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QD-TYPE METHODS FOR QUASISEPARABLE MATRICES*

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Abstract. In the last few years many numerical techniques for computing eigenvalues of structured rank matrices have been proposed. Most of them are based on *QR* iterations since, in the symmetric case, the rank structure is preserved and high accuracy is guaranteed. In the unsymmetric case, however, the *QR* algorithm destroys the rank structure, which is instead preserved if *LR* iterations are used. We consider a wide class of quasiseparable matrices which can be represented in terms of the same parameters involved in their Neville factorization. This class, if assumptions are made to prevent possible breakdowns, is closed under *LR* steps. Moreover, we propose an implicit shifted *LR* method with a linear cost per step, which resembles the qd method for tridiagonal matrices. We show that for totally nonnegative quasiseparable matrices the algorithm is stable and breakdowns cannot occur, if the Laguerre shift, or other shift strategy preserving nonnegativity, is used. Computational evidence shows that good accuracy is obtained also when applied to symmetric positive definite matrices.

Key words. qd algorithms, LR for eigenvalues, quasiseparable matrices.

AMS subject classifications. 65F15

1. Introduction. In the recent literature quasiseparable matrices have received a great deal of interest (see [7, 9, 3] and references therein). In fact, matrices with this structure appear naturally in many application fields such as systems theory, signal processing or integral equations. Also covariance matrices, or matrices involved in multivariate statistics or discretization of elliptic PDEs have often the quasiseparable structure.

The class of quasiseparable matrices includes many important matrices such as companion matrices of polynomials, tridiagonal matrices and their inverses (Green's quasiseparable), unitary Hessenberg, banded matrices. In [7] the class is proved to be closed under inversion, and a linear complexity inversion method is proposed.

An interesting research topic is the development of fast algorithms, both for the solution of linear systems and for eigenvalue and eigenvector computation, taking advantage of the representation of the matrix in terms of a small number of parameters.

The main purpose of this paper is to propose an *LR* scheme for eigenvalue computation of a quasiseparable matrix not necessarily Hermitian. In fact, for unsymmetric quasiseparable matrices, it is well know that the *QR* algorithm destroys the rank structure with an increase of the cost of the computation of the eigenvalues. The *LR* algorithm, on the contrary, maintains the rank structure providing a valid alternative once the stability is guaranteed. The main objection to the use of *LR* iterations is the possible instability. However, Fernando and Parlet [10] and Parlett in [17], suggested to apply the *LR* algorithm to symmetric positive definite tridiagonal matrices, showing the good performance and stability of the qd-type methods over the standard *QR* method. The idea behind qd-type algorithms, first proposed by Rutishauser [20], is to represent tridiagonal matrices as the product of the bidiagonal factors of the *LU* factorization, and to update the bidiagonal factors with formulas requiring only quotients and sums. The algorithm is highly accurate and has become one of LAPACK's main tool for computing eigenvalues of symmetric tridiagonal matrices. Since many interesting algorithms for semiseparable and quasiseparable matrices have been derived from similar techniques employed on tridiagonal matrices (see for example [16, 19, 22]), our idea is to design an algorithm inspired by the qd-type algorithms. While these algorithms for tridiagonals perform well on symmetric positive definite matrices, it turns out that the methods we propose in this paper achieve a high accuracy and stability when applied to totally nonnegative matrices.

The association between totally nonnegative and quasiseparable matrices, was recently done by Dopico, Bella and Olshevsky in two different talks [5], [6] and by Gemignani in [14]. They presented necessary and sufficient conditions to verify if a quasiseparable matrix is totally nonnegative, and proposed fast and stable algorithms for the solution of linear systems.

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A historical example of a totally nonnegative and quasiseparable matrix is the influence function matrux for a string with both ends fastened [11].

For totally nonnegative matrices, we are able to prove that the algorithms here proposed for the computation of the eigenvalues are subtraction free and turn out to be very effective when used with the Laguerre shift strategy. The formulation of the algorithms in terms of recurrences, where some intermediate variable are introduced to avoid possible cancellations, makes these methods similar to the qd-type algorithms for tridiagonals matrices. For a quasiseparable, totally nonnegative matrices Gemignani in [14], following an idea of Koev [15], sketched an algorithm for the reduction into a similar tridiagonal form. We extend this algorithm for the matrices that we call Neville-representable[1], showing the effectiveness when associated with a qd scheme.

The paper is organized as follows. In Section 2 some preliminary definitions and results are provided. In Section 3 the class of Neville-representable quasiseparable matrices is introduced, and structural results for the the L and R factors of the LU factorization of matrices in this class are given. A complete characterization of the class of the Neville-representable quasiseparable matrices is given in terms of the generators of the quasiseparable matrix. Section 4 contains a description of the shifted LR-iterations, and theoretical results about the preservation of the structure. In Section 6, as an alternative for the computation of the eigenvalue, we show a tridiagonalization procedure that can be followed by qd-type iterations as well as any other eigensolver for unsymmetric tridiagonal matrices. Section 7 contains the numerical experiments. In particular, we tested our methods both on random unsymmetric matrices, and on totally nonnegative matrices. The results show a good performance, in terms of time required and accuracy achieved, also for matrices not totally nonnegative. A comparison, for symmetric matrices with `EIGSSD` routine[2] implementing implicit QR steps is performed, showing the better behavior of our methods still achieving a comparable accuracy.

2. Preliminary results. In this section we present some preliminary results useful in the remaining part of the paper.

DEFINITION 1. *An $n \times n$ matrix S is called a semiseparable matrix if the following properties are satisfied:*

$$\operatorname{rank} S(i:n,1:i) \leq 1, \quad \operatorname{rank} S(1:i,i:n) \leq 1, \quad \textit{for} \quad i = 1,\ldots,n-1.$$

All semiseparable matrices $S = s_{ij}$ can be represented by using six vectors $\mathbf{u},\mathbf{v},\mathbf{t},\mathbf{p},\mathbf{q}$ and $\mathbf{r}$ in this way (see Def 2.14 in [24]):

$$s_{ij} = \begin{cases} u_i t_{i-1} t_{i-2} \cdots t_j v_j, & 1 \leq j < i \leq n, \\ u_i v_i = p_i q_i, & 1 \leq j = i \leq n, \\ p_i r_i r_{i+1} \cdots r_{j-1} q_j, & 1 \leq i < j \leq n. \end{cases} \tag{2.1}$$

If S is irreducible, $\mathbf{t}$ and $\mathbf{r}$ can be chosen as unit vectors, thus the representation is made up with the four vectors $\mathbf{u},\mathbf{v},\mathbf{p}$ and $\mathbf{q}$, called generators, and S is said to be generator-representable. If some t_i or r_i is zero, S is reducible. However, if S is reducibile but symmetric or triangular, then it can always be expressed as the direct sum of two or more generator-representable matrices. See [2] for the details.

In this paper a generalization of the semiseparable plus diagonal matrices is considered, that is the class of quasiseparable matrices introduced in [8, 21].

There are many definition of quasiseparable matrix [24]. The most general is the following.

DEFINITION 2. *A $n \times n$ matrix S is called a quasiseparable matrix if the following conditions are satisfied:*

$$\operatorname{rank} S(i+1:n,1:i) \leq 1, \quad \operatorname{rank} S(1:i,i+1:n) \leq 1, \quad \textit{for} i = 1,\ldots,n-1.$$

This definition captures semiseparable matrices, tridiagonal matrices and semiseparable plus diagonal matrices. Note that also noninvertible matrices as well as block diagonal matrices are included in the class, while this does not happen if other definitions are chosen.

[1] We call Neville-representable, the matrices for which the Neville elimination process can be completed

[2] EIGSSD is a Matlab function included in the package SSPack developed by the group at K. U. Leuven.

A very convenient way to represent quasiseparable matrices is the one introduced in [4, 8]. The Givens-vector representation as well as the generator representation can be both be considered as special cases of this quasiseparable representation [24]. An unsymmetric quasiseparable matrix A can be expressed by means of $7n-8$ parameters, as follows

$$A = \begin{pmatrix} \delta_1 & q_2p_1 & q_3r_2p_1 & q_4r_{3:2}p_1 & \cdots & q_nr_{n-1:2}p_1 \\ u_2v_1 & \delta_2 & q_3p_2 & q_4r_3p_2 & \cdots & q_nr_{n-1:3}p_2 \\ u_3t_2v_1 & u_3v_2 & \delta_3 & q_4p_3 & \cdots & q_nr_{n-1:4}p_3 \\ u_4t_{3:2}v_1 & u_4t_3v_2 & u_4v_3 & \ddots & & \vdots \\ \vdots & \vdots & \vdots & & \delta_{n-1} & q_np_{n-1} \\ u_nt_{n-1:2}v_1 & u_nt_{n-1:3}v_2 & u_nt_{n-1:4}v_3 & \cdots & u_nv_{n-1} & \delta_n \end{pmatrix}, \tag{2.2}$$

where $t_{i:j} = t_it_{i-1}t_{i-2}\cdots t_j$, for $i > j$. Note that the redundancy of parameters allows to express quasiseparable matrices with zeros subblocks. The relevance of this representation is proved by the following theorem [24].

THEOREM 1. *A matrix A is quasiseparable if and only if is representable as in* (2.2).

In the following simple results are reported, about representations of quasiseparable matrices, which will be useful in the following sections.

COROLLARY 2. *A quasiseparable matrix A can be decomposed as $A = S^{(u)} + Q$, where*

$$S^{(u)} = \left[\begin{array}{c|ccc} 0 & & & \\ \vdots & & S_{n-1} & \\ 0 & & & \\ \hline 0 & 0 & \cdots & 0 \end{array}\right],$$

where S_{n-1} is a $(n-1)\times(n-1)$ symmetric semiseparable matrix, representable with parameters $\mathbf{q} = (q_2,\ldots,q_n)^T$, $\mathbf{p} = (p_1,\ldots,p_{n-1})^T$ and $\mathbf{r} = (r_2,\ldots,r_{n-1})^T$ as in (2.1)*, and Q is a lower triangular matrix. Similarly $A = S^{(l)} + P$, where $S^{(l)}$ embeds a symmetric semiseparable matrix of size $n-1$ with zeros in the first row and in the last column, and P is an upper triangular.*

Proof. From (2.2) we see that the upper right $(n-1)\times(n-1)$ minor of A has a semiseparable structure (2.1) in the upper triangular part. We set $S_{n-1} = \mathrm{triu}(A,1) + \mathrm{tril}(A^T,-2)$. Matrix Q is defined as the difference between A and $S^{(u)}$, and it is easy to see that it is lower triangular. □

LEMMA 2.1. *If a quasiseparable matrix A is such that all the $r_i \neq 0$, $i = 2,\ldots,n-1$ in the representation* (2.2)*, we have*

$$A = \hat{\mathbf{p}}\hat{\mathbf{q}}^T + K,$$

with K lower triangular.

