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Existence, Uniqueness and Algorithms for Matrix Unitary Reduction to Semiseparable Form

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Abstract

This paper concerns the study of a unitary transformation from a generic symmetric matrix A into a semiseparable matrix. The problem is studied both theoretically and from an algorithmic point of view. In particular, we first give a proof of the existence of such a transformation and then we discuss the uniqueness of such transformation proving an Implicit-Q Theorem for semiseparable matrices. Finally, we study structural properties of the factors of the QR-decomposition of a semiseparable matrix. These properties allows us to design a method based on the QR iterations applied to a semiseparable matrix for reducing a symmetric matrix to semiseparable form. This method has the same asymptotic cost of the reduction of a symmetric matrix to tridiagonal form. Once the transformation has been accomplished, if one is interested in computing the eigenvalues each further QR iteration can be done in linear time.

Keywords. Eigenvalues, QR iteration, semiseparable matrices, unitary reduction.
AMS subject classification. 65F15, 15A18

1 Introduction

Recently the class of semiseparable matrices has aroused much interest in several authors [9][10][12][6] [15][4]. In fact, matrices of this form appear in many different fields such as in linear system theory [8], in the discretization of differential and integral equations [14] as well as in certain problems of image modelling [7]. Moreover, the inverse of an irreducible tridiagonal matrix is a semiseparable matrix. In view of the relevance of this class of matrices, fast algorithms have been proposed for the solution of linear systems with semiseparable structure [16][4], and for the computation of the eigenvalues [6]. Since the cost of operating with semiseparable matrices is comparable with that of working with tridiagonal ones, it is interesting to see if such class can have the same role of the class of tridiagonal matrices in the computation of the eigenvalues. In fact, the QR algorithm for the computation of the eigenvalues of a symmetric dense matrix is usually preceded by a preprocessing phase where the original matrix is reduced to a similar symmetric tridiagonal one by means of an orthogonal transformation. This reduction allows one to perform each QR step in $O(n)$ flops instead of the $O\left(n^3\right)$ flops required applying directly the method to the original dense matrix. The preprocessing step is however expensive since it takes $4/3n^3 + O\left(n^2\right)$ flops.

Very recently, Van Barel, Vandebril and Mastronardi [2], proposed to transform a generic symmetric matrix in a semiseparable one as a preprocessing phase for the computation of the eigenvalues. They gave an algorithm which has the same cost of the reduction of the matrix to tridiagonal form. Moreover, they show that after the reduction, the dominant eigenvalues are already well approximated. In fact, they proved that the partial execution of their algorithm computes a semiseparable matrix whose eigenvalues are the Ritz-values of the Lanczos process applied to the original matrix. This fact represents a strong motivation for further investigating this type of reduction as an alternative to the classical tridiagonal reduction.

In the first part of the paper we focus on the question of the existence and uniqueness of the reduction to semiseparable form. In particular, we give a proof of the existence of a unitary transformation which reduces a symmetric matrix to a semiseparable matrix or to a block diagonal with semiseparable blocks. Moreover, we prove the essential uniqueness of the unitary matrix (Implicit-Q Theorem), and therefore of the semiseparable matrix, once the first column of the transformation has been chosen. In the second part of the paper, we deal with algorithmic issues and we highlight some structural proprieties of semiseparable matrices which are used to design an algorithm for reducing a symmetric matrix to semiseparable form in $4/3n^3 + O\left(n^2\right)$ flops. The proposed method is an n-step procedure where the current matrix is expressed as the sum of a semiseparable part and of a correction matrix which shrinks progressively until it vanishes. Each step consists in the application of a unitary transformation where the unitary matrix is the Q factor of the QR-decomposition of the semiseparable part of the matrix. As a consequence of the essential uniqueness of the unitary reduction, we note that our method yields the same semiseparable matrix obtained by the method in [2]—provided that the algorithm in [2] is rewritten in terms of columns instead of rows. Actually, a deeper insight of our method reveals that our algorithm is essentially the one proposed in [2]. However, the two methods originate from different points of view. In fact, while the method of Van Barel et al. [2] acts directly on the given matrix by means of orthogonal similarity transformations, our method applies QR steps to the semiseparable part of a suitable additive decomposition of the current matrix. In this respect, our method is motivated by structural properties of semiseparable matrices.

The paper is organized as follows. Section 2 contains definitions and notation as well as some known properties of semiseparable matrices. In Section 3 we present some new results relating singularity and reducibility of semiseparable matrices. In Section 4 we prove the existence of a similarity unitary transformation to reduce a matrix in semiseparable form or in block diagonal form where the blocks are semiseparable and we prove a theorem which clarifies the essential uniqueness of the semiseparable reduction once the first column of the transformation has been specified. In Section 5 we give some rank properties of the Q and R factors of semiseparable matrices. Section 6 is devoted to the description of the algorithm. In particular some theoretical insights on the algorithm are given in Section 6.1, while Section 6.2 presents the actual algorithm for transforming a matrix into semiseparable form. Two algorithm for computing a QR iteration of a semiseparable matrix and their cost are given in Section 6.3, and the complete analysis of the cost of the algorithm is done in Section 6.4. Finally, Section 7 contains some conclusions and highlights some further developments.

2 Definitions, Notation and Properties

A symmetric semiseparable matrix is constructed from the lower triangular part of a rank-one matrix. In particular we have the following definition.

Definition 2.1 A symmetric matrix S is semiseparable if there are two vectors $\mathbf{u}$ and $\mathbf{v}$ such that

$$S = \begin{bmatrix} u_1v_1 & u_2v_1 & \cdots & u_{n-1}v_1 & u_nv_1 \\ u_2v_1 & u_2v_2 & \cdots & u_{n-1}v_2 & u_nv_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ u_{n-1}v_1 & u_{n-1}v_2 & \cdots & u_{n-1}v_{n-1} & u_{n-1}v_n \\ u_nv_1 & u_nv_2 & \cdots & u_nv_{n-1} & u_nv_n \end{bmatrix}.$$

We call the vectors $\mathbf{u}$ and $\mathbf{v}$ the *representatives* of S. $\square$

Note that this definition differs from that given in [2], where semiseparable matrices are defined in terms of rank properties of submatrices. We prefer the definition 2.1 because it allows to work directly with the representatives of S.

The class of semiseparable matrices has important connections with the class of tridiagonal matrices. This duality allows one to state the following well known properties [5][12].

1. The inverse of a nonsingular, irreducible symmetric tridiagonal matrix is a symmetric semiseparable matrix.

2. The inverse of a nonsingular, reducible symmetric tridiagonal matrix is block diagonal with symmetric semiseparable blocks.

3. $\det(S) = u_n v_1 \prod_{i=1}^{n-1}(v_{i+1}u_i - u_{i+1}v_i)$, hence, S is singular iff $u_n = 0$ or $v_1 = 0$ or there exists an index k such that $v_{k+1}u_k - u_{k+1}v_k = 0$. In any case, singular semiseparable matrices have two consecutive rows and columns linearly dependent.

4. Any nonsingular symmetric semiseparable matrix has simple eigenvalues.

For better understanding the results obtained in this paper, it is useful to define what zero-headed and zero-tailed matrices are.

Definition 2.2 A matrix whose first k columns and rows are equal to zero will be denoted as k*-zero-headed* matrix, similarly, a matrix whose last k columns and rows are zero will be named k*-zero-tailed*. □

In the rest of the paper we will use the standard MATLAB colon notation in order to represent submatrices and portions of vectors.

3 Structural Properties of Symmetric Semiseparable Matrices

In this section we present some results which relate singularity and reducibility of semiseparable matrices. In particular, we note that singular semiseparable matrices are also reducible. This relation is interesting since it is not true for tridiagonal matrices.

Lemma 3.1 *Let S be a symmetric semiseparable matrix whose representatives are the vectors $\mathbf{u}$ and $\mathbf{v}$. S is reducible iff one of the following cases is true*

1) S is zero-tailed,

2) S is zero-headed,

3) there exists an index i, such that u_i and v_i are simultaneously zero.

Proof. If S is zero-tailed or zero-headed the matrix is obviously reducible since it is already in its reduced form.

It is well known that a matrix is irreducible iff the associated graph is strongly connected. We first prove that if there is an index i such that both u_i and v_i are equal to zero, the matrix is reducible. Since $\mathbf{u}$ and $\mathbf{v}$ are the representatives of S, $u_i = 0$ and $v_i = 0$, implies that the matrix S has the i-th column and row equal to zero. The associated graph is not strongly connected since there is no way to reach node i.

