\boldsymbol{\zeta}\right] \mathcal{G}_{n-1}\cdots\mathcal{G}_1 P$$

or

$$\left[\mathbf{0}|\widehat{Y}\right] \mathcal{G}_1^H\cdots\mathcal{G}_{n-1}^H = \left[\boldsymbol{y}_1|\ldots|\boldsymbol{y}_{n-1}|\boldsymbol{\zeta}\right]. \tag{12}$$

Inspired by (11) and (12), let us introduce the vectors $\tilde{\boldsymbol{y}}_i$ and $\tilde{\boldsymbol{x}}_i$ by means of the relations

$$[\boldsymbol{x}_1|\ldots|\boldsymbol{x}_{k-1}|\tilde{\boldsymbol{x}}_k]^H = (\mathcal{G}_{k-1}\cdots\mathcal{G}_1)([1:k],[1:k])\,[\boldsymbol{g}_1|\hat{\boldsymbol{x}}_1|\ldots|\hat{\boldsymbol{x}}_{k-1}]^H,$$

and

$$\left[\boldsymbol{y}_1|\ldots|\boldsymbol{y}_{k-1}|\tilde{\boldsymbol{y}}_k\right] = \left[\mathbf{0}|\hat{\boldsymbol{y}}_1|\ldots|\hat{\boldsymbol{y}}_{k-1}\right](\mathcal{G}_1^H\cdots\mathcal{G}_{k-1}^H)([1:k],[1:k]).$$

The Givens rotations $\mathcal{G}_1,\ldots,\mathcal{G}_{n-1}$ can be computed by using the relation (10) without performing the triangularization of P directly. This enables the computation of Q given $\widehat{Q}$ to be performed at a linear rather than a quadratic cost. At the first step we want to determine G_1 such that

$$G_1\begin{bmatrix} d_1^{(1)} & 0 \\ 0 & d_1^{(2)}+\hat{\boldsymbol{x}}_1^H\hat{\boldsymbol{y}}_1\end{bmatrix} G_1^H\begin{bmatrix}1\\0\end{bmatrix} = G_1\,[\boldsymbol{g}_1|\hat{\boldsymbol{x}}_1]^H\,[\mathbf{0}|\hat{\boldsymbol{y}}_1]\,G_1^H\begin{bmatrix}1\\0\end{bmatrix} + \begin{bmatrix}d_1^{(2)}\\0\end{bmatrix}$$

which can be rewritten as

$$\begin{bmatrix} d_1^{(1)} & 0 \\ 0 & d_1^{(2)}+\hat{\boldsymbol{x}}_1^H\hat{\boldsymbol{y}}_1\end{bmatrix} G_1^H\boldsymbol{e}_1 = [\boldsymbol{g}_1|\hat{\boldsymbol{x}}_1]^H\,[\mathbf{0}|\hat{\boldsymbol{y}}_1]\,G_1^H\boldsymbol{e}_1 + d_1^{(2)}G_1^H\boldsymbol{e}_1,$$

where $\boldsymbol{e}_1 = \begin{bmatrix}1\\0\end{bmatrix}$. In this way we obtain

$$\begin{bmatrix} d_1^{(1)}-d_1^{(2)} & -\boldsymbol{g}_1^H\hat{\boldsymbol{y}}_1 \\ 0 & 0\end{bmatrix} G_1^H\boldsymbol{e}_1 = \mathbf{0}$$

which enables the computation of G_1.

At the kth step G_k operates on the 2×2 matrix

$$(\mathcal{G}_{k-1}\cdots\mathcal{G}_1\left[\begin{array}{c|c} d_1^{(1)} & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{D}_2+\widehat{S}\end{array}\right]\mathcal{G}_1^H\cdots\mathcal{G}_{k-1}^H)([k:k+1],[k:k+1]) =$$

$$= \begin{bmatrix} \theta_k & \vartheta_k \\ \hat{\boldsymbol{x}}_k^H\tilde{\boldsymbol{y}}_k & d_k^{(2)}+\hat{\boldsymbol{x}}_k^H\hat{\boldsymbol{y}}_k\end{bmatrix}.$$

