A QR–method for computing the singular values via semiseparable matrices.

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In this paper we propose a new method for computing the singular value decomposition of a real matrix. In a first phase, an algorithm for reducing the matrix A into an upper triangular semiseparable matrix by means of orthogonal transformations is described. A remarkable feature of this phase is that, dependding on the distribution of the singular values, after few steps of the reduction, the large singular values are already computed with a precision depending on the gaps between the singular values.

An efficient implementation of the implicit QR–method for upper triangular semiseparable matrices is derived and applied to the latter matrix for computing its singular values.

The numerical tests show that the proposed method can compete with the methods available in the literature for computing the singular values of a matrix.

Keywords : SVD decomposition, QR-like algorithms, semiseparable matrices, bidiagonal matrices, singluar values.
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A *QR*–method for computing the singular values via semiseparable matrices*

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22nd August 2003

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1 Introduction

The standard procedure to compute the singular value decomposition of a dense matrix [4] £rst reduces it into a bidiagonal one by means of orthogonal transformations.

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Once the bidiagonal matrix has been computed, the QR–method is considered to reduce the latter matrix into a diagonal one (see, for instance, [5, 9, 7, 3] and the references therein).

In this paper we consider a new method for computing the singular value decomposition of a real matrix $A \in \mathbb{R}^{m \times n}$. In a £rst phase, an algorithm for reducing the matrix A into an upper triangular semiseparable matrix by means of orthogonal transformations is described, whose computational complexity is the same as for the standard reduction of a $m \times n$ matrix into a bidiagonal one by orthogonal transformations [5]. A remarkable feature of this phase is that, after few steps of the reduction, the large singular values are already computed with a precision depending on the gaps between the singular values and also depending on the spreading of the singular values. Indeed, it is showed that the latter reduction can be considered as a kind of subspace–like iteration method, where the size of the subspace increases by one dimension at each step of the reduction. Moreover it is also stated that the singular values have a very close connection to the Lanczos Ritz values, hereby interfering with the convergence behaviour of the subspace iteration.

Therefore, it turns out that the proposed reduction of a dense matrix into an upper triangular semiseparable (UTSS) one is an algorithm that can be ef£ciently used to compute an approximation of the largest singular values and the associated subspaces of the singular vectors. Such problems arise in many different areas, such as, principal component analysis, data mining, magnetic resonance spectroscophy, microarray data analysis, gene expression data, ... (see, for instance, [6, 14, 13, 17, 18] and the references therein).

In a second phase, once a UTSS matrix has been computed, an iterative method is derived and applied to the latter matrix in order to reduce it into a block diagonal one. It is proven that each iteration of the method is equivalent to an implicit QR–iteration. Hence, we derive an ef£cient implementation of the implicit QR–method for UTSS matrices.

The paper is organized as follows. A short introduction to the standard procedure for computing the singular values of a matrix is described in § 2. The de£nition and basic concepts of semiseparable matrices are introduced in § 3. The algorithm for reducing real matrices into UTSS ones is described in § 4 followed by the analysis of its "*convergence*" properties, discussed in § 5. In § 6, § 7 and § 8 the implicit QR-method is described. Moreover, the equivalence of the proposed method with the QR–method for semiseparable matrices is proven in § 8.

The implementation issues of the method are described in § 9.

The numerical experiments are shown in § 10 followed by the conclusions and future work.

2 The standard QR–method

In this section a brief explanation of the standard QR–method [5, p. 448–460] for calculating the singular values of an m by n matrix is given.

Let $A \in \mathbb{R}^{m \times n}$. Without loss of generality, one can assume that $m \geq n$. In a £rst phase the matrix A is transformed into a bidiagonal one by using orthogonal transformations U_B and V_B to the left and to the right, respectively, i.e.,

$$U_B^T A V_B = \begin{pmatrix} B \\ 0 \end{pmatrix}, \text{ with } B = \begin{pmatrix} d_1 & f_1 & 0 & \cdots & 0 \\ 0 & d_2 & \ddots & \ddots & \vdots \\ & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & f_{n-1} \\ 0 & \cdots & & 0 & d_n \end{pmatrix}.$$

Computed B, the QR–method is applied to it. The latter method generates a sequence of bidiagonal matrices converging to a block diagonal one.

Here a short description of one iteration of the QR method is considered. More details can be found in [5, p. 452–456].