Assume now that S is reducible but none of the above cases is true. This means that S is not zero-tailed or zero-headed and if $u_i = 0$ then $v_i \neq 0$. However, since S is reducible the associated graph is not strongly connected, for instance, there is no path from node i to node j, where $i \geq j$. This means that $s_{ij} = u_i v_j = 0$. s_{ij} can be equal to zero because u_i, v_j or both u_i and v_j are zero. We show that the three possibilities lead to a contradiction.

Case 1. $u_i = 0$ while $v_j \neq 0$. Since u_i and v_i cannot be both zero, we have $v_i \neq 0$. Since S is not zero-tailed, $u_n \neq 0$, then $s_{nj} = u_n v_j \neq 0$, and $s_{in} = s_{ni} = u_n v_i \neq 0$. This is a contradiction since it means that there is a path from node i to node j, passing trough node n.

Case 2. $u_i = 0$ and $v_j = 0$ while both v_i and u_j are different from zero. Since S is not zero-tailed, we have $u_n \neq 0$, then $s_{ni} = u_n v_i \neq 0$. Moreover, $s_{j1} = u_j v_1 \neq 0$ since S is not zero-headed, and $s_{n1} = u_n v_1 \neq 0$. Then there is a path from i to j passing trough nodes n and 1, which contradicts the hypothesis.

Case 3. $u_i \neq 0$, $v_j = 0$. Since $u_j \neq 0$ and S is not zero-headed, $s_{j1} = u_j v_1 \neq 0$ and $s_{i1} = u_i v_1 \neq 0$. This means there is a path from i to j passing trough node 1, which is a contradiction. □

From previous lemma it turns out that a semiseparable reducible matrix is also singular.

Theorem 3.2 *Let S be a symmetric, nonsingular, semiseparable matrix. Then, S is irreducible.*

Proof. Since S is nonsingular then, for Lemma 3.1, S is also irreducible, since any reducible matrix is singular because it has at least a row and a column equal to zero. □

Note that the contrary is not true that is, there are semiseparable singular matrices which are also irreducible.

4 Existence and Uniqueness

The following Theorem gives us a theoretical proof of the existence of a similarity transformation which maps symmetric matrices into the class of semiseparable matrices.

Theorem 4.1 *For every symmetric matrix A there exists a matrix S and an orthogonal matrix Q such that*

$$A = Q^T S Q,$$

where S is either semiseparable or block diagonal with semiseparable blocks.

Proof. We have two cases. First case: A is nonsingular. Then we know [13], that by means of an orthogonal transformation H we can reduce A^{-1} to a tridiagonal matrix T, that is

$$A^{-1} = H^T T H.$$

If T is irreducible, which means that its sub diagonal entries are nonzero, then, we can set $S = T^{-1}$ and $Q = H$. In the case T is reducible, its inverse is not semiseparable but is block diagonal with semiseparable blocks. Second case: A is singular. Let k be the algebraic multiplicity of the eigenvalue $\lambda = 0$. By means of an orthogonal transformation P, we can transform A in a k-zero-tailed matrix, where the principal leading $(n-k) \times (n-k)$ minor $\tilde{A}$ is nonsingular, that is

$$A = P^T \left[\begin{array}{cc} \tilde{A} & O \\ O & O \end{array} \right] P.$$

Then we can reason as before on the nonsingular matrix $\tilde{A}$, and we have

$$\tilde{A} = \tilde{Q}^T \tilde{S} \tilde{Q}.$$

Setting $Q = \left[\begin{array}{cc} \tilde{Q} & O \\ O & I \end{array} \right] P$, and $S = \left[\begin{array}{cc} \tilde{S} & O \\ O & O \end{array} \right]$ we get $A = Q^T S Q$.

□

From previous theorem, it turns out that a matrix with multiple eigenvalues cannot be transformed in a semiseparable matrix but only in a block diagonal matrix with semiseparable blocks.

As underlined in Section 2 the class of semiseparable matrices is strictly related to the class of tridiagonal matrices. For this reason, it is obvious to try to generalize theoretical as well as computational results to the class of semiseparable matrices. In particular, for the class of tridiagonal matrices it holds a theoretical unicity theorem, namely the Implicit-Q Theorem [13]. This theorem ensures that, up to the signs, we cannot find two different tridiagonal matrices similar to A obtained from two different orthogonal transformation sharing the first column.

Because of the duality between tridiagonal matrices and semiseparable matrices, we started working on proving a similar result for semiseparable symmetric matrices. In fact if a similar result is true also for semiseparable matrices, then we are guaranteed that given a matrix A there exists a unique semiseparable matrix similar to A once the first column of the orthogonal transformation is specified.

For nonsingular semiseparable matrices the analogue of the Implicit-Q Theorem [13] can be proved straightforward by using their inverses which are tridiagonal. In particular we have the following

Theorem 4.2 *Let A be a nonsingular symmetric matrix. Let Q and V be orthogonal matrices such that $Q^T AQ = S_1$ and $V^T AV = S_2$, where S_1 and S_2 are semiseparable and $Q\mathbf{e}_1 = V\mathbf{e}_1$. Then $Q\mathbf{e}_i = d_i V\mathbf{e}_i$, for $i = 1, 2, \ldots, n$, $d_i = \pm 1$, and $S_1 D = DS_2$, where $D = diag(d_1, \ldots, d_n)$.*

Proof. Let $T_1 = S_1^{-1}$ and $T_2 = S_2^{-1}$. Note that T_1 and T_2 are irreducible, otherwise S_1 and S_2 would not be semiseparable (but only block diagonal with semiseparable blocks). So we can directly apply the Implicit-Q theorem to A^{-1} where $Q^T A^{-1} Q = T_1$ and $V^T A^{-1} V = T_2$, and we get the thesis. $\Box$

However, Theorem 4.2 is not true for singular matrices under the same hypothesis. Let us consider the following example.

Example 4.1 Consider the singular matrix

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix},$$

and the two orthogonal matrices Q and V such that $Q = I$ and

$$V = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2^{-1/2} & 2^{-1/2} \\ 0 & 2^{-1/2} & -2^{-1/2} \end{bmatrix}.$$

We have that $Q\mathbf{e}_1 = V\mathbf{e}_1$ but

$$V^T AV = \begin{bmatrix} 2 & 2^{1/2} & 0 \\ 2^{1/2} & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

which is different from $Q^T AQ = A$. So we get two different semiseparable matrices by means of two different orthogonal transformations with the same first column. $\Box$

However, it is possible to prove that two singular semiseparable matrices similar to a given matrix A, coincides up to a certain row and column, for example in the above case, the semiseparable matrices $Q^T AQ$ and $V^T AV$ coincide for the entry $(1, 1)$. In order to prove the main theorem we need some technical lemmas.

Lemma 4.3 *Let S be a singular symmetric semiseparable matrix. Then it is possible to find an orthogonal matrix P and a symmetric zero-tailed semiseparable matrix S_1 such that*

$$S = P^T S_1 P.$$

Moreover, let k be the smallest index such that $\det S(k-1:k, k-1:k) = 0$, *then* $P = \begin{bmatrix} I_{k-2} & 0 \\ 0 & \tilde{P} \end{bmatrix}$.

Proof. Let $\mathbf{u}$ and $\mathbf{v}$ be the representatives of S. If S is already zero-tailed the theorem is true with $P = I_n$. In any other case we have $2 \le k \le n$ and it is easy to show that, by means of a single Givens rotation $G = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$ acting on rows $k-1, k$ by a sutable angle α, it is possible to transform the matrix S to a similar matrix $\hat{S} = GSG^T$ whose representatives $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ are such that

$$\hat{u}_i = \begin{cases} u_i & i \le k-2 \\ cu_{k-1} - su_k & i = k-1 \\ 0 & i = k \\ u_i & i \ge k+1; \end{cases} \qquad \hat{v}_i = \begin{cases} v_i & i \le k-2 \\ cv_{k-1} - sv_k & i = k-1 \\ sv_{k-1} + sv_k & i = k \\ v_i & i \ge k+1; \end{cases} \qquad i = 1, 2, \ldots, n,$$

where $c = \cos\alpha$, and $s = \sin\alpha$.

