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Two fast algorithms for solving diagonal-plus-semiseparable linear systems☆

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Abstract

In this paper we discuss the structure of the factors of a QR- and a URV-factorization of a diagonal-plus-semiseparable matrix. The Q-factor of a QR-factorization has the diagonal-plus-semiseparable structure. The $U^{\rm T}$ - and V-factor of a URV-factorization are semiseparable lower Hessenberg orthogonal matrices. The strictly upper triangular part of the R-factor of a QR- and of a URV-factorization is the strictly upper triangular part of a rank-2 matrix. This latter fact provides a tool to construct a fast QR-solver and a fast URV-solver for linear systems of the form (D+S)x=b.

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1. Introduction

In this paper we consider two fast and stable algorithms for solving linear systems (D+S)x=b involving diagonal-plus-semiseparable matrices. Exploiting the structure of such matrices, algorithms with $\mathcal{O}(n)$ computational complexity can be developed, where n is the size of the considered problems.

The algorithms we propose are divided into two steps, sharing the first one. The first step transforms the initial linear system into an equivalent one with upper Hessenberg coefficient matrix \tilde{H}_{D+S} by means of n-1 Givens rotations. Instead of applying directly the n-1 Givens rotations to both the right- and the left-hand side of the linear system, we explicitly construct the matrix product $\tilde{G}_{2,\dots,n}$ of the latter Givens rotations. We show that $\tilde{G}_{2,\dots,n}$ can be written as the product of a diagonal matrix D_M and a lower Hessenberg matrix $G_{2,\dots,n}$ which upper triangular part is the upper triangular part of a rank-1 matrix. Moreover, the upper Hessenberg matrix \tilde{H}_{D+S} can be factorized as the product of D_M and an upper Hessenberg matrix H_{D+S} which upper triangular part is the upper triangular part of a rank-2 matrix. Hence, it turns out that $D+S=G_{2,\dots,n}^{-1}H_{D+S}$. This factorization allows to further speed-up the algorithm. When H_{D+S} is computed, the aim of the second step of both the algorithms is to reduce the matrix H_{D+S} into an upper triangular one, by means of Givens rotations. This can be accomplished either applying n-1 Givens rotations to the left (first algorithm), obtaining a URV-factorization of D+S, or applying n-1 Givens rotations to the right (second algorithm), obtaining a URV-factorization of D+S.

Due to the particular structure of the matrices involved in both factorizations, we show that the computational complexity of the corresponding system solvers is O(n). Furthermore, the Q-factor of the QR-factorization of D+S is still a diagonal-plus-semiseparable matrix.

Very recently, some fast algorithms for the QR- and URV-factorization of diagonal-plus-semiseparable matrices, based on [8] which itself is included in a more extended work [2], have been proposed by several authors [1,3–6]. In particular, a more general class of structured matrices, has been analyzed in [2,5]. Diagonal-plus-semiseparable matrices can be considered as a simplification of this more general class. The reason why this subclass itself is important, is because every symmetric matrix can be reduced to a similar semiseparable one by orthogonal similarity transformations (cf. [7]) instead of to a tridiagonal one. Hence the QR-algorithm of a semiseparable matrix can be used to calculate the eigenvalues of the original matrix. The basis of this QR-algorithm is the QR-factorization of a diagonal-plus-semiseparable matrix, which is studied in this paper.

When we apply the QR-algorithm, a sequence of similar semiseparable matrices is constructed which converges to a block-diagonal matrix. Hence problems with numerical stability can occur (cf. [7]). Therefore, we also look at the QR- and URV-factorization when an alternative definition and representation for diagonal-plus-semiseparable matrices are used, in order to preserve the numerical stability.

The basic idea of the backward stable algorithm proposed in [1], and further extended in [6], is to annihilate, at each step of the algorithm, all the entries in the last row, with the exception of that one in the last column of the matrix, by means of orthogonal transformations. Hence, the last unknown can be computed, since the equation made by the last row involves only this unknown. Then the size of the problem is reduced by one, neglecting the last row and column of the matrix and the corresponding entry of the right-hand side. The latter algorithm can be shown to be equivalent to first factorize the initial diagonal-plus-semiseparable matrix into a URV-decomposition, where U^T

and V are semiseparable lower Hessenberg orthogonal and R is upper triangular, and then solving the three derived linear systems. The URV-solver we propose gains a bit of efficiency exploiting the particular structure of \tilde{G}_{2-n} .

The paper is organized as follows. In Section 2 we define a diagonal-plus-semiseparable matrix. Sections 3 and 4 focus on the specific structure of the factors of a QR- and a URV-factorization respectively. In Section 5 we construct a fast QR- and a fast URV-solver for diagonal-plus-semiseparable linear systems. Section 6 is about the computational complexity of the two solvers proposed in the previous section and Section 7 shows some numerical experiments. In Section 8 we have a look at the QR- and URV-solver when another definition and representation for diagonal-plus-semiseparable matrices are used. Section 9 contains the conclusions.

2. Preliminaries

Definition 1. A semiseparable matrix S of semiseparability rank I is a matrix formed by the strictly upper triangular part of a rank-1 matrix and the lower triangular part of another rank-1 matrix. More precisely, let $u = [u_1, u_2, ..., u_n]^T$, $v = [v_1, v_2, ..., v_n]^T$ with $v_n \neq 0$, $p = [p_1, p_2, ..., p_n]^T$ and $q = [q_1, q_2, ..., q_n]^T$, then

$$S = \text{tril}(vu^{T}, 0) + \text{triu}(pq^{T}, 1).$$

The vectors u, v, p and q are called the generating vectors of S. With tril(A, s) we denote the lower triangular portion of A by setting all its entries above the sth diagonal equal to zero (s=0 is the main diagonal, s > 0 is above the main diagonal and s < 0 is below the main diagonal). Analogously, triu(A, s) is formed by the upper triangular portion of A where all entries below the sth diagonal are set to zero.

Remark. If v_n would be zero, the last row of S would be zero and this trivial case for solving linear systems as we will do in part 5, we exclude.