Let $\hat{V}_1$ be the Givens rotation

$$\hat{V}_1 = \begin{pmatrix} c_1 & s_1 \\ -s_1 & c_1 \end{pmatrix}, \text{ such that } \hat{V}_1^T \begin{pmatrix} d_1^2 - \kappa \\ d_1 f_1 \end{pmatrix} = \begin{pmatrix} \times \\ 0 \end{pmatrix},$$

where κ is a shift[1]. Let $V_1 = diag(\hat{V}_1, I_{n-2})$, with $I_k, k \geq 1$, the identity matrix of order k. The matrix B is multiplied to the right by V_1, introducing the bulge denoted by "$+$" in the matrix BV_1,

$$BG_1 = \begin{pmatrix} \times & \times & 0 & \cdots & & \\ + & \times & \times & 0 & \cdots & \\ 0 & 0 & \times & \times & 0 & \cdots \\ & & & \ddots & \ddots & \end{pmatrix}.$$

The rest of the iteration is completed applying $2n-3$ Givens rotations, $U_1, \ldots, U_{n-1}$, $V_2, \ldots, V_{n-1}$ in order to move the bulge downward the bidiagonal structure and eventually remove it,

$$U^T BV \equiv (U_{n-1}^T \cdots U_1^T) B (V_1 V_2 \cdots V_{n-1}) = \begin{pmatrix} \times & \times & & & \\ & \times & \times & & \\ & & \times & \times & \\ & & & \times & \times \\ & & & & \times \end{pmatrix}.$$

Hence, the bidiagonal structure is preserved after one iteration of the QR–method. It can be proved that $Ve_1 = V_1 e_1$,where e_1 is the £rst vector of the canonical basis. Moreover, if Q and R are the orthogonal factor and the upper triangular factor of the QR factorization of $B^T B - \kappa I_n$, respectively, then Q and V are essentially the same, i.e.,

$$V = diag(\pm 1, \ldots, \pm 1) Q. \quad (1)$$

Furthermore, $T = Q^T B^T B Q$ is a symmetric tridiagonal matrix. Taking the following theorem into account, it turns out that each iteration of the QR–method is essentially uniquely determined by the £rst column of Q, i.e., by the the £rst column of V_1.

[1] Usually κ is chosen as the eigenvalue of $S(n-1:n, n-1:n)$ closest to $S(n,n)$ (Wilkinson shift), where $S = B^T B$.

Theorem 1 *[5, p. 416]***(Implicit Q Theorem)** *Suppose $Q = [q_1, \ldots, q_n]$ and $V = [v_1, \ldots, v_n]$ are orthogonal matrices with the property that both $Q^T AQ = T$ and $V^T AV = S$ are tridiagonal where $A \in \mathbb{R}^{n\times n}$ is symmetric. Let k denote the small positive integer for which $t_{k+1,k} = 0$ with the convention that $k = n$ if T is irreducible. If $v_1 = q_1$, then $v_i = \pm q_i$ and $|t_{i,i-1}| = |s_{i,i-1}|$ for $i = 2, \ldots, k$. Moreover, if $k < n$, then $s_{k+1,k} = 0$.*

Summarizing, the *QR*–method for computing the SVD of a matrix $A \in \mathbb{R}^{m\times n}$ can be divided into two phases.

Phase 1 Reduction of A into a bidiagonal matrix B by means of orthogonal transformations.

Phase 2 The *QR*–method is applied to B.

3 The new method via semiseparable matrices

Bidiagonal matrices play the main role in the standard procedure for computing the SVD of a matrix described in the previous section. In the new method, this role is played by upper triangular semiseparable matrices.

De£nition 1.1 *S is called a semiseparable matrix of semiseparability rank r if there exist two matrices R_1 and R_2 both of rank r, such that*

$$S = triu(R_1) + tril(R_2),$$

where $triu(R_1)$ and $tril(R_2)$ denote respectively the upper triangular part of the matrix R_1 and the strictly lower triangular part of the matrix R_2. When $r = 1$, R_1 and R_2 are two rank one matrices. Hence they can both be written as the outer product of two vectors, respectively u and v for R_1 and s and t for R_2. These vectors are also called the generators of the semiseparable matrix S.

In the sequel a semiseparable matrix of semiseparability rank 1 will be referred to as a semiseparable matrix.

Similarly to the *QR*–method described in § 1, the new method is divided into two phases.

Phase 1 Reduction of A into an upper triangular semiseparable matrix (UTSS) S_u by means of orthogonal transformations.

Phase 2 The new iterative method is applied to S_u preserving the upper triangular semiseparable structure.

In the next section an algorithm to reduce matrices into UTSS ones is described. An important feature of this algorithm is that the largest singular values are already computed with enough precision after few steps of the reduction, when the distribution of the singular values satisfy some mild conditions.

4 Reduction of a matrix to an upper triangular semiseparable one

The algorithm given here makes use of orthogonal transformations, i.e., Givens and Householder transformations, to reduce the matrix A into a UTSS matrix. The algorithm is based on the following result that can easily be adapted to transform arbitrary matrices into lower triangular semiseparable form.