Consider now the permutation

$$q_i = \begin{cases} i & i \le k-1 \\ i+1 & k+1 \le i \le n-1 \\ k & i = n, \end{cases} \qquad i = 1, 2, \ldots, n,$$

and let Q be the permutation matrix induced by q. We have that the matrix $S_1 = Q\hat{S}Q^T$ is a zero-tailed semiseparable matrix represented by $Q\hat{\mathbf{u}}$ and $Q\hat{\mathbf{v}}$. Then $S_1 = QGSG^TQ^T$, and $P = QG$, where $P(1:k-2, 1:k-2) = I_{k-2}$. $\square$

If $\operatorname{rank}(S) = n-h$, where $h > 1$, we can apply h times the above lemma to the leading principal submatrix. So, we have the following lemma.

Lemma 4.4 *Let S be a singular symmetric semiseparable matrix and let $\operatorname{rank}(S) = n-h$. Then it is possible to find an orthogonal matrix P and a symmetric h-zero-tailed semiseparable matrix S_1 such that*

$$S = P^T S_1 P.$$

Moreover, let k be the smallest index such that $\det S(k-1:k, k-1:k) = 0$, then $P = \begin{bmatrix} I_{k-2} & 0 \\ 0 & \tilde{P} \end{bmatrix}$.

Next lemma shows that there exists a unique h-zero-tailed semiseparable matrix similar to a singular matrix A with rank $n-h$.

Lemma 4.5 *Let A be a symmetric singular matrix, and let $\operatorname{rank}(A) = n-h$. Let Q and V be orthogonal matrices such that $Q^TAQ = S_1$ and $V^TAV = S_2$, where S_1 and S_2 are semiseparable h-zero-tailed matrices and $Q\mathbf{e}_1 = V\mathbf{e}_1$. Then $Q\mathbf{e}_i = d_iV\mathbf{e}_i$, for $i = 1, 2, \ldots, n-h$, $d_i = \pm 1$. Moreover, $\tilde{S}_1 D = D\tilde{S}_2$, where $\tilde{S}_1$ and $\tilde{S}_2$ are the leading $(n-h) \times (n-h)$ principal submatrices of S_1 and S_2 respectively and $D = diag(d_1, \ldots, d_{n-h})$.*

Proof. Since $A = QS_1Q^T$ and $A = VS_2V^T$, we have $WS_1 = S_2W$ where $W = V^TQ$. Moreover, $W\mathbf{e}_1 = \mathbf{e}_1$. Writing in block form the above equation relating S_1 with S_2, we have

$$\begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix} \begin{bmatrix} \tilde{S}_1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} \tilde{S}_2 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix},$$

which means

$$\begin{bmatrix} W_{11}\tilde{S}_1 & 0 \\ W_{21}\tilde{S}_1 & 0 \end{bmatrix} = \begin{bmatrix} \tilde{S}_2 W_{11} & \tilde{S}_2 W_{12} \\ 0 & 0 \end{bmatrix}$$

from which it follows $W_{21} = 0$, $W_{12} = 0$, and

$$W_{11}\tilde{S}_1 = \tilde{S}_2 W_{11}.$$

Since $\tilde{S}_1$ and $\tilde{S}_2$ are nonsingular and $W_{11}\mathbf{e}_1 = \mathbf{e}_1$ the theorem is proved applying Theorem 4.2. $\square$

Once we have proved the above lemmas we are ready for stating the following Theorem.

Theorem 4.6 *Let A be a symmetric singular matrix. Let Q and V be orthogonal matrices such that $U^TAU = G$ and $V^TAV = H$, where G and H are semiseparable matrices and $U\mathbf{e}_1 = V\mathbf{e}_1$. Let $k_G = \min\{i : \det(G(i-1 : i, i-1 : i)) = 0\}$, $k_H = \min\{i : \det(H(i-1 : i, i-1 : i)) = 0\}$ and $k = \min\{k_G, k_H\}$. Then $U\mathbf{e}_i = d_i V\mathbf{e}_i$, for $i = 1, 2, \ldots, k-2$, $d_i = \pm 1$, and $G_k D = DH_k$, where $G_k = G(1 : k-2, 1 : k-2)$, $H_k = H(1 : k-2, 1 : k-2)$ and $D = diag(d_1, \ldots, d_{k-2})$.*

Proof. Since A is singular, G and H are singular as well. Let $\mathrm{rank}(A) = \mathrm{rank}(G) = \mathrm{rank}(H) = n-h$. From Lemma 4.4, for the matrix G there exist an orthogonal matrix P of the form

$$P = \begin{bmatrix} I_{k_G-2} & 0 \\ 0 & \tilde{P} \end{bmatrix}$$

and a semiseparable h-zero-tailed matrix S_1 such that $G = PS_1P^T$. Similarly, for the matrix H we have an orthogonal matrix Q and a semiseparable h-zero-tailed matrix S_2 such that $H = QS_2Q^T$, where

$$Q = \begin{bmatrix} I_{k_H-2} & 0 \\ 0 & \tilde{Q} \end{bmatrix}.$$

From the relation between G, H and A we have

$$WS_1 = S_2W,$$

where $W = QV^TUP^T$. Note that W is orthogonal since it is the product of orthogonal matrices. Moreover, for the block diagonal form of P and Q we have

$$W\mathbf{e}_1 = QV^TUP^T\mathbf{e}_1 = QV^TU\mathbf{e}_1 = Q\mathbf{e}_1 = \mathbf{e}_1.$$

For Lemma 4.5 we then have that the matrices S_1 and S_2 coincides up to the sign and $W(1 : n-h, 1 : n-h) = I_{n-h}$. Since $G = PS_1P^T$, $H = QS_2Q^T$, and $P(1 : k-2, 1 : k-2) = Q(1 : k-2, 1 : k-2) = I_{k-2}$, we have the thesis. $\square$

Summarizing Theorem 4.2 and Theorem 4.6 we get the following general result.

Theorem 4.7 (Implicit-Q Theorem) *Let A be a symmetric matrix. Let Q and V be orthogonal matrices such that $U^T AU = G$ and $V^T AV = H$, where G and H are semiseparable matrices and $U\mathbf{e}_1 = V\mathbf{e}_1$. Let $k_G = \min\{i : \det(G(i-1 : i, i-1 : i)) = 0\}$, $k_H = \min\{i : \det(H(i-1 : i, i-1 : i)) = 0\}$ and $k = \min\{k_G, k_H\}$ with the convention that $k = n+2$ if A is nonsingular. Then $U\mathbf{e}_i = d_i V\mathbf{e}_i$, for $i = 1, 2, \ldots, k-2$, $d_i = \pm 1$, and $G_k D = DH_k$, where $G_k = G(1 : k-2, 1 : k-2)$, $H_k = H(1 : k-2, 1 : k-2)$ and $D = diag(d_1, \ldots, d_{k-2})$.*

The above theorem states the essential uniqueness up to row and column $k-2$. Note that this result is tight in the sense that we cannot obtain a stronger result proving the uniqueness of the semiseparable submatrix of order larger than $k-2$ (see Example 4).

5 General Results on the QR applied to Semiseparable Matrices

In this section we give some theoretical structural properties of the QR-decomposition of semiseparable matrices. These structural consideration are essential for the design of linear time algorithms for the computation of the QR-decomposition of semiseparable matrix and moreover are important also in the construction of our method for reducing a symmetric matrix to semiseparable form.

Theorem 5.1 *Let S be a semiseparable matrix, then its QR-decomposition can be obtained by means of $n-1$ Givens rotations. Moreover, the factor Q obtained in this way is lower Hessenberg.*

Proof. Since S is a symmetric semiseparable matrix, there exist two vectors $\mathbf{u} = (u_i)$ and $\mathbf{v} = (v_i)$ such that

$$S = \begin{bmatrix} u_1 v_1 & u_2 v_1 & \cdots & u_n v_1 \\ u_2 v_1 & u_2 v_2 & \cdots & u_n v_2 \\ \vdots & \vdots & \ddots & \vdots \\ u_n v_1 & u_n v_2 & \cdots & u_n v_n \end{bmatrix}. \tag{1}$$

For $i = n, n-1, \ldots, 2$, let $R^{(n)} = S$ and $R^{(i-1)} = G_i R^{(i)}$, where G_i is the Givens rotation acting on rows $i-1$ and i of $R^{(i)}$ annihilating the entries in positions $(i, 1), (i, 2) \ldots, (i, i-1)$ of $R^{(i)}$.