Definition 2. A *diagonal-plus-semiseparable matrix* then is the sum of a diagonal matrix and a semiseparable one. Let us denote the diagonal-plus-semiseparable matrix throughout this paper in the following way:

$$D+S = \begin{pmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_n \end{pmatrix} + \begin{pmatrix} u_1v_1 & p_1q_2 & p_1q_3 & \dots & p_1q_n \\ u_1v_2 & u_2v_2 & p_2q_3 & \dots & p_2q_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ u_1v_n & u_2v_n & u_3v_n & \dots & u_nv_n \end{pmatrix}$$

Remark. In [1,5] diagonal-plus-semiseparable matrices are defined with zeros on the main diagonal of the semiseparable matrix. Given a diagonal-plus-semiseparable matrix in this form, it can always be transformed into a diagonal-plus-semiseparable one as in our definition. Therefore we only need

to adapt the diagonal matrix by subtracting $u_i v_i$ of d_i for i = 1, ..., n and this costs 2n flops.

3. A QR-factorization

In this section, we prove that the R-factor and the Q-factor of a QR-factorization of a diagonal-plus-semiseparable matrix have some special structure, namely:

Theorem 1. The strictly upper triangular part of the R-factor of a QR-factorization of a diagonal-plus-semiseparable matrix is the strictly upper triangular part of a rank-2 matrix. The Q-factor is again a diagonal-plus-semiseparable matrix. More precisely, it is the product of a lower Hessenberg matrix, which lower triangular part is the lower triangular part of a rank-1 matrix, and an upper Hessenberg matrix, which upper triangular part is the upper triangular part of another rank-1 matrix.

The proof of this theorem is constructive and consists of two steps.

Starting from a diagonal-plus-semiseparable matrix D+S the first step is to reduce the semiseparable matrix S to an upper triangular matrix \tilde{S} by n-1 (with n the dimension of the matrix S) Givens rotations \tilde{G}_i . After applying the same n-1 Givens rotations on the rows of D, the diagonal matrix is transformed into an upper Hessenberg one \tilde{D} . At this point we show that the upper triangular matrix \tilde{S} is the upper triangular part of a rank-2 matrix and that the upper triangular part of the upper Hessenberg matrix \tilde{D} comes from a rank-1 matrix which has one generating vector in common with the rank-2 matrix. Hence the sum of \tilde{D} and \tilde{S} is an upper Hessenberg matrix $\tilde{H}_{D+S} = \tilde{D} + \tilde{S}$. Its upper triangular part is the upper triangular part of a rank-2 matrix (cf. Proposition 2).

The next step is to apply another n-1 Givens rotations \hat{G}_i on \tilde{H}_{D+S} in order to delete the subdiagonal. These last Givens rotations do not change the rank of the strictly upper triangular part (cf. Proposition 3) and so the final matrix, which is the *R*-factor of the *QR*-factorization of the matrix D+S, will have a strictly upper triangular part of some rank-2 matrix.

The structure of the Q-factor is a consequence of the fact that this Q-factor is the product of the 2n-2 Givens rotations \tilde{G}_i and \hat{G}_i . The product of the n-1 Givens rotations \tilde{G}_i is an upper Hessenberg matrix whose upper triangular part is the upper triangular part of a rank-1 matrix (cf. Proposition 2) and the product of the n-1 Givens rotations \hat{G}_i is a lower Hessenberg matrix whose lower triangular part is the lower triangular part of another rank-1 matrix (cf. Proposition 3).

Before working out our proposed strategy, we introduce some notation which we use throughout this paper: $\tau_i = v_i^2 + \cdots + v_n^2$ for $i = 1, \dots, n$.

3.1. The first step

3.1.1. The semiseparable matrix

First we apply n-1 Givens rotations \tilde{G}_i on the semiseparable matrix S from bottom to top. In order to annihilate the first element of the last row, we apply a Givens rotation on the rows n and

n-1 of the form

$$ilde{G}_n = I_{n-2} \oplus \left(egin{array}{ccc} rac{v_{n-1}}{\sqrt{ au_{n-1}}} & rac{v_n}{\sqrt{ au_{n-1}}} \ rac{-v_n}{\sqrt{ au_{n-1}}} & rac{v_{n-1}}{\sqrt{ au_{n-1}}} \end{array}
ight).$$

Because of the structure of a semiseparable matrix also the other elements of the last row, except the last element, become zero. In fact, the last two elements of each column, different from the last column, are of the form u_iv_{n-1} and u_iv_n and the Givens rotation \tilde{G}_n is built in such a way that it turns the vector $(v_{n-1}, v_n)^T$ into the vector $(\sqrt{\tau_{n-1}}, 0)^T$ so the whole last row, except the last element, is annihilated.

Analogously we annihilate the i-1 first elements of the ith row by the Givens rotation

$$ilde{G}_i = I_{i-2} \oplus \left(egin{array}{cc} rac{v_{i-1}}{\sqrt{ au_{i-1}}} & rac{\sqrt{ au_i}}{\sqrt{ au_{i-1}}} \ rac{-\sqrt{ au_i}}{\sqrt{ au_{i-1}}} & rac{v_{i-1}}{\sqrt{ au_{i-1}}} \end{array}
ight) \oplus I_{n-i}.$$

After these group of Givens rotations the matrix S is transformed into an upper triangular matrix \tilde{S} which, by straightforward calculation, can be written as the upper triangular part of the rank-2 matrix