We have

$$G_k \begin{bmatrix} \theta_k & \vartheta_k \\ \hat{\boldsymbol{x}}_k^H \tilde{\boldsymbol{y}}_k & d_k^{(2)} + \hat{\boldsymbol{x}}_k^H \hat{\boldsymbol{y}}_k \end{bmatrix} G_k^H \boldsymbol{e}_1 = G_k \left[\tilde{\boldsymbol{x}}_k | \hat{\boldsymbol{x}}_k\right]^H \left[\tilde{\boldsymbol{y}}_k | \hat{\boldsymbol{y}}_k\right] G_k^H \boldsymbol{e}_1 + \begin{bmatrix} d_k^{(2)} \\ 0 \end{bmatrix}$$

which gives

$$\begin{bmatrix} \theta_k - d_k^{(2)} - \tilde{\boldsymbol{x}}_k^H \tilde{\boldsymbol{y}}_k & \vartheta_k - \tilde{\boldsymbol{x}}_k^H \hat{\boldsymbol{y}}_k \\ 0 & 0 \end{bmatrix} G_k^H \boldsymbol{e}_1 = \boldsymbol{0}. \tag{13}$$

At the end of the process a factored form of the unitary matrix Q and a generator representation of the order-p quasiseparable matrix M are available at the cost of $O(n)$ flops. Due to computations performed in the updating procedure the generators in the strictly upper triangular part of M can have length greater than p. In this case a compression scheme [2] requiring additional $O(n)$ flops must be carried out to recover a condensed representation for the whole matrix M. Once M is known, then the last column $\boldsymbol{r}_n$ of $R = (r_{i,j})$ can efficiently be computed by solving the linear system

$$(M - d_n^{(2)} I)\boldsymbol{r}_n = X^H \boldsymbol{h}_n.$$

Moreover, by using $\boldsymbol{r}_n$ we can determine $\boldsymbol{y}_n$ by the last column of the relation $YR = H$, i.e, $Y\boldsymbol{r}_n = \boldsymbol{h}_n$ or

$$r_{n,n}\boldsymbol{y}_n = \boldsymbol{h}_n - \sum_{i=1}^{n-1} r_{i,n}\boldsymbol{y}_i.$$

However, this relation clearly shows that the norm of the vectors $\boldsymbol{y}_j^{(k)}$ which generate the lower triangular part of the matrix S_k can not be bounded from above since, for instance, large vectors are expected if $r_{n,n}$ is almost zero. The growth of the magnitude of these vectors generally leads to numerical difficulties and poorly accurate results as discussed in the next example.

Example 3.1 *Let $p = 1$ and $n = 4$. Consider the Cauchy matrix $C \in \mathbb{R}^{4\times 4}$ defined by the set of generators $\boldsymbol{g} = [1, 1, 1, 0]$, $\boldsymbol{h} = [1, 1, 1, 1]$, $D_1 = \mathrm{diag}[2\cos(\frac{(2i-1)\pi}{9})]_{1\le i\le 4}$, and $D_2 = \mathrm{diag}[2\cos(\frac{2i\pi}{9})]_{1\le i\le 4}$. By using Matlab we get*

$$C = \begin{bmatrix} 2.8794 & 0.6527 & 0.3473 & 0.2660 \\ -1.8794 & 1.5321 & 0.5000 & 0.3473 \\ -0.5321 & -1.4397 & 1.5321 & 0.6527 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Since the 3×3 leading principal submatrix of C is nonsingular, we find that the QR factorization of C is essentially unique. The internal MATLAB function

$[Q, R] = qr(C)$ returns

$$Q = \begin{bmatrix} -0.8276 & -0.3219 & 0.4599 & 0 \\ 0.5401 & -0.6798 & 0.4961 & 0 \\ 0.1529 & 0.6590 & 0.7365 & 0 \\ 0 & 0 & 0 & 1.0000 \end{bmatrix},$$

from which we obtain

$$S = Q^T D_1 Q - D_2 = \begin{bmatrix} 0.0387 & 0.0985 & -0.4864 & 0 \\ 0.0985 & 0.1588 & -0.7840 & 0 \\ -0.4864 & -0.7840 & 1.4553 & 0 \\ 0 & 0 & 0 & 0.3473 \end{bmatrix}.$$

One easily deduces that the lower triangular part of S can not be represented as the lower triangular part of a rank-one matrix or, differently saying, we are not able to find two vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^4$ such that $(S)_{i,j} = x_i y_j$ for $1 \leq j \leq i \leq 4$. Although the rank properties of the matrix S are verified the representation used is too week to capture the structure of S correctly. If we perturb the vector $\boldsymbol{g}$ and thereby set $\boldsymbol{g} = \boldsymbol{g}(\epsilon) = [1, 1, 1, \epsilon]$, then $C = C(\epsilon)$ is nonsingular and the method described above works. However, since we are dealing with a nearly degenerate situation poor results and ill-conditioning problems can be expected. For $\epsilon = 10^{-8}$ we find that $\dfrac{\max |y_i|}{\min |y_i|} \simeq 3.6e + 07$.