For $i = n$ the situation is as follows

$$R^{(n-1)} = G_n S^{(n)} = \begin{bmatrix} u_1 v_1 & u_2 v_1 & \cdots & u_{n-1} v_1 & u_n v_1 \\ u_2 v_1 & u_2 v_2 & \cdots & u_{n-1} v_2 & u_n v_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ u'_{n-1} v_1 & u'_{n-1} v_2 & \cdots & u'_{n-1} v_{n-1} & u_n v'_{n-1} \\ 0 & 0 & \cdots & 0 & u_n v'_n \end{bmatrix}.$$

We can repeat the same reasoning on the $(n-1) \times (n-1)$ leading principal submatrix of $R^{(n-1)}$, and for the semiseparable structure of the leading principal submatrices at each step we annihilate the entries in positions $(i,1), (i,2) \ldots, (i, i-1)$ without introducing non-zeros in the rows already set to zero. In particular after step i-th we have that the matrix $R^{(n-i)}$ coincides with S in the first $n-i-1$ rows and is upper triangular in the last $i+1$ rows.

After $n-1$ Givens rotations $R^{(1)} = R$ is an upper triangular matrix and the matrix $Q = G_n^T G_{n-1}^T \cdots G_3^T G_2^T$ is orthogonal because it is the product of orthogonal matrices. Moreover, since each G_i acts only on rows $i-1$ and i, it is easy to prove by induction on the number of Givens rotations that Q is lower Hessenberg. $\square$

Remark 5.2 *It is well known that the QR-decomposition of a matrix is not unique. While for nonsingular matrices the factorizations differs for phase matrices, in the singular case, we can get Q and R factors which do not differ for a phase transformation. In our case, if S is singular, the algorithm modelling the above proof, enforces the factor Q to be lower Hessenberg while other structures are possible.*

In the next Theorem we show that the lower triangular part of the Q factor of a semiseparable matrix is semiseparable as well. The proof is given for a generic lower Hessenberg orthogonal matrix.

Theorem 5.3 *Let Q be an orthogonal, irreducible, lower Hessenberg matrix. Then there exist two vectors $\mathbf{r}$ and $\mathbf{s}$ such that* $\mathrm{tril}\,(Q) = \mathrm{tril}\,(\mathbf{r}\mathbf{s}^{\mathbf{T}})$.

Proof. Note that the assumption that Q is irreducible means that the upper diagonal entries of Q, $q_{i,i+1}$ are not zero. Consider the 2×2 block matrix obtained embedding Q as follows

$$X = \begin{bmatrix} \mathbf{e_1^T} & 0 \\ Q & \mathbf{e}_n \end{bmatrix}.$$

Since Q is lower Hessenberg, the above matrix X is lower triangular and is invertible since its diagonal elements are either 1 or $q_{i,i+1}$ which are different form zero by assumption. We can use an inversion formula [18][17] based on the

Schur complement of X. In particular we get that the block structure of X^{-1} is as follows

$$X^{-1} = \begin{bmatrix} \mathbf{p}_{11} & P_{12} \\ p_{21} & \mathbf{p}_{22}^T \end{bmatrix}$$

where $\mathbf{p}_{11}$ and $\mathbf{p}_{22}$ are n-dimensional vectors, p_{21} is a nonzero scalar and P_{12} is a $n \times n$ strict lower triangular matrix since X^{-1} must be lower triangular. From the structure of the inverse of X and by using the Schur complement formula, it follows that

$$Q^{-1} = Q^T = P_{12} - 1/p_{21}\, \mathbf{p}_{11}\mathbf{p}_{22}^T. \tag{2}$$

But since Q^T must be upper Hessenberg then we have $\mathrm{tril}\,(Q) = \mathrm{tril}\left(\mathbf{r}\mathbf{s}^T\right)$ where we set $\mathbf{r} = \mathbf{p}_{22}$ and $\mathbf{s} = -1/p_{21}\mathbf{p}_{11}$. □

Remark 5.4 *From equation* (2) *it turns out that* $P_{12} = Q^T - \mathbf{s}\mathbf{r}^T$. *Since* Q^T *is upper Hessenberg, and* P_{12} *is strictly lower triangular,*

$$\mathrm{tril}\,(P_{12}, -2) = -\mathrm{tril}\left(\mathbf{s}\mathbf{r}^T, -2\right).$$

The above relation allows one to express the upper diagonal entries of Q *in terms of the representatives of the lower triangular part of* Q.

Theorem 5.3 requires the irreducibility of the matrix Q in order to be applied. Next lemma, gives us a necessary and sufficient condition for this to happen in the case Q is the orthogonal factor of the QR-decomposition of a semiseparable matrix.

Lemma 5.5 *The* Q *factor of the* QR*-decomposition of a symmetric semiseparable matrix* S *is reducible iff* S *is zero-tailed.*

Proof. Assume Q is reducible. Since Q is orthogonal and lower Hessenberg, then Q is block diagonal, that is

$$Q = \begin{bmatrix} Q_1 & O \\ O & Q_2 \end{bmatrix},$$

where Q_1, Q_2 are Hessenberg orthogonal. Moreover, Q_1 can be supposed irreducible, so, by Theorem 5.3, $\mathrm{tril}\,(Q_1) = \mathrm{tril}\left(\mathbf{r}_1\mathbf{s}_1^T\right)$. Rewriting the upper triangular factor R in block form as

$$R = \begin{bmatrix} R_{11} & R_{12} \\ O & R_{22} \end{bmatrix}$$

we get that QR should have the block in position (2,1) equal to zero, which is not possible if S has the semiseparable structure unless S has the form

$$S = \begin{bmatrix} S_{11} & O \\ O & O \end{bmatrix},$$

that is S is zero-tailed.

Vice versa, if S is zero-tailed, a Q and R factors can be

$$Q = \begin{bmatrix} Q_1 & O \\ O & I \end{bmatrix}, \quad R = \begin{bmatrix} R_{11} & O \\ O & O \end{bmatrix}, \tag{3}$$

where $Q_1 R_1 = S_{11}$. $\square$

Note that using the algorithm for obtaining the QR decomposition of a symmetric semiseparable matrix as described in Theorem 5.1 we always obtain either irreducible Q factors or in the form (3) (see Remark 6.5 below).

Theorem 5.6 *The R factor of the QR-decomposition of a symmetric semiseparable matrix S, is the upper triangular part of a rank-2 matrix.*

Proof. Assume first that Q is irreducible, then by Theorems 5.1 and 5.3, Q^T is upper Hessenberg and (from equation (2)) can be expressed as

$$Q^T = P_{12} + \mathbf{s}\mathbf{r}^T, \tag{4}$$

with P_{12} strictly lower triangular. So we have

$$R = P_{12} S + \mathbf{s}\mathbf{t}^T,$$

where $\mathbf{t} = S\mathbf{r}$. Now we observe that $\operatorname{triu}(P_{12}S) = \operatorname{triu}\left(P_{12}\mathbf{v}\mathbf{u}^T\right)$ and we get

$$\operatorname{triu}(R) = \operatorname{triu}\left(\mathbf{z}\mathbf{u}^T + \mathbf{s}\mathbf{t}^T\right),$$

where $\mathbf{z} = P_{12}\mathbf{v}$.

If Q is reducible, as underlined after Lemma 5.5, we know that Q and R should have the structure as in equation (3). Then we can find the vectors $\mathbf{z}_1, \mathbf{u}_1, \mathbf{s}_1$ and $\mathbf{t}_1$ such that

$$\operatorname{triu}(R_{11}) = \operatorname{triu}\left(\mathbf{z}_1\mathbf{u}_1^T + \mathbf{s}_1\mathbf{t}_1^T\right),$$

and we obtain the vectors $\mathbf{z}, \mathbf{u}, \mathbf{s}, \mathbf{t}$ padding the representatives of R_{11} with zeros. $\square$

An important feature of the QR method for eigenvalues computation of semiseparable matrices is the conservation of the semiseparable structure after the RQ step. A proof of this fact for positive definite semiseparable, based on the equivalence between QR and LR methods has been obtained by Fasino [11]. In the following we give an alternative proof which uses only the rank properties of the Q and R factors of the decomposition and holds for any symmetric semiseparable matrix.