$$\begin{pmatrix} \frac{1}{\sqrt{\tau_{1}}} \\ \frac{v_{1}}{\sqrt{\tau_{2}}\sqrt{\tau_{1}}} \\ \frac{v_{2}}{\sqrt{\tau_{3}}\sqrt{\tau_{2}}} \\ \vdots \\ \frac{v_{n-2}}{\sqrt{\tau_{n-1}}\sqrt{\tau_{n-2}}} \end{pmatrix} \begin{pmatrix} u_{1}\tau_{1} \\ (v_{1}p_{1})q_{2} + u_{2}\tau_{2} \\ \vdots \\ \left(\sum_{l=1}^{j-1}v_{l}p_{l}\right)q_{j} + u_{j}\tau_{j} \\ \vdots \\ \left(\sum_{l=1}^{j-1}v_{l}p_{l}\right)q_{n} + u_{n}\tau_{n} \end{pmatrix} + \begin{pmatrix} \frac{0}{\sqrt{\tau_{1}}} \\ \frac{-\tau_{1}p_{1}}{\sqrt{\tau_{2}}\sqrt{\tau_{1}}} \\ \frac{-v_{1}p_{1}v_{2} - \tau_{2}p_{2}}{\sqrt{\tau_{3}}\sqrt{\tau_{2}}} \\ \vdots \\ \frac{-(\sum_{l=1}^{i-2}v_{l}p_{l})v_{i-1} - \tau_{i-1}p_{i-1}}{\sqrt{\tau_{i}}\sqrt{\tau_{i-1}}} \\ \vdots \\ \frac{-(\sum_{l=1}^{n-2}v_{l}p_{l})v_{n-1} - \tau_{n-1}p_{n-1}}{\sqrt{\tau_{n-1}}v_{n}} \end{pmatrix}^{T}$$

3.1.2. The diagonal matrix

Of course we also need to apply the same n-1 Givens rotations \tilde{G}_i to the diagonal matrix of the original D+S. Straightforward calculation shows that D is transformed into an upper Hessenberg

matrix \tilde{D} with upper triangular part the upper triangular part of a rank-1 matrix, namely

$$\begin{pmatrix} \frac{1}{\sqrt{\tau_1}} \\ \frac{v_1}{\sqrt{\tau_2}\sqrt{\tau_1}} \\ \frac{v_2}{\sqrt{\tau_3}\sqrt{\tau_2}} \\ \vdots \\ \frac{v_{n-1}}{\sqrt{\tau_{n-1}}v_n} \end{pmatrix} (d_1v_1 \quad d_2v_2 \quad \dots \quad d_nv_n)$$

and subdiagonal $\tilde{s} = \left[\frac{-d_1\tau_2}{\sqrt{\tau_2}\sqrt{\tau_1}}, \frac{-d_2\tau_3}{\sqrt{\tau_3}\sqrt{\tau_2}}, \dots, \frac{-d_{n-1}\tau_n}{\sqrt{\tau_{n-1}}v_n}\right]$

3.1.3. The original matrix D + S

The n-1 Givens rotations from bottom to top change the original matrix D+S into the sum \tilde{H}_{D+S} of an upper Hessenberg matrix \tilde{D} and an upper triangular one \tilde{S} . When we have a closer look at the matrices \tilde{D} and \tilde{S} , we remark that the upper triangular part of \tilde{S} and of \tilde{D} have one of the generating vectors in common. Hence:

Proposition 2. The n-1 Givens rotations from bottom to top change the original matrix D+S into an upper Hessenberg matrix \tilde{H}_{D+S} with an upper triangular part which is the upper triangular part of the rank-2 matrix $\tilde{T}=$

$$\begin{pmatrix} \frac{1}{\sqrt{\tau_{1}}} \\ \frac{v_{1}}{\sqrt{\tau_{2}}\sqrt{\tau_{1}}} \\ \frac{v_{2}}{\sqrt{\tau_{3}}\sqrt{\tau_{2}}} \\ \vdots \\ \frac{v_{n-2}}{\sqrt{\tau_{n-1}}\sqrt{\tau_{n-2}}} \end{pmatrix} \begin{pmatrix} u_{1}\tau_{1} + d_{1}v_{1} \\ (v_{1}p_{1})q_{2} + u_{2}\tau_{2} + d_{2}v_{2} \\ \vdots \\ \left(\sum_{l=1}^{j-1}v_{l}p_{l}\right)q_{j} + u_{j}\tau_{j} + d_{j}v_{j} \\ \vdots \\ \left(\sum_{l=1}^{m-1}v_{l}p_{l}\right)q_{j} + u_{j}\tau_{j} + d_{j}v_{j} \\ \vdots \\ \left(\sum_{l=1}^{m-1}v_{l}p_{l}\right)v_{i-1} - \tau_{i-1}p_{i-1} \\ \vdots \\ \left(\sum_{l=1}^{m-1}v_{l}p_{l}\right)q_{n} + u_{n}\tau_{n} + d_{n}v_{n} \end{pmatrix} + \begin{pmatrix} \frac{0}{\sqrt{\tau_{1}}} \\ \frac{-\tau_{1}p_{1}}{\sqrt{\tau_{2}}\sqrt{\tau_{1}}} \\ \vdots \\ \frac{-(\sum_{l=1}^{m-2}v_{l}p_{l})v_{n-1} - \tau_{n-1}p_{n-1}}{\sqrt{\tau_{n-1}}v_{n}} \end{pmatrix} \begin{pmatrix} q_{1} \\ q_{2} \\ \vdots \\ q_{n} \end{pmatrix}^{T}$$

and subdiagonal $\tilde{s} = \left[\frac{-d_1 \tau_2}{\sqrt{\tau_2} \sqrt{\tau_1}}, \frac{-d_2 \tau_3}{\sqrt{\tau_3} \sqrt{\tau_2}}, \dots, \frac{-d_{n-1} \tau_n}{\sqrt{\tau_{n-1}} v_n} \right]$

The product $\tilde{G}_{2,\dots,n} = \tilde{G}_2 \tilde{G}_3 \dots \tilde{G}_n$ of the n-1 Givens rotations is an upper Hessenberg matrix of the following form:

