Orthogonal similarity transformation of a symmetric matrix into a diagonal-plus-semiseparable one with free choice of the diagonal

Raf Vandebril,
Ellen Van Camp,
Marc Van Barel,
Nicola Mastronardi

Report TW 398, August 2004

Katholieke Universiteit Leuven
Department of Computer Science
Celestijnenlaan 200A – B-3001 Heverlee (Belgium)

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Abstract

In this paper we describe an orthogonal similarity transformation for transforming arbitrary symmetric matrices into a diagonal-plus-semiseparable matrix, where we can freely choose the diagonal. Very recently an algorithm was proposed for transforming arbitrary symmetric matrices into similar semiseparable ones. This reduction is strongly connected to the reduction to tridiagonal form. The class of semiseparable matrices can be considered as a subclass of the diagonal-plus-semiseparable matrices. Therefore we can interpret the proposed algorithm here as an extension of the reduction to semiseparable form.

It will be proved that for special choices of the diagonal, the algorithm has some spectrum revealing properties.

A numerical experiment is performed comparing thereby the accuracy of this reduction algorithm with respect to the accuracy of the traditional reduction to tridiagonal form, and the reduction to semiseparable form. The experiment indicates that all three reduction algorithms are equally accurate. Moreover it is shown in the experiments that asymptotically all the three approaches have the same complexity, i.e. that they have the same factor preceding the n^3 term in the computational complexity. Finally we illustrate that special choices of the diagonal create a specific convergence behavior.

Keywords : Orthogonal similarity transformation, semiseparable plus diagonal matrix, symmetric matrix.
AMS(MOS) Classification : Primary : 15A21, Secondary : 15A18, 65F15.

Orthogonal similarity transformation of a symmetric matrix into a diagonal-plus-semiseparable one with free choice of the diagonal *

Raf Vandebril[†], Ellen Van Camp[‡], Marc Van Barel[§], Nicola Mastronardi[¶]

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Abstract

In this paper we describe an orthogonal similarity transformation for transforming arbitrary symmetric matrices into a diagonal-plus-semiseparable matrix, where we can freely choose the diagonal. Very recently an algorithm was proposed for transforming arbitrary symmetric matrices into similar semiseparable ones. This reduction is strongly connected to the reduction to tridiagonal form. The class of semiseparable matrices can be considered as a subclass of the diagonal-plus-semiseparable matrices. Therefore we can interpret the proposed algorithm here as an extension of the reduction to semiseparable form.

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1 Introduction

Nowadays a lot of attention is paid to the class of semiseparable and diagonal-plus-semiseparable matrices. Especially the class of diagonal-plus-semiseparable matrices is very interesting as it covers also the class of semiseparable matrices, and it arises in different fields e.g. statistics [16, 11], the field of orthogonal rational functions [17], vibrational systems [9], time-varying systems [4]. Also different algorithms already exist for this class of matrices, ranging from solving equations with a diagonal-plus-semiseparable matrix as coefficient matrix [19], eigenvalue solvers [2, 13], algorithms connected to inverse eigenvalue problems [7], inversion formulas [5, 14] and also theoretical considerations connected to the eigenvalues of subblocks of these matrices exist, for example [6]. The

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[†]Email:raf.vandebril@cs.kuleuven.ac.be

[‡]Email:ellen.vancamp@cs.kuleuven.ac.be

[§]Email:marc.vanbarel@cs.kuleuven.ac.be

[¶]Email:nicola.mastronardi@cs.kuleuven.ac.be

definition and the representation of semiseparable matrices is studied in [21]. Moreover it is interesting to know that there exist reduction algorithms to transform diagonal-plus-semiseparable matrices to tridiagonal form [8, 12], but no algorithm exists in the other direction, i.e. there is no orthogonal reduction algorithm for transforming a symmetric tridiagonal matrix into a similar diagonal-plus-semiseparable one.

It is also well-known how any symmetric matrix can be transformed into a similar tridiagonal one [10, 15]. This orthogonal similarity transformation forms the basic step for various algorithms. For example if one wants to compute the eigenvalues of a symmetric matrix, one can first transform it into a similar tridiagonal one and then compute the eigenvalues of this tridiagonal matrix by means of a QR-algorithm [22, 23] or divide and conquer algorithms [3].

Very recently an algorithm was developed for transforming an arbitrary symmetric matrix, via orthogonal similarity transformations into a similar semiseparable one [18]. This reduction costs $9n^2$ operations more than the reduction to tridiagonal form. This extra cost creates however an extra convergence behavior, namely a subspace iteration step which is performed in each step of the reduction process on the already semiseparable part of the matrix. This reduction to semiseparable form, can be used, similarly like in the tridiagonal case as a basic step for calculating for example the eigenvalues. There exist QR-algorithms [1, 20] as well as divide-and-conquer algorithms [2, 13] to compute the eigendecomposition of symmetric semiseparable matrices.

In this paper we present an extension of the algorithm presented in [18]. The class of semiseparable matrices can be considered as a subclass of the class of diagonal-plus-semiseparable matrices, namely these matrices having as diagonal zero. The algorithm presented reduces via orthogonal similarity transformations symmetric matrices into similar diagonal-plus-semiseparable ones, with a free choice of the diagonal. Moreover, also QR-algorithms exist for diagonal-plus-semiseparable matrices [1] as well as divide and conquer algorithms [13]. This algorithm solves a gap in the orthogonal transformations that exists for transforming symmetric, tridiagonal, semiseparable and diagonal-plus-semiseparable matrices into each other.

The computational complexity of this reduction algorithm differs only with a term $n(n-1)$ of the reduction to semiseparable form. Moreover it will be shown that for special choices of the diagonal, if one for example has already information about the spectrum, convergence behavior occurs, thereby revealing properties of the spectrum of the matrix.

The paper is organized as follows. Section 2 describes the most important part of the paper, namely the reduction to diagonal-plus-semiseparable form, with a free choice of the diagonal. The third section describes a little change in this algorithm, such that another orthogonal similarity transformation is performed and the outcome is again a diagonal-plus-semiseparable matrix, with the same diagonal as in section 2 but a different semiseparable part. Section 4 describes briefly the convergence behavior of the reduction algorithm connected with special choices of the diagonal. Examples show that if eigenvalues appear in the top left part of the diagonal matrix, the reduction algorithm will reveal them in the resulting diagonal-plus-semiseparable matrix. In Section 5 numerical experiments are performed comparing three reduction algorithms w.r.t. accuracy and complexity.

2 The algorithm

In this section, we will prove the following theorem by constructing an algorithm which fulfills the demands of the theorem.

Theorem 1 *Let A be an $n \times n$ arbitrary symmetric matrix and $d = [d_1, d_2, \ldots, d_n]$ an arbitrary n-dimensional vector. Then there exists an orthogonal similarity transformation which transforms the symmetric matrix A into a diagonal-plus-semiseparable matrix $D + S$ with $D = \mathrm{diag}(\mathrm{d})$:*

$$Q^T A Q = D + S.$$

2.1 Notation

Before starting to construct an algorithm that transforms an arbitrary symmetric matrix into a diagonal-plus-semiseparable one, we introduce some definitions and notation.

Definition 1 *When any submatrix of the upper-, or the lower-, triangular part of a symmetric matrix S has rank at most one, this matrix is called a* semiseparable matrix.