Lemma 5.7 *Let $S = QR$ be the QR-decomposition of a symmetric semiseparable matrix. Then, the matrix $S_1 = RQ$ is still symmetric and semiseparable.*

Proof. Since $S_1 = Q^T SQ$, S_1 is symmetric. If Q is irreducible, from (4), we have $S_1 = RQ = R(P_{12}^T + \mathbf{rs}^T)$, taking into account that RP_{12}^T is strictly upper triangular, we get $\mathrm{tril}\,(S_1) = \mathrm{tril}\left(R\mathbf{rs}^T\right)$. Since S_1 is symmetric this proves that is also semiseparable.

Assume now that Q is reducible, then from (3), S is zero-tailed. The matrix $S_1 = RQ$ is

$$S_1 = RQ = \left[\begin{array}{cc} R_{11}Q_1 & O \\ O & O \end{array} \right],$$

which is semiseparable since Q_1 is irreducible. Moreover S_1 is zero-tailed. □

Remark 5.8 *Note that S_1 if the Q factor of S is reducible then is zero-tailed.*

6 Description of the Unitary Reduction

In this section we propose a procedure of reducing A to a similar semiseparable matrix S. Our method consists of an n steps algorithm where at each step we write the current matrix as the sum of a semiseparable and a correction matrix. The correction matrix shrinks at each step until it disappears as we get the semiseparable matrix S. In this way we get a sequence of $n-1$ semiseparable matrices each one "designed" on the first row and the first column of the current matrix, each one approximating better the semiseparable S.

6.1 Decomposition of A

In this section we give the theoretical properties which allow us to construct a method for reducing a symmetric matrix to a semiseparable or to a block diagonal with semiseparable blocks.

Next Theorem shows how we can always decompose a generic matrix as the sum of a semiseparable plus a zero-headed correction matrix.

Theorem 6.1 *Let A be a symmetric matrix. Then, we can decompose A as the sum of a symmetric semiseparable matrix S and a symmetric zero-headed matrix P; that is $A = S + P$.*

Proof. Without loss of generality we assume that at least one entry in the first column of A is nonzero. Otherwise, since A is symmetric we set $S = 0$ and $P = A$ and we get the thesis.

If the first column of A is nonzero, we choose the representatives of S as the vector $\mathbf{u} = A(:,1)$ and a generic vector $\mathbf{v}$ such that $v(1) = 1$. It is easy to show that the matrix $P = A - S$ has the first row and column equal to zero. □

As proved in Theorem 4.1, it is not always possible to reduce a generic A to a semiseparable form but sometimes we obtain only a block diagonal matrix with semiseparable blocks. The following lemma gives us necessary and sufficient conditions for this to happen.

Lemma 6.2 *Let $B = S + C$, Where S is symmetric semiseparable h-zero-tailed ($h \geq 0$), and C is symmetric k-zero-headed where $1 \leq k \leq n-1$. B is not block-diagonal iff $k + h < n$.*

Proof. The matrix C can be represented as

$$C = \begin{bmatrix} O & O \\ O & C_1 \end{bmatrix}, \tag{5}$$

where C_1 is $(n-k) \times (n-k)$. If S is not zero-tailed, the Lemma is true since $h = 0$, while $k < n$.

Assume now that S is h-zero-tailed, that is

$$S = \begin{bmatrix} S_1 & O \\ O & O \end{bmatrix},$$

where $S_1 \in \mathbb{R}^{(n-h)\times(n-h)}$. Then, from (5), the matrix $B = S + C$ is not block-diagonal iff the diagonal blocks of S and C do overlap, which means $k < n - h$. $\square$

The last two results show how we can start our $n-1$ steps procedure to compute a similar semiseparable matrix S and give us a condition for obtaining a matrix which is not semiseparable but only block diagonal with semiseparable blocks. Next theorem is the core of our algorithm which works as follows: we first write A as the sum of a semiseparable matrix plus a correction zero-headed matrix (see Theorem 6.1). Then we apply a QR iteration to the semiseparable matrix. By means of this orthogonal transformation we obtain (see Theorem 6.3) a new semiseparable matrix and a new correction matrix to which we can apply again this procedure. At each step we obtain a semiseparable matrix which is "more and more" similar to A because the correction matrix has at each step a new row and column of zeros.

Theorem 6.3 *Let $A = S + C$, where S is symmetric semiseparable and C is symmetric k-zero-headed. If A is not block-diagonal and $S = QR$ is a QR decomposition of S with Q lower Hessenberg, then the matrix $B = Q^T AQ$ can be expressed as*

$$B = \tilde{S} + \tilde{C},$$

where $\tilde{S}$ is symmetric semiseparable and $\tilde{C}$ is symmetric l-zero-headed, with $l \geq k+1$.

Proof. Since A is not block-diagonal, by Lemma 6.2, we know that if S is $h-$zero-tailed, then $h < n - k$. Moreover, for Lemma (5.5), if $h \neq 0$, the Q and R factors of the QR decomposition of S have the block structure given in equation (3).

Let $B = S_1 + C_1$, where $S_1 = RQ$ and $C_1 = Q^TCQ$. From Lemma 5.7 we know that S_1 is symmetric semiseparable.

We analyze separately the cases, $h = 0$, that is when S is not zero-tailed, and the case $1 \leq h < n-k$. If $h = 0$, for Lemma 5.5, the matrix Q is irreducible, and, from (4)

$$\operatorname{tril}(S_1) = \operatorname{tril}\left(R\mathbf{r}\mathbf{s}^T\right).$$

Moreover, since Q is irreducible, from (4) $Q = P_{12}^T + \mathbf{r}\mathbf{s}^T$, we have also

$$\operatorname{tril}(C_1)(:, 1 : k+1) = \operatorname{tril}\left(Q^TCP_{12}^T + Q^TC\mathbf{r}\mathbf{s}^T\right)(:, 1 : k+1).$$

Note that $\operatorname{tril}\left(Q^TCP_{12}^T\right)(:, 1 : k+1) = O$, as a consequence of the structures of C and P_{12}, so the following equation holds

$$\operatorname{tril}(C_1)(:, 1 : k+1) = \operatorname{tril}\left(Q^TC\mathbf{r}\mathbf{s}^T\right)(:, 1 : k+1). \tag{6}$$

and therefore

$$\operatorname{tril}(B)(:, 1 : k+1) = \operatorname{tril}\left(S_1 + Q^TC\mathbf{r}\mathbf{s}^T\right)(:, 1 : k+1) = \operatorname{tril}\left(\tilde{\mathbf{r}}\mathbf{s}^T\right)(:, 1 : k+1), \tag{7}$$

where $\tilde{\mathbf{r}} = (R + Q^TC)\mathbf{r}$. Let $\tilde{S}$ be the symmetric semiseparable matrix defined by the vectors $\tilde{\mathbf{r}}$ and $\tilde{\mathbf{s}}$, where $\tilde{\mathbf{s}}(1 : k+1) = \mathbf{s}(1 : k+1)$, i.e.

$$\operatorname{tril}\left(\tilde{S}\right) = \operatorname{tril}\left(\tilde{\mathbf{r}}\tilde{\mathbf{s}}^T\right).$$

We can write

$$B = \tilde{S} + \tilde{C},$$

where $\tilde{C} = S_1 - \tilde{S} + C_1$. This matrix is at least $(k+1)$-zero-headed, since

$$\begin{aligned}\operatorname{tril}\left(\tilde{C}\right)(:, 1 : k+1) &= \operatorname{tril}\left(S_1 - \tilde{S}\right)(:, 1 : k+1) + \operatorname{tril}(C_1)(:, 1 : k+1)\\ &= \operatorname{tril}\left((R\mathbf{r} - \tilde{\mathbf{r}})\tilde{\mathbf{s}}^T\right)(:, 1 : k+1) + \operatorname{tril}(C_1)(:, 1 : k+1) = O,\end{aligned}$$

by using the definition of $\tilde{\mathbf{r}}$ and (6).