$$\tilde{G}_{2,\dots,n} = \begin{pmatrix} \frac{v_1}{\sqrt{\tau_1}} & \frac{v_2}{\sqrt{\tau_1}} & \frac{v_3}{\sqrt{\tau_1}} & \cdots & \frac{v_{n-2}}{\sqrt{\tau_1}} & \frac{v_{n-1}}{\sqrt{\tau_1}} & \frac{v_n}{\sqrt{\tau_1}} \\ -\frac{\tau_2}{\sqrt{\tau_2}\sqrt{\tau_1}} & \frac{v_1v_2}{\sqrt{\tau_2}\sqrt{\tau_1}} & \frac{v_1v_3}{\sqrt{\tau_2}\sqrt{\tau_1}} & \cdots & \frac{v_1v_{n-2}}{\sqrt{\tau_2}\sqrt{\tau_1}} & \frac{v_1v_{n-1}}{\sqrt{\tau_2}\sqrt{\tau_1}} & \frac{v_1v_n}{\sqrt{\tau_2}\sqrt{\tau_1}} \\ -\frac{\tau_3}{\sqrt{\tau_3}\sqrt{\tau_2}} & \frac{v_2v_3}{\sqrt{\tau_3}\sqrt{\tau_2}} & \cdots & \frac{v_2v_{n-2}}{\sqrt{\tau_3}\sqrt{\tau_2}} & \frac{v_2v_{n-1}}{\sqrt{\tau_3}\sqrt{\tau_2}} & \frac{v_2v_n}{\sqrt{\tau_3}\sqrt{\tau_2}} \\ & \ddots & & \vdots & \vdots \\ -\frac{\tau_{n-1}}{\sqrt{\tau_{n-1}}\sqrt{\tau_{n-2}}} & \frac{v_{n-2}v_{n-1}}{\sqrt{\tau_{n-1}}\sqrt{\tau_{n-2}}} & \frac{v_{n-2}v_n}{\sqrt{\tau_{n-1}}\sqrt{\tau_{n-2}}} \\ & & -\frac{\tau_n}{\sqrt{\tau_{n-1}}v_n} & \frac{v_{n-1}v_n}{\sqrt{\tau_{n-1}}v_n} \end{pmatrix}.$$

Note that the upper triangular part of $\tilde{G}_{2,\dots,n}$ is the upper triangular part of a rank-1 matrix.

3.2. The second step

Next we need to annihilate the subdiagonal of \tilde{H}_{D+S} in order to get a complete upper triangular matrix. Therefore we apply another n-1 Givens rotations \hat{G}_i but now from top to bottom. (Remark that we first applied Givens rotations \tilde{G}_i on the semiseparable matrix and on the diagonal one separately and now on the sum of them!)

When we apply \hat{G}_1 to \tilde{H}_{D+S} , it is sufficient to apply it only on the first element of the subdiagonal \tilde{s} and on the two generating column vectors of the rank-2 matrix \tilde{T} . So, except for the first diagonal element, the upper triangular part of $\hat{G}_1\tilde{H}_{D+S}$ is still the upper triangular part of a rank-2 matrix.

The other Givens rotations \hat{G}_i are also applied to an element of the subdiagonal \tilde{s} and on the two column vectors of the modified rank-2 matrix. They all annihilate an element of the subdiagonal and create a modified upper triangular part which is still the upper triangular part of a rank-2 matrix except for the first i elements on the diagonal.

This justifies the next proposition:

Proposition 3. The (n-1) Givens rotations \hat{G}_i from top to bottom change the upper Hessenberg matrix \tilde{H}_{D+S} into an upper triangular matrix which strictly upper triangular part is the strictly upper triangular part of a rank-2 matrix. The product $\hat{G}_{1,\dots,n-1} = \hat{G}_{n-1} \dots \hat{G}_2 \hat{G}_1$ of the n-1 Givens rotations is a lower Hessenberg matrix whose lower triangular part is the lower triangular part of a rank-1 matrix.

The latter is straightforward because the product $\hat{G}_{1,\dots,n-1}$ is built by Givens rotations applied on the rows and from top to bottom.

3.3. Proof of Theorem 1

Every Givens rotation is an orthogonal matrix and the product of orthogonal matrices is again an orthogonal matrix. Hence Propositions 2 and 3 give us a way to construct a *QR*-factorization of a diagonal-plus-semiseparable matrix and show that the strictly upper triangular part of the *R*-factor is the strictly upper triangular part of a rank-2 matrix.

Because $\tilde{G}_{2,\dots,n}$ is an upper Hessenberg matrix whose upper triangular part is the upper triangular part of a rank-1 matrix, and $\hat{G}_{1,\dots,n-1}$ is a lower Hessenberg matrix whose lower triangular part is the lower triangular part of another rank-1 matrix, their product $Q = \hat{G}_{1,\dots,n-1}\tilde{G}_{2,\dots,n}$ has the diagonal-plus-semiseparable structure. The latter is very easy to see if you look at $\tilde{G}_{2,\dots,n}$ as the sum of an uppertriangular matrix and a subdiagonal matrix and at $\hat{G}_{1,\dots,n-1}$ as the sum of a lower triangular matrix and a supdiagonal one. The product of the sup- and subdiagonal leads to a diagonal matrix and the rest of the product to a semiseparable matrix of semiseparability rank 1.

4. A URV-factorization

In this section, we prove that the R-, U- and V-factor of a URV-factorization of a diagonal-plus-semiseparable matrix have a special structure as well, namely:

Theorem 2. The strictly upper triangular part of the R-factor of a URV-factorization of a diagonal-plus-semiseparable matrix is the strictly upper triangular part of a rank-2 matrix. The orthogonal matrix U is equal to $\tilde{G}_{2,...,n}$. The orthogonal matrix V is lower Hessenberg and its lower triangular part is the lower triangular part of a rank-1 matrix.

The proof of this theorem again consists of two steps.

The first step is the same as for the QR-factorization, so by means of the same n-1 Givens rotations \tilde{G}_i the diagonal-plus-semiseparable matrix D+S is transformed into an upper Hessenberg matrix \tilde{H}_{D+S} with subdiagonal \tilde{s} and which upper triangular part is the upper triangular part of the rank-2 matrix \tilde{T} (cf. Proposition 2).

In the next step we want to annihilate the subdiagonal, but instead of doing this by means of n-1 Givens rotations on the rows of the upper Hessenberg matrix \tilde{H}_{D+S} (as for the QR-factorization), we now apply n-1 Givens rotations H_i on the columns of \tilde{H}_{D+S} , starting from the last column up to the first one. In this way we create a URV-factorization. The product $\tilde{G}_{2,\dots,n}$ is equal to the U-factor, so the structure of the U-factor is already known (cf. Proposition 2), and the product $H_{1,\dots,n-1}$ of the Givens rotations H_i forms the V-factor.