Proof. Using Corollary 2, $A = S^{(u)} + Q$. If $r_i \neq 0$, we can define the the vectors $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ as follows

$$\begin{cases} \hat{q}_1 = 0 \\ \hat{q}_2 = q_2 \\ \hat{q}_i = q_ir_{i-1}r_{i-2}\cdots r_2, \quad i = 2,\ldots,n, \end{cases} \qquad \begin{cases} \hat{p}_1 = p_1 \\ \hat{p}_i = p_i/(r_ir_{i-1}\cdots r_2) \quad i = 1,\ldots,n-1 \\ \hat{p}_n = 0. \end{cases}$$

We have $S^{(u)} = \hat{\mathbf{p}}\,\hat{\mathbf{q}}^T + Z$, where Z is a lower triangular matrix. Then $A = \hat{\mathbf{p}}\,\hat{\mathbf{q}}^T + K$ with $K = Q + Z$. □

3. The Neville representation. Neville elimination is a classical elimination technique which, differently from the standard Gaussian method, uses consecutive rows (columns) to reduce a matrix into an upper (lower) triangular form. When this elimination can be completely accomplished over rows and columns to reduce the matrix to diagonal form without interchanges, its formulation in terms of Gauss elementary matrices allows to represent the matrix as the product of $O(n)$ bidiagonal matrices: these factors give the *Neville representation* of the matrix, which is called *Neville-representable*. Neville elimination for rank-structured matrices is considered in [14].

In this section we introduce a subclass of quasiseparable matrices which are Neville-representable.

First, we present some general results about LU factorization of quasiseparable matrices, then we consider the Neville representation for quasiseparable matrices, showing conditions for its existence.

We will refer as LU factorization the usual factorization of a matrix into the product of a unit lower triangular and an upper triangular. Usually, in the following, we will denote with L unit lower triangular and with R unit upper triangular matrices.

THEOREM 3. *Let A be a quasiseparable matrix, and assume there exist L, R and D such that $A = LDR$ where L and R are unit lower and upper triangular and D is diagonal. Then L and R can be chosen having quasiseparable structure. Moreover, L and R can be represented, according to (2.2), with the same parameters u_i, t_i, q_i, r_i appearing in the representation of A.*

Proof. Since A is LU-factorizable, if A is nonsingular then it is also strongly nonsingular, and the thesis follows from a known result, which states that in this case L and R must be quasiseparable (see [24], p. 171).
In the case A is singular, we have that at least one of the d_i's is zero. Writing $A = S^{(l)} + P$, where $S^{(l)}$ is strictly lower triangular and quasiseparable, and P is upper triangular, we have $LD = AR^{-1} = S^{(l)}R^{-1} + PR^{-1}$, and looking at the $\mathrm{tril}(LD,-1) = \mathrm{tril}(S^{(l)}R^{-1},-1)$, we see that LD is quasiseparable, and the generators can be expressed in terms of the generators of A. In detail, denote by $\mathbf{u},\mathbf{v},\mathbf{t}$ the generators of the lower triangular part of A, by $\tilde{\mathbf{u}},\tilde{\mathbf{v}},\tilde{\mathbf{t}}$ the generators of $\mathrm{tril}(LD,-1)$ and by w_{ij} the (i,j) entry of R^{-1}, we have

$$\tilde{u}_i = u_i, \quad \tilde{t}_i = t_i, \quad \tilde{v}_i = \sum_{j=1}^{i} t_{i:j+1} v_j w_{ji}.$$

Thus L can be chosen, in infinitely many ways, as a unit lower triangular semiseparable matrix, generated by the same $\tilde{\mathbf{u}},\tilde{\tilde{\mathbf{v}}},\tilde{\mathbf{t}}$, where $\tilde{\tilde{v}}_i d_i = \tilde{v}_i$.

Similarly, R can be chosen as a unit upper triangular semiseparable matrix, generated by the same $\mathbf{q},\mathbf{r}$ generating the upper triangular part of A. □

Now we will consider a set of quasiseparable matrices which are Neville-representable. A Neville-representable matrix, can be expressed as a product of this form, see [12]:

$$L^{(n-1)} \cdots L^{(1)} D R^{(1)} \cdots R^{(n-1)},$$

where D is diagonal, and the factors $L^{(i)}$, $R^{(i)}$ are unit bidiagonal, lower and upper respectively, with zero entries in these positions:

$$L^{(i)}_{k+1,k} = R^{(i)}_{k,k+1} = 0, \quad \text{for} \quad k = 1,\dots,i-1.$$

DEFINITION 3. *Let $\mathcal{S}$ be the set of matrices A admitting the following factorization:*

$$A = L_s L_1 D R_1 R_s, \tag{3.1}$$

where

$$L_s^{-1} = \begin{pmatrix} 1 & & & & \\ -x_1 & 1 & & & \\ & -x_2 & 1 & & \\ & & \ddots & \ddots & \\ & & & -x_{n-1} & 1 \end{pmatrix} \quad L_1 = \begin{pmatrix} 1 & & & & \\ -a_1 & 1 & & & \\ & -a_2 & 1 & & \\ & & \ddots & \ddots & \\ & & & -a_{n-1} & 1 \end{pmatrix}$$

$$R_1 = \begin{pmatrix} 1 & -b_1 & & & \\ & 1 & -b_2 & & \\ & & \ddots & \ddots & \\ & & & 1 & -b_{n-1} \\ & & & & 1 \end{pmatrix} \quad R_s^{-1} = \begin{pmatrix} 1 & -y_1 & & & \\ & 1 & -y_2 & & \\ & & \ddots & \ddots & \\ & & & 1 & -y_{n-1} \\ & & & & 1 \end{pmatrix}$$

and D is a diagonal matrix. It is straightforward to see that the matrices introduced by Definition 3 are LU-factorizable and semiseparable. Moreover, they are also Neville-representable, because if we set

$$\begin{aligned} &L^{(i)} = I + \mathrm{diag}(x_i\mathbf{e}_i, -1), \quad R^{(i)} = I + \mathrm{diag}(y_i\mathbf{e}_i, 1), \quad i = n-1, \dots, 2, \\ &L^{(1)} = (I + \mathrm{diag}(x_1\mathbf{e}_1, -1))L_1, \quad R^{(1)} = R_1(I + \mathrm{diag}(y_1\mathbf{e}_1, 1)), \end{aligned}$$

where $\mathbf{e}_i$ is the i-th vector of the canonical basis of $\mathbf{R}^{n-1}$, we have

$$A = L_s L_1 D R_1 R_s = L^{(n-1)} \cdots L^{(1)} D R^{(1)} \cdots R^{((n-1))},$$

that is the Neville representation of A. Therefore (3.1) can be seen as a variant of the Neville reprentation. The factorization (3.1) is not unique: even when A is strongly nonsingular and the products $L = L_s L_1$ and $R = R_1 R_s$ are uniquely determined, there are infinely many values of x_1, a_1, b_1, y_1 giving the same matrices $L^{(1)}$ and $R^{(1)}$, and therefore the same A: they can be freely chosen according to the conditions $x_1 - a_1 = l_{21}$ and $y_1 - b_1 = r_{12}$.

Nevertheless there are LU-factorizable quasiseparable matrices which are not Neville-representable. For instance, the matrix

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

is factorizable $A = LDR$, where

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix},$$

but we cannot find any x_i and a_i such that $L_s L_1 = L$.

The matrices in $\mathcal{S}$ can be recognized also as the LU-factorizable quasiseparable matrices which admit a representation (2.2) satisfying the following conditions:

a) $u_i \neq 0$, for $i = 2, 3, \dots n$;

b) $q_i \neq 0$, for $i = 1, 2, \dots, n-1$.

Let us call $\mathcal{S}_1$ the set of these matrices.

REMARK 1. One can see some ambiguity in the definition of $\mathcal{S}_1$, due to the fact that the same semiseparable matrix has infinitely many representations (2.2). For instance, a semiseparable matrix having zero entries only in the last row is in $\mathcal{S}_1$, because it can represented according to (2.2) with $u_n = 1$, $t_{n-1} = v_{n-1} = \delta_n = 0$, but it can also be represented with $u_n = \delta_n = 0$, for arbitrary choices of t_{n-1} and v_{n-1}. Two simple characterizing prescriptions for matrices in $\mathcal{S}_1$ are the following:

c) if there is an entry $a_{ij} = 0$ in the strictly lower triangular part, then $a_{kj} = 0$ for $k = i+1, \dots, n$;

d) if there is an entry $a_{ij} = 0$ in the strictly upper triangular part, then $a_{ik} = 0$ for $k = j+1, \dots, n$.

A quasiseparable matrix which violates (c) or (d) cannot be represented with all nonzero u_i and q_i. We could overcome the question by saying that the matrices in $\mathcal{S}_1$ are all those that admit a representation (2.2) with $u_i = q_i = 1$, for every i, as we will see in Corollary 5.

THEOREM 4. *The class $\mathcal{S}$ coincides with the class $\mathcal{S}_1$.*

Proof. We prove the theorem by showing that the $\mathcal{S} \subseteq \mathcal{S}_1$ and $\mathcal{S}_1 \subseteq \mathcal{S}$.

Let us start by proving that if $A \in \mathcal{S}$, then $A \in \mathcal{S}_1$. First, A is factorizable $A = LDR$ with $L = L_s L_1$ and $R = R_1 R_s$. To prove that A is quasiseparable it is sufficient to prove that it is quasiseparable in the lower and upper triangular parts.

Observe that L_s is semiseparable, in fact the rank-one structure propagates to the main diagonal. We distinguish two cases, according with the possible reducibility of L_s.

If L_s is irreducible, then all $x_i \neq 0$. Hence it can be written as $L_s = \bar{\mathbf{u}}\bar{\mathbf{v}}^T + P$, where $\bar{u}_i = \prod_{k=1}^{i-1} x_k$, $\bar{v}_i = \bar{u}_i^{-1}$, P is a strictly upper triangular matrix with superdiagonal entries $p_{i,i+1} = x_i^{-1}$. Writing the bidiagonal matrix L_1 as $L_1 = I - \mathrm{diag}(\mathbf{a}, -1)$, we have

$$\begin{aligned} A &= (\bar{\mathbf{u}}\bar{\mathbf{v}}^T + P)(I - \mathrm{diag}(\mathbf{a}, -1))DR \\ &= (\bar{\mathbf{u}}\bar{\mathbf{v}}^T + P - \bar{\mathbf{u}}\bar{\mathbf{v}}^T \mathrm{diag}(\mathbf{a}, -1) - P\,\mathrm{diag}(\mathbf{a}, -1))DR \\ &= \bar{\mathbf{u}}(\bar{\mathbf{v}}^T - \bar{\mathbf{v}}^T \mathrm{diag}(\mathbf{a}, -1))DR + (P - P\,\mathrm{diag}(\mathbf{a}, -1))DR. \end{aligned}$$

Setting $\tilde{\mathbf{v}}^T = (\bar{\mathbf{v}}^T - \bar{\mathbf{v}}^T \operatorname{diag}(\mathbf{a},-1))DR$, and $\tilde{P} = (P - P\operatorname{diag}(\mathbf{a},-1))DR$ we have that $A = \bar{\mathbf{u}}\tilde{\mathbf{v}}^T + \tilde{P}$. $\tilde{P}$ is an upper triangular matrix having $-a_i d_i x_i^{-1}$ as i-th diagonal entry. So A is the sum of a rank-one matrix and an upper triangular matrix, and hence is quasiseparable in the lower triangular part. In a similar way we can show that A is quasiseparable in the upper triangular part. Note that all the entries of $\bar{\mathbf{u}}$ are nonzero, since $\bar{u}_i\bar{v}_i = 1$. Hence, condition a) of definition of class $\mathcal{S}_1$ is satisfied.