Theorem 2 *Let $A \in \mathbb{R}^{m\times n}$, $m \geq n$. There exist two orthogonal matrices U and V such that*

$$UAV = \begin{pmatrix} S_u \\ 0 \end{pmatrix},$$

where S_u is an upper triangular semiseparable matrix.

PROOF:
The proof given here is a constructive one. We prove the existence of such a transformation by reducing the matrix A to the appropriate form by using Givens and Householder transformations.

The proof is given by induction. For an easy understanding and without loss of generality, the proof is restricted to a matrix $A \in \mathbb{R}^{m\times n}$, with $m = 6$ and $n = 5$. The side on which the operations are performed plays a very important role.

The following notation is introduced: $A^{(l)}_{k,j}$ denotes the matrix A at step l. Moreover, k denotes the number of operations performed to the left of the matrix $A^{(l)}_{0,0}$, and j denotes the number of operations performed to the right of the matrix $A^{(l)}_{0,0}$. $A^{(l)}_{0,0}$ will be also denoted by $A^{(l)}$. $U^{(l)}_k$ stands for the kth operation to the left at step l, and $V^{(l)}_j$ for the jth operation to the right in step l. These operations are Givens and Householder transformations.

- Step 1. In this £rst step of the algorithm two orthogonal matrices $U^{(1)}_1$ and $V^{(1)}_1$ are to be found, such that the matrix $A^{(2)} = U^{(1)}_1 A^{(1)} V^{(1)}_1$, with $A^{(1)} = A$, has the following properties: the £rst two rows of the matrix $A^{(2)}$ satisfy already the semiseparable structure and the £rst column of $A^{(2)}$ is zero below the £rst element. As mentioned before we prove the theorem considering a matrix of size $m = 6$ and $n = 5$. A Householder transformation $V^{(1)}_1$ is applied to the right of $A^{(1)} = A^{(1)}_{0,0}$ in order to annihilate all the elements in the £rst row except for the £rst one. $\otimes$ denote the elements to be annihilated, and $\boxtimes$ denote the part of the matrix having already a semiseparable structure.

$$A^{(1)} = \begin{pmatrix} \times & \otimes & \otimes & \otimes & \otimes \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{pmatrix} \xrightarrow{A^{(1)}_{0,0}V^{(1)}_1} A^{(1)}_{0,1} = \begin{pmatrix} \times & 0 & 0 & 0 & 0 \\ \times & \times & \times & \times & \times \\ \otimes & \times & \times & \times & \times \\ \otimes & \times & \times & \times & \times \\ \otimes & \times & \times & \times & \times \\ \otimes & \times & \times & \times & \times \end{pmatrix}$$

A Householder transformation $U_1^{(1)}$ is now applied to the left of $A_{0,1}^{(1)}$ in order to annihilate all the elements in the £rst column except the £rst two ones, $A_{0,1}^{(1)} = A_{0,0}^{(1)} V_1^{(1)}$, followed by a Givens transformation $U_2^{(1)}$ applied to the left of $A_{1,1}^{(1)}$ in order to annihilate the second element in the £rst column. As a consequence, the £rst two rows of $A_{2,1}^{(1)}$ have already a semiseparable structure.

$$U_1^{(1)} A_{0,1}^{(1)} = \begin{pmatrix} \times & 0 & 0 & 0 & 0 \\ \otimes & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \end{pmatrix} \quad \xrightarrow{U_2^{(1)} A_{1,1}^{(1)}} \quad A_{2,1}^{(1)} = \begin{pmatrix} \times & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \end{pmatrix}$$

Then we put

$$A^{(2)} = A_{2,1}^{(1)}.$$

.

- Step $k > 1$. By induction, the £rst k rows of $A^{(k)}$ have a semiseparable structure and the £rst $k-1$ columns are already in an upper triangular form. Without loss of generality, let us assume $k = 3$. This means that $A^{(3)}$ has the following structure:

$$A^{(3)} = \begin{pmatrix} \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & \times \end{pmatrix}. \tag{2}$$

The aim of this step is to make the upper triangular semiseparable stucture in the £rst 4 rows and the £rst 3 columns of the matrix. To this end, a Householder transformation $V_1^{(3)}$ is applied to the right of $A^{(3)}$, chosen in order to annihilate the last two elements of the £rst row of $A^{(3)}$. Note that because of the dependency between the £rst three rows, $V_1^{(3)}$ annihilates the last two entries of the second and third row, too. Furthermore, a Householder transformation is performed to the left of the matrix $A_{0,1}^{(3)}$ to annihilate the last two elements in column 3.