This kind of structure can be embedded in a lager one, more precisely:

Definition 2 *A matrix has* semiseparable structure of dimension m*, when the $m \times m$ lower-right block is a semiseparable matrix. The rank of every matrix one can take out of the last m columns up to and including the main diagonal must be at most one and, by symmetry, every matrix one can take out of the last m rows up to and including the main diagonal has rank at most one as well. The elements belonging to this semiseparable structure are denoted by $\boxtimes$:*

$$
\begin{array}{cc}
 & \begin{array}{ccccc|ccccc} & & & & & \multicolumn{5}{c}{\overbrace{\hphantom{\boxtimes\quad\boxtimes\quad\cdots\quad\boxtimes\quad\boxtimes}}^{m}} \end{array} \\
\begin{array}{r} \\ \\ \\ \\ \\ m\left\{\begin{array}{c} \\ \\ \\ \\ \\ \end{array}\right. \end{array} &
\left(\begin{array}{ccccc|ccccc}
 & & & & & \boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes \\
 & & & & & \boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes \\
 & & A_m & & & \vdots & \vdots & & \vdots & \vdots \\
 & & & & & \boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes \\
 & & & & & \boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes \\ \hline
\boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes \\
\vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
\boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes
\end{array}\right).
\end{array}
$$

With $S_0^{(m)}$ we denote a matrix with semiseparable structure of dimension m. $\times$ denotes an arbitrary element of a matrix, $\otimes$ an element which we will annihilate, $+$ a changed element and elements denoted with a $\square$ around it, belong to the semiseparable structure.

A Givens transformation working on the ith and $(i+1)$th row of a matrix, in order to annihilate an element on the ith row, is denoted by $\hat{G}_i^T$:

$$\hat{G}_i^T \begin{bmatrix} \times \\ \times \end{bmatrix} = \begin{bmatrix} 0 \\ \times \end{bmatrix}.$$

When $\hat{G}_i^T$ is embedded in the identity matrix, we use the notation G_i^T.

The algorithm proposed in this section will add at each step one row and column to the semiseparable structure of a matrix $S_0^{(k)}$ which will become the semiseparable part S of the requested diagonal-plus-semiseparable matrix and will add at each step one diagonal element to a matrix $D_0^{(k)}$ which will become the requested diagonal part D.

During each step, we will construct two sequences of matrices $S_{i-1}^{(k)}$ and $D_{i-1}^{(k)}$ for $i = 1, \ldots, n$. The matrix $S_0^{(k)}$ we start with, is one with semiseparable structure of dimension k. Next the aim is to annihilate the elements of each row which belong to the semiseparable structure, starting from the first down to the last row by means of Givens transformations $G_i^{(k)^T}$. When applying the transpose of these Givens transformations a new semiseparable structure is built but of dimension $k+1$.

For the sequence of diagonal matrices $D_{i-1}^{(k)}$, we want it to change into the same diagonal as the matrix $D_0^{(k)}$, we started that step with, but with the elements shifted one place up to the left-upper corner and with d_{k+1} added as last diagonal element.

In order to achieve this form of diagonal matrix, during the whole algorithm we will switch between $S_{i-1}^{(k)} + D_{i-1}^{(k)}$ and $\hat{S}_{i-1}^{(k)} + \hat{D}_{i-1}^{(k)}$ which are, as a sum, equal to each other. The reason for this is that we want the diagonal part to remain unchanged under the application of a Givens transformation $G_i^{(k)^T}$ and its transpose $G_i^{(k)}$. Therefore, the ith and $(i+1)$th diagonal elements of the diagonal part must be equal. This will be achieved by changing the ith element of $D_{i-1}^{(k)}$ and this adapted diagonal matrix is denoted by $\hat{D}_{i-1}^{(k)}$. Now, also the (i,i)th element of $S_{i-1}^{(k)}$ must be changed in order the keep the same matrix and this adapted part is denoted by $\hat{S}_{i-1}^{(k)}$. Hence,

$$G_i^{(k)^T}(S_{i-1}^{(k)} + D_{i-1}^{(k)})G_i^{(k)} = G_i^{(k)^T}(\hat{S}_{i-1}^{(k)} + \hat{D}_{i-1}^{(k)})G_i^{(k)} = S_i^{(k)} + D_i^{(k)}$$

with $D_i^{(k)} = \hat{D}_{i-1}^{(k)}$.

Also important to note is that the elements belonging to the rank one structure of $\hat{S}_i^{(k)}$ will be the same as the ones belonging to the rank one structure in $S_i^{(k)}$.

2.2 The first step

Starting with the arbitrary symmetric matrix A, the last row and column of course form a semiseparable structure of dimension one. Even when subtracting the element d_1 of the element $A(n,n)$, the semiseparable structure remains. Hence, we can write A as the sum of a matrix $S_0^{(1)}$ with semiseparable structure of dimension one and a diagonal matrix $D_0^{(1)}$:

$$A = S_0^{(1)} + D_0^{(1)} := \left(\begin{array}{ccc|c} \times & \dots & \times & \boxtimes \\ \vdots & & \vdots & \vdots \\ \times & \dots & \times & \boxtimes \\ \hline \boxtimes & \dots & \boxtimes & \boxplus \end{array}\right) + \left(\begin{array}{ccc|c} 0 & \dots & 0 & 0 \\ \vdots & & \vdots & \vdots \\ 0 & \dots & 0 & 0 \\ \hline 0 & \dots & 0 & d_1 \end{array}\right)$$

with $\boxplus = A(n,n) - d_1$.

First all the elements of the last column of A (or of $S_0^{(1)}$) are annihilated up to row $n-2$ by means of the product of $n-2$ Givens transformations $G_{1:n-2}^{(1)^T} := G_{n-2}^{(1)^T} \dots G_2^{(1)^T} G_1^{(1)^T}$ and the application of $G_{1:n-2}^{(1)}$ on the columns will zero out the last row of $S_0^{(1)}$ up to the last but two elements:

$$S_{n-2}^{(1)} + D_{n-2}^{(1)} := G_{1:n-2}^{(1)^T}(S_0^{(1)} + D_0^{(1)})G_{1:n-2}^{(1)}$$

$$= \left(\begin{array}{cccc|c} \times & \dots & \times & \times & 0 \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \times & 0 \\ \times & \dots & \times & \times & \boxtimes \\ \hline 0 & \dots & 0 & \boxtimes & \boxplus \end{array}\right) + \left(\begin{array}{ccc|c} 0 & \dots & 0 & 0 \\ \vdots & & \vdots & \vdots \\ 0 & \dots & 0 & 0 \\ 0 & \dots & 0 & 0 \\ \hline 0 & \dots & 0 & d_1 \end{array}\right).$$

The former transformations $G_{1:n-2}^{(1)}$ and $G_{1:n-2}^{(1)^T}$ did not change the matrix $D_0^{(1)}$.