When we apply H_1 to \tilde{H}_{D+S} , it is sufficient to apply it only on the last element of the subdiagonal \tilde{s} and on the two generating row vectors of the rank-2 matrix \tilde{T} . So, except for the last diagonal element, the upper triangular part of $(\tilde{H}_{D+S})H_1$ is still the upper triangular part of a rank-2 matrix because only the generating row vectors change.

The other Givens rotations H_i are also applied to an element of the subdiagonal \tilde{s} and on the two row vectors of the modified rank-2 matrix. They all annihilate an element of the subdiagonal and create a modified upper triangular part which is still the upper triangular part of a rank-2 matrix except for the last i elements on the diagonal.

This justifies the next proposition:

Proposition 5. The (n-1) Givens rotations H_i applied from the last column to the first, change the upper Hessenberg matrix \tilde{H}_{D+S} into an upper triangular matrix which strictly upper triangular part is the strictly upper triangular part of a rank-2 matrix. The product $H_{1,\dots,n-1}$ of H_i , and hence the V-factor of a URV-factorization, is lower Hessenberg and its lower triangular part is the lower triangular part of a rank-1 matrix.

The latter is straightforward because the product $H_{1,\dots,n-1}$ is built by Givens rotations applied on the columns, starting from the last ones.

5. Construction of two fast algorithms for solving linear diagonal-plus-semiseparable systems

The aim is to solve a linear system of the form (D+S)x=b. The previous sections give us a tool to solve such systems in $\mathcal{O}(n)$ flops with n equal to the dimension of (D+S). To this end we use the QR-factorization of Section 3 and the URV-factorization of Section 4 of D+S to get an upper triangular system and then the fact that the strictly upper triangular part comes from a rank-2 matrix in both cases. We give two algorithms.

5.1. Construction of a fast QR-solver

First we apply the n-1 Givens rotations \tilde{G}_i of Section 3.1 on the left-hand side (D+S)x and on the right-hand side b in order to get the upper triangular part of a rank-2 matrix \tilde{T} and some extra subdiagonal \tilde{s} .

In order to reduce the computational complexity, we have a closer look at Proposition 2, more precisely at the two rank-1 matrices of \tilde{T} , the subdiagonal \tilde{s} and the product $\tilde{G}_{2,\dots,n}$ of the Givens rotations \tilde{G}_i . Hence we notice that they all have the same denominators. These denominators can be put outside by means of a diagonal matrix D_M which we define in the following way: $D_M = \text{diag}([1/\sqrt{\tau_1}, 1/\sqrt{\tau_2}\sqrt{\tau_1}, \dots, 1/\sqrt{\tau_{n-1}}v_n])$.

Hence the product $\tilde{G}_{2,\dots,n}$ is written as follows: $\tilde{G}_{2,\dots,n} = D_M G_{2,\dots,n}$ with

$$G_{2,...,n} := egin{pmatrix} v_1 & v_2 & v_3 & \dots & v_{n-2} & v_{n-1} & v_n \ - au_2 & v_1v_2 & v_1v_3 & \dots & v_1v_{n-2} & v_1v_{n-1} & v_1v_n \ & - au_3 & v_2v_3 & \dots & v_2v_{n-2} & v_2v_{n-1} & v_2v_n \ & & \ddots & & dots & dots \ & & - au_{n-1} & v_{n-2}v_{n-1} & v_{n-2}v_n \ & & & - au_n & v_{n-1}v_n \end{pmatrix},$$

the rank-2 matrix $\tilde{T} = D_M T$ with

$$T := \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ \vdots \\ v_{n-1} \end{pmatrix} \begin{pmatrix} u_1\tau_1 + d_1v_1 \\ (v_1p_1)q_2 + u_2\tau_2 + d_2v_2 \\ \vdots \\ \sum_{l=1}^{j-1} v_lp_lq_j + u_j\tau_j + d_jv_j \\ \vdots \\ \vdots \\ (\sum_{l=1}^{n-1} v_lp_l \end{pmatrix} + \begin{pmatrix} 0 \\ -\tau_1p_1 \\ -v_1p_1v_2 - \tau_2p_2 \\ \vdots \\ -\left(\sum_{l=1}^{i-2} v_lp_l\right)v_{i-1} - \tau_{i-1}p_{i-1} \\ \vdots \\ q_n \end{pmatrix}^{\mathsf{T}} \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \end{pmatrix}^{\mathsf{T}}$$

and the subdiagonal \tilde{s} such that $\operatorname{diag}(\tilde{s}, -1) = D_M \operatorname{diag}(s, -1)$ with

$$s := [-d_1\tau_2, -d_2\tau_3, \dots, -d_{n-1}\tau_n].$$

Here $\operatorname{diag}(a, -1)$ denotes a matrix with a on the subdiagonal and all zeros elsewhere.

This implies that the upper Hessenberg matrix \tilde{H}_{D+S} can be written as the product of D_M and another upper Hessenberg matrix $H_{D+S} = \text{triu}(T) + \text{diag}(s, -1)$, where T still is a rank-2 matrix, and that the original matrix D + S can be factorized as $D + S = G_{2,...,n}^{-1} H_{D+S}$. Hence the linear system (D+S)x = b is equivalent with $H_{D+S}x = G_{2,...,n}b$.

In the next step the last n-1 Givens rotations \hat{G}_i are applied to the right- and left-hand side such that the subdiagonal of H_{D+S} is annihilated and only the transformed upper triangular matrix R remains. (Remark that the matrix R is not the R-factor of the QR-decomposition of D+S because we have dropped the denominators.)

The last step is to solve the system $Rx = \hat{b}$ where the strictly upper triangular part of the upper triangular matrix R comes from a rank-2 matrix. This system can be solved starting from bottom to top in $\mathcal{O}(n)$ flops (cf. [5]). For the sake of completeness we mention the following Proposition:

Proposition 6. An upper triangular linear system Ax = b where the strictly upper triangular part of A is the upper triangular part of a rank-r matrix with r independent of the dimension n of A, can be solved using (4r + 1)n - 5r flops.