$$A_{0,0}^{(3)} V_1^{(3)} = \begin{pmatrix} \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\ 0 & \boxtimes & \boxtimes & 0 & 0 \\ 0 & 0 & \boxtimes & 0 & 0 \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & \otimes & \times & \times \\ 0 & 0 & \otimes & \times & \times \end{pmatrix} \quad \xrightarrow{U_1^{(3)} A_{0,1}^{(3)}} \quad A_{1,1}^{(3)} = \begin{pmatrix} \times & \boxtimes & \boxtimes & 0 & 0 \\ 0 & \boxtimes & \boxtimes & 0 & 0 \\ 0 & 0 & \boxtimes & 0 & 0 \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix}$$

The Givens transformation $U_2^{(3)}$ is now applied d to the left of the matrix $A_{1,1}^{(3)}$, annihilating the element marked with a circle.

$$A_{1,1}^{(3)} = \begin{pmatrix} \times & \boxtimes & \boxtimes & 0 & 0 \\ 0 & \boxtimes & \boxtimes & 0 & 0 \\ 0 & 0 & \boxtimes & 0 & 0 \\ 0 & 0 & \otimes & \times & \times \\ 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix} \xrightarrow{U_2^{(3)} A_{1,1}^{(3)}} A_{2,1}^{(3)} = \begin{pmatrix} \times & \boxtimes & \boxtimes & 0 & 0 \\ 0 & \boxtimes & \boxtimes & 0 & 0 \\ 0 & 0 & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix}$$

Dependency is now created between the fourth and the third row. Nevertheless, as it can be seen in the £gure above, the upper part does not satisfy the semiseparable structure, yet. A chasing technique is used in order to chase the non semiseparable structure upwards and away, by means of Givens transformations. Applying $V_2^{(3)}$ to the right to annihilate the entry $(2,3)$ of $A_{2,1}^{(3)}$, a nonzero element is introduced in the third row on the second column. Because of the semiseparable structure, this operation introduces two zeros in the third column, too. Annihilating the element just created in the third row with a Givens transformation to the left, the semiseparable structure holds between the second and the third row.

$$A_{2,1}^{(3)} V_2^{(3)} = \begin{pmatrix} \times & \boxtimes & 0 & 0 & 0 \\ 0 & \boxtimes & 0 & 0 & 0 \\ 0 & \otimes & \times & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix} \xrightarrow{U_3^{(3)} A_{2,2}^{(3)}} A_{3,2}^{(3)} = \begin{pmatrix} \times & \boxtimes & 0 & 0 & 0 \\ 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix}$$

This upchasing of the semiseparable structure can be repeated to create a complete upper semiseparable part starting from row 4 to row 1. This is shown in the next £gure:

$$A_{3,2}^{(3)} V_3^{(3)} = \begin{pmatrix} \times & 0 & 0 & 0 & 0 \\ \times & \times & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix} \xrightarrow{U_4^{(3)} A_{3,3}^{(3)}} A_{4,3}^{(3)} = \begin{pmatrix} \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix}$$

Then we pose

$$A^{(4)} = A_{4,3}^{(3)}.$$

This proves the induction step.

- Step $n+1$. Finally, a Householder transformation has to be performed to the left to have a complete upper triangular semiseparable structure. In fact, suppose, the matrix has already the separable structure in the £rst n rows, then one single Householder transformation is needed to annihilate all the elements in the n–th column below the n–th row. (see the £gure).

$$A^{(5)} = \begin{pmatrix} \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \boxtimes & \boxtimes \\ 0 & 0 & 0 & 0 & \boxtimes \\ 0 & 0 & 0 & 0 & \times \end{pmatrix} \xrightarrow{U_1^{(5)} A_{0,0}^{(5)}} A_{1,0}^{(5)} = \begin{pmatrix} \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & \boxtimes & \boxtimes & \boxtimes \\ 0 & 0 & 0 & \boxtimes & \boxtimes \\ 0 & 0 & 0 & 0 & \boxtimes \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

After the latter Householder transformation, the desired upper triangular semiseparable structure is created and the theorem is proved.

■

The reduction just described is obtained applying Givens and Householder transformations to A. The computational complexity of the algorithm is computed considering only the multiplications by Householder transformations, since the cost of the multiplications by Givens rotations are negligible with respect to that one of the latter ones. Hence, it turns out that the computational complexity of the algorithm is $4mn^2 - 4/3n^3$, that is the same computational complexity of the standard procedure that reduces matrices into bidiagonal form by Householder transformations [5].