Let us assume now $1 \leq h < n-k$. From equation (3), since Q is reducible, it turns out that S_1 is $h-$zero-tailed as well. In particular, since Q_1 is irreducible, $Q_1 = \hat{P}_{12} + \hat{\mathbf{r}}\hat{\mathbf{s}}^T$, where the $\hat{\mathbf{r}}$ and $\hat{\mathbf{s}}$ are $n-h$ entries vectors. Setting $\mathbf{r} = [\hat{\mathbf{r}}, \mathbf{0}]^T$ and $\mathbf{s} = [\hat{\mathbf{s}}, \mathbf{0}]^T$, we have

$$\operatorname{tril}(S_1) = \operatorname{tril}\left(R\mathbf{r}\mathbf{s}^T\right).$$

Note that because of the reducibility of Q we have

$$Q(:, 1 : k+1) = \begin{bmatrix} \hat{P}_{12}^T(:, 1 : k+1) + \hat{\mathbf{r}}\hat{\mathbf{s}}^T(1 : k+1) \\ O \end{bmatrix},$$

then,

$$\begin{aligned}\operatorname{tril}(C_1)(:,1:k+1) &= \operatorname{tril}\left(Q^T C Q(:,1:k+1)\right)\\ = \operatorname{tril}\left(Q^T C \begin{bmatrix} \hat{P}_{12}^T(:,1:k+1) \\ O \end{bmatrix}\right) &+ \operatorname{tril}\left(Q^T C \begin{bmatrix} \hat{\mathbf{r}}\hat{\mathbf{s}}^T(:,1:k+1) \\ O \end{bmatrix}\right).\end{aligned}$$

Since C is $k-$zero-headed and $\hat{P}_{12}^T$ is strictly upper triangular,

$$\operatorname{tril}\left(Q^T C \begin{bmatrix} \hat{P}_{12}^T(:,1:k+1) \\ O \end{bmatrix}\right) = O,$$

so we get

$$\operatorname{tril}(C_1)(:,1:k+1) = \operatorname{tril}\left(Q^T C \mathbf{r}\mathbf{s}^T(1:k+1)\right).$$

We have

$$\operatorname{tril}(B)(:,1:k+1) = \operatorname{tril}\left(S_1 + Q^T C \mathbf{r}\mathbf{s}^T(1:k+1)\right) = \operatorname{tril}\left(\tilde{\mathbf{r}}\mathbf{s}^T(:,1:k+1)\right),$$

where $\tilde{\mathbf{r}} = (R + Q^T C)\mathbf{r}$. Proceeding as in the case Q irreducible, we set $\tilde{\mathbf{s}}(1:k+1) = \hat{\mathbf{s}}(1:k+1)$, and

$$\operatorname{tril}\left(\tilde{S}\right) = \operatorname{tril}\left(\tilde{\mathbf{r}}\tilde{\mathbf{s}}^T\right).$$

We have $B = \tilde{S} + \tilde{C}$, where $C = S_1 - \tilde{S} + C_1$. It is straightforward to prove that

$$\operatorname{tril}\left(\tilde{C}\right)(:,1:k+1) = O.$$

□

Remark 6.4 *Theorem 6.3 holds true also under weaker assumptions, namely when the QR-decomposition of S is not completely accomplished; that is, if $S = QR$, where Q has the Hessenberg structure for the first $k+1$ columns and R is triangular only for the first $k+1$ columns. In this case, RQ is no more semiseparable, but the semiseparable structure is maintained in the first $k+1$ rows and columns. This property is sufficient for ensuring the possibility of reiterate the procedure (see the details in the proof of Theorem 6.3).*

6.2 Description of the Algorithm

Theorems 6.1 and 6.3 suggest a possible algorithm for the computation of a symmetric, semiseparable matrix similar to the initial matrix A.

For better understanding, we describe our algorithm in terms of the matrices involved without working with the representatives of the semiseparable matrices appearing during the computation. However, from a computational point of

Figure 1: The Algorithm `reduce` applied to a symmetric matrix A, by means of orthogonal matrices, transforms A into a similar symmetric, semiseparable or block-diagonal with semiseparable blocks matrix S. In the case we find a block diagonal matrix we split the problem applying the procedure to each block, obtaining then a block diagonal matrix with semiseparable blocks.

`S=reduce(A)`

1. Find a symmetric semiseparable matrix S and a zero-headed matrix C such that A=S+C.
2. Let $A_1 = A$, $S_1 = S$, $C_1 = C$.
3. For $k = 1, 2, \ldots, n-1$ do
4.   If A_k is not block diagonal do
5. $[A_{k+1}, S_{k+1}, C_{k+1}]=\texttt{step}(A_k, S_k, C_k)$.
6.   else
7.   let $A_k = \text{blkdiag}(A_1^{(k)}, A_2^{(k)}, \ldots, A_p^{(k)})$
8.   for i=1:p do
9. $S^{(i)} = \texttt{reduce}(A_i^{(k)})$
10. If none of the matrices A_k was block-diagonal, return $S = S_n$, else return the block diagonal matrix whose diagonal blocks are the semiseparable matrices $S^{(i)}$.

Figure 2: The procedure `step` performs a step of the algorithm in Figure 1. Given a matrix A_k decomposed as the sum of a semiseparable matrix S_k and of a k-zero-headed matrix C_k returns a matrix B, similar to A_k and a decomposition of B as the sum of a semiseparable matrix $\tilde{S}$ and of a l-zero-headed matrix $\tilde{C}$, $l \geq k+1$.

$[B, \tilde{S}, \tilde{C}]$= $\texttt{step}(A_k, S_k, C_k)$

1. $[Q, R] = QR(S_k)$.
2. Compute $S_1 = Q^T S Q$
3. Compute $C_1 = Q^T C_k Q$
4. Extract from the first $k+1$ columns of C_1 the semiseparable matrix S_2. Return $\tilde{C} = C_1 - S_2$.
5. Return $\tilde{S} = S_1 + S_2$, and $B = \tilde{S} + \tilde{C}$.

---

view it is essential to work with a different representation of the semiseparable matrix.

Some authors [2][3] pointed out that working with the representative vectors of a semiseparable matrix as defined in Definition 2 does not lead to stable methods. In order to have more stable algorithms they suggest a different representation of the semiseparable matrices involved, which has not these drawbacks. The algorithm that we present in this section in matrix form requires the same number of operations when working with the different representatives.

The algorithm `reduce`, described in detail in Figure 1 and 2, after the initial decomposition of the original matrix A as the sum of a semiseparable matrix S and a correction matrix C, consists in a cycle repeated $n-1$ times, where at each time it is checked if the current matrix is not block-diagonal (testing the condition given in Lemma 6.2). If this is the case, the procedure `step` is called, which executes a QR iteration on the semiseparable matrix and returns a new semiseparable and a new correction matrix with a more row and column equal to zero. Note that the QR-decomposition of the semiseparable must satisfied conditions given in Theorem 6.3, in particular the Q factor must be in Hessenberg form. Details on the computation of such decomposition are given in Section 6.3. The new semiseparable matrix returned is the combination of the semiseparable obtained as the product RQ (see Lemma 5.7) and of the semiseparable that can be extracted from the unitary transformation applied to the correction matrix. In the case the current matrix is block-diagonal the algorithm is applied to each block and in this case we do not get a semiseparable matrix but a block-diagonal where the semiseparable structure appears in the blocks.

As we will see in Section 6.4, the obtained algorithm has the same cost of the reduction of a matrix to tridiagonal form, that is $2n^3 + O\left(n^2\right)$ flops if Givens rotations are used, and $4/3n^3 + O\left(n^2\right)$ flops when using Householder reflections to decompose the semiseparable matrix.

Note that the computation of the QR-decomposition of the semiseparable matrix designed on the first k rows and columns of A, coincides with the application of the orthogonal transformation of Van Barel et al. [2] to the matrix obtained from A after k of their steps. In fact, as it will be shown in next section, the two transformations involve the same matrices.

6.3 Cost Analysis of a QR Step on Semiseparable Matrices

In this section we describe two linear cost algorithms for performing an iteration of the QR method on a semiseparable matrix. Such iterations are used by procedure `step`. Moreover, once we have completed the transformation into semiseparable form, such iterations can be used for approximating the eigenvalues. The existence of a linear cost algorithm for the QR iteration on a semiseparable matrix, appears to be already known [1][11] but, to the best of our knowledge, there is no published paper which addresses this point. We describe explicitly our algorithms also because the analysis of procedure `step` requires the knowledge of the structure of the Q factor in terms of Givens or Householder matrices. In particular, we show that working with the representatives of the semiseparable S, the algorithm based on Givens rotations proposed in Theorem 5.1 has a linear cost, and we give a linear cost method for computing a partial QR decomposition which uses Householder reflections.