Proof. Because the strictly upper triangular part of A comes from a rank-r matrix, it can be written as $triu(A^{n\times n}, 1) = triu(B^{n\times r}C^{r\times n}, 1)$. Hence the ith equation is of the form:

$$A_{i,i}x_i + \sum_{k=i+1}^n B_{i,:}C_{:,k}x_k = b_i$$

where $B_{i,:}$ is the Matlab-style notation for the *i*th row of B and $C_{:,k}$ denotes the kth column of C. This implies that

$$x_i = \frac{b_i - B_{i,:} \sum_{k=i+1}^{n} C_{:,k} x_k}{A_{i,i}}.$$

Now we apply backward substitution, which is the standard way to solve an upper triangular system, and rewrite the sum in the formula for x_i as $C_{:,i+1}x_{i+1} + \sum_{k=i+2}^{n} C_{:,k}x_k$. Hence the calculation of x_i can be done in 4r+1 flops because $\sum_{k=i+2}^{n} C_{:,k} x_k$ is already calculated in order to find x_{i+1} . \square

5.2. Construction of a fast URV-solver

As for the QR-solver, we first apply the n-1 Givens rotations \tilde{G}_i of Section 3.1 on the left-hand side (D+S)x and on the right-hand side b. Also here we reduce the computational complexity by neglecting the matrix D_M and just looking at H_{D+S} and $G_{2,\dots,n}b$.

In the next step the subdiagonal of H_{D+S} is annihilated. Because the left-hand side is of the form $H_{D+S}x$, we can not just apply the n-1 Givens rotations H_i to H_{D+S} in order to transform it into an upper triangular matrix R, but we also have to apply their inverse to the unknown x. Denote $(H_1 \dots H_{n-1})^T x$ by y. (Remark that the matrix R is not the R-factor of the URV-decomposition of D + S because we have neglected the denominators.)

The following step is to solve the system $Rv = \hat{b}$ where the strictly upper triangular part of the upper triangular matrix R comes from a rank-2 matrix. This system can be solved starting from bottom to top in $\mathcal{O}(n)$ flops because of Proposition 6.

Solving $x = (H_1 ... H_{n-1})y$ is the last step of this algorithm.

5.3. The algorithms

Next we give the two algorithms.

OR-solver.

As input we give the diagonal of the matrix D, the four generating vectors u, v, p and q of S and the vector b. The output is the solution of the linear system (D+S)x=b.

- I. Transform D+S by means of n-1 Givens rotations \tilde{G}_i into an upper Hessenberg matrix H_{D+S} which is built by a rank-2 matrix $T = \eta \rho^{T} + vq^{T}$ and a subdiagonal s. (Remark that we neglect the matrix D_M in both cases.)
 - A. compute the elements of the vectors τ and σ :
 - $\bullet \ \tau_i = v_i^2 + \dots + v_n^2,$
 - $\sigma_i = \sqrt{\tau_i}$
 - B. construct the generating vectors η, ρ and ν of the rank-2 matrix $T = \eta \rho^{T} + \nu q^{T}$:

 - $\eta = [1, v_1, v_2, \dots, v_{n-1}]^T$ $\rho_i = (\sum_{l=1}^{i-1} v_l p_l) q_i + u_i \tau_i + d_i v_i$

$$v_i = (-\sum_{l=1}^{i-2} v_l p_l) v_{i-1} - \tau_{i-1} p_{i-1}$$

C. construct the elements of the subdiagonal s:

$$s_i = -d_i \tau_{i+1}$$

- D. apply the product $G_{2,\dots,n}$ to the right-hand side b:
 - $\bullet \ \widetilde{b}_i = \left(\sum_{l=i}^n v_l b_l\right) v_{i-1} \tau_i b_{i-1}$ $\bullet \ \widetilde{b}_1 = \sum_{l=1}^n v_l b_l$

II. Transform the upper Hessenberg matrix $H_{D+S} = \text{triu}(T) + \text{diag}(s, -1)$ into an upper triangular matrix by means of n-1 Givens rotations \hat{G}_i to the left and store the new diagonal elements in a vector r:

$$\hat{G}_i = \text{Givens}(\eta_i \rho_i + v_i q_i, s_i)$$

- apply \hat{G}_i on η ,
- apply \hat{G}_i on v,
- apply \hat{G}_i on the right-hand side \tilde{b} .

Remark that it is sufficient to apply the Givens rotations only on the vectors η and v because $T = \eta \rho^{T} + vq^{T}$.

III. Solve the upper triangular linear system by backward substitution and the way proposed in the proof of Proposition 6.

URV-solver.

As input we give again the diagonal of the matrix D, the four generating vectors u, v, p and q of S and the vector b. The output is the solution of the linear system (D+S)x=b.

- I. Equivalent to step I. of the *QR*-solver.
- II. Transform the upper Hessenberg matrix $H_{D+S} = triu(T) + diag(s, -1)$ into an upper triangular matrix by means of n-1 Givens rotations H_i to the right and store the new diagonal elements in a vector r:

$$H_i = \text{Givens}(\eta_i \rho_i + v_i q_i, s_i)$$

- apply H_i on ρ ,
- apply H_i on q.

Remark that it is sufficient to apply the Givens rotations only on the vectors ρ and q because $T = \eta \rho^{T} + vq^{T}$.

- III. Solve the upper triangular linear system by backward substitution and the way proposed in the proof of Proposition 6. Remark that this solution is y instead of x because we did not apply the inverse of the Givens rotations H_i to x yet.
- IV. Solve $x = (H_1 ... H_{n-1})y$:
 - apply H_i on y.

6. Complexity

With an *n*-dimensional matrix D+S, the QR-solver and the URV-solver both only need 54n-44 flops and n-1 square roots. The quantity of memory places needed is 13n+9 for the QR-solver and 15n+9 for the URV-solver. The QR-solver proposed in [2] uses 58n flops and the URV-solver of [1] 57n flops, so in both cases our constructed algorithms are a little bit faster.

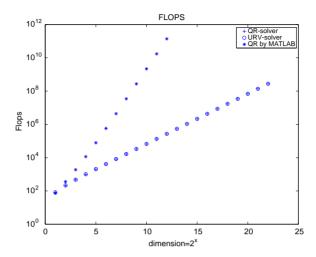


Fig. 1. Number of Flops used by the QR-solver, the URV-solver and the QR by MATLAB.