If L_s is reducible, then one or more $x_i = 0$. For simplicity let us consider only the case we have $x_i = 0$ and $x_j \neq 0$ for all $j \neq i$. The generalization to multiple blocks is straightforward. We already observed that reducible triangular semiseparable matrices can be expressed as the direct sum of generator representable semiseparable matrices. In this case $L_s = L_s^{(1)} \oplus L_s^{(2)}$ where $L_s^{(1)}$ and $L_s^{(2)}$ are generator representable semiseparable irreducible matrices of sizes n_1 and n_2 respectively, and hence $L_s^{(1)} = \mathbf{u}^{(1)}\mathbf{v}^{(1)^T} + P_1$, and $L_s^{(2)} = \mathbf{u}^{(2)}\mathbf{v}^{(2)^T} + P_2$, with P_1 and P_2 strictly upper triangular matrices. Moreover, $\mathbf{u}^{(1)}$ and $\mathbf{u}^{(2)}$ have no zero entries, since $u_i^{(1)}v_i^{(1)} = 1$, $u_i^{(2)}v_i^{(2)} = 1$. Let us partition the matrix according with the partition on L_s, thus we have $D = \operatorname{blkdiag}(D_1, D_2)$, and

$$R = R_1 R_s = \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}.$$

In the same way as before we get

$$A = \begin{bmatrix} \mathbf{u}^{(1)}\mathbf{w}^{(1)^T} & 0 \\ \kappa\mathbf{u}^{(2)}\mathbf{e}_{n_1}^T & \mathbf{u}^{(2)}\mathbf{w}^{(2)^T} \end{bmatrix} + \begin{bmatrix} P_{11} & P_{12} \\ 0 & P_{22} \end{bmatrix},$$

where $\mathbf{e}_{n_1}$ is the n_1-th vector of the canonical basis in $\mathbf{R}^{n_1}$, $\kappa = -v_1^{(2)} d_{n_1} a_i$, $\mathbf{w}^{(1)^T} = (\mathbf{v}^{(1)^T} - \mathbf{v}^{(1)^T}\operatorname{diag}(\mathbf{a}(1:i-1),-1))D_1 R_{11}$ and $\mathbf{w}^{(2)^T} = (\mathbf{v}^{(2)^T} - \mathbf{v}^{(2)^T}\operatorname{diag}(\mathbf{a}(i+1:n-1),-1))D_2 R_{22} + \kappa\mathbf{e}_{n_1}^T R_{12}$. Moreover, P_{11} and P_{22} are upper triangular matrices. Note that the block in position $(2,1)$ is null except for the last column, and this column is proportional to $\mathbf{u}^{(2)}$. Then $\operatorname{tril}(A)$ is quasiseparable and the following is a possible choice of generators for A:

$$t_j = \begin{cases} 0 & \text{for } j = i \\ 1 & \text{for } j \neq i \end{cases}, \quad u_j = \begin{cases} u_j^{(1)} & \text{for } 1 \le j \le i \\ u_{j-i}^{(2)} & \text{for } i+1 \le j \le n \end{cases}, \quad v_j = \begin{cases} w_j^{(1)} & \text{for } 1 \le j < i \\ \kappa & \text{for } j = i \\ w_{j-i}^{(2)} & \text{for } j+1 \le j \le n \end{cases}.$$

Clearly all u_j's are nonzero. A similar proof can be given for the upper triangular part of A.
Let us prove that $\mathcal{S}_1 \subseteq \mathcal{S}$, that is for every quasiseparable, LU-factorizable matrix with $u_i \neq 0$ and $q_i \neq 0$ we can find parameters $\mathbf{x}, \mathbf{a}, \mathbf{b}, \mathbf{y}, \mathbf{d}$ such that $A = L_s L_1 D R_1 R_s$.
By assumption we have $A = LDR$, where L is unit lower triangular, D diagonal and R is unit upper triangular. We want to prove that it is possible to factorize L as $L_s L_1$ and R as $R_1 R_s$. By Theorem 3, we have that L and R can be chosen quasiseparable, so, in detail

$$L = \begin{pmatrix} 1 & & & & & \\ \tilde{u}_2\tilde{v}_1 & 1 & & & & \\ \tilde{u}_3\tilde{t}_2\tilde{v}_1 & \tilde{u}_3\tilde{v}_2 & 1 & & & \\ \tilde{u}_4\tilde{t}_{3:2}\tilde{v}_1 & \tilde{u}_4\tilde{t}_3\tilde{v}_2 & \tilde{u}_4\tilde{v}_3 & 1 & & \\ \vdots & \vdots & \vdots & & \ddots & \\ \tilde{u}_n\tilde{t}_{n-1:2}\tilde{v}_1 & \tilde{u}_n\tilde{t}_{n-1:3}\tilde{v}_2 & \tilde{u}_n\tilde{t}_{n-1:4}\tilde{v}_3 & \cdots & \tilde{u}_n\tilde{v}_{n-1} & 1 \end{pmatrix},$$

where $\tilde{u}_i \neq 0$ since $\tilde{u}_i = u_i$, which are assumed to be nonzero. Is now easy to prove that L can be factorized as the product of L_s and L_1 by observing that the Neville elimination can be applied to the rows of L. In particular, L_s is the inverse of the bidiagonal matrix $I - \operatorname{diag}(\mathbf{x},-1)$ having the Neville multipliers as codiagonal entries, i.e. $x_{i-1} = -\tilde{u}_i\tilde{t}_{i-1}/\tilde{u}_{i-1}$, $i = 3,\ldots,n$.
Reasoning in the same way for the upper triangular part of A we can complete the proof. □
The following corollary weakens the redundancy of the representation (2.2) for matrices in $\mathcal{S}$.

COROLLARY 5. *If $A \in \mathcal{S}$, then it can be represented, according to (2.2), with $u_i = q_i = 1$, $i = 2,\ldots,n$, $t_i = x_i$, $r_i = y_i$, $i = 2,\ldots,n-1$.*

Proof. By direct inspection, a simple choice for the parameters involved in the representations of the semiseparable matrices L and R of the factorization $A = LDR$ is the following:

$$u_i = 1,\ v_i = x_i - a_i,\ i = 2,\dots,n,\ t_i = x_i,\ i = 2,\dots,n-1,\ \text{for } L,$$

$$q_i = 1,\ p_i = y_i - b_i,\ i = 2,\dots,n,\ r_i = y_i,\ i = 2,\dots,n-1,\ \text{for } R.$$

Theorem 3 says that the parameters u_i, t_i, q_i and r_i for A can be taken from the represention of L and R. □

It is easy to prove that $\mathcal{S}$ contains all quasiseparable and Neville-representable matrices.

THEOREM 6. *Any quasiseparable Neville-representable matrix is in $\mathcal{S}$.*

Proof. Since $\mathcal{S} = \mathcal{S}_1$, we show that a Neville-representable quasiseparable matrix must be in $\mathcal{S}_1$. Assume by contradiction this is not true, then by Remark 1, one of conditions (c),(d) would not be obeyed, say (c). This means that there exist, in the strictly lower triangular part, some $a_{ij} = 0$ with $a_{i+1,j} \neq 0$, and, as a consequence of the rank structure, all the entries in the i-th row of the strictly lower triangular part would be zero. Then the i-th row could not be used to eliminate the $(i+1)$-th one, and the Neville row elimination would fail. But this would cause a contradiction. □

3.1. Quasiseparable Totally nonnegative matrices. Neville elimination is deeply connected with totally nonnegative matrices [15, 12, 13].

DEFINITION 4. *A matrix A is called totally nonnegative (TN) if all its minor of any order are nonnegative.*

THEOREM 7. *If $A \in \mathcal{S}$ and $x_i, y_i \geq 0$, $a_i, b_i \leq 0$ and $d_i \geq 0$ then A is totally nonnegative.*

Proof. The theorem holds for nonsingular matrices as proved in [14]. In the case A is nonsingular also the converse is true. If A is a singular matrix in $\mathcal{S}$, with $x_i, y_i \geq 0$, $a_i, b_i \leq 0$ and $d_i \geq 0$, then A is TN since product of TN matrices. □

REMARK 2. We can easily recognize matrices in $\mathcal{S}$ diagonally similar to TN matrices. The general condition is that $x_i y_i \geq 0$, $d_i \geq 0$, $a_i b_i \geq 0$ with $a_i x_i \leq 0$.

The class of totally nonnegative matrices has nice properties that resemble those of positive semidefinite Hermitian matrices, in particular its eigenvalues are real and nonnegative. Another similarity between the two classes of matrices is that also for TN matrices we can give an interlacing Theorem [11, 1].

THEOREM 8. *Let A be TN with eigenvalues $\lambda_1 \geq \lambda_2 \cdots \geq \lambda_n$. Suppose A_k is a $k \times k$ submatrix of A lying in rows and columns with consecutive indices and having eigenvalues $\tilde{\lambda}_1 \geq \tilde{\lambda}_2 \cdots \geq \tilde{\lambda}_k$. Then*

$$\lambda_i \geq \tilde{\lambda}_i \geq \lambda_{i+n-k}, \quad i = 1,\dots,k.$$

4. On the shifted LR-algorithm. In this section we present the shifted *LR* algorithm acting implicitly on the representation (3.1) of A. The shifted *LR* method proceeds iteratively as follows[3], let $A^{(0)} = A$, we obtain the sequence of matrices $A^{(k)}$ in this way:

$$\begin{cases} A^{(k)} = L^{(k)} D^{(k)} R^{(k)}, \\ A^{(k+1)} = {L^{(k)}}^{-1} A^{(k)} L^{(k)} - \sigma_{k+1} I = D^{(k)} R^{(k)} L^{(k)} - \sigma_{k+1} I, \quad k = 0,1,\dots, \end{cases} \tag{4.1}$$

where, for every k, the parameter $\sigma^{(k+1)}$ is chosen in accordance with some shift strategy to accelerate convergence [4]. Usually, instead of computing explicitly the factorization of $A^{(k)}$, and multiplying the factors in reverse order according to (4.1), we proceed implicitly performing the transition $A^{(k)} \to A^{(k+1)}$ in terms of their Neville representations. Note that $A^{(k+1)}$ is no more similar to $A^{(k)}$ because the at each step we subtract off a shift, but we never restore it. This means that we have to accumulate the shifts during

[3]The superscript notation $\cdot^{(i)}$ will be used only for depicting *LR*-steps performed on matrices. We will omit this superscript as much as possible, not to overload the notation.

[4]In section 4.3 we describe in detail the choice of the Laguerre shift, that is particularly suited when dealing with totally nonnegative matrices.

the computation and add them back once the approximation of each eigenvalue becomes available. An important result is that the quasiseparable structure is preserved under *LR* step.

THEOREM 9. *The quasiseparable structure is preserved under LR steps.*

Proof. Let $A = LDR$, we want to prove that the matrix $A^{(1)} = DRL$ is still quasiseparable, although the possible symmetry of A is not preserved. By Corollary 2, there exists a symmetric semiseparable matrix $S^{(u)}$, and a lower triangular matrix Q such that $A = S^{(u)} + Q$, so we have $A^{(1)} = L^{-1}AL = L^{-1}(S^{(u)} + Q)L$. As remarked in Section 2, if $S^{(u)}$ is irreducible, then it is is generator representable, otherwise it is the direct sum of generator representable matrices. Assume that $S^{(u)}$ is irreducible, therefore $S^{(u)} = \mathbf{p}\mathbf{q}^T + X$, where X is a strictly lower triangular matrix. Then $A^{(1)} = L^{-1}\mathbf{p}\mathbf{q}^T L + L^{-1}XL + L^{-1}QL$. Setting $\tilde{\mathbf{p}} = L^{-1}\mathbf{p}$, $\tilde{\mathbf{q}} = L^T\mathbf{q}$, $\tilde{Q} = L^{-1}(X+Q)L$, we have $A^{(1)} = \tilde{\mathbf{p}}\tilde{\mathbf{q}} + \tilde{Q}$. Then the minors taken out of the strictly upper triangular part of $A^{(1)}$ have rank at most one. In the case $S^{(u)}$ is reducible, we can use the same arguments for each of the irreducible diagonal blocks, obtaining that $A^{(1)}$ is reducible too and is quasiseparable in the upper triangular part.