When the next Givens transformation $G_{n-1}^{(1)^T}$ would be applied to $S_{n-2}^{(1)} + D_{n-2}^{(1)}$ in order to annihilate $S_{n-2}^{(1)}(n-1,n)$, the diagonal part $D_{n-2}^{(1)}$ would change. In order to avoid this, we change the matrix $D_{n-2}^{(1)}$ into the form $\hat{D}_{n-2}^{(1)} = [0,\dots,0,d_1,d_1]$ and hence, the matrix $S_{n-2}^{(1)}$ must be adapted into $\hat{S}_{n-2}^{(1)}$:

$$
\begin{aligned}
S^{(1)}_{n-2} + D^{(1)}_{n-2} &= \left(\begin{array}{cccc|c} \times & \dots & \times & \times & 0 \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \times & 0 \\ \times & \dots & \times & \times & \boxtimes \\ \hline 0 & \dots & 0 & \boxtimes & \boxplus \end{array}\right) + \left(\begin{array}{ccc|c} 0 & \dots & 0 & 0 \\ \vdots & & \vdots & \vdots \\ 0 & \dots & 0 & 0 \\ 0 & \dots & 0 & 0 \\ \hline 0 & \dots & 0 & d_1 \end{array}\right) \\
&= \left(\begin{array}{cccc|c} \times & \dots & \times & \times & 0 \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \times & 0 \\ \times & \dots & \times & + & \boxtimes \\ \hline 0 & \dots & 0 & \boxtimes & \boxplus \end{array}\right) + \left(\begin{array}{ccc|c} 0 & \dots & 0 & 0 \\ \vdots & & \vdots & \vdots \\ 0 & \dots & 0 & 0 \\ 0 & \dots & d_1 & 0 \\ \hline 0 & \dots & 0 & d_1 \end{array}\right) := \hat{S}^{(1)}_{n-2} + \hat{D}^{(1)}_{n-2}
\end{aligned}
$$

with $+ = S^{(1)}_{n-2}(n-1, n-1) - d_1$. So, the matrix $\hat{D}^{(1)}_{n-2}$ will not change under the similarity transformation based on $G^{(1)}_{n-1}$.

When applying now the Givens transformation $G^{(1)^T}_{n-1}$ on the last two rows in order to annihilate the last but one element of the last column, we get the following situation for the matrix $\hat{S}^{(1)}_{n-2}$:

$$
\begin{array}{c} \\ \\ \\ \rightarrow \\ \rightarrow \end{array}
\begin{pmatrix} \times & \dots & \times & \times & 0 \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \times & 0 \\ \times & \dots & \times & + & \otimes \\ 0 & \dots & 0 & \boxtimes & \boxplus \end{pmatrix} \longrightarrow \begin{pmatrix} \times & \dots & \times & \times & 0 \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \times & 0 \\ \boxtimes & \dots & \boxtimes & \times & 0 \\ \boxtimes & \dots & \boxtimes & \times & \times \end{pmatrix}
$$

i.e., the last two rows are proportional with the exception of the entries in the last two columns.

When applying the transpose $G^{(1)}_{n-1}$ of the former transformation on the last two columns, the last two columns become linearly dependent above and on the main diagonal. Because of symmetry, the last two rows become linearly dependent below and on the main diagonal as well:

$$
\begin{array}{c} \begin{array}{ccccc} & & & \downarrow & \downarrow \end{array} \\ \begin{pmatrix} \times & \dots & \times & \times & 0 \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \times & 0 \\ \boxtimes & \dots & \boxtimes & \times & 0 \\ \boxtimes & \dots & \boxtimes & \times & \times \end{pmatrix} \end{array} \longrightarrow \begin{pmatrix} \times & \dots & \times & \boxtimes & \boxtimes \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \boxtimes & \boxtimes \\ \boxtimes & \dots & \boxtimes & \boxtimes & \boxtimes \\ \boxtimes & \dots & \boxtimes & \boxtimes & \boxtimes \end{pmatrix}
$$

Hence, the orthogonal similarity transformation based on $G^{(1)}_{n-1}$ has transformed the matrix $\hat{S}^{(1)}_{n-2} + \hat{D}^{(1)}_{n-2}$ into a matrix $S^{(1)}_{n-1} + D^{(1)}_{n-1} := G^{(1)^T}_{n-1}(\hat{S}^{(1)}_{n-2} + \hat{D}^{(1)}_{n-2})G^{(1)}_{n-1}$ with $S^{(1)}_{n-1}$ of semiseparable structure of dimension two and $D^{(1)}_{n-1} = \hat{D}^{(1)}_{n-2}$ the diagonal matrix $diag[0, \dots, 0, d_1, d_1]$:

$$
S^{(1)}_{n-1} + D^{(1)}_{n-1} = \begin{pmatrix} \times & \dots & \times & \boxtimes & \boxtimes \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \boxtimes & \boxtimes \\ \boxtimes & \dots & \boxtimes & \boxtimes & \boxtimes \\ \boxtimes & \dots & \boxtimes & \boxtimes & \boxtimes \end{pmatrix} + \begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & 0 & & \\ & & & d_1 & \\ & & & & d_1 \end{pmatrix}.
$$

Because the element in the lower-right corner does not influence the semiseparable structure, we can change the element $S^{(1)}_{n-1}(n,n)$ into $\hat{S}^{(1)}_{n-1}(n,n) = S^{(1)}_{n-1}(n,n) + d_1 - d_2$ and so $\hat{D}^{(1)}_{n-1}(n,n)$ becomes d_2. Now, the 2×2 block in the lower-right corner of $\hat{S}^{(1)}_{n-1} + \hat{D}^{(1)}_{n-1}$ will have the following structure:

$$\hat{S}^{(1)}_{n-1} + \hat{D}^{(1)}_{n-1} = \begin{pmatrix} \times & \dots & \times & \boxtimes & \boxtimes \\ \vdots & & \vdots & \vdots & \vdots \\ \times & \dots & \times & \boxtimes & \boxtimes \\ \boxtimes & \dots & \boxtimes & \boxtimes & \boxtimes \\ \boxtimes & \dots & \boxtimes & \boxtimes & \boxplus \end{pmatrix} + \begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & 0 & & \\ & & & d_1 & \\ & & & & d_2 \end{pmatrix},$$

with $\boxplus$ the adapted element $\hat{S}^{(1)}_{n-1}(n,n) = S^{(1)}_{n-1}(n,n) - d_1 + d_2$. At last, we put $S^{(2)}_0 + D^{(2)}_0 := \hat{S}^{(1)}_{n-1} + \hat{D}^{(1)}_{n-1}$ because we have constructed the sum of a matrix with semiseparable structure 2 and of a diagonal matrix where d_1 has gone up one place and which contains the two first elements of d now.

2.3 The kth step

Suppose that after $k-1$ steps, we have a matrix $S^{(k)}_0 + D^{(k)}_0$ with $S^{(k)}_0$ of semiseparable structure of dimension k and $D^{(k)}_0 = \mathrm{diag}([0,\dots,0,\mathrm{d_1},\mathrm{d_2},\dots,\mathrm{d_{k-1}},\mathrm{d_k}])$:

$$\begin{array}{c} \\ S^{(k)}_0 + D^{(k)}_0 = \end{array} \begin{array}{c} \begin{array}{ccccccc} & & & \overset{n-k+1}{\downarrow} & & & \end{array} \\ \begin{pmatrix} \times & \dots & \times & \boxtimes & \dots & \boxtimes \\ \vdots & & \vdots & \vdots & & \vdots \\ \times & \dots & \times & \boxtimes & \dots & \boxtimes \\ \boxtimes & \dots & \boxtimes & \boxtimes & \dots & \boxtimes \\ \vdots & & \vdots & \vdots & \ddots & \vdots \\ \boxtimes & \dots & \boxtimes & \boxtimes & \dots & \boxtimes \end{pmatrix} \end{array} + \begin{pmatrix} 0 & & & & & \\ & \ddots & & & & \\ & & 0 & & & \\ & & & d_1 & & \\ & & & & \ddots & \\ & & & & & d_k \end{pmatrix}.$$

In this step we will transform $S^{(k)}_0 + D^{(k)}_0$ into a matrix $S^{(k+1)}_0 + D^{(k+1)}_0$ with $S^{(k+1)}_0$ of semiseparable structure of dimension $k+1$ and $D^{(k+1)}_0 = \mathrm{diag}([0,\dots,0,\mathrm{d_1},\dots,\mathrm{d_k},\mathrm{d_{k+1}}])$.