7. Numerical results

The numerical tests were performed on a Linux-pc, running MATLAB-5.3. ¹

For the QR-solver, the URV-solver and the QR-solution generated by MATLAB, we calculated the number of flops by means of the MATLAB-command FLOPS. Fig. 1 shows that our QR-and URV-solver indeed have linear complexity and that their amount of flops is comparable. Even for very low dimensions, the algorithms proposed in this article are faster than the QR-solver of MATLAB.

The second test shows that the two solvers we propose in this article are backward stable for the problems we solve. We built diagonal-plus-semiseparable matrices having condition number $10^i, i=1,2,\ldots,16$ and for each condition number matrices of dimension $2^j, j=1,2,\ldots,17$. For these 272 test matrices we calculated the relative residuals $\|\tilde{b}-b\|/\|b\|$ with b the exact right-hand side of the linear system we want to solve and \tilde{b} equals $A\tilde{x}$ where \tilde{x} are the solutions we calculated with our QR-, respectively URV-solver. As shown in the histograms of Fig. 2, all the relative residuals are of the order of 10^{-15} .

8. A more general class of diagonal-plus-semiseparable matrices

The definition (Definition 2) we gave for a diagonal-plus-semiseparable matrix is theoretically very useful and many algorithms for diagonal-plus-semiseparable matrices are written in terms of the generating vectors d, u, v, p and q. When the components of these generating vectors are given with high relative precision, the elements of the diagonal-plus-semiseparable matrix they generate, are also reconstructed with high relative precision.

¹ MATLAB is a trademark of the MathWorks, Inc.

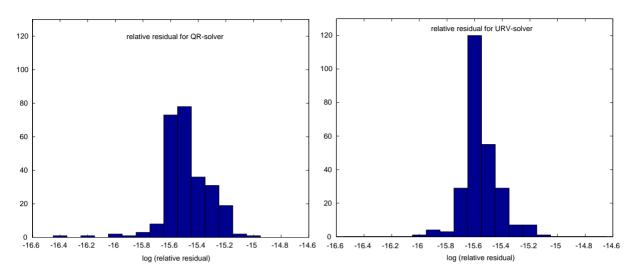


Fig. 2. Histograms of the relative residuals for the QR- and the URV-solver.

If we start from a semiseparable matrix, however, and apply the QR-algorithm, for example, to calculate the eigenvectors, a sequence of similar semiseparable matrices is constructed which converges to a block-diagonal matrix. Hence a loss of numerical stability can occur. For example, suppose we have the following 5×5 semiseparable matrix:

Example 1.

$$\begin{pmatrix} 1.2738 & 2.8264 \cdot 10^{-1} & 3.8483 \cdot 10^{-1} & 7.4397 \cdot 10^{-3} & 5.1648 \cdot 10^{-11} \\ -5.7004 \cdot 10^{-1} & 2.2236 & 8.6760 \cdot 10^{-3} & 1.6773 \cdot 10^{-4} & 1.1644 \cdot 10^{-12} \\ 1.2664 \cdot 10^{-1} & -4.9398 \cdot 10^{-1} & 2.5026 & 6.2603 \cdot 10^{-4} & 4.3461 \cdot 10^{-11} \\ -1.6459 \cdot 10^{-4} & 6.4202 \cdot 10^{-4} & -3.2527 \cdot 10^{-3} & 1.0000 \cdot 10^{2} & 4.5647 \cdot 10^{-17} \\ 1.5753 \cdot 10^{-12} & -1.5858 \cdot 10^{-13} & 1.5679 \cdot 10^{-12} & 4.8030 \cdot 10^{-8} & 1.0000 \cdot 10^{5} \end{pmatrix}$$

Representing the lower triangular part of this matrix with the generators u and v gives us the following vectors:

$$u = (1.5753 \cdot 10^{-12} - 1.5858 \cdot 10^{-13} 1.5679 \cdot 10^{-12} 4.8030 \cdot 10^{-8} 1.0000 \cdot 10^{5})^{T},$$

 $v = (8.0861 \cdot 10^{11} - 3.6187 \cdot 10^{11} 8.0391 \cdot 10^{10} - 1.0448 \cdot 10^{8} 1.0000)^{T}.$

Because the first element of u is of order 10^{-12} and is constructed by summations of elements of order 1, we can expect that this element has a precision of only 4 significant decimal digits left. Using this number to reconstruct the elements within the matrix only give these elements with a limited number of exact digits.

Hence a more stable way of representing diagonal-plus-semiseparable matrices is needed. For a diagonal-plus-semiseparable matrix D + S of dimension n, this new representation consists of

a diagonal $d = [d_1, \ldots, d_n]$ to construct the diagonal matrix D, a sequence of Givens rotations $G^l = [G_1^l, \ldots, G_{n-1}^l]$ and a vector $d^l = [d_1^l, \ldots, d_n^l]$ to construct the lower triangular part of the semiseparable matrix S, and another sequence of Givens rotations $G^u = [G_1^u, \ldots, G_{n-2}^u]$ and a vector $d^u = [d_1^u, \ldots, d_{n-1}^u]$ for the strictly upper triangular part of the semiseparable matrix S. An important remark is that this way of representing diagonal-plus-semiseparable matrices is as cheap as the representation with generating vectors in memory use.

The following figures denote how the lower triangular part of the semiseparable matrix S can be constructed. The elements denoted by \boxtimes form already a semiseparable part. Initially one starts on the first 2 rows of the matrix. The element d_1^l is placed in the upper left position, then a Givens transformation G_1^l is applied, and finally to complete the first step element d_2^l is added in position (2,1). Only the first two columns and rows are shown here.

$$egin{pmatrix} d_1^l & 0 \ 0 & 0 \end{pmatrix}
ightarrow G_1^l egin{pmatrix} d_1^l & 0 \ 0 & 0 \end{pmatrix} + egin{pmatrix} 0 & 0 \ 0 & d_2^l \end{pmatrix}
ightarrow egin{pmatrix} oxtimes & 0 \ oxtimes & d_2^l \end{pmatrix}.$$