Similarly, we can prove that $A^{(1)}$ has the quasiseparable structure in the strictly lower triangular part. □

In this section we present two different methods. The first, presented in Section 4.1 works on the parameters a_i, b_i, x_i, y_i and d_i, the second one, described in Section 4.2, considers the aggregated parameters $m_i = x_i y_i$ and takes advantage on the fact that there are some quantities that are invariant during the steps as explained in the following Corollary.

COROLLARY 10. *Let A be a quasiseparable matrix in $\mathcal{S}$. If $x_i \neq 0$ and $y_i \neq 0$, for $i = 1, \ldots, n-1$ we can define the quantities*

$$h_i = \frac{a_i d_i}{x_i}, \quad k_i = \frac{b_i d_i}{y_i}, \quad i = 1, \ldots, n-1. \tag{4.2}$$

These quantities are invariant under LR steps without shift.

Proof. By Corollary 5, in the representation (2.2) of A we have that $r_i \neq 0$ for $i = 2, \ldots, n-1$. By Lemma 2.1, $A = \hat{\mathbf{p}}\hat{\mathbf{q}}^T + K$, where K is lower triangular. Consider the diagonal entries of A, that for the previous equality, are given by the sum of the diagonal entries of $\hat{\mathbf{p}}\hat{\mathbf{q}}^T$ and the diagonal entries of K, say k_i. This means $\delta_i = p_i q_i + k_i$. The diagonal entries of the new quasiseparable matrix $A^{(1)} = L^{-1}AL = L^{-1}(\hat{\mathbf{p}}\hat{\mathbf{q}}^T + K)L$, since L is unit lower triangular, we have that the diagonal entries of the lower triangular term $L^{-1}KL$ are still equal to k_i, which then remain constant during all the iterative steps.

Let denote by $\Delta = \mathrm{diag}(K)$. The matrix $B = A - \Delta$ has a semiseparable structure in the upper triangular part, which extends to the main diagonal. Since $A = L_s L_1 D R_1 R_s$, B can be expressed as

$$B = A - \Delta = L_s T R_s, \tag{4.3}$$

where $T = L_1 D R_1 - L_s^{-1} \Delta R_s^{-1}$ is tridiagonal. The upper triangular matrix R_s is irreducible semiseparable, therefore by Lemma 2.1 it can be written as $R_s = \tilde{\mathbf{p}}\tilde{\mathbf{q}}^T + \tilde{K}$, where $\tilde{K}$ is strictly lower triangular. Substituting in (4.3) we find

$$B = L_s T \tilde{\mathbf{p}}\tilde{\mathbf{q}}^T + L_s T \tilde{K},$$

thus we see that the diagonal of B agrees with the one-rank structure in the upper triangular part only if the lower triangular matrix $L_s T \tilde{K}$ has all zeros as diagonal entries, and this happens only if T is lower bidiagonal. So we readily obtain $k_i = \frac{d_i b_i}{y_i}$.

Repeating the same reasoning for the lower triangular part of A we obtain the that $h_i = \frac{d_i a_i}{x_i}$ are invariants too. □

4.1. A qd-type method. In this section we show how to obtain, starting from a matrix $A = A^{(k)}$ in $\mathcal{S}$, expressed as $A = L_s L_1 D R_1 R_s$ the new representation of $A^{(k+1)} = D R_1 R_s L_s L_1 - \sigma_{k+1} I$ in terms of the updated parameters, that is $A^{(k+1)} = \bar{\bar{L}}_s \bar{\bar{L}}_1 \bar{\bar{D}} \bar{\bar{R}}_1 \bar{\bar{R}}_s$, under the assumption that $A^{(k+1)} \in \mathcal{S}$.

The entire procedure consists in updating the parameters x_i, y_i, d_i, a_i, b_i which define quasiseparable matrices in $\mathcal{S}$. The updating process starts with the computation of $\tilde{A} = D R_1 R_s L_s L_1$, and replaces products

of the type RL with products of the type LDR, with D diagonal. In particular, we have

$$\tilde{A} = DR_1\,(R_sL_s)\,L_1 = DR_1(\bar{L}_s E\bar{R}_s)\,L_1 \tag{4.4}$$
$$= (DR_1\bar{L}_s)\,E\bar{R}_s\,L_1 = (\bar{\bar{L}}_S F\bar{R}_1)E\bar{R}_s\,L_1 \tag{4.5}$$
$$= \bar{\bar{L}}_S F\bar{R}_1\,(E\bar{R}_s\,L_1) = \bar{\bar{L}}_S\,F\bar{R}_1(\bar{L}_1 G\bar{\bar{R}}_s) \tag{4.6}$$

where D,E,F and G are diagonal matrices. Equations (4.4), (4.5), (4.6) make sense if the intermediate matrices R_sL_s, $DR_1\bar{L}_s$, and $E\bar{R}_s\,L_1$ are all LU-factorizable. Anyway, if the procedure described by equations (4.4), (4.5), (4.6) can be carried on and $A^{(k+1)} = \tilde{A} - \sigma_{k+1}I$ is LU-factorizable too, then

$$A^{(k+1)} = \bar{\bar{L}}_S F\bar{R}_1\bar{L}_1 G\bar{\bar{R}}_S - \sigma_{k+1}I = \bar{\bar{L}}_S\bar{\bar{L}}_1\bar{\bar{D}}\bar{\bar{R}}_1\bar{\bar{R}}_S, \tag{4.7}$$

where $\bar{\bar{D}}$ is diagonal.
The assumptions required by the updating equations (4.4), (4.5), (4.6), besides the preliminary request for $A^{(k+1)}$ to be in $\mathcal{S}$, are satisfied in case A is a TN matrix and the shift is properly chosen, as we will see later.

Let us describe the updating process described by equality (4.4). Set

$$\bar{L}_s E\bar{R}_s = R_sL_s,$$

for a suitable nonsingular diagonal matrix E. If we rewrite the above equation as $\bar{R}_s^{-1}E^{-1}\bar{L}_s^{-1} = L_s^{-1}R_s^{-1}$, where all the matrices involved are bidiagonal or diagonal, and define the auxiliary variables

$$\begin{cases} \alpha_i = e_i^{-1} - x_{i-1}y_{i-1}, & i = 1,\dots,n-1 \\ \alpha_n = 1, \end{cases}$$

we obtain the following recurrences:

$$\begin{cases} e_i^{-1} = \alpha_i + x_{i-1}y_{i-1}, & i = n,\dots,2 \\ \alpha_{i-1} = \alpha_i/e_i^{-1}, & i = n,\dots,2, \\ e_1^{-1} = \alpha_1. \end{cases}$$

Then, we can compute the entries of $\bar{L}_s^{-1}$ and $\bar{R}_s^{-1}$ as follows

$$\begin{aligned} \bar{x}_i &= x_i/e_{i+1}^{-1}, \quad i = 1,\dots,n-1 \\ \bar{y}_i &= y_i/e_{i+1}, \quad i = 1,\dots,n-1. \end{aligned}$$

The updating described in (4.5) consists of

$$\bar{\bar{L}}_S F\bar{R}_1 = DR_1\bar{L}_s,$$

for a suitable nonsingular diagonal matrix F. Again we can use the fact that the inverse of matrices of type L_s is bidiagonal. We have $F\bar{R}_1\bar{L}_s^{-1} = \bar{\bar{L}}_S^{-1}DR_1$, and setting

$$\beta_i = 1 - b_i\bar{x}_i, \quad i = 1,\dots,n-1,$$

we obtain the following recurrences for the diagonal entries of F:

$$\begin{cases} f_1 = d_1\beta_1, \\ f_i = d_i\beta_i/\beta_{i-1}, & i = 2,\dots,n-1, \\ f_n = d_n/\beta_{n-1}, \end{cases}$$

and the final $\bar{\bar{x}}_i$ describing $\bar{\bar{L}}_s$

$$\bar{\bar{x}}_i = \bar{x}_i f_{i+1}/d_i, \quad i = 1,\dots,n-1.$$

The intermediate entries of $\bar{R}_1$ are

$$\begin{cases} \bar{b}_1 = b_1/\beta_1, \\ \bar{b}_i = b_i\beta_i/\beta_{i-1}, & i = 2,\dots,n-1. \end{cases}$$

Let us describe step (4.6), that is

$$\bar{L}_1 G \bar{\bar{R}}_S = E \bar{R}_s L_1.$$

If we re-write the above equation as $\bar{R}_s^{-1} E^{-1} \bar{L}_1 = L_1 G \bar{\bar{R}}_S^{-1}$, and defining the auxiliary variables

$$\gamma_i = 1 - \bar{y}_i a_i, \; i = 1, \dots, n-1,$$

we obtain the following recurrences for the diagonal entries of G:

$$\begin{cases} g_1 = \gamma_1 / e_1^{-1}, \\ g_i = \gamma_i / (\gamma_{i-1} e_i^{-1}), \quad i = 2, \dots, n-1, \\ g_n = 1/(\gamma_{n-1} e_n^{-1}). \end{cases}$$

The final entries of $\bar{\bar{R}}_s$ are computed as follows

$$\bar{\bar{y}}_i = \bar{y}_i g_{i+1} / e_{i+1}^{-1}, \quad i = 1, \dots, n-1,$$

while the intermediate entries of $\bar{L}_1$ are

$$\bar{a}_i = a_i / (e_{i+1}^{-1} g_i), \quad i = 1, \dots, n-1.$$

It remains to describe the final updating which involves the terms in the brackets in (4.7). If no shift is chosen, then $A^{(k+1)} = A^{(1)}$, so $\bar{\bar{L}}_1$, $\bar{\bar{D}}$, and $\bar{\bar{R}}_1$ have to be found such that

$$\bar{\bar{L}}_1 \bar{\bar{D}} \bar{\bar{R}}_1 = F \bar{R}_1 \bar{L}_1 G. \tag{4.8}$$

The final matrices $\bar{\bar{L}}_1$ and $\bar{\bar{R}}_1$ can be computed introducing auxiliary variables δ_i defined as

$$\begin{cases} \delta_i = \bar{\bar{d}}_i - \bar{a}_i \bar{b}_i f_i g_i, \quad i = 1, \dots, n-1 \\ \delta_n = \bar{\bar{d}}_n. \end{cases}$$

We have the following recurrences for the final $\bar{\bar{D}}$

$$\begin{cases} \delta_1 = f_1 g_1, \\ \bar{\bar{d}}_i = \delta_i + \bar{a}_i \bar{b}_i f_i g_i, \quad i = 1, \dots, n-1 \\ \delta_{i+1} = \delta_i f_{i+1} g_{i+1} / \bar{\bar{d}}_i, \quad i = 1, \dots, n-1, \\ \bar{\bar{d}}_n = \delta_n. \end{cases} \tag{4.9}$$

The entries of $\bar{\bar{L}}_1$ and $\bar{\bar{R}}_1$ can be then obtained as follows

$$\bar{\bar{a}}_i = \bar{a}_i f_{i+1} g_i / \bar{\bar{d}}_i, \quad i = 1, \dots, n-1 \tag{4.10}$$

$$\bar{\bar{b}}_i = \bar{b}_i f_i g_{i+1} / \bar{\bar{d}}_i, \quad i = 1, \dots, n-1. \tag{4.11}$$