First we annihilate the elements in the $(n-k+1)$th column up to row $n-k-1$ by means of a product $G^{(k)^T}_{1:n-k-1} = G^{(k)^T}_{n-k-1} \dots G^{(k)^T}_2 G^{(k)^T}_1$ of $n-k-1$ Givens transformations. Because of the semiseparable structure of dimension k, the upper-right $(n-k) \times k$ block has rank at most one. Hence, not only the elements of the $(n-k+1)$th column will be annihilated, but also the first $n-k-1$ elements of all last k columns. Applying the same transformation $G^{(k)}_{1:n-k-1}$ to the columns, the elements 1 up to $n-k-1$ of the last k rows will be annihilated. Also here $G^{(k)}_{1:n-k-1}$ and its transpose do not influence $D^{(k)}_0$. The resulting matrix is denoted by $S^{(k)}_{n-k-1} + D^{(k)}_{n-k-1}$:

$$G^{(k)^T}_{1:n-k-1}(S^{(k)}_0 + D^{(k)}_0)G^{(k)}_{1:n-k-1} \quad = \quad S^{(k)}_{n-k-1} + D^{(k)}_{n-k-1} =$$

$$\begin{array}{rc} 1 & \rightarrow \\ & \\ n-k-1 & \rightarrow \\ n-k & \rightarrow \\ n-k+1 & \rightarrow \\ & \\ n & \rightarrow \end{array} \begin{pmatrix} \times & \dots & \times & \times & 0 & \dots & 0 \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ \times & \dots & \times & \times & 0 & \dots & 0 \\ \times & \dots & \times & \times & \boxtimes & \dots & \boxtimes \\ 0 & \dots & 0 & \boxtimes & \boxtimes & \dots & \boxtimes \\ \vdots & & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \boxtimes & \boxtimes & \dots & \boxtimes \end{pmatrix} + \begin{pmatrix} 0 & & & & & & \\ & \ddots & & & & & \\ & & 0 & & & & \\ & & & 0 & & & \\ & & & & d_1 & & \\ & & & & & \ddots & \\ & & & & & & d_k \end{pmatrix}.$$

When we want to annihilate the last k elements of the $(n-k)$th row of $S^{(k)}_{n-k-1}$ by means of a Givens transformation $G^{(k)^T}_{n-k}$, $D^{(k)}_{n-k-1}$ would change. Therefore, we add d_1 to $D^{(k)}_{n-k-1}(n-k,n-k)$

and rename this as $\hat{D}^{(k)}_{n-k-1} = \mathrm{diag}([0,\ldots,0,\mathrm{d}_1,\mathrm{d}_1,\ldots,\mathrm{d}_\mathrm{k}])$ such that $\hat{D}^{(k)}_{n-k-1}$ remains the same under the Givens transformation $G^{(k)}_{n-k}$ and its transpose. Hence, the element $S^{(k)}_{n-k-1}(n-k,n-k)$ must be adapted as follows: $S^{(k)}_{n-k-1}(n-k,n-k) - d_1$. This changed matrix will be denoted by $\hat{S}^{(k)}_{n-k-1}$ and we have the following situation:

$$\hat{S}^{(k)}_{n-k-1} + \hat{D}^{(k)}_{n-k-1} = \begin{array}{c} \begin{matrix} 1 & & & n-k & & & n \\ \downarrow & & & \downarrow & & & \downarrow \end{matrix} \\ \begin{pmatrix} \times & \ldots & \times & \times & 0 & \ldots & 0 \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ \times & \ldots & \times & \times & 0 & \ldots & 0 \\ \times & \ldots & \times & \boxplus & \boxtimes & \ldots & \boxtimes \\ 0 & \ldots & 0 & \boxtimes & \boxtimes & \ldots & \boxtimes \\ \vdots & & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \ldots & 0 & \boxtimes & \boxtimes & \ldots & \boxtimes \end{pmatrix} \end{array} + \begin{pmatrix} 0 & & & & & & \\ & \ddots & & & & & \\ & & 0 & & & & \\ & & & d_1 & & & \\ & & & & d_1 & & \\ & & & & & \ddots & \\ & & & & & & d_k \end{pmatrix}$$

with $\boxplus = S^{(k)}_{n-k-1}(n-k,n-k) - d_1$. Because we changed an element on the main diagonal of $S^{(k)}_{n-k-1}$ in the upper-left corner of a semiseparable block, the dependency is not changed by this adaptation.

Now the orthogonal similarity transformation based on $G^{(k)}_{n-k}$ can be performed on $\hat{S}^{(k)}_{n-k-1} + \hat{D}^{(k)}_{n-k-1}$:

$$S^{(k)}_{n-k} + D^{(k)}_{n-k} := G^{(k)^T}_{n-k}(\hat{S}^{(k)}_{n-k-1} + \hat{D}^{(k)}_{n-k-1})G^{(k)}_{n-k}$$

with $D^{(k)}_{n-k} = \hat{D}^{(k)}_{n-k-1}$. Figure 1 only shows the transformation of the matrix $\hat{S}^{(k)}_{n-k-1}$ into $S^{(k)}_{n-k}$. Remark that now also in the first elements of the $(n-k)$th row and column appear dependencies, in contrast with the starting matrix $S^{(k)}_0$ where there is only dependency in the last k rows and columns. This is why at the end of the kth step we will have a semiseparable structure of dimension $k+1$.

Next the element on the superdiagonal at the $(n-k+1)$th row, and because of the semiseparable structure also the other elements of that row belonging to the rank one part, should be annihilated. But once again we want the diagonal part to remain the same after the transformation, so $D^{(k)}_{n-k}$ will be changed into $\hat{D}^{(k)}_{n-k} = \mathrm{diag}([0,\ldots,0,\mathrm{d}_1,\mathrm{d}_2,\mathrm{d}_2,\ldots,\mathrm{d}_\mathrm{k}])$ such that the elements on the $(n-k+1)$th and $(n-k+2)$th row are equal. $S^{(k)}_{n-k}$ will be adapted into $\hat{S}^{(k)}_{n-k}$ too:

$$\hat{S}^{(k)}_{n-k} + \hat{D}^{(k)}_{n-k} = \begin{array}{c} \begin{matrix} 1 & & & & n-k+1 & & & n \\ \downarrow & & & & \downarrow & & & \downarrow \end{matrix} \\ \begin{pmatrix} \times & \ldots & \times & \boxtimes & \boxtimes & 0 & \ldots & 0 \\ \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots \\ \times & \ldots & \times & \boxtimes & \boxtimes & 0 & \ldots & 0 \\ \boxtimes & \ldots & \boxtimes & \boxtimes & \boxtimes & 0 & \ldots & 0 \\ \boxtimes & \ldots & \boxtimes & \boxtimes & \boxplus & \boxtimes & \ldots & \boxtimes \\ 0 & \ldots & 0 & 0 & \boxtimes & \boxtimes & \ldots & \boxtimes \\ \vdots & & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \ldots & 0 & 0 & \boxtimes & \boxtimes & \ldots & \boxtimes \end{pmatrix} \end{array} + \begin{pmatrix} 0 & & & & & & & \\ & \ddots & & & & & & \\ & & 0 & & & & & \\ & & & d_1 & & & & \\ & & & & d_2 & & & \\ & & & & & d_2 & & \\ & & & & & & \ddots & \\ & & & & & & & d_k \end{pmatrix}$$

with $\boxplus = S^{(k)}_{n-k}(n-k+1,n-k+1) + d_1 - d_2$. Also here this adaptation does not change the dependency because it works on the upper-left element of a semiseparable block.