The second step consists of applying the Givens transformation G_2^l on the second and the third row, furthermore d_3^l is added in position (3,3). Here only the first three columns are shown and the second and third row. This leads to:

$$\left(egin{array}{cccc}oxtom{igotimes} & d_2^l & 0 \ 0 & 0 & 0 \end{array}
ight)
ightarrow G_2^l \left(egin{array}{cccc}oxtom{igotimes} & d_2^l & 0 \ 0 & 0 & 0 \end{array}
ight) + \left(egin{array}{cccc} 0 & 0 & 0 \ 0 & 0 & d_3^l \end{array}
ight)
ightarrow \left(egin{array}{cccc}oxtom{igotimes} & oxtom{igotimes} & 0 \ oxtom{igotimes} & oxtom{igotimes} & d_3^l \end{array}
ight).$$

This process can be repeated by applying the Givens transformation G_3^l on the third and the fourth row of the matrix, and afterwards adding the diagonal element d_4^l . After applying all the n-1 Givens transformations G^l and adding all the diagonal elements d^l , the lower triangular part of a semiseparable matrix is constructed.

The construction of the strictly upper triangular part of the semiseparable matrix S is similar: apply the same n-2 steps on d^u and G^u as for the lower triangular part, but with multiplying by G_i^{uT} to the right at the *i*th step instead of to the left.

At last the diagonal matrix D = diag(d) is added and hence the diagonal-plus-semiseparable matrix D + S is constructed.

Suppose the Givens and vector representation of a diagonal-plus-semiseparable matrix D+S is known. When denoting the Givens transformations as

$$G_i^l = \begin{pmatrix} c_i^l & -s_i^l \\ s_i^l & c_i^l \end{pmatrix}$$
 and $G_i^u = \begin{pmatrix} c_i^u & -s_i^u \\ s_i^u & c_i^u \end{pmatrix}$.

The elements D + S(i, j) are calculated in the following way:

$$D + S(i,j) = c_i^l s_{i-1}^l s_{i-2}^l \cdots s_j^l d_j^l \quad \text{for } j < i < n,$$

$$D + S(i,j) = c_j^u s_{j-1}^u s_{j-2}^u \cdots s_i^u d_i^u \quad \text{for } i < j < n,$$

$$D + S(n,i) = s_i^l s_{i-1}^l s_{i-2}^l \cdots s_j^l d_j^l \quad \text{for } j < i = n,$$

$$D + S(i,n) = s_j^u s_{j-1}^u s_{j-2}^u \cdots s_i^u d_i^u \quad \text{for } i < j = n,$$

$$D + S(i,i) = c_i^l d_i^l + d(i) \quad \text{for } i = j \le n.$$

The elements of the semiseparable matrix can therefore be calculated in a stable way. Looking back at Example 1,

Example 2 (Example 1 continued). The Givens-vector representation of the matrix in Example 1 is the following: (In the first row of G^l the elements c_1^l, \ldots, c_4^l are stored and in the second row the elements s_1^l, \ldots, s_4^l . Similar for G^u .)

$$G^{l} = \begin{pmatrix} 9.0903 \cdot 10^{-1} & 9.7620 \cdot 10^{-1} & 9.9999 \cdot 10^{-1} & 1.0000 \\ -4.1672 \cdot 10^{-1} & -2.1686 \cdot 10^{-1} & -1.2997 \cdot 10^{-3} & 4.8030 \cdot 10^{-10} \end{pmatrix},$$

$$d^{l} = \begin{pmatrix} 1.4012 & 2.2778 & 2.5026 & 1.0000 \cdot 10^{2} & 1.0000 \cdot 10^{5} \end{pmatrix},$$

$$G^{u} = \begin{pmatrix} 5.9187 \cdot 10^{-1} & 9.9981 \cdot 10^{-1} & 1.0000 \cdot 10^{-1} \\ 8.0603 \cdot 10^{-1} & 1.9329 \cdot 10^{-2} & 6.9423 \cdot 10^{-8} \end{pmatrix},$$

$$d^{u} = \begin{pmatrix} 4.7753 \cdot 10^{-1} & 8.67764 \cdot 10^{-3} & 6.2603 \cdot 10^{-4} & 4.5647 \cdot 10^{-7} \end{pmatrix}.$$

All the elements of the semiseparable matrix can be reconstructed now with high relative precision.

The class of matrices that can be built with this new representation is even larger than the class of diagonal-plus-semiseparable matrices defined in Definition 2. More precisely, this new representation can represent all diagonal-plus-semiseparable matrices defined as follows:

Definition 3. A matrix D + S is called a diagonal-plus-semiseparable matrix of semiseparability rank 1 if all sub-matrices which can be taken out of the strictly lower, respectively strictly upper triangular part, of the matrix D + S have rank ≤ 1 and there exists at least one sub-matrix having exact rank 1.

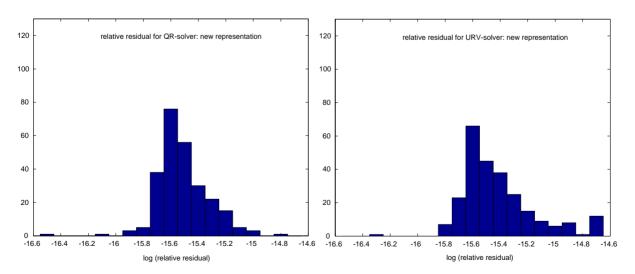


Fig. 3. Histograms of the relative residuals for the QR- and the URV-solver with new representation.

It can be shown that this larger class of diagonal-plus-semiseparable matrices as defined in Definition 3 is the pointwise closure of the class of diagonal-plus-semiseparable matrices according to Definition 2.

For more details about this new representation, see [7].

For the QR- and URV-solver presented in this paper, we also made a non-trivial implementation for this new representation. The computational complexity is still linear and, as the numerical experiments applied on the same test matrices as we used for the representation with generating vectors show, the backward stability is preserved (see Fig. 3). The software is available at www.cs.kuleuven.ac.be/ \sim marc.

9. Conclusions

By exploiting the specific structure of the factors of a *QR*-and a *URV*-factorization of diagonal-plus-semiseparable matrices, we constructed two fast and backward stable solvers for diagonal-plus-semiseparable linear systems, defined by Definition 2 as well as for the more general class defined by Definition 3.

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