In case of shift $\sigma = \sigma_{k+1}$, note that $A^{(k+1)} = A^{(1)} - \sigma I$ can be expressed as

$$\bar{\bar{L}}_S F \bar{R}_1 \bar{L}_1 G \bar{\bar{R}}_S - \sigma I = \bar{\bar{L}}_S (F \bar{R}_1 \bar{L}_1 G - \sigma \bar{\bar{L}}_S^{-1} \bar{\bar{R}}_S^{-1}) \bar{\bar{R}}_S.$$

So we must modify only the updating of the variables $\bar{\bar{a}}_i, \bar{\bar{b}}_i$ and $\bar{\bar{d}}_i$ described by equations (4.10), (4.11) and (4.9). In particular equation (4.8) becomes

$$\bar{\bar{L}}_1 \bar{\bar{D}} \bar{\bar{R}}_1 = F \bar{R}_1 \bar{L}_1 G - \sigma \bar{\bar{L}}_S^{-1} \bar{\bar{R}}_S^{-1},$$

and $\bar{\bar{L}}_1$, $\bar{\bar{D}}$ and $\bar{\bar{R}}_1$ can be computed by means of the following recurrences, where δ_i is defined as before as

$$\begin{cases} \delta_i = \bar{\bar{d}}_i - \bar{a}_i \bar{b}_i f_i g_i, \quad i = 1, \dots, n-1 \\ \delta_n = \bar{\bar{d}}_n. \end{cases}$$

The recurrences replacing (4.9) are

$$\begin{cases} \delta_1 = f_1 g_1 - \sigma, \\ \bar{\bar{d}}_i = \delta_i + \bar{a}_i \bar{b}_i f_i g_i, \quad i = 1, \ldots, n-1, \\ \delta_{i+1} = f_{i+1} g_{i+1} \delta_i / \bar{\bar{d}}_i - \sigma(1 + \bar{\bar{x}}_i(\bar{\bar{y}}_i - \bar{\bar{b}}_i) - f_{i+1} g_i \bar{a}_i \bar{\bar{y}}_i / \bar{\bar{d}}_i), \quad i = 1, \ldots, n-1, \\ \bar{\bar{d}}_n = \delta_n. \end{cases} \tag{4.12}$$

The new $\bar{\bar{a}}_i$ and $\bar{\bar{b}}_i$ can be obtained as follows

$$\bar{\bar{a}}_i = (\bar{a}_i f_i g_{i+1} - \sigma \bar{\bar{x}}_i)/\bar{\bar{d}}_i, \quad i = 1, \ldots, n-1, \tag{4.13}$$

$$\bar{\bar{b}}_i = (\bar{b}_i f_{i+1} g_i - \sigma \bar{\bar{y}}_i)/\bar{\bar{d}}_i, \quad i = 1, \ldots, n-1 \tag{4.14}$$

Alternatively, one can first compute $\bar{\bar{a}}_i$ and $\bar{\bar{b}}_i$ with(4.13), and (4.14) and then express δ_{i+1}, as

$$\delta_{i+1} \; = \; f_{i+1} g_{i+1} \delta_i / \bar{\bar{d}}_i - \sigma(1 + \bar{\bar{y}}_i(\bar{\bar{x}}_i - \bar{\bar{a}}_i) - f_i g_{i+1} \bar{b}_i \bar{\bar{x}}_i / \bar{\bar{d}}_i), \quad i = 1, \ldots, n-1.$$

REMARK 3. We denoted the method described in this section as belonging to the family of qd algorithms [20, 10, 17]. The reason is that it has similar characteristics, since the definition of the auxiliary variables, α_i, δ_i makes it possible, with some sign hypotheses (see Theorem 12), to get rid of subtractions which are hidden in the auxiliary parameters: only divisions, multiplications and sums are needed (except for the shift).

4.2. Working with invariants: another qd-type method. In Corollary 10 we proved that if $x_i \neq 0$ and $y_i \neq 0$ for all $i = 1, \ldots, n-1$, then the quantities h_i and k_i defined as in (4.2) are invariant under *LR* steps. This observation allows to rewrite the previous recurrences using these quantities. The new algorithm, described by Algorithm 1, although applicable only to a subclass of matrices in $\mathcal{S}$, has a lower computational cost as we will see in section 5.

The new recurrences consider the aggregated quantities $m_i = x_i y_i$, the invariants k_i, h_i and the diagonal entries d_i. Once we want to recover the Neville representation of $A^{(k)}$, we can assign arbitrary nonzero values say to the x_i, compute $y_i = m_i/x_i$ and find a_i, b_i using the formulas for the invariants. Note that the use of invariants allows to simplify the recurrences since we have only to update the values m_i and the new diagonal entries d_i. This procedure should be combined with an effective shift strategy. A particularly convenient choice for the shift is described in Section 4.3.

As in the recurrences presented in Section 4.1 we see that we still need auxiliary variables α_i and δ_i, but the aggregation of parameters x_i and y_i into m_i allows to reduce the number of recurrences. This method has not a natural matrix formulation but it is easy to verify its correctness by merging the recurrences for the updating of x_i and y_i to get the updating formula for m_i.

4.3. The Laguerre shift. The choice of an adequate shift strategy is always of crucial importance for the convergence. Various shift strategies have been proposed, ranging from the classical Rayleigh shift defined as the entry in position (n,n), or the Wilkinson shift in the case the matrix might have complex eigenvalues [26]. In this section we describe in detail a shift technique known as Laguerre shift [26, 18] which has shown to be effective in the case of quasiseparable matrices with real positive eigenvalues.

In particular the shift $\sigma = \sigma_{k+1}$ in (4.12) is chosen in accordance with the following formula

$$\sigma = \frac{n}{s_1^{(k)} + \sqrt{(n-1)(n s_2^{(k)} - (s_1^{(k)})^2}}, \tag{4.15}$$

where $s_1^{(k)} = \mathrm{trace}((A^{(k)})^{-1})$ and $s_2 = \mathrm{trace}((A^{(k)})^{-2})$. The choice of the Laguerre shift guarantees that the eigenvalues are computed in an ordered way since $0 < \sigma \leq \mu_n$, where μ_n is the smallest eigenvalues of $A^{(k)}$. If μ_n is simple, then $\sigma < \mu_n$.
We start from $A^{(k)}$ factorized as

$$A^{(k)} = L_s L_1 D R_1 R_s,$$

Algorithm 1 $[\bar{\bar{m}},\bar{\bar{h}},\bar{\bar{k}},\bar{\bar{d}}] \leftarrow \texttt{LRstep}(m,h,k,d,\sigma)$

$\alpha_n \leftarrow 1$;
for $i = n$ to 2 **do**
  $e_i^{-1} \leftarrow \alpha_i - m_{i-1}$; {Auxiliary variables}
  $\alpha_{i-1} \leftarrow \alpha_i / e_i^{-1}$;
end for
$e_1^{-1} \leftarrow \alpha_1$;
for $i = 1$ to $n-1$ **do**
  $p_i \leftarrow \left(1 - \frac{k_i m_i}{d_i e_{i+1}^{-1}}\right)\left(1 - \frac{h_i m_i}{d_i e_{i+1}^{-1}}\right)$; {Auxiliary variables}
end for
for $i = 1$ to $n-1$ **do**
  $\bar{\bar{m}}_i \leftarrow m_i p_{i+1} d_{i+1} / (p_i d_i e_{i+1}^{-2})$; {Updating of m_i}
end for
$\delta_1 \leftarrow p_1 d_1 / e_1^{-1} - \sigma$;
for $i = 1$ to $n-1$ **do**
  $\bar{\bar{d}}_i \leftarrow \delta_i + h_i k_i m_i / (d_i e_{i+1}^{-1})$; {Updating of d_i}
  $\delta_{i+1} \leftarrow \delta_i p_{i+1} d_{i+1} / (p_i \bar{\bar{d}}_i e_{i+1}^{-1}) - \sigma(1 + \bar{\bar{m}}_i(1 + (\sigma - (h_i + k_i))/\bar{\bar{d}}_i))$;
end for
$\bar{\bar{d}}_n \leftarrow \delta_n$; {Updating of the last d_n}
for $i = 1$ to $n-1$ **do**
  $\bar{\bar{h}}_i \leftarrow h_i - \sigma$;
  $\bar{\bar{k}}_i \leftarrow k_i - \sigma$.
end for

so we need the diagonal entries c_{ii} of

$$C = (A^{(k)})^{-1} = R_s^{-1} R_1^{-1} D^{-1} L_1^{-1} L_s^{-1}.$$

In the case $x_i, y_i \neq 0$, using the invariants[5] by direct computation, we have

$$\begin{cases} c_{nn} = d_n^{-1}, \\ c_{n-1,n-1} = d_{n-1}^{-1} + d_n^{-1} m_{n-1}(h_{n-1} d_{n-1}^{-1} - 1)(k_{n-1} d_{n-1}^{-1} - 1), \\ c_{ii} = d_i^{-1} + (d_{i+1}^{-1} + \sum_{r=i+1}^{n-1} (\prod_{j=i+1}^{r} m_j h_j k_j d_j^{-2}) d_{r+1}^{-1}) m_i (h_i d_i^{-1} - 1)(k_i d_i^{-1} - 1), \ i = n-2, \dots, 1. \end{cases}$$

Setting

$$\begin{cases} t_{n-1} = d_n^{-1} m_{n-1}, \\ t_i = (d_{i+1}^{-1} + \sum_{r=i+1}^{n-1} (\prod_{j=i+1}^{r} m_j h_j k_j d_j^{-2}) d_{r+1}^{-1}) m_i, \ i = n-2, \dots, 1, \end{cases}$$

the requested trace s_1 can be computed with about $14n$ flops in this way:

$$\begin{cases} c_{nn} = d_n^{-1}, \\ t_{n-1} = d_n^{-1} m_{n-1}, \\ t_i = (t_{i+1} h_{i+1} k_{i+1} d_{i+1}^{-1} + 1) m_i d_{i+1}^{-1}, \quad i = n-2, \dots, 1, \\ c_{ii} = d_i^{-1} + t_i (h_i d_i^{-1} - 1)(k_i d_i^{-1} - 1), \quad i = n-1, \dots, 1, \\ s_1 = \mathrm{trace}(C) = \sum_i^n c_{ii}. \end{cases}$$

Since $s_2 = \mathrm{trace}(C^2) = \sum_{i=1}^n c_{ii} + 2\sum_{j=1}^{n-1} \sum_{i=j+1}^n c_{ij} c_{ji}$, the sum of all the products $c_{ij} c_{ji}$ has to be computed.

[5] We have different formulas in the case some x_i or y_i are zero. We choose here to present only this case because it is simpler, but other formulas when working with the full set of parameters can be found.