Now the Givens transformations $G^{(k)^T}_{n-k+1}$ and $G^{(k)}_{n-k+1}$ can be applied to $\hat{S}^{(k)}_{n-k} + \hat{D}^{(k)}_{n-k}$.

The same idea is repeated for $j = n-k+1,\ldots,n-1$. At each time, the aim is to annihilate the elements belonging to the rank one structure of the jth row of $S^{(k)}_{j-1} + D^{(k)}_{j-1}$ by means of a Givens

$$
\begin{array}{r}
\\ \\ \\ \\
n-k \rightarrow \\
n-k+1 \rightarrow \\
\\ \\ \\
\end{array}
\begin{pmatrix}
\times & \times & \cdots & \times & \times & 0 & 0 & \cdots & 0 \\
\times & \times & \cdots & \times & \times & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & & \vdots \\
\times & \times & \cdots & \times & \times & 0 & 0 & \cdots & 0 \\
\times & \times & \cdots & \times & \times & \otimes & \otimes & \cdots & \otimes \\
0 & 0 & \cdots & 0 & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes \\
0 & 0 & \cdots & 0 & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes \\
\vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes
\end{pmatrix}
\xrightarrow{G_{n-k}^{(k)^T} \hat{S}_{n-k-1}^{(k)}}
\begin{array}{c}
\begin{array}{ccccccccc}
 & & & & n-k & n-k+1 & & & \\
 & & & & \downarrow & \downarrow & & &
\end{array} \\
\begin{pmatrix}
\times & \times & \cdots & \times & \times & 0 & 0 & \cdots & 0 \\
\times & \times & \cdots & \times & \times & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & & \vdots \\
\times & \times & \cdots & \times & \times & 0 & 0 & \cdots & 0 \\
\boxtimes & \boxtimes & \cdots & \boxtimes & \times & 0 & 0 & \cdots & 0 \\
\boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes \\
0 & 0 & \cdots & 0 & \otimes & \boxtimes & \boxtimes & \cdots & \boxtimes \\
\vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & \otimes & \boxtimes & \boxtimes & \cdots & \boxtimes
\end{pmatrix}
\end{array}
$$

$$
\xrightarrow{G_{n-k}^{(k)^T} \hat{S}_{n-k-1}^{(k)} G_{n-k}^{(k)T}}
\begin{pmatrix}
\times & \times & \cdots & \times & \boxtimes & \boxtimes & 0 & \cdots & 0 \\
\times & \times & \cdots & \times & \boxtimes & \boxtimes & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & & \vdots \\
\times & \times & \cdots & \times & \boxtimes & \boxtimes & 0 & \cdots & 0 \\
\boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes & \boxtimes & 0 & \cdots & 0 \\
\boxtimes & \boxtimes & \cdots & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \cdots & \boxtimes \\
0 & 0 & \cdots & 0 & 0 & \boxtimes & \boxtimes & \cdots & \boxtimes \\
\vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & 0 & \boxtimes & \boxtimes & \cdots & \boxtimes
\end{pmatrix}.
$$

Figure 1: Transformation of $\hat{S}_{n-k-1}^{(k)}$ into $S_{n-k}^{(k)}$

transformation $G_j^{(k)^T}$ working on the rows j and $j+1$. Because we want the diagonal part $D_{j-1}^{(k)}$ to remain unchanged, the jth and $(j+1)$th element must be the same and therefore we change $D_{j-1}^{(k)} = \mathrm{diag}([0,\ldots,0,\mathrm{d}_1,\ldots,\mathrm{d}_\mathrm{l},\mathrm{d}_\mathrm{l},\mathrm{d}_{\mathrm{l}+1},\ldots,\mathrm{d}_\mathrm{k}])$ into $\hat{D}_{j-1}^{(k)} = \mathrm{diag}([0,\ldots,0,\mathrm{d}_1,\ldots,\mathrm{d}_\mathrm{l},\mathrm{d}_{\mathrm{l}+1},\mathrm{d}_{\mathrm{l}+1},\ldots,\mathrm{d}_\mathrm{k}])$ with $l = j-n+k$. Hence, the matrix $S_{j-1}^{(k)}$ must be adapted as follows:

$$\hat{S}_{j-1}^{(k)}(j,j) = S_{j-1}^{(k)}(j,j) + d_l - d_{l+1}.$$

Because the element we adapt is the upper-left element of a semiseparable block, the existing dependencies do not change.

Next the similarity transformation based on $G_j^{(k)}$ can be applied in order to annihilate the last elements of the jth row. But as indicated in Figure 1, the elements of the jth row and column will be added to the rank one part.

$$S_j^{(k)} + D_j^{(k)} := G_j^{(k)^T} (\hat{S}_{j-1}^{(k)} + \hat{D}_{j-1}^{(k)}) G_j^{(k)}$$

$$\begin{array}{cc}
 & \begin{array}{cccccccccc} & & & n-k & & j & j+1 & & & \\ & & & \downarrow & & \downarrow & \downarrow & & & \end{array} \\
\begin{array}{c} \\ \\ \\ n-k \quad \rightarrow \\ \\ j \quad \rightarrow \\ j+1 \quad \rightarrow \\ \\ \\ \\ \end{array} &
\begin{pmatrix}
\times & \dots & \times & \boxtimes & \dots & \boxtimes & \boxtimes & 0 & \dots & 0 \\
\vdots & & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\
\times & \dots & \times & \boxtimes & \dots & \boxtimes & \boxtimes & 0 & \dots & 0 \\
\boxtimes & \dots & \boxtimes & \boxtimes & \dots & \boxtimes & \boxtimes & 0 & \dots & 0 \\
\vdots & & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\
\boxtimes & \dots & \boxtimes & \boxtimes & \dots & \boxtimes & \boxtimes & 0 & \dots & 0 \\
\boxtimes & \dots & \boxtimes & \boxtimes & \dots & \boxtimes & \boxtimes & \boxtimes & \dots & \boxtimes \\
0 & \dots & 0 & 0 & \dots & 0 & \boxtimes & \boxtimes & \dots & \boxtimes \\
\vdots & & \vdots & \vdots & & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \dots & 0 & 0 & \dots & 0 & \boxtimes & \boxtimes & \dots & \boxtimes
\end{pmatrix}
\end{array}$$

After $k-1$ similarity transformations applied in the way we just described, we will obtain that the last $k+1$ rows and columns of $S_{n-1}^{(k)}$ will belong to a semiseparable structure.

As a last small step, the last element of $D_{n-1}^{(k)}$ will be changed into d_{k+1} and $S_{n-1}^{(k)}$ will become $\hat{S}_{n-1}^{(k)}$ with $\hat{S}_{n-1}^{(k)}(n,n) = S_{n-1}^{(k)}(n,n) - d_k + d_{k+1}$. Also here this adaptation does not influence the dependencies already existing in $S_{n-1}^{(k)}$ because only the last element on the main diagonal is changed.

Hence, we have transformed $S_0^{(k)} + D_0^{(k)}$ into a matrix $\hat{S}_{n-1}^{(k)}$ with a semiseparable structure of dimension $k+1$ and a diagonal part $\hat{D}_{n-1}^{(k)} = \mathrm{diag}([0, \dots, 0, \mathrm{d_1}, \dots, \mathrm{d_k}, \mathrm{d_{k+1}}])$ as requested. So, we can define $S_0^{(k+1)} + D_0^{(k+1)} := \hat{S}_{n-1}^{(k)} + \hat{D}_{n-1}^{(k)}$.