4 The Second Solution Method: A QL-Based Approach

The algorithm in the previous section computes the unitary Hessenberg matrix $\widetilde{Q} = \mathcal{G}_1 \cdots \mathcal{G}_{n-1}$ which solves (10) by making use of a generator-based representation for the quasiseparable matrices involved. In this section we present a different solution method which works under less restrictive assumptions and is suited to employ more robust quasiseparable parametrizations yet retaining low complexity estimates.

The starting point is the relation (10) which, for notational convenience, is rewritten as

$$\widetilde{Q}\widetilde{A}\widetilde{Q}^H = A, \tag{14}$$

where

$$\widetilde{A} = \left[\begin{array}{c|c} d_1^{(1)} & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{D}_2 + \widehat{S} \end{array}\right], \quad A = \left[\begin{array}{c|c} \widehat{D}_2 & \mathbf{0} \\ \hline \mathbf{0}^H & \widehat{d}_n^{(2)} \end{array}\right] + S.$$

The direct problem addressed in the previous section consists in computing the matrix A given in input the matrix $\widetilde{A}$. Let us consider now the reverse problem. Since the first eigenvalue $d_1^{(1)}$ of $\widetilde{A}$, and, a fortiori, of A, is given and, moreover, we know that the QR (QL) iteration maintains the quasiseparable properties of the input matrix [3,9,20,2], then it is quite natural to look at the action of the shifted QL iteration applied to the matrix A with ultimate shift $d_1^{(1)}$. The result should be a certain matrix B defined by

$$\begin{cases} A - d_1^{(1)} I_n = \widetilde{Q}\widetilde{L}, \\ B = \widetilde{L}\widetilde{Q} + d_1^{(1)} I_n \end{cases} \tag{15}$$

and suitably related to $\widetilde{A}$.

The scheme (15) can be run backwards in order to recover the matrix A from B. The computation essentially amounts to the LQ factorization of the matrix $B - d_1^{(1)} I_n$. Inspired by this consideration, we are going to investigate the properties of LQ factorizations of the matrix $\widetilde{A} - d_1^{(1)} I_n$. Notice that the matrix is singular and, therefore, its LQ factorization is not unique. In what follows we relate the unitary factor of a certain LQ factorization of $\widetilde{A} - d_1^{(1)} I_n$ to the sought unitary matrix $\widetilde{Q}$. The first result describes the structure of the matrix

$$E = (\widetilde{A} - d_1^{(1)} I_n)\widetilde{Q}^H. \tag{16}$$

Observe that $\widetilde{Q}^H = \mathcal{G}_1^H \cdots \mathcal{G}_{n-1}^H$ is a upper unitary Hessenberg matrix specified by its Schur parametrization [13,15].

Theorem 4.1 *Let $\widetilde{E} = E([2:n],[2:n])$ be the $(n-1) \times (n-1)$ trailing principal submatrix of the matrix E defined in (16). Then $\widetilde{E}$ has an order-p upper quasiseparable structure including the main diagonal, that is,*

$$p \geq \max_{1 \leq k \leq n-1} \text{rank} \widetilde{E}[1\colon k, k\colon n-1].$$

PROOF. We show that $\widetilde{Q}(\widetilde{A} - d_1^{(1)} I_n)$ has an order$-p$ lower quasiseparable structure including the main diagonal. In the case of real nodes this implies immediately the thesis. In the case of nodes located on the unit circle it suffices to apply the result to the conjugate Cauchy-like matrix $\bar{C}$. ¿From (3) we find that

$$\widetilde{Q} \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q}^H \end{array}\right] (D_1 - d_1^{(1)} I_n) \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{Q} \end{array}\right] = R(D_2 - d_1^{(1)} I_n)P^{-1} + (Q^H G) \cdot (H P^{-1}),$$

where P is the irreducible upper Hessenberg matrix defined by (7) and (8). This implies that

$$\widetilde{Q}(\widetilde{A} - d_1^{(1)} I_n) = R(D_2 - d_1^{(1)} I_n)P^{-1} + (Q^H G) \cdot (HP^{-1}).$$

The thesis now follows by observing that the first column of the matrix on the left-hand side is zero and, moreover, the inverse of an irreducible upper Hessenberg matrix admits an order-1 lower quasiseparable structure including the main diagonal.