Let us start from those involving co-diagonal entries $c_{i,i-1}c_{i-1,i}$, which have the following form

$$\begin{cases} c_{n,n-1}c_{n-1,n} = m_{n-1}(h_{n-1}d_{n-1}^{-1}-1)(k_{n-1}d_{n-1}^{-1}-1)d_n^{-2}, \\ c_{n-1,n-2}c_{n-2,n-1} = (1+h_{n-1}m_{n-1}d_n^{-1}(k_{n-1}d_{n-1}^{-1}-1))(1+k_{n-1}m_{n-1}d_n^{-1}(h_{n-1}d_{n-1}^{-1}-1)) \\ \qquad m_{n-2}(h_{n-2}d_{n-2}^{-1}-1)(k_{n-2}d_{n-2}^{-1}-1)d_{n-1}^{-2}, \\ c_{i,i-1}c_{i-1,i} = (1+h_im_i(k_id_i^{-1}-1)(d_{i+1}^{-1}+\sum_{r=i+1}^{n-1}d_{r+1}^{-1}\prod_{j=i+1}^{r}m_jh_jk_jd_j^{-1})) \\ \qquad (1+k_im_i(h_id_i^{-1}-1)(d_{i+1}^{-1}+\sum_{r=i+1}^{n-1}d_{r+1}^{-1}\prod_{j=i+1}^{r}m_jh_jk_jd_j^{-1})) \\ \qquad m_{i-1}(h_{i-1}d_{i-1}^{-1}-1)(k_{i-1}d_{i-1}^{-1}-1)d_i^{-2}, \quad i=n-2,\dots,2. \end{cases}$$

If we set

$$\begin{cases} t'_{n-1} = (1+h_{n-1}m_{n-1}d_n^{-1}(k_{n-1}d_{n-1}^{-1}-1)), \\ t''_{n-1} = (1+k_{n-1}m_{n-1}d_n^{-1}(h_{n-1}d_{n-1}^{-1}-1)), \\ t'_i = (1+h_im_i(k_id_i^{-1}-1)(d_{i+1}^{-1}+\sum_{r=i+1}^{n-1}d_{r+1}^{-1}\prod_{j=i+1}^{r}m_jh_jk_jd_j^{-1})), \quad i=n-2,\dots,2, \\ t''_i = (1+k_im_i(h_id_i^{-1}-1)(d_{i+1}^{-1}+\sum_{r=i+1}^{n-1}d_{r+1}^{-1}\prod_{j=i+1}^{r}m_jh_jk_jd_j^{-1})), \quad i=n-2,\dots,2, \end{cases}$$

all co-diagonal entries products $c_{i,i-1}c_{i-1,i}$ can be computed according to the following scheme, with $18n$ flops:

$$\begin{cases} t'_{n-1} = (1+h_{n-1}m_{n-1}d_n^{-1}(k_{n-1}d_{n-1}^{-1}-1)), \\ t''_{n-1} = (1+k_{n-1}m_{n-1}d_n^{-1}(h_{n-1}d_{n-1}^{-1}-1)), \\ t'_i = h_{i+1}m_{i+1}d_{i+2}(1+t'_{i+1}k_{i+1}d_{i+2}), \quad i=n-2,\dots,2, \\ t''_i = k_{i+1}m_{i+1}d_{i+2}(1+t''_{i+1}h_{i+1}d_{i+2}), \quad i=n-2,\dots,2, \\ z_{n-1} = d_n^{-2}, \\ z_i = (1+t'_{i+1}(k_{i+1}d_{i+1}^{-1}-1))(1+t''_{i+1}(h_{i+1}d_{i+1}^{-1}-1)), \quad i=n-2,\dots,1, \\ c_{i,i-1}c_{i-1,i} = z_{i-1}m_{i-1}(h_{i-1}d_{i-1}^{-1}-1)(k_{i-1}d_{i-1}^{-1}-1), \quad i=n,\dots,2. \end{cases}$$

The sums $\varepsilon_j = \sum_{i=j+2}^{n} c_{ij}c_{ji}$, $j=n-2,\dots,1$ can be computed in this way:

$$\begin{cases} w_{n-1} = 0, \\ w_j = (w_{j+1}+z_{j+1})m_{j+1}h_{j+1}k_{j+1}d_{j+1}^{-2}, \quad j=n-2,\dots,1, \\ \varepsilon_j = w_jm_j(h_jd_j^{-1}-1)(k_jd_j^{-1}-1), \quad j=n-2,\dots,1. \end{cases}$$

Finally the sum $\sum_{j=1}^{n-1}\sum_{i=j+1}^{n} c_{ij}c_{ji}$ which is required to complete the computation of s_2 can be expressed as

$$\sum_{j=1}^{n-1}\sum_{i=j+1}^{n} c_{ij}c_{ji} = c_{n,n-1}c_{n-1,n} + \sum_{j=1}^{n-2}(\varepsilon_j + c_{j+1,j}c_{j,j+1}) = \sum_{j=1}^{n-1}(w_j+z_j)m_j(h_jd_j^{-1}-1)(k_jd_j^{-1}-1),$$

and costs $9n$ flops more.

In the case we deal with a restricted class of matrices, for example, when dealing with tridiagonal or semiseparable matrices, we can simplify this procedure and compute the shift with a lower number of operations. In Section 7 for example we simplified the computation of the shift when our method is applied to tridiagonal matrices, obtaining the Laguerre shift with a lower number of flops.

5. Stability and computational cost. In Section 4.1 and 4.2 we described the implicit *LR* algorithm acting on the Neville representation of the matrix, assuming that the algorithm proceeds without incurring in situations requiring the algorithm to stop. However, it is well known [26] that *LR* algorithm occurs in a breakdown if, at step k, the matrix $A^{(k)}$ is no more LU-factorizable. In practical cases, to overcome this situation and resume the iterative process, one can change the value of the shift σ_k and hopefully the problem does not present on the new matrix. When our method is applied however, as observed in Section 4.1, we can have that the process halts also because one of the quantities appearing in the denominator of the recurrences in Section 4.1 or 4.2 annihilates. We will refer to this anomalous situation as a breakdown too.

In this section we first show that the class of Neville representable quasiseparable matrices is closed under shifted *LR* steps, then we analyze stability, structure preservation of the method when applied to

totally nonnegative matrices. Moreover, we show that both breakdown situations do not occur when the algorithm is applied to totally nonnegative matrices.

We first observe that the following Corollary holds.

COROLLARY 11. *Let $A \in \mathcal{S}$, if each LR-step does not occur in breakdown, then each $A^{(k)}$ in* (4.1) *is still in $\mathcal{S}$.* The proof is based on the observation that, if we do not occur in breakdowns, at each step, we can construct a matrix $A^{(k+1)}$ similar to $A^{(k)} - \sigma_{k+1} I$, by means of the updating of the parameters involved in the Neville representation as described in Section 4.1 or 4.2.

The natural class to which the proposed algorithm can be applied is the class of TN matrices.

THEOREM 12. *Each LR-step applied to a TN quasiseparable matrix $A^{(k)}$, with $d_i > 0$, without shift or with a shift which preserves the positivity of the eigenvalues:*

1. *does not occur in breakdowns, and the updated parameters involved in the representation are all nonnegative,*
2. *produces a new matrix which is still quasiseparable TN, with $d_i > 0$,*
3. *does not contain subtractions (except a subtraction for the shift).*

Proof. For a totally nonnegative matrix $A^{(k)}$, from Theorem 7 we know that $x_i, y_i \geq 0$, $a_i, b_i \leq 0$. If we assume $x_i, y_i \neq 0$, we have equivalently $m_i > 0$, $h_i, k_i \leq 0$. The shift σ_{k+1} is such that $0 < \sigma_{k+1} < \mu_n$, where μ_n is the smallest eigenvalue of $A^{(k)}$.

1. We see immediately, by induction on i, that $e_i^{-1} \geq \alpha_i > 0$; as a consequence: $\bar{x}_i, \bar{y}_i \geq 0$, $\beta_i, \gamma_i \geq 1$, $f_i, g_i > 0$, $\bar{\bar{x}}_i, \bar{\bar{y}}_i \geq 0$, $\bar{a}_i, \bar{b}_i \leq 0$. Similarly, if we assume $x_i, y_i \neq 0$ and we refer to the formulation introduced in Section 4.1 and used in Algorithm 1, we find that $p_i \geq 1$ and $\bar{\bar{m}}_i \geq 0$.
   If there is no shift, then $\bar{\bar{d}}_i \geq \delta_i > 0$, $i = 1, \ldots, n-1$, again by induction on i, and, as a consequence, $\bar{\bar{a}}_i, \bar{\bar{b}}_i \leq 0$.
   In the case of shift, we have by hypothesis that at each step σ_{k+1} is such that $0 < \sigma_{k+1} < \mu_n$. We have to show that also in this case $\bar{\bar{d}}_i > 0$. We know that
   $$A^{(k+1)} = L^{(k)} A^{(k)} L^{(k)^{-1}} - \sigma_{k+1} I = \bar{\bar{L}}_S T \bar{\bar{R}}_S,$$
   where $T = F \bar{R}_1 \bar{L}_1 G - \sigma_{k+1} \bar{\bar{L}}_S^{-1} \bar{\bar{R}}_S^{-1}$ is tridiagonal. Now, let T_j be the j-th leading principal minor of T, observe that for each j, $\det(T_j) > 0$, since T_j is similar to $A_j^{(k)} - \sigma_{k+1} I_j$ where $A_j^{(k)}$ is the j-th leading principal minor of $A^{(k)}$. From the interlacing property for TN matrices (Theorem 8) we have that $0 < \mu_n - \sigma_{k+1} \leq \mu_i^{(j)} - \sigma_{k+1}$, where $\mu_i^{(j)}$ is an eigenvalue of $A_j^{(k)}$. This means that $\det(T_j) > 0$, so T is strongly nonsingular, and in its LU factorization $T = \bar{\bar{L}}_1 \bar{\bar{D}} \bar{\bar{R}}_1$ the entries $\bar{\bar{d}}_i$ are all positive. Moreover, $\bar{\bar{a}}_i, \bar{\bar{b}}_i \leq 0$, as shown by (4.13) and (4.14).
   No breakdown happens, because no division by zero can occur in computing the quantities α_i, f_i, g_i, p_i, δ_i.
2. $A^{(k+1)}$ is still TN, because it is Neville-representable, with nonnegative parameters. In particular, all $\bar{\bar{d}}_i$ are positive.
3. It is easy to check that the updating formulas in Section 4.1 and Algorithm 1 described in Section 4.2 do not contain subtractions when applied to TN matrices, with the exception of a subtraction for the computation of δ_{i+1}. In fact, e_i^{-1}, β_i, γ_i are sums of nonnegative quantities, and p_i in the second loop of Algorithm 1 is the product of sums of nonnegative quantities, since $k_i, h_i \leq 0$, and the other factors are positive. Moreover, by induction we can prove that, in case no shift is applied, $\delta_i > 0$ and hence each $\bar{\bar{d}}_i$ is obtained as the sum of two nonnegative quantities, δ_i and $\bar{a}_i \bar{b}_i f_i g_i$, or $k_i h_i m_i / (d_i e_{i+1}^{-1})$ in Algorithm 1.
   In the case of shift, assume by way of contradiction that for a given i, $\delta_i \leq 0$. It is easy to see that, if this is the case, $\delta_j \leq 0$ for all $j > i$, since δ_{i+1} is computed as the sum of two negative quantities, in (4.12) and in the third loop of Algorithm 1 as well. But this is a contradiction since $\bar{\bar{d}}_n = \delta_n > 0$, as already proved. The updating of the invariants does not involve subtractions since $h_i, k_i \leq 0$ and $\sigma_{k+1} > 0$.

□

The approximation of distinct eigenvalues in increasing order is a well known property of *LR* convergence in the real positive case, if the shift strategy preserves the ordering, as for Laguerre shift. More in

detail, for nonsingular quasiseparable TN matrices the Laguerre shift σ_{k+1} is such that $0 < \sigma_{k+1} \leq \mu_n$, thus the shift is generally multiplied by a factor slightly less than one, also to prevent the effect of rounding errors which could destroy the TN structure.