5 Convergence properties of the reduction.

5.1 Subspace iteration

At each step of the algorithm introduced in Theorem 2, one more row (column) is added to the set of the rows (columns) of the matrix already proportional to each other by means of orthogonal transformations. In this section, using arguments similar to those considered in [16, 15], we show that this algorithm can be interpreted as a kind of nested subspace iteration method [5], where the size of the vector subspace is increased by one and a change of coordinate system is made at each step of the algorithm. As a consequence, the upper triangular blocks along the main diagonal in the part of the matrix already semiseparable, give information on the largest singular values of the matrix.

Given a matrix $\hat{A}$ and an initial subspace $\mathcal{S}^{(0)}$, the subspace iteration method [5] can be described as follows

$$\mathcal{S}^{(i)} = \hat{A}\mathcal{S}^{(i-1)}, \ \ i = 1,2,3,\ldots$$

Under weak assumptions on A and $\mathcal{S}^{(0)}$, the sequence $\{\mathcal{S}^{(i)}\}$ converges to an invariant subspace, corresponding to the largest eigenvalues in modulus.

The reduction algorithm of a dense matrix to a UTSS matrix can be seen as such a kind of subspace iteration, where the size of the subspace grows by one dimension at each step of the algorithm.

Let $A^{(1)} \equiv A$. Let $U_1^{(1)}, U_2^{(1)}$ and $V_1^{(1)}$ be the orthogonal matrices, described in step 1 of the proof of Th. 2. Hence the matrix

$$A^{(2)} = U_2^{(1)} U_1^{(1)} A^{(1)} V_1^{(1)} \tag{3}$$

has the upper triangular semiseparable structure in the £rst two rows and in the £rst column.

De£ne $\hat{U}^{(1)^T} \equiv U_2^{(1)} U_1^{(1)}$, and let $\hat{U}^{(1)} = [\hat{u}_1^{(1)}, \hat{u}_2^{(1)}, \ldots, \hat{u}_m^{(1)}]$. Then, because $A^{(1)}V^{(1)} = \hat{U}^{(1)}A^{(2)}$ has the £rst row, except for the £rst element equal to zero (see Theorem 2) we get:

$$A^{(1)}A^{(1)^T} = \hat{U}^{(1)}A^{(2)}A^{(2)^T}\hat{U}^{(1)^T} = \hat{U}^{(1)} \begin{pmatrix} \times & \times & \cdots & \times \\ 0 & \times & \cdots & \times \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \times & \cdots & \times \end{pmatrix} \equiv \hat{U}^{(1)} R_1. \qquad (4)$$

Let $e_1, \ldots, e_n$ be the standard basis vectors of $\mathbb{R}^n$. From (4), because of the structure of R_1, it turns out that:

$$A^{(1)}A^{(1)^T} < e_1 > = < \hat{u}_1^{(1)} >,$$

where $< x, y, z, \ldots >$ denotes the subspace spanned by the vectors $x, y, z, \ldots$. This means that the £rst column of $A^{(1)}A^{(1)^T}$ and $\hat{u}_1^{(1)}$ span the same one–dimensional space. In fact, one subspace iteration step is performed on the vector e_1.

The £rst step of the algorithm is completed when the following orthogonal transformation is performed,

$$A^{(2)} = \hat{U}^{(1)^T} A^{(1)} V_1^{(1)} \Leftrightarrow A^{(2)}A^{(2)^T} = \hat{U}^{(1)^T} A^{(1)} A^{(1)^T} \hat{U}^{(1)}$$

The latter transformation can be interpreted as a change of coordinate system: $A^{(1)}$ and $A^{(2)}$ represent the same linear transformation with respect to different coordinate systems. Let $y \in \mathbb{R}^n$. Then y is represented in the new system by $\hat{U}^{(1)^T} y$. This means that for the vector $\hat{u}_1^{(1)}$ we get $\hat{U}^{(1)^T}\hat{u}_1^{(1)} = e_1$. Summarizing, this means that one step of subspace iteration on the subspace $< e_1 >$ is performed, resulting in a new subspace $\hat{u}_1^{(1)}$, and then, by means of a coordinate transformation, it is transformed back into the subspace $< e_1 >$. So, instead of working with a £xed matrix and changing subspaces, we work with £xed subspaces and changing matrices. Therefore, let $z^{(i)}$ denote the singular vector corresponding to the largest singular value of $A^{(i)}$, $i = 1, 2, \ldots$, the sequence $\left\{ z^{(i)} \right\}$ converges to e_1, and, consequently, the entry $A^{(i)}(1,1)$ converges to the largest singular value of A. The second step can be interpreted in a completely analogous way.