The upper quasiseparable structure of $\widetilde{E}$ in Theorem 4.1 can efficiently be exploited to generate in linear time a unitary matrix U such that $\widetilde{E}U$ is lower triangular [8]. More specifically, it is possible to show that U can further be decomposed as $U = V \cdot T$, where V and T are unitary, T is lower banded with bandwidth $p - 1$ and, moreover,

$$V = \left[\begin{array}{c|c} I_{p-1} & \mathbf{0}^H \\ \hline \mathbf{0} & \widehat{V} \end{array}\right],$$

where $\widehat{V}$ is upper banded with bandwidth p. In this way we obtain that

$$(\widetilde{A} - d_1^{(1)} I_n)\mathcal{G}_1^H \cdot (\mathcal{G}_2^H \cdots \mathcal{G}_{n-1}^H) \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & U \end{array}\right] = \text{lower triangular}. \tag{17}$$

Observe that

$$\mathcal{G}_2^H \cdots \mathcal{G}_{n-1}^H = \mathcal{G}_1 \widetilde{Q}^H = \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & G \end{array}\right],$$

where G is a unitary upper Hessenberg matrix.

Since the $(n-1) \times (n-1)$ trailing principal submatrix of $(\widetilde{A} - d_1^{(1)} I_n)$ is nonsingular and the same clearly holds for the corresponding submatrix of $(\widetilde{A} - d_1^{(1)} I_n)\mathcal{G}_1^H$ we conclude that $G \cdot U$ is the essentially unique unitary factor in the LQ factorization of the trailing principal submatrix of order $n - 1$ of $(\widetilde{A} - d_1^{(1)} I_n)\mathcal{G}_1^H$. Therefore, if we assume to know the matrix $\mathcal{G}_1$ then the computation of G and, hence, of $\widetilde{Q}$ might be performed by means of the following two-step procedure.

(1) Firstly we compute an LQ factorization of $(\widetilde{A} - d_1^{(1)} I_n)\mathcal{G}_1^H = \widetilde{L}\widetilde{S}^H$ with $\widetilde{S}$ unitary of the form $\widetilde{S} = \left[\begin{array}{c|c} 1 & \mathbf{0}^H \\ \hline \mathbf{0} & S \end{array}\right]$.

(2) Secondly, in view of (17) we recover the matrix G from a suitable refactorization of S as product of unitary matrices with specified shapes. More precisely, we have

$$S = G \cdot U = G \cdot V \cdot T, \tag{18}$$

where G is unitary upper Hessenberg and V and T are specified as above.

This procedure is eligible for computing the right matrix G provided that the decomposition (18) is essentially unique. Conditions for the uniqueness are proved in the next result.

Theorem 4.2 *Assume that all the entries in the last nonzero subdiagonal of T and in the last nonzero superdiagonal of $\widehat{V}$ are nonzero. Then the factors G, V and T in the decomposition of S are essentially unique whenever we have fixed the first $p-1$ and the last p Givens rotations in the Schur decomposition of G.*

PROOF. Let us first consider the factorization of the matrix S as the product of $G \cdot V = P$ and T. Observe that P is unitary and T is unitary lower banded with bandwidth $p-1$. Let

$$\widetilde{T} = \left[\begin{array}{c|c} \begin{matrix} I_{p-1} \\ 0_{(n-p)\times(p-1)} \end{matrix} & T \\ \hline 0_{p-1} & 0_{(p-1)\times(n-p)} \end{array}\right],$$

be the upper triangular matrix obtained from T by an appropriate bordering. Introduce also the corresponding bordered unitary matrix $\widetilde{P}$ defined by

$$\widetilde{P} = \left[\begin{array}{c|c} 0_{(p-1)\times(n-1)} & I_{p-1} \\ \hline P & 0_{(n-1)\times(p-1)} \end{array}\right].$$

We have

$$\widetilde{P} \cdot \widetilde{T} = \left[\begin{array}{c|c} 0_{p-1} & 0_{(p-1)\times(n-1)} \\ \hline P \begin{bmatrix} I_{p-1} \\ 0_{(n-p)\times(p-1)} \end{bmatrix} & S \end{array}\right].$$