As a consequence of the shift strategy the eigenvalues are computed in increasing order, so the deflation criterion is based only on the magnitude of the off-diagonal entries in the last row and column of $A^{(k)}$.

The cost of Algorithm 1 is of $17n$ flops without shift and of $27n$ in the case a shift strategy is applied. The cost doubles if one works without invariants, and decreases, if one deals, for example, with tridiagonal matrices, because the parameters x_i and y_i are not neeeded.

6. Reduction to tridiagonal form. The Neville representation of quasiseparable matrices makes it easy to describe also an $O(n^2)$ algorithm for the reduction into tridiagonal form of a matrix in $\mathcal{S}$. A tridiagonalization procedure for TN matrices with the generalized quasiseparable structure has been described by Gemignani in [14] and inspires to the algorithm of Koev designed for a generic TN matrix [15]. However,

Algorithm 2 Tridiagonalization procedure

$\hat{x} \leftarrow x$; $\hat{y} \leftarrow y$, $\hat{a} \leftarrow a$; $\hat{b} \leftarrow b$; $\hat{d} \leftarrow d$;
for $j = 1$ to n-1 **do**
  for $i = n-1$ to j **do**
    $[\hat{x}, \hat{y}, \hat{a}, \hat{b}, \hat{d}] \leftarrow \texttt{swap}(\hat{x}, \hat{y}, \hat{a}, \hat{b}, \hat{d}, i)$; {Annihilates row i}
    $[\hat{x}, \hat{y}, \hat{a}, \hat{b}, \hat{d}] \leftarrow \texttt{swap}(\hat{y}, \hat{x}, \hat{b}, \hat{a}, \hat{d}, i)$; {Annihilates column i}
  end for
end for

Algorithm 3 $[\hat{x}, \hat{y}, \hat{a}, \hat{b}, \hat{d}] \leftarrow \texttt{swap}(x, y, a, b, d, i)$

Require: $i <= n-1$
$\alpha \leftarrow x(i)$ {The Gauss transformation acting on rows i and $i+1$ is $E = \begin{bmatrix} 1 & 0 \\ \alpha & 1 \end{bmatrix}$}
$\hat{x} \leftarrow x$, $\hat{y} \leftarrow y$, $\hat{a} \leftarrow a$, $\hat{b} \leftarrow b$, $\hat{d} \leftarrow d$; {Parameter initialization}
$\hat{x}(i) \leftarrow 0$;
$w \leftarrow 1 + \alpha y(i)$; {The new Gauss transformation acting on the left of R_s is $E^{(1)} = \begin{bmatrix} w & 0 \\ \alpha & 1/w \end{bmatrix}$}
$\hat{y}(i-1) \leftarrow w y(i-1)$, $\hat{y}(i) \leftarrow y(i)/w$;
$k \leftarrow w - \alpha b(i)$ {The new Gauss transformation acting on the left of R_1 is $E^{(2)} = \begin{bmatrix} k & 0 \\ \alpha & 1/k \end{bmatrix}$}
$\hat{b}(i-1) \leftarrow w b(i-1)$; $\hat{b}(i) \leftarrow k b(i)/w$;
if $i \neq n-1$ **then**
  $\hat{b}(i+1) \leftarrow k b(i+1)$
end if
$\hat{d}(i) \leftarrow k d(i)$; $\hat{d}(i+1) \leftarrow d(i+1)/k$;
$\hat{a}(i) \leftarrow a(i) - (\alpha d(i+1)/d(i))$;
if $i \neq n-1$ **then**
  $\delta \leftarrow (\alpha d(i+1)/d(i)) a(i+1)/a(i)$, {The Gauss transformation acting on rows $i+1, i+2$ on the left of L_1 is
$$E^{(3)} = \begin{bmatrix} 1 & 0 \\ \delta & 1 \end{bmatrix}\}$$
  $\hat{a}(i+1) \leftarrow a(i+1) + \delta$;
end if
if $i \neq n-1$ **then**
  $\hat{x}(i+1) \leftarrow \delta - x(i+1)$
end if

it is possible to see that the algorithm can be extended also to matrix not TN but belonging to the class $\mathcal{S}$.

TABLE 7.1
Results for totally nonnegative random matrices.

n	niter	$E^{(abs)}$	$E^{(rel)}$	$E^{(rel2)}$	QS-qd(sec)
10	37	3.3526e-15	4.8898e-16	1.4517e-14	0.38
50	239	5.6901e-14	3.5140e-15	1.0133e-14	0.56
100	488	1.3217e-13	6.0148e-15	1.5512e-13	1.65
200	993	2.2589e-13	7.3909e-15	1.5067e-13	4.62
300	1546	3.1303e-13	8.7152e-15	1.5241e-13	10.61
400	2080	3.0187e-13	7.6370e-15	6.3569e-13	19.29
500	2576	3.8896e-13	8.6375e-15	2.9228e-13	33.69
700	3812	6.1653e-13	1.1881e-14	3.2559e-12	68.83
1000	5689	9.5412e-13	1.4728e-14	8.9376e-13	135.19

In the case the tridiagonalization process is applied to TN matrices the stability of the process is guaranteed since it is subtraction free, and no breakdown can occur since there are no divisions by zero. Let us describe the process of tridiagonalization of a matrix $A \in \mathcal{S}$ using the representation in terms of parameters x_i, y_i, a_i, b_i, d_i. The algorithm can be described as follows.

To understand the tridiagonalization procedure, note that each time we apply the `swap` procedure with parameter i, we annihilate the entry x_i or y_i appearing in the representation of the quasiseparable matrix. We need to annihilate each x_i several time, since the swap procedure creates a bulge that has to be removed with more Gauss transformations. In particular, we have to apply `swap` on row i for each column, then we have a total of $n(n-1)$ calls to `swap`. The `swap` function, with parameter i, acts on rows i, $i+1$ and annihilates x_i, multiplying by a Gauss elementary matrix G_i on the right and by its inverse on the left. We have, $G_i^{-1} A G_i = G_i^{-1} L_s L_1 D R_1 R_s G_i$, where $G_i = I_{i-1} \oplus E \oplus I_{n-i-1}$, and $E = \begin{bmatrix} 1 & 0 \\ x(i) & 1 \end{bmatrix}$. Reasoning similarly to what done for deriving the recurrences in Section 4.1, the Gauss transformation G_i acting on the right is moved inside as follows:

$$\begin{aligned} G_i^{-1} A G_i &= G_i^{-1} L_s L_1 D R_1 (R_s G_i) = L_s^{(1)} L_1 D R_1 G_i^{(1)} \hat{R}_s \\ &= L_s^{(1)} L_1 D (R_1 G_i^{(1)}) \hat{R}_s = L_s^{(1)} L_1 D G_i^{(2)} \hat{R}_1 \hat{R}_s \\ &= L_s^{(1)} G_{i+1}^{(3)} \hat{L}_1 \hat{D} \hat{R}_1 \hat{R}_s = \hat{L}_s \hat{L}_1 \hat{D} \hat{R}_1 \hat{R}_s. \end{aligned}$$

In particular, with the same notation of the pseudocode in Algorithm 3, we have $G_i^{(1)} = I_{i-1} \oplus E^{(1)} \oplus I_{n-i-1}$, with $E^{(1)} = \begin{bmatrix} w & 0 \\ x(i) & 1/w \end{bmatrix}$, $G_i^{(2)} = I_{i-1} \oplus E^{(2)} \oplus I_{n-i-1}$, with $E^{(2)} = \begin{bmatrix} k & 0 \\ x(i) & 1/k \end{bmatrix}$, and finally $G_{i+1}^{(3)} = I_i \oplus E^{(3)} \oplus I_{n-i-2}$, with $E^{(3)} = \begin{bmatrix} 1 & 0 \\ \delta & 1 \end{bmatrix}$. Since $G_i^{(1)} L_s$ has the only effect of annihilating the i-th row, when we multiply on the right by $G_{i+1}^{(3)}$, this will only update the entry $i+1$ of the vector describing $L_s^{(1)}$.

The swap procedure costs 19 flops, hence the cost of the tridiagonalization procedure is $19n^2$. Once the tridiagonal matrix is available, one can apply one of the well known techniques for tridiagonal matrices. For example, since we already have the LU factorization, we can proceed applying our method described in Section 4.1 pruned of the unnecessary recurrences related to the updating of the parameters x_i and y_i, that now are zero. Similarly one can apply the dqds algorithm [17]. Another possible way is to symmetrize the tridiagonal matrix first, then apply the QR or the LL^H method. The cost of dqds algorithm is about 6n flops plus the cost of the shift, that is $31n$ if Laguerre shift is applied using a simplified version of the formulas proposed in Section 4.3.

7. Numerical experiments. In this section we report some numerical results obtained using our methods for the computation of all eigenvalues of a possible unsymmetric quasiseparable matrix. The experiments where done using MATLAB 2006b on a Mac Powerbook, running OS X.5.

We denote by $\lambda = [\lambda_1, \lambda_2, \ldots, \lambda_n]$ the vector containing the exact eigenvalues and by $\tilde{\lambda} = [\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_n]$ the vector of the computed ones, sorted in such a way $\tilde{\lambda}_i$ is an approximation of λ_i. The error criteria for

TABLE 7.2
$A = (ones(n) + diag(0:n-1))^{-1}$. A is an arrowhead symmetric matrix

n	niter	$E^{(abs)}$	$E^{(rel)}$	$E^{(rel2)}$	QS−qd(sec)
10	39	7.6328e-16	1.7383e-16	1.0623e-15	0.18
50	222	3.8659e-15	6.5444e-16	4.1704e-14	0.34
100	444	1.0880e-14	1.6580e-15	3.5737e-14	1.28
200	883	1.3769e-14	1.9065e-15	6.8910e-14	4.32
300	1314	1.1747e-14	1.5437e-15	3.0430e-13	9.56
500	2162	1.3649e-14	1.6849e-15	2.0812e-13	27.06

TABLE 7.3
Random sspd matrix. Comparison with QS−qd *and* EIGSSD

n	$E^{(abs)}$	$E^{(rel)}$	QS−qd(sec)	$E^{(abs)}$	$E^{(rel)}$	EIGSSD(sec)
10	2.7732e-15	1.0333e-15	0.08	1.0151e-14	3.7824e-15	0.14
50	4.6343e-13	7.5474e-14	0.39	7.4737e-14	1.2172e-14	0.94
100	2.7996e-13	3.1850e-14	1.36	2.7323e-13	3.1085e-14	3.29
200	3.0727e-12	2.3750e-13	5.25	1.0149e-12	7.8444e-14	12.59
300	2.4134e-12	1.4828e-13	14.80	8.9760e-12	5.5147e-13	32.64
500	6.9054e-12	3.5405e-13	35.29	2.6940e-12	1.3812e-13	78.63

measuring accuracys are as follows:

$$E^{(abs)} = \|\lambda - \tilde{\lambda}\|_\infty = \max_i \left\{ |\lambda_i - \tilde{\lambda}_i| \right\}, \qquad E^{(rel)} = \max_i \left\{ \frac{|\lambda_i - \tilde{\lambda}_i|}{|\lambda_i|} \right\}.$$

We also use the infinity norm relative criterion defined as

$$E^{(rel2)} = \frac{\|\lambda - \tilde{\lambda}\|_\infty}{\|\lambda\|_\infty}.$$

Note that $E^{(rel)} <$ tol guarantees that all eigenvalues have been computed with a relative error lower than the tolerance tol, while this is not true when $E^{(rel2)}$ is considered. In our experiments we compared the eigenvalues computed with our method (denoted as QS−qd for quasiseparable-qd) with MATLAB eig, and we used a cutting criterion of 10^{-16} as deflation tolerance. We know that, for rank structured matrices, it is often more convenient to compute the eigenvalues applying directly an iterative method without the preliminary reduction to tridiagonal or Hessenberg form [23]. In fact, the possibility of representing the matrices with a low number of parameters, and the closure under *GR*-type [25] steps, makes it convenient to apply directly an implicit method acting on the representation of the rank structured matrix. The overhead of the computation of the tridiagonal structure is, in fact, not rewarded by the efficiency of the tridiagonal eigensolver. The purpose of our experimentation is to show that good accuracy and efficiency can be obtained applying QS−qd directly on the representation of a quasiseparable matrix.