The next figure shows the complete 3th step on a 6×6 matrix:

$$S_0^{(3)} + D_0^{(3)} = \begin{pmatrix}
\times & \times & \times & \boxtimes & \boxtimes & \boxtimes \\
\times & \times & \times & \boxtimes & \boxtimes & \boxtimes \\
\times & \times & \times & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & 0 & & & \\
& & & d_1 & & \\
& & & & d_2 & \\
& & & & & d_3
\end{pmatrix}$$

$$\downarrow \quad G_{1:2}^{(3)}$$

$$S_2^{(3)} + D_2^{(3)} = \begin{pmatrix}
\times & \times & \times & 0 & 0 & 0 \\
\times & \times & \times & 0 & 0 & 0 \\
\times & \times & \times & \boxtimes & \boxtimes & \boxtimes \\
0 & 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
0 & 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
0 & 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & 0 & & & \\
& & & d_1 & & \\
& & & & d_2 & \\
& & & & & d_3
\end{pmatrix}$$

$$||$$

$$\hat{S}_2^{(3)} + \hat{D}_2^{(3)} = \begin{pmatrix}
\times & \times & \times & 0 & 0 & 0 \\
\times & \times & \times & 0 & 0 & 0 \\
\times & \times & \times - d_1 & \otimes & \otimes & \otimes \\
0 & 0 & \otimes & \boxtimes & \boxtimes & \boxtimes \\
0 & 0 & \otimes & \boxtimes & \boxtimes & \boxtimes \\
0 & 0 & \otimes & \boxtimes & \boxtimes & \boxtimes
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & d_1 & & & \\
& & & d_1 & & \\
& & & & d_2 & \\
& & & & & d_3
\end{pmatrix}$$

$$
\begin{aligned}
& \downarrow \quad G_3^{(3)} \\
S_3^{(3)} + D_3^{(3)} &= \begin{pmatrix}
\times & \times & \boxtimes & \boxtimes & 0 & 0 \\
\times & \times & \boxtimes & \boxtimes & 0 & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
0 & 0 & 0 & \boxtimes & \boxtimes & \boxtimes \\
0 & 0 & 0 & \boxtimes & \boxtimes & \boxtimes
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & d_1 & & & \\
& & & d_1 & & \\
& & & & d_2 & \\
& & & & & d_3
\end{pmatrix} \\
& \,|| \\
\hat{S}_3^{(3)} + \hat{D}_3^{(3)} &= \begin{pmatrix}
\times & \times & \boxtimes & \boxtimes & 0 & 0 \\
\times & \times & \boxtimes & \boxtimes & 0 & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes + d_1 - d_2 & \otimes & \otimes \\
0 & 0 & 0 & \otimes & \boxtimes & \boxtimes \\
0 & 0 & 0 & \otimes & \boxtimes & \boxtimes
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & d_1 & & & \\
& & & d_2 & & \\
& & & & d_2 & \\
& & & & & d_3
\end{pmatrix} \\
& \downarrow \quad G_4^{(3)} \\
S_4^{(3)} + D_4^{(3)} &= \begin{pmatrix}
\times & \times & \boxtimes & \boxtimes & \boxtimes & 0 \\
\times & \times & \boxtimes & \boxtimes & \boxtimes & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
0 & 0 & 0 & 0 & \boxtimes & \boxtimes
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & d_1 & & & \\
& & & d_2 & & \\
& & & & d_2 & \\
& & & & & d_3
\end{pmatrix} \\
& \,|| \\
\hat{S}_4^{(3)} + \hat{D}_4^{(3)} &= \begin{pmatrix}
\times & \times & \boxtimes & \boxtimes & \boxtimes & 0 \\
\times & \times & \boxtimes & \boxtimes & \boxtimes & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes + d_2 - d_3 & \otimes \\
0 & 0 & 0 & 0 & \otimes & \boxtimes
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & d_1 & & & \\
& & & d_2 & & \\
& & & & d_3 & \\
& & & & & d_3
\end{pmatrix} \\
& \downarrow \quad G_5^{(3)} \\
S_5^{(3)} + D_5^{(3)} &= \begin{pmatrix}
\times & \times & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\times & \times & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & d_1 & & & \\
& & & d_2 & & \\
& & & & d_3 & \\
& & & & & d_3
\end{pmatrix} \\
& \,|| \\
\hat{S}_5^{(3)} + \hat{D}_5^{(3)} &= \begin{pmatrix}
\times & \times & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\times & \times & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\
\boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes + d_3 - d_4
\end{pmatrix} + \begin{pmatrix}
0 & & & & & \\
& 0 & & & & \\
& & d_1 & & & \\
& & & d_2 & & \\
& & & & d_3 & \\
& & & & & d_4
\end{pmatrix}
\end{aligned}
$$

2.4 The last step

The last step starts with a matrix $S_0^{(n-1)} + D_0^{(n-1)}$ where $S_0^{(n-1)}$ has a semiseparable structure of dimension $n-1$ and $D_0^{(n-1)} = \mathrm{diag}([0, \mathrm{d}_1, \ldots, \mathrm{d}_{n-1}])$:

$$S_0^{(n-1)} + D_0^{(n-1)} = \begin{pmatrix} \times & \boxtimes & \ldots & \boxtimes \\ \boxtimes & \boxtimes & \ldots & \boxtimes \\ \vdots & \vdots & \ddots & \vdots \\ \boxtimes & \boxtimes & \ldots & \boxtimes \end{pmatrix} + \begin{pmatrix} 0 & & & \\ & d_1 & & \\ & & \ddots & \\ & & & d_{n-1} \end{pmatrix}.$$

For each j, with $j = 1, \ldots, n-1$, we want to annihilate the superdiagonal element $(j, j+1)$ of the jth row, and because of the semiseparable structure of dimension $n-1$, also all elements right from the superdiagonal, by means of a Givens transformation $G_j^{(n-1)^T}$ on the jth and $(j+1)$th row. First the diagonal part $D_{j-1}^{(n-1)}$ will be updated into $\hat{D}_{j-1}^{(n-1)} = \mathrm{diag}([\mathrm{d}_1, \ldots, \mathrm{d}_j, \mathrm{d}_j, \mathrm{d}_{j+1}, \ldots, \mathrm{d}_{n-1}])$ such that $\hat{D}_{j-1}^{(n-1)}$ remains the same under the orthogonal similarity transformation based on $G_j^{(n-1)}$. The adaptation of $S_{j-1}^{(n-1)}$ is also as explained in the kth step, more precisely, $\hat{S}_{j-1}^{(n-1)}(j,j) = S_{j-1}^{(n-1)}(j,j) + d_{j-1} - d_j$ if $j \neq 1$ and $\hat{S}_{j-1}^{(n-1)}(j,j) = S_{j-1}^{(n-1)}(j,j) - d_j$ if $j = 1$. Also now the existing structure of $S_{j-1}^{(n-1)}$ is not changed. Hence, the Givens transformations $G_j^{(n-1)^T}$ and $G_j^{(n-1)}$ will be performed.

After these $n-1$ transformations, we have the following situation:

$$S_{n-1}^{(n-1)} + D_{n-1}^{(n-1)} = \begin{pmatrix} \boxtimes & \boxtimes & \ldots & \boxtimes \\ \boxtimes & \boxtimes & \ldots & \boxtimes \\ \vdots & \vdots & \ddots & \vdots \\ \boxtimes & \boxtimes & \ldots & \boxtimes \end{pmatrix} + \begin{pmatrix} d_1 & & & & \\ & d_2 & & & \\ & & \ddots & & \\ & & & d_{n-1} & \\ & & & & d_{n-1} \end{pmatrix}.$$

Only the last diagonal element is not of the requested form, but we can change it into d_n and subtract it from $S_{n-1}^{(n-1)}(n,n)$. This last subtraction does not destroy the semiseparable structure and hence we have transformed an arbitrary symmetric matrix A into a similar diagonal-plus-semiseparable one with the diagonal equal to d. This finishes the algorithm.