The use of Givens rotations is the most natural choice to factor a semiseparable matrix. In fact, a straightforward application of Householder method do not lead to a linear cost algorithm. In the proof of Theorem 5.1 it has been shown the Hessenberg form of the Q factor obtained as the product of $n-1$ Givens matrices $Q = G_n^T G_{n-1}^T \cdots G_2^T$. However, in order to compute the new semiseparable matrix $S_1 = RQ$, the matrix Q is not actually formed, since

$$S_1 = Q^T S Q = G_2 G_3 \cdots G_n S G_n^T \cdots G_3^T G_2^T.$$

We can construct the representatives $\mathbf{u}^{\text{new}}$ and $\mathbf{v}^{\text{new}}$ of the new semiseparable matrix S_1 modifying the representatives of S a component at a time since each Givens matrix acts locally on two rows and two columns. In particular, if

$$G_n = \begin{bmatrix} I & 0 & 0 \\ O & c_1 & -s_1 \\ O & s_1 & c_1 \end{bmatrix},$$

by performing simple calculation, we have

$$G_n S G_n^T = \begin{bmatrix} u_1 v_1 & u_2 v_1 & \cdots & u'_{n-1} v_1 & 0 \\ u_2 v_1 & u_2 v_2 & \cdots & u'_{n-1} v_2 & \vdots \\ \vdots & \vdots & \ddots & \vdots & 0 \\ u'_{n-1} v_1 & u'_{n-1} v_2 & \cdots & u'_{n-1} \tilde{v}_{n-1} & z_n \\ 0 & \cdots & 0 & z_n & c_1 u_n v'_n \end{bmatrix},$$

where $u'_{n-1} = c_1 u_{n-1} - s_1 u_n$, $v'_n = s_1 v_{n-1} + c_1 v_n$, $\tilde{v}_{n-1} = c_1 v_{n-1} - s_1 u_n (c_1 v_{n-1} - s_1 v_n)/u'_{n-1}$ and $z_n = -s_1 u_n v'_n$. Then we can set $u_n^{\text{new}} = c_1 u_n$ and $v_n^{\text{new}} = v'_n$. After the transformation by means of the Givens matrix G_{n-1} defined in terms of s_2 and c_2 and acting on rows and columns $n-2$ and $n-1$, we have the following situation:

$$G_{n-1} G_n S G_n^T G_{n-1}^T = \begin{bmatrix} u_1 v_1 & u_2 v_1 & \cdots & u'_{n-1} v_1 & 0 & 0 \\ u_2 v_1 & u_2 v_2 & \cdots & u'_{n-2} v_2 & 0 & \vdots \\ \vdots & \vdots & \ddots & \vdots & 0 & 0 \\ u'_{n-2} v_1 & u'_{n-2} v_2 & \cdots & u'_{n-2} \tilde{v}_{n-2} & z_{n-1} & -s_2 z_n \\ 0 & \cdots & 0 & z_{n-1} & c_2 u'_{n-1} v'_{n-1} & c_2 z_n \\ 0 & \cdots & 0 & -s_2 z_n & c_2 z_n & u_n^{\text{new}} v_n^{\text{new}} \end{bmatrix}, \quad (8)$$

where $u'_{n-2} = c_2 u_{n-2} - s_2 u'_{n-1}$, $v'_{n-1} = s_2 v_{n-2} + c_2 \tilde{v}_{n-2}$, $\tilde{v}_{n-2} = c_2 v_{n-2} - s_2 u'_{n-1}(c_2 v_{n-2} - s_2 \tilde{v}_{n-1})/u'_{n-2}$ and $z_{n-1} = -s_2 u'_{n-1} v'_{n-1}$. Then we can set $v_{n-1}^{\text{new}} = c_2 z_n / u_n^{\text{new}}$ and $u_{n-1}^{\text{new}} = c_2 u'_{n-1} v'_{n-1} / v_{n-1}^{\text{new}}$. Note that the case in which one of the denominators of the above formulas becomes zero can be treated separately since it corresponds either to the case we do not need any rotation or we execute an exchange of two sequent rows. Since the leading $(n-2) \times (n-2)$ matrix obtained in (8) is still semiseparable, we can repeat inductively the same reasoning on the leading principal matrix of dimension $n-2$ and obtain after i steps the last i entries of the vectors $\mathbf{u}^{\text{new}}$ and $\mathbf{v}^{\text{new}}$. Note that the entries that are zero in the last rows and columns of the matrix in (8), may be non-zero in the final matrix S_1. However, we need to compute explicitly only the entry z_i in position $(i, i-1)$, that is necessary to split the diagonal entry and determine v_{i-1}^{new}. The other entries can be recovered from the semiseparable structure of S_1 once the computation of its representatives has been completed. The cost of the above procedure is given by the solution of the following recurrence:

$$T(n) = T(n-1) + k,$$

where k is a constant accounting for the computation of u'_{n-1}, $\tilde{v}_{n-1}$, z_n, $u_n^{\text{new}} = c u_n$ and $v_n^{\text{new}} = v'_n$. We then have $T(n) = O(n)$.

Remark 6.5 *Assume to apply the above algorithm to a singular semiseparable matrix S. Let k be an index such that the submatrix $S(k : k+1, k : k+1)$ is singular. The semiseparable matrix S_1 obtained applying the above algorithm is such that the singular submatrix is shifted down of one position, in particular $S_1(k+1 : k+2, k+1 : k+2)$ is singular. This means that after $n-k-1$ steps the singular submatrix is positioned in the right-lower corner. A more Givens transformation is sufficient to kill the last row and column.*

This means that if $\operatorname{rank}(S) = n - k$, *after at most n QR iterations of the above method, we obtain a k-zero-tailed semiseparable matrix similar to S.*

Another way of computing the QR decomposition of a matrix is by using Householder reflections instead of Givens matrices. Unfortunately, for the class of semiseparable matrices, the usual column-wise method does not produce a linear cost algorithm because we do not completely exploit the structure of the matrix. However, it is easy to see that it is sufficient to apply a single Householder reflection to decompose a rank-one matrix into its Q and R factors. This observation leads to an $O(n)$ algorithm which combines Householder and Givens matrices and allows one to compute a partial decomposition of a semiseparable matrix, which is sufficient for our purposes (see Remark 6.4). For example, assume we would like to compute the QR partial decomposition of the first h columns of S, we may proceed as follows.

1. Construct the Householder matrix $H = I - \beta \mathbf{w}\mathbf{w}^T$ such that the vector $H\mathbf{s}_{h+1}$ has the last $n-h-1$ entries equal to zero, where $\mathbf{s}_{h+1}$ is the $(h+1)$-th column of the semiseparable matrix S.

2. Compute $\hat{R} = HS$, and note that $\hat{R}(h+2:n, 1:h+1) = 0$. Moreover, $\hat{R}(1:h+1, 1:h+1)$ is semiseparable.

3. Apply h Givens rotations in order to factor QR the matrix $\hat{R}(1:h+1, 1:h+1)$. Let $\hat{R}(1:h+1, 1:h+1) = \tilde{G}_2^T \tilde{G}_3^T \ldots \tilde{G}_{h+1}^T \tilde{R}$.