For symmetric semiseparable plus diagonal matrices (both TN or not) we compared the results obtained with our solver both in terms of accuracy and CPU time with the results obtained by using the *QR* solver implemented by the routine EIGSSD by the group at K.U. Leuven which is available online. On TN quasiseparable matrices, a comparison with the method (denoted by TridLR) described in Section 6, that first reduces the matrix in tridiagonal form, and then applies the method dqds [17] for tridiagonal matrices, are reported. We run tests also on arrowhead matrices, and on unsymmetric TN matrices. Table 7.1 reports the results obtained by our method on instances of random generated totally nonnegative matrices of different sizes. The time in seconds of our implementation is reported as well. We see that the absolute and relative errors are quite good, and the increase of time respect to the size shows, as expected, a quadratic behavior. To show the effectiveness of QS−qd also for matrices that are not totally nonnegative, we report some results in Tables 7.2 and 7.3. In particular in Table 7.2 are reported the results obtained

TABLE 7.4
Comparison for totally nonnegative sspd matrices between `QS-qd` *and* `EIGSSD`

n	$E^{(abs)}$	$E^{(rel)}$	`QS-qd`(sec)	$E^{(abs)}$	$E^{(rel)}$	`EIGSSD`(sec)
10	1.8438e-14	1.8196e-15	0.10	2.4170e-14	2.3852e-15	0.17
50	7.5067e-14	4.2194e-15	1.98	1.4532e-13	1.2172e-14	4.39
100	6.4859e-14	3.0592e-15	6.40	2.0281e-12	9.5658e-14	16.66
200	3.5978e-13	9.3222e-15	10.05	1.5309e-12	3.9668e-14	31.09
300	4.4886e-13	8.2383e-15	10.71	1.2081e-12	2.2174e-14	22.60
400	4.6996e-13	8.9675e-15	21.38	1.6238e-12	3.0985e-14	48.55
500	6.4709e-13	1.0402e-14	39.42	6.0125e-10	9.6647e-12	76.97

TABLE 7.5
For totally nonegative matrices, comarispon between the two approaches proposed in this paper. The `TriLR` *first applies the tridiagonalization procedure of Section 6 and the steps of* `dqds` *algorithm.*

n	$E^{(abs)}$	$E^{(rel)}$	`TriLR`(sec)	$E^{(abs)}$	$E^{(rel)}$	`QS-qd`(sec)
10	3.3562e-15	7.2967e-16	0.17	6.2538e-15	1.3596e-15	0.10
50	3.7408e-14	3.1866e-15	0.78	3.6114e-14	3.0764e-15	0.38
100	9.8449e-14	4.4702e-15	2.26	1.1809e-13	5.3618e-15	1.35
200	2.1553e-13	7.0867e-15	8.74	2.5090e-13	8.2494e-15	4.69
400	2.4226e-13	6.3467e-15	39.96	3.1101e-13	8.1479e-15	21.79
600	3.3020e-13	6.5145e-15	80.22	4.8100e-13	9.4897e-15	49.92
800	3.9049e-13	7.1229e-15	149.61	7.0710e-13	1.2898e-14	91.31
1000	4.9826e-13	7.8901e-15	263.43	1.0501e-12	1.6629e-14	136.11

on a particular arrowhead matrix, with well distributed eigenvalues. The algorithm, in this case is fast and accurate. The behavior of our method on random symmetric semiseparable plus diagonal matrices is reported in Table 7.3. We compare of our method with the `EIGSSD` routine proposed by the group at K.U. Leuven, which represents the state of the art of the *QR* implementation for symmetric semiseparable plus diagonal matrices. In this case, our algorithm performs a little worst from the point of view of accuracy, but is faster, requiring almost half the time required by the *QR* routine. To make a fair comparison, the time for the conversion from our representation to the Givens-vector representation used by the `EIGSSD` routine is not accounted for.

As we pointed out in Section 5, the stability of `QS-qd` is not guaranteed for a generic symmetric matrix. However, the only potentially dangerous subtraction of Algorithm 1 can occur in the computation of the p_i at early steps of the process, since at convergence m_i goes to zero.

In the case the matrix is totally nonnegative, our algorithm performs better also in terms of accuracy, and we gain a digit over the *QR* implementation as can be observed from the results in Table 7.4.

In Section 6 we described a tridiagonalization procedure for quasiseparable, Neville-representable matrices. The comparison between the flops required by the tridiagonalization procedure followed by standard qd technique for tridiagonals (denoted, as mentioned before, as `TridLR`), and `QS-qd`, seems to suggest that it is more convenient to reduce the matrix into tridiagonal form. However, if one compares the time required by the two algorithms, reported in Table 7.5, we note that the times obtained are not those expected, and the accuracy is comparable. This suggests that, together with flops count, a comparison of the times is also interesting since the interpreter or compiler - depending on the language the code is written in -can optimize the code to get faster execution times.

8. Conclusions. In this paper two approaches for the computation of the eigenvalues of a quasiseparable Neville representable matrix have been proposed. The first one is a qd-type algorithm inspired by the qd methods for tridiagonal matrices, the second idea is to reduce the matrix to tridiagonal form and then apply a method for tridiagonal matrices, for instance the same qd algorithm.

We have presented several theoretical results showing the closeness of the class of Neville representable matrices under *LR* steps. For totally nonnegative matrices we proved also, that the proposed

algorithms are subtraction free, do not occur in breakdown and if a shift preserving positivity is adopted, then each *LR* step produces a new matrix still totally nonnegative.

An extensive numerical testing has been performed showing the effectiveness of this approach.

REFERENCES

[1] T. ANDO, *Totally positive matrices*, Lin. Alg. and its Appl., 90 (1987), pp. 165–219.

[2] M. VAN BAREL, R. VANDEBRIL, AND N. MASTRONARDI, *A note on the representation and definition of semiseparable matrices*, Numerical Linear Algebra with Applications, 12 (2005), pp. 839–858.

[3] T. BELLA, Y. EIDELMAN, I. GOHBERG, AND V. OLSHEVSKY, *Computations with quasiseparable polynomials and matrices*, Theoretical Computer Science, 409 (2008), pp. 158–179.

[4] D. A. BINI, L. GEMIGNANI, AND V. Y. PAN, *QR-like algorithms for generalized semiseparable matrices*, Tech. Report 1470, Department of Mathematics, University of Pisa, 2003.

[5] F. DOPICO, T. BELLA, AND V. OLSHEVSKY, *Fast and accurate computations with some classes of quasiseparable matrices*. SIAM conference on Applied Linear Algebra, Monterey, October 2009.

[6] ———, *Fast and accurate computations with totally nonnegative quasiseparable matrices*. Multidisciplinary International Symposium on Positive Systems: Theory and Applications, September 2009.

[7] Y. EIDELMAN AND I. GOHBERG, *On a new class of structured matrices*, Integr. equ. oper. theory, 34 (1999), pp. 293–324.

[8] ———, *On a new class of structured matrices*, Integral Equations Operator Theory, 34 (1999), pp. 293–324.

[9] Y. EIDELMAN, I. GOHBERG, AND V. OLSHEVSKY, *The qr iteration method for hermitian quasiseparable matrices of an arbitrary order*, Lin. Alg. and its Appl., 404 (2005), pp. 305–324.

[10] K. V. FERNANDO AND B. N. PARLETT, *Accurate singular values abd differential qd algorithms*, Numerische Mathematik, 67 (1994), pp. 191–229.

[11] F. R. GANTMACHER AND M. G. KREIN, *Oszillationsmatrizen, Oskillationskerne und Kleine Schwingungen Mechanischer Systeme*, Akademie-Verlag, Berlin, 1960.

[12] M. GASCA AND J. M. PEÑA, *A matricial description of Neville elimination with applications to total positivity*, Lin. Alg. and its Appl., 202 (1994), pp. 33–53.

[13] ———, *On factorization of totally positive matrices*, in Total Positivity and its Applications, M. Gasca and C. A. Micchelli, eds., Kluwer Acad. Pub, 1996, pp. 109–132.

[14] L. GEMIGNANI, *Neville elimination for rank-structured matrices*, Lin. Alg. and its Appl., 428 (2008), pp. 9078–991.

[15] PLAMEN KOEV, *Accurate eigenvalues and svds of totally nonnegative matrices*, SIAM Journal on Matrix Analysis and Applications, 27 (2005), pp. 1–234.

[16] N. MASTRONARDI AND S. CHANDRASEKARAN ANS S. VAN HUFFEL, *Fast and stable two-way algorithm for diagonal plus semi-separable systems of linear equations*, Numer. Linear Algebra Appl., 8 (2001), pp. Fast and stable two–way algorithm for diagonal plus semi–separable systems of linear equations.

[17] B. N. PARLETT, *The new qd algorithms*, Acta Numerica, 4 (1995), pp. 459–491.

[18] B. PLESTENJAK, M. VAN BAREL, AND E. VAN CAMP, *A cholesky lr algorithm for the positive definite symmetric diagonal-plus-semiseparable eigenproblem*, Linear Algebra and its Applications, 428 (2008), pp. 586 – 599.

[19] P. RÓZSA, R. BEVILACQUA, F. ROMANI, AND P. FAVATI, *On the inverse of block tridiagonal matrices with application to the inverses of band matrices and block band matrices*, Oper. Theory Adv. Appl., 40 (1989), pp. 447–469.

[20] H. RUTISHAUSER, *Solution of eigenvalue problem with the LR-transformation*, Nat. Bur. Standards Appl. Math. Series, 49 (1958), pp. 47–81.

[21] E. E. TYRTYSHNIKOV, *Mosaic ranks for weakly semiseparable matrices*, in Large-Scale Scientific Computations of Engineering and Enviromental Problems II, M. Griebel, S. Margenov, and P. Y. Yalamov, eds., vol. 73 of Notes on numerical fluid mechanics, Vieweg, 2000, pp. 36–41.

[22] R. VANDEBRIL, M. VAN BAREL, AND N. MASTRONARDI, *An implicit qr-algorithm for symmetric semiseprable matrices*, Numer. Linear Algebra Appl., 12 (2005), pp. 625–658.

[23] ———, *Matrix Computations and Semiseparable Matrices, Volume 2: Eigenvalue and Singular Value methods*, Johns Hopkins University Press, Baltimore, Maryland, USA, 2008.

[24] RAF VANDEBRIL, MARC VAN BAREL, AND NICOLA MASTRONARDI, *Matrix Computations and Semiseparable Matrices, Volume I: Linear Systems*, Johns Hopkins University Press, Baltimore, Maryland, USA, 2008.

[25] D. S. WATKINS, *The Matrix Eigenvalue Problem: GR and Krylov Subspace Methods*, SIAM, Philadelphia, Pennsylvania, USA, 2007.

[26] J. H. WILKINSON, *The Algebraic Eigenvalue Problem*, Oxford University Press, London, 1965.