3 A second algorithm

The theorem proven in the former section can be formulated even stronger:

Theorem 2 *Let A be an $n \times n$ arbitrary symmetric matrix and $d = [d_1, d_2, \ldots, d_n]$ an arbitrary n-dimensional vector. Then there exists another orthogonal similarity transformation which transforms the symmetric matrix A into a diagonal-plus-semiseparable matrix $D + S$ with $D = \mathrm{diag}(\mathrm{d})$:*

$$Q^T A Q = D + S.$$

The construction of such a similarity transformation is quite similar to the former one. When we apply the former algorithm up to the last step, but with the diagonal starting from d_2 instead of d_1, so with $\tilde{d} = [d_2, d_3, \ldots, d_{n-1}, d_n, *]$, where $*$ is an arbitrary element of $\mathbb{R}$, we get

$$S_0^{(n-1)} + D_0^{(n-1)} = \begin{pmatrix} \times & \boxtimes & \ldots & \boxtimes \\ \boxtimes & \boxtimes & \ldots & \boxtimes \\ \vdots & \vdots & \ddots & \vdots \\ \boxtimes & \boxtimes & \ldots & \boxtimes \end{pmatrix} + \begin{pmatrix} 0 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{pmatrix}.$$

In the first algorithm, for the last step we repeated the same idea as we used in all former steps, but at this point we can also change the first diagonal element of $D_0^{(n-1)}$ into d_1 such that the diagonal part is the requested diagonal matrix D. The first element of $S_0^{(n-1)}$ must be adapted too, but this element, whatever its value is, can be included in the semiseparable structure. Now the requested form is reached without the last step of the former algorithm:

$$\left(\begin{array}{cccc} \boxplus & \boxtimes & \dots & \boxtimes \\ \boxtimes & \boxtimes & \dots & \boxtimes \\ \vdots & \vdots & \ddots & \vdots \\ \boxtimes & \boxtimes & \dots & \boxtimes \end{array}\right) + \left(\begin{array}{cccc} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{array}\right),$$

with $\boxplus = \times - d_1$ and as a consequence, $Qe_1 = e_1$ because we did not apply any transformation on the first row. This ends the construction of a similarity transformation as requested in Theorem 2.

4 Convergence properties of the reduction algorithm.

In this section we will briefly indicate some interesting convergence results connected with the reduction algorithm. In [18] an algorithm was proposed for reducing arbitrary symmetric matrices to semiseparable form, moreover a detailed convergence analysis of this reduction algorithm was included. It was shown that the matrices in the reduction algorithm contained the Lanczos Ritz values connected to starting vector e_1, in the part of the matrix already in semiseparable form. Moreover it was also shown that on this already reduced part at each step of the algorithm a step of subspace iteration was performed. This leads to a kind of nested subspace iteration. An analysis of both of these convergence behaviors led to the observation that the subspace iteration tended to converge to clusters if the eigenvalues of the already reduced part (these are the Lanczos Ritz values) approximated well enough the real dominant eigenvalues of the matrix.

As the reduction to semiseparable form can be seen as a special case of the reduction to diagonal-plus-semiseparable form (we can freely choose the diagonal to be zero), the convergence behavior of the latter case is a special case of a more general convergence behavior related to the reduction to diagonal-plus-semiseparable form. The analysis of this reduction is however not so straightforward as the one in [18]. First of all, the Krylov subspace convergence behavior is replaced by a more general form of Rational Krylov subspace convergence behavior (see e.g. [6]). Also the analysis of the subspace iteration is not straightforward anymore. In the reduction to semiseparable form, it could be interpreted as a QR-step without shift, in this reduction it should be seen as a QR-step with a special type of multi-shift. As the analysis of both of these convergence behaviors and their interaction are extended, technical and detailed we do not cover them in this publication, but in a forthcoming paper. Nevertheless to illustrate the power of this convergence behavior, we illustrate a simple fact by some numerical experiments. We show that if eigenvalues of the original matrix are present in the upper left part of the diagonal, used for the reduction to diagonal-plus-semiseparable form, then the algorithm will reveal these eigenvalues. This behavior results from teh specific reduction technique used, as we will give also as an example a diagonal-plus-semiseparable matrix, not coming from the reduction algorithm, which also has eigenvalues on the left upper corner, but does not reveal them.

5 Numerical Experiments

In this section three numerical experiments are performed. In a first experiment the accuracy of the reduction algorithm is compared w.r.t. the orthogonal similarity reduction to tridiagonal and semiseparable form. In a second experiment the computational complexity of these three reduction algorithms is compared and in the final experiment the reduction algorithm is examined for special choices of the diagonal, in correspondence with the previously given theorems. All the experiments are performed in Matlab [1], and the software can be freely downloaded from the

[1] Matlab is a registered trademark of the Mathwork Inc.

website:
http://www.cs.kuleuven.ac.be/∼marc/software

For the first experiment a set of test matrices was generated of dimensions 2^i for $i = 3, \ldots, 11$. The symmetric matrices were constructed in such a way that they have as eigenvalues $[1 : 2^i]$ for each choice of i. In Figure 2 the relative accuracy of the eigenvalues of the reduced matrices w.r.t. the original matrices is given. Denote the original eigenvalues with λ_i and the computed ones with $\tilde{\lambda}_i$, then the relative accuracy is calculated as

$$\frac{\max_i |\lambda_i - \tilde{\lambda}_i|}{\max_i |\lambda_i|}$$

It can be seen clearly that all three approaches are equally accurate.

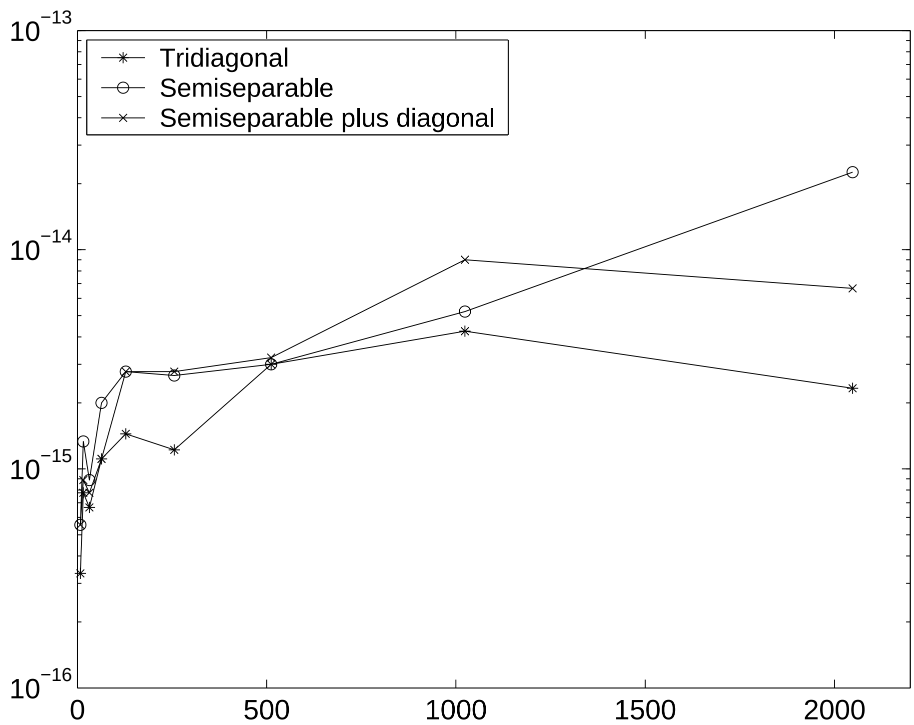

Figure 2: Relative residual of the eigenvalues.