Let

$$A^{(3)} = \hat{U}^{(2)^T} A^{(2)} V_1^{(2)}, \qquad (5)$$

where $\hat{U}^{(2)}$ and $V_1^{(2)}$ are orthogonal matrices such that $A^{(3)}$ is a UTSS matrix in the £rst three rows and the £rst two columns. Denote $\hat{U}^{(2)} = [\hat{u}_1^{(2)}, \hat{u}_2^{(2)}, \ldots, \hat{u}_m^{(2)}]$. From (5), $A^{(2)}A^{(2)^T}$ can be written as follows,

$$A^{(2)}A^{(2)^T} = \hat{U}^{(2)}A^{(3)}A^{(3)^T}\hat{U}^{(2)^T} = \hat{U}^{(2)} \begin{pmatrix} \times & \times & \cdots & \times & \times \\ 0 & \times & \cdots & \times & \times \\ 0 & 0 & \times & \cdots & \times \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \times & \cdots & \times \end{pmatrix} \equiv \hat{U}^{(2)} R_2.$$

Considering the subspace $< e_1, e_2 >$ and using the same notation as above, we have,

$$A^{(2)} {A^{(2)}}^T < e_1, e_2 > = < \hat{u}_1^{(2)}, \hat{u}_2^{(2)} > .$$

This means that the second step of the algorithm is a step of subspace iteration performed on a slightly grown subspace. For every new dependency that is created in the matrix $A^{(i)}$, the dimension of the subspace is increased by one.

This means that from step i, $i = 1, \ldots, n$, (so there is dependency between the rows 1 upto i), all the consecutive steps perform subspace iterations on the subspace of dimension i. From [16], we know that these consecutive iterations on subspaces tend to create block upper triangular matrices. Furthermore, the process works for all the nested subspaces at the same time, and so our semiseparable matrix will tend to become more and more block upper triangular, where the blocks contain the singular values of the same value. This explains why the upper–right block already gives a good estimate of the largest singular values, as they are connected to a subspace on which were performed the most subspace iterations.

This insight also opens a lot of new perspectives. In a lot of problems, only few largest singular values need to be computed. In such cases, the proposed algorithm gives the required information after only few steps, without running the algorithm to the completion. Moreover, because the matrices generated at each step of the algorithm converges to a block upper triangular matrix, the original problem can be divided into smaller independent subproblems. Furthermore, if the UTSS reduction is "iterated", the sequence of UTSS matrices generated converges to a block upper triangular matrix.

We £nish this section with a theorem from [16] concerning the speed of convergence of subspace iterations. (Theorem 5.4 [16])

De£nition 2.1 *Denote with $\mathcal{S}$ and $\mathcal{T}$ two subspaces, then the distance $d(\mathcal{S}, \mathcal{T})$ between these two subspaces is de£ned in the following way:*

$$d(\mathcal{S}, \mathcal{T}) = \sup_{s \in \mathcal{S}, \|s\|_2 = 1} \inf_{t \in \mathcal{T}} \|s - t\|_2$$

Using this de£nition, we can state the following convergence theorem:

Theorem 3 *Let $A \in \mathbb{C}^{n \times n}$, and let p be a polynomial of degree $\leq n$. Let $\lambda_1, \ldots, \lambda_n$ denote the eigenvalues of A, ordered so that $|p(\lambda_1)| \geq |p(\lambda_2)| \geq \cdots \geq |p(\lambda_n)|$. Suppose k is a positive integer less than n for which $|p(\lambda_k)| > |p(\lambda_{k+1})|$. Let (p_i) be a sequence of polynomials of degree $\leq n$ such that $p_i \to p$ as $i \to \infty$ and $p_i(\lambda_j) \neq 0$ for $j = 1, \ldots, k$ and all i. Let $\rho = |p(\lambda_k)|/|p(\lambda_{k+1})|$. Let $\mathcal{T}$ and $\mathcal{U}$ be the invariant subspaces of A associated with $\lambda_1, \ldots, \lambda_k$ and $\lambda_{k+1}, \ldots, \lambda_n$ respectively. Consider the nonstationary subspace iteration*

$$\mathcal{S}_i = p_i(A)\mathcal{S}_{i-1}$$

where $\mathcal{S}_0$ is a k-dimensional subspace of $\mathbb{C}^n$ satisfying $\mathcal{S} \cap \mathcal{U} = \{0\}$. Then for every $\hat{\rho}$ satisfying $\rho < \hat{\rho} < 1$ there exists a constant $\hat{C}$ such that

$$d(\mathcal{S}_i, \mathcal{T}) \leq \hat{C}\hat{\rho}^i, \quad i = 1, 2, 3, \ldots$$

In our case Theorem 3 can be applied with the polynomials $p_i(z)$ and $p(z)$ chosen in the following sense: $p_i(z) = p(z) = z$.