Observe that the first $p-1$ columns of P coincide with the first $p-1$ columns of G which are completely determined by the Givens rotations $\mathcal{G}_2, \ldots, \mathcal{G}_p$. It follows that

$$\widetilde{T}^H \cdot \widetilde{T} = (\widetilde{P} \cdot \widetilde{T})^H \cdot (\widetilde{P} \cdot \widetilde{T}) = \left[\begin{array}{c|c} I_{p-1} & [I_{p-1}, 0_{(p-1)\times(n-p)}]G^H S \\ \hline S^H G \begin{bmatrix} I_{p-1} \\ 0_{(n-p)\times(p-1)} \end{bmatrix} & I_{n-1} \end{array}\right],$$

which provides the Cholesky decomposition of the positive semidefinite matrix on the right hand-side. If the main diagonal of $\widetilde{T}$ is nonzero except for the entries in the last $p-1$ positions, then we can conclude that T and, therefore, P are essentially unique. The same reasoning can be applied to prove the essential uniqueness of the factors G and V in the decomposition of P.

Generally speaking, this theorem says that, if we know the first $p-1$ and the last p Givens rotations in the Schur decomposition of G then under quite mild assumptions we are able to determine the matrix G completely by refactoring S as the product of suitable unitary matrices. All these factorizations can be computed in linear time by using numerically stable methods. Furthermore, the required Givens rotations can also be obtained in linear time in the triangularization of the matrix P in (8). Finally, by using (14) we can update in linear time the parametrization of $\widetilde{A}$ to obtain a parametrization for the larger matrix A.

Example 4.3 *Let $C = C(\epsilon)$ be the matrix defined in the previous example for $\epsilon = 10^{-8}$. We find that*

$$(\widetilde{A} - d_1^{(1)} I_4) \cdot \mathcal{G}_1^H = \begin{bmatrix} 0.7277 & -0.4937 & 0 & 0 \\ 0.5498 & 0.8105 & -0.3531 & 0.0000 \\ 0.1982 & 0.2922 & -2.1267 & 0.0000 \\ -0.0000 & -0.0000 & 0.0000 & -3.4115 \end{bmatrix},$$

and

$$G = \begin{bmatrix} -0.5735 & -0.8192 & 0.0000 \\ -0.8192 & 0.5735 & -0.0000 \\ -0.0000 & 0.0000 & 1.0000 \end{bmatrix}, \quad U = \begin{bmatrix} -0.1985 & 0.9801 & 0 \\ -0.9801 & -0.1985 & 0.0000 \\ 0.0000 & 0.0000 & 1.0000 \end{bmatrix}.$$

Observe that the entry in position $(2,3)$ of $U = U(\epsilon)$ becomes smaller and smaller as ϵ approaches zero. Since in this case $U = V = \widehat{V}$, according to Theorem 4.2 this behavior can indicate a connection between the rank structure of $\widetilde{A}$ and the properties of the factorization (18)

Remark 4.4 *The computational effort of the LQ-based method can be further reduced by avoiding the explicit computation of the factors in the LQ factorization of $\widetilde{A} - d_1^{(1)} I_n$. In particular, Theorem 4.1 implies that, starting from the matrix $\widetilde{A} - d_1^{(1)} I_n$ having quasiseparable structure in its strictly upper triangular part, applying the factor $Q^H = \mathcal{G}_1^H \cdots \mathcal{G}_{n-1}^H$ to the columns will result in the matrix $E = (\widetilde{A} - d_1^{(1)} I_n)\widetilde{Q}^H$ in* (16) *having quasiseparable structure including* *the main diagonal. It turns out that under some mild conditions, this characterization is sufficient to obtain the required Givens rotations* $G_1^H, \ldots, G_{n-1}^H$ *directly, except for the first and the last* p *Givens rotations. An implementation of such an idea will be described in a forthcoming paper.*

5 Conclusion and Discussion

In this paper we establish the theoretical basis of fast methods to find the QR factorization of a Cauchy-like matrix C, as a means of computing a UTV decomposition of a displacement structured matrix A efficiently. Our approach is based on the characterization of the unitary factor Q as the eigenvector matrix of a partially given quasiseparable matrix M suitably related to C. This enables the computation of Q to be reduced to solving an inverse eigenvalue problem for the matrix M. Two methods are presented which are suited to exploit the quasiseparable structure of M. The first method makes use of a condensed representation of M via generators which can be prone to numerical instabilities and difficulties. The second method reduces to computing a sequence of QR factorizations of quasiseparable matrices, or to some more efficient version of this scheme (cf. Remark 4.4). Therefore, this method can in principle be made more robust by using appropriate condensed representations for these matrices. Details concerning the implementation of these methods as well as the results of numerical experiments will be the subject of a forthcoming paper.

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