In the second experiment the computational complexity of the three approaches was compared. The computational complexity of the reduction to tridiagonal and semiseparable form differs in an extra $9n^2$ operations that need to be performed to get the semiseparable structure. The reduction to diagonal-plus-semiseparable form needs an extra $\sum_{j=1}^{n} 2j = n(n-1)$ operations for the extra additions and substractions needed for making the matrix semiseparable with that specific diagonal. Figure 3 shows the computer time in seconds (the Matlab command *cputime* was used) divided by the third power of the problem size. What one expects is that all three curves, as they have the same factor preceding the n^3 term in the computational cost, tend to the same value for large n. This can be observed clearly in the figure. Moreover one can see that for computational timings the extra $n(n-1)$ operations performed by the reduction to diagonal-plus-semiseparable, w.r.t. the reduction to diagonal are negligible.

In this last experiment we have created a symmetric matrix with eigenvalues $1, 2, 3, 4, 5$ and performed different reductions of this matrix to a diagonal-plus-semiseparable matrix, thereby varying the diagonal. The different resulting matrices are shown, and it can be seen clearly, that if an eigenvalue is present on the top left, it is revealed, by the reduction algorithm. On top the

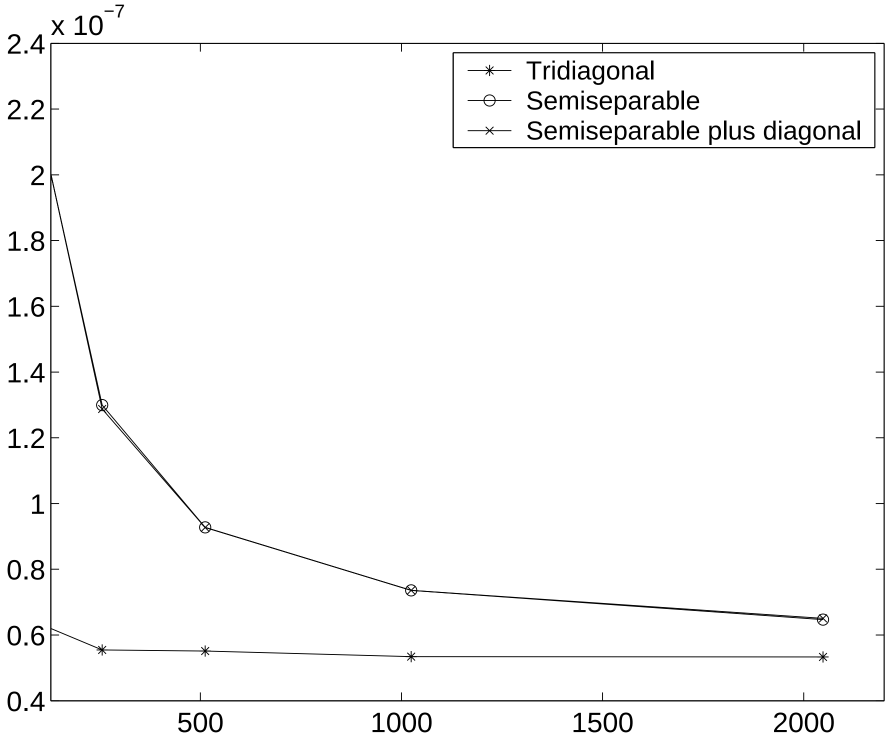

Figure 3: Computational complexity

diagonal d used for the reduction is shown, and below the resulting semiseparable matrix. The reader can generate much more examples indicating this convergence behavior, as the software can be downloaded. The last matrix shows that this behavior is related to the reduction algorithm as also a diagonal-plus-semiseparable matrix will be given, having as a diagonal eigenvalues in the upper left positions, but the eigenvalues are not revealed.

$$d = [5, 4, 8.3812e-01, 1.9640e-02, 6.8128e-01]$$

$$S = \begin{pmatrix} 5 & 1.0864e-15 & -2.7746e-15 & -1.7157e-15 & -5.3996e-16 \\ 1.0864e-15 & 4 & 8.8505e-17 & 5.4728e-17 & 1.7224e-17 \\ -2.7746e-15 & 8.8505e-17 & 1.7780e+00 & 5.8117e-01 & 1.8291e-01 \\ -1.7157e-15 & 5.4728e-17 & 5.8117e-01 & 1.4985e+00 & 4.6543e-01 \\ -5.3996e-16 & 1.7224e-17 & 1.8291e-01 & 4.6543e-01 & 2.7235e+00 \end{pmatrix}$$

$$d = [1, 5.0281e-01, 2, 3, 7.0947e-01]$$

$$S = \begin{pmatrix} 1 & 3.0611e-15 & 8.4210e-16 & -3.4843e-16 & 1.2741e-16 \\ 3.0611e-15 & 2.2405e+00 & 4.7803e-01 & -1.9779e-01 & 7.2327e-02 \\ 8.4210e-16 & 4.7803e-01 & 2.9501e+00 & -3.9313e-01 & 1.4376e-01 \\ -3.4843e-16 & -1.9779e-01 & -3.9313e-01 & 4.0160e+00 & -3.7151e-01 \\ 1.2741e-16 & 7.2327e-02 & 1.4376e-01 & -3.7151e-01 & 4.7934e+00 \end{pmatrix}$$

$$d = [1, 2, 3, 4, 5]$$

$$S = \begin{pmatrix} 1 & 2.3560e-15 & 1.8142e-15 & -9.8031e-16 & 6.4328e-16 \\ 2.3560e-15 & 2 & -5.9863e-16 & 3.2347e-16 & -2.1226e-16 \\ 1.8142e-15 & -5.9863e-16 & 3 & -1.1084e-15 & 7.2736e-16 \\ -9.8031e-16 & 3.2347e-16 & -1.1084e-15 & 4 & 2.4364e-16 \\ 6.4328e-16 & -2.1226e-16 & 7.2736e-16 & 2.4364e-16 & 5 \end{pmatrix}$$

This last example shows a semiseparable matrix, not coming from the reduction algorithm. Moreover it is shown that even though the diagonal contains eigenvalues of the complete diagonal-plus-semiseparable matrix in the upper left positions, they are not revealed.

$$d = [1, 2, 3, 8, 7]$$

$$S = \begin{pmatrix} 0.3156 & -0.9067 & -0.1277 & 0.3125 & -0.0830 \\ -0.9067 & 1.7095 & 0.2408 & -0.5891 & 0.1564 \\ -0.1277 & 0.2408 & -0.2081 & 0.5091 & -0.1352 \\ 0.3125 & -0.5891 & 0.5091 & -3.9552 & 1.0501 \\ -0.0830 & 0.1564 & -0.1352 & 1.0501 & -3.8619 \end{pmatrix}$$

6 Conclusion and future work

In this paper we presented an algorithm to transform any symmetric matrix by means of an orthogonal similarity transformation into a similar diagonal-plus-semiseparable matrix with free choice of the diagonal. When the first elements of the diagonal are eigenvalues of the original matrix, the upper-left block of the diagonal-plus-semiseparable matrix will be a diagonal block with these eigenvalues on the diagonal. This leads to some interesting convergence behavior which needs further investigation.

The computational complexity is comparable with the one of the algorithms reducing into tridiagonal and semiseparable form.

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