4. Compute $Q = HG_2^T G_3^T \cdots G_{h+1}^T$ and $R = Q^T S$, where

$$G_i = \begin{bmatrix} \tilde{G}_i & 0 \\ 0 & I \end{bmatrix}. \tag{9}$$

As underlined earlier in this section, we do not want to compute the factor R but we would like to construct the new semiseparable matrix S_1 through its representatives. Moreover, at step h of our method we need only the first $h+1$ columns of S_1 (see Remark 6.4) which can be completed arbitrarily because of the presence of the correction matrix C. This means that we want to compute the vector $\mathbf{u}^{\text{new}}$ and the first $h+1$ entries of $\mathbf{v}^{\text{new}}$. So, we are interested in the cost of the computation of $S_1(:, 1:h+1) = G_2 G_3 \cdots G_{h+1} HSHG_{h+1}^T \cdots G_3^T G_2^T(:, 1:h+1)$. Let $\hat{S} = HSH$. Note that because $H = \begin{bmatrix} I_h & 0 \\ 0 & \tilde{H} \end{bmatrix}$, we have

$$\hat{S} = \begin{bmatrix} I_h & 0 \\ 0 & \tilde{H} \end{bmatrix} \begin{bmatrix} S_{11} & S_{12}^T \\ S_{12} & S_{22} \end{bmatrix} \begin{bmatrix} I_h & 0 \\ 0 & \tilde{H} \end{bmatrix} = \left[\begin{array}{c|c} S_{11} & \mathbf{x} \quad 0 \\ \hline \mathbf{x}^T & \\ 0 & \tilde{H} S_{22} \tilde{H} \end{array}\right].$$

Moreover, the vector $\mathbf{x}$ is such that $x_i = \tilde{u}_{h+1} v_i$, for $i = 1, 2, \ldots, h+1$, where $\tilde{u}_{h+1} = \text{norm}(u(h+1:n))$. Let $\mathbf{y} = [\alpha, \hat{\mathbf{y}}]^T$ be the first column of $\tilde{H} S_{22} \tilde{H}$. For the structure of $\tilde{H}$, we have

$$\mathbf{y} = v_1 \mathbf{u} - \beta w_1 \mathbf{z} - (\beta v_1 \mathbf{w}^T \mathbf{u} - \beta^2 w_1 \mathbf{w}^T \mathbf{z}) \mathbf{w}, \tag{10}$$

where $\mathbf{z} = S_{22} \mathbf{w}$. Then, $\hat{S}$ can be rewritten as

$$\hat{S} = \left[\begin{array}{cc|c} S_{11} & \mathbf{x} & 0 \\ \mathbf{x}^T & \alpha & \hat{\mathbf{y}}^T \\ \hline 0 & \hat{\mathbf{y}} & \tilde{H} S_{22} \tilde{H}(2:n-h, 2:n-h) \end{array}\right],$$

and the leading $(h+1) \times (h+1)$ submatrix $\tilde{S}_{11} = \begin{bmatrix} S_{11} & \mathbf{x} \\ \mathbf{x}^T & \alpha \end{bmatrix}$ is still semiseparable.

From equation (9), it turns out that the matrix $G = G_2 G_3 \cdots G_{h+1}$ is block-diagonal with the following structure

$$G = \begin{bmatrix} \tilde{G} & 0 \\ 0 & I_{n-h-1} \end{bmatrix},$$

hence

$$S_1 = G\hat{S}G^T = \left[\begin{array}{cc} \tilde{G}\tilde{S}_{11}\tilde{G}^T & \mathbf{g}\hat{\mathbf{y}}^T \\ \hat{\mathbf{y}}\mathbf{g}^T & \tilde{H}S_{22}\tilde{H}(2:n-h, 2:n-h) \end{array} \right],$$

where $\mathbf{g}$ is the last column of the matrix $\tilde{G}$. The representatives $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ of $\tilde{G}S_{11}\tilde{G}^T$ can be computed in linear time by using the algorithm which uses the Givens rotations.

Since we are interested only in the first $h+1$ columns of S_1, we have that the vector $\mathbf{u}^{(\text{new})}$ and the first $h+1$ entries of $\mathbf{v}^{(\text{new})}$ can be computed in linear time since $\mathbf{y}$ can be computed in linear time by means of equation (10), and $\mathbf{v}^{(\text{new})}(1:h+1) = \hat{\mathbf{v}}$ and $\mathbf{u}^{(\text{new})} = [\hat{\mathbf{u}}; \gamma\,\hat{\mathbf{y}}]$ where γ is such that $\hat{\mathbf{v}} = \gamma\,\mathbf{g}$.

6.4 Cost Analysis of the Algorithm

In this section we analyze the computational cost of algorithm `reduce` in Figure 1. Let us first analyze the computational cost of the procedure `step`. We have seen in Section 6.3 that the Q factor of S can be obtained as the product of $n-1$ Givens matrices or as the product of an Householder matrix and a suitable number of Givens matrices. In both cases, the cost of the computation in line 1 and 2 is accomplished in linear time.

The analysis of the cost depends on the algorithm used to decompose the semiseparable matrix S. If it is accomplished by means of only Givens rotations, the computation of C_1 in line 3, corresponds to the matrix product

$$C_1 = G_2G_3\cdots G_nCG_n^T\cdots G_3^TG_2^T.$$

The cost depends on the structure of C. Assume for example, that C is h-zero-headed. Since each G_i acts only on rows and columns $i-1$ and i, the computation of

$$\hat{C} = G_{h+2}G_{h+3}\cdots G_nCG_n^T\cdots G_{h+3}^TG_{h+2}^T \tag{11}$$

can be accomplished in $6(n-h)(n-h-1)$ flops. Once we have $\hat{C}$, which is still h-zero-headed, we need only to compute two vectors which represent the first $h+1$ columns of C_1, because the first $h+1$ columns of C_1 present a semiseparable structure (see the proof of Theorem 6.3). This has a linear cost in the size of the matrix and hence, step 3 costs $6(n-h)^2 + O(n)$.

Observe that in the case we compute the partial QR factorization of S in line 1, we have

$$C_1 = G_2G_3\cdots G_{h+1}\hat{C}G_{h+1}^T\cdots G_3^TG_2^T,$$

where $\hat{C} = HCH$, and H is the Householder orthogonal transformation, annihilating the entries from $h+2$ to n of column $h+1$ of the matrix S. The main difference is that, the Givens rotations in equation (11), operating on the rows of S annihilate the last $n-(h+2)$ rows of S, while by using Householder reflections only the submatrix of indices $(h+2:n, 1:h+2)$ it is set to zero.

The cost of the computation of $\hat{C}$ becomes in this case $4(n-h)^2 + O(n)$ flops.

Steps 4. and 5. have a linear cost since every operation can be carried on with the representatives of the semiseparable matrices.

In the first line of procedure `reduce`, we have to extract from A a semiseparable matrix S. This can be accomplished in various ways. A possibility is that of setting the representatives of S to be respectively the first column of A and the first vector of the canonical basis $\mathbf{e}_1$. In this case the matrix C will be 1-zero-headed, and will coincide with A in the other entries, that is $C(2:n, 2:n) = A(2:n, 2:n)$ and $C(1,:) = \mathbf{0}, C(:,1) = \mathbf{0}^T$. Once we have settled the additive decomposition of A, in line 3, we call $n-1$ times the procedure step, every time with a matrix C_k which is k-zero-headed. The total cost of the procedure becomes

$$\sum_{k=1}^{n-1} 6(n-k)^2 + O(n) = 2n^3 + O\left(n^2\right),$$

if Givens rotations are used, while it becomes

$$\sum_{k=1}^{n-2} 4(n-k)^2 + O(n) = \frac{4}{3}n^3 + O\left(n^2\right),$$

when Householder reflections are used.

Note that the lower Hessenberg structure of the factor Q is not guaranteed when using Householder reflections. However, it is easy to show that Theorem 6.3 remains true also under weaker hypotheses. In fact, at step h, if Q is obtained using an Householder matrix, we still need h Givens rotations to compute C_1. Then the matrix Q will have the lower Hessenberg structure for the first $h+1$ columns of Q, and this is sufficient to prove Theorem 6.3.

7 Conclusion and Further Work

This paper addresses the general question of the existence and uniqueness of a unitary reduction of a generic symmetric matrix to semiseparable form. In particular we show that, under suitable assumptions, the reduced form is unique. In the second part of the paper, we propose an algorithm which takes $4/3n^3 + O\left(n^2\right)$ flops for transforming a symmetric matrix into semiseparable form. Our method is a reformulation of the one proposed in [2]. In order to devise the algorithm we deeply investigated the structure of a semiseparable matrix and of the Q and R factors of its QR-decomposition. In particular, the proposed algorithm is strongly related to the rank properties of the Q factor of the semiseparable matrices. For completeness, we sketched an algorithm which performs in linear time a QR iteration on semiseparable matrices and another linear cost method which computes a partial QR-decomposition of semiseparable matrices.

We are currently investigating the possibility of modifying our algorithm in order to obtain a semiseparable plus diagonal matrix. In this way we work with matrices belonging to a wider class, and we have a larger number of degree of freedom which could be spent to devise less expensive methods. In fact, it appears [15] that working with semiseparable plus diagonal matrices takes the same cost of working with semiseparable matrices. This kind of reduction might be also used to introduce a diagonal correction with the objective of a better approximation of the spectrum.

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