5.2 The Lanczos-Ritz values

In an analogues way as in the previous subsection one can show that the intermediate matrices $A^{(i)}$ satisfy the following property. The matrices $A^{(i)}A^{(i)^T}$ have in the upper left $i \times i$ block the eigenvalues equal to the Ritz Values, corresponding with the starting vector e_1. The proof of this statement is a combination of a proof given in [10] and the proof of the subspace iteration above. It will not be given here, because it is easy to reconstruct.

As mentioned before, the interaction between the Lanczos-Ritz value behaviour, and the subspace iteration is the following. The subspace iteration, will start converging as soon as the Lanczos-Ritz values have converged close enough to the dominant eigenvalues. We will not go into the details, because a thourough study of the interaction between the two behaviours was already made in the Technical report [10]. The interested reader can £nd there answers to all the questions concerning the proofs, theorems and interactions between these two convergence behaviours.

6 The new method

As described in § 2, a crucial point of one iteration of the QR–method applied to bidiagonal matrices is the knowledge of the £rst column of the orthogonal factor of the QR–factorization of $B^T B - \kappa I$. Moreover, after each iteration of the QR–method the bidiagonal structure of the involved matrices is preserved.

Similarly, in § 8 we will prove that one iteration of the implicit QR method applied to an upper semiseparable matrix S_u is uniquely determined by the £rst column of the orthogonal factor Q of the QR factorization of

$$S_u^T S_u - \kappa I, \tag{6}$$

where κ is a suitable shift. Expoiting the particular structure of matrix (6), we will show how the £rst column of Q can be computed without explictly computing $S_u^T S_u$.

Moreover, in § 8, we will prove that an implicit Q–theorem similar to Th. 1 holds also for semiseparable matrices. Hence we will show that each iteration of the new method is actually an iteration of the implicit QR–method applied to semiseparable matrices.

In this section we describe how the £rst column of the orthogonal factor of the QR factorization of (6) can be determined.

Denote by u and v the generators of the matrix S_u,

$$S_u = \begin{pmatrix} u_1v_1 & u_2v_1 & u_3v_1 & \cdots & u_nv_1 \\ 0 & u_2v_2 & u_3v_2 & \cdots & u_nv_2 \\ & 0 & u_3v_3 & \cdots & u_nv_3 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & \cdots & & 0 & u_nv_n \end{pmatrix}. \tag{7}$$

Let $\tau_i = \sum_{k=1}^{i} v_k^2,\ i = 1,\ldots,n$. An easy calculation reveals that

$$S = S_u^T S_u = \begin{pmatrix} u_1 u_1 \tau_1 & u_2 u_1 \tau_1 & u_3 u_1 \tau_1 & \cdots & u_n u_1 \tau_1 \\ u_2 u_1 \tau_1 & u_2 u_2 \tau_2 & u_3 u_2 \tau_2 & & u_n u_2 \tau_2 \\ u_3 u_1 \tau_1 & u_3 u_2 \tau_2 & u_3 u_3 \tau_3 & & \vdots \\ \vdots & & & \ddots & \\ u_n u_1 \tau_1 & u_n u_2 \tau_2 & \cdots & & u_n v_n \tau_n \end{pmatrix} \qquad (8)$$

is a symmetric semiseparable matrix.

Let us denote the generators for this symmetric S by $\hat{u}$ and $\hat{v}$,

$$\begin{aligned} \hat{u} = u &= (u_1, u_2, u_3, \cdots, u_n) \\ \hat{v} &= (u_1\tau_1, u_2\tau_2, u_3\tau_3, \cdots, u_n\tau_n). \end{aligned}$$

Therefore $S - \kappa I$ is a diagonal plus semiseparable matrix.
The Q factor of the QR factorization of a diagonal plus semiseparable matrix of order n, can be given by the product of $2n-2$ Givens rotations (see [11] for the details).

Due to the structure of the matrix involved, the £rst $n-1$ Givens rotations, $G_i, i = 1,\ldots,n-1$, applied from bottom to top (G_1^T acts on the last two rows of the matrix, annihilating all the elements in the last row of S below the main diagonal, G_2^T acts on the rows $n-2$ and $n-1$ of $G_1^T S$, annihilating all the elements in row $n-1$ below the main diagonal, G_{n-1}^T acts on the £rst two rows of $G_{n-2}^T \cdots G_1^T S$, annihilating the element in position $(2,1)$) reduce the semiseparable matrix S into an upper triangular one and the diagonal matrix κI into an upper Hessenberg one, respectively. Moreover let $\hat{Q} = G_1 G_2 \cdots G_{n-1}$, it can be easily checked that $S_l = S_u \hat{Q}$ is a lower triangular semiseparable matrix.

Let $H = \hat{Q}^T(S - \kappa I)$. The QR–factorization of H can be computed by means of $n-1$ Givens rotations $G_n, G_{n+1}, \ldots, G_{2n-2}$ such that G_n^T acts on the £rst two rows of H, annihilating the entry $(2,1)$, G_{n+1}^T acts on the rows 2 and 3 of $G_n^T H$, annihilating the entry $(3,2)$, ..., G_{2n-2}^T acts on the last two rows of $G_{2n-3}^T \cdots G_n^T H$, annihilating the entry $(n, n-1)$.

Taking into account that S_l is a lower triangular matrix, $\hat{Q}^T e_1 = G_{n-1}^T e_1$, and

$$\begin{aligned} H &= \hat{Q}^T(S - \kappa I) \\ &= \hat{Q}^T S_u^T S_u - \kappa \hat{Q}^T \\ &= S_l^T S_u - \kappa \hat{Q}^T, \end{aligned}$$

then

$$He_1 = S_l(1,1) S_u(1,1) e_1 - \kappa G_{n-1}^T e_1.$$

Moreover,

$$G_1 G_2 \cdots G_{n-1} G_n G_{n+1} \cdots G_{2n-2} e_1 = G_1 G_2 \cdots G_{n-1} G_n e_1$$

since $G_i e_1 = e_1,\ i = n+1,\ldots,2n-2$. This means that the £rst column of the Q factor of the QR–factorization of $S - \kappa I$ depends only on the product $G_1 G_2 \cdots G_{n-1} G_n$. Furthermore, let

$$\hat{S}_l = S_u G_1 G_2 \cdots G_{n-1} G_n = S_l G_n. \qquad (9)$$

7 Chasing the bulge

The matrix (9) differs form a lower triangular semiseparable matrix for a bulge in position $(1,2)$. In order to retrieve the lower triangular semiseparable structure an algorithm is presented in this section. At each step of the algorithm the bulge is chased downward one position along the super diagonal, by applying orthogonal transformations to $\hat{S}_l$. Only orthogonal transformations with the £rst column equal to e_1 are applied to the right of $\hat{S}_l$. Indeed, imposing this constraint, the £rst column of $G_1 \cdots G_n$ is not modi£ed if multiplied to the right by one of the latter orthogonal matrices.

Before describing the algorithm, we consider the following theorem.

Theorem 4 *Let*

$$C = \begin{pmatrix} u_1 v_1 & \alpha & 0 \\ u_2 v_1 & u_2 v_2 & u_2 v_3 \end{pmatrix} \tag{10}$$

with u_1, u_2, v_1, v_2, v_3 all different from zero. Then there exists a Givens transformation G such that,

$$\hat{C} = C \begin{pmatrix} 1 & 0 \\ 0 & G \end{pmatrix} \tag{11}$$

has a linear dependency between the £rst two columns of $\hat{C}$.

PROOF:
The theorem is proven by explicitly constructing the Givens matrix G. Denote the Givens transformation G in the following way,

$$G = \frac{1}{\sqrt{1+t^2}} \begin{pmatrix} t & -1 \\ 1 & t \end{pmatrix}. \tag{12}$$

Taking (10) and (12) into account, (11) can be written in the following way,

$$\hat{C} = \begin{pmatrix} u_1 v_1 & \frac{t\alpha}{\sqrt{1+t^2}} & \frac{-\alpha}{\sqrt{1+t^2}} \\ u_2 v_1 & \frac{t u_2 v_2 + u_2 v_3}{\sqrt{1+t^2}} & \frac{-u_2 v_2 + t u_2 v_3}{\sqrt{1+t^2}} \end{pmatrix}.$$

Dependency between the £rst two columns leads to the following condition on the coef£cients of the previous matrix:

$$\frac{t\alpha}{\sqrt{1+t^2}\, u_1 v_1} = \frac{t u_2 v_2 + u_2 v_3}{\sqrt{1+t^2}\, u_2 v_1}.$$

Simpli£cation leads to:

$$\frac{t\alpha}{u_1} = \frac{t u_2 v_2 + u_2 v_3}{u_2}$$

Extracting the factor t out of the previous equation proves the existence of the Givens transformation G.

$$t = \frac{v_3}{\left(\frac{\alpha}{u_1} - v_2\right)}$$

■

The next theorem yields the algorithm that transforms $\hat{S}_l$ into a lower triangular semiseparable matrix.

Theorem 5 *Let $\hat{S}_l$ be a matrix whose lower triangular part is semiseparable with generators u and v and the strictly upper triangular part is zero except for the entry $(1,2)$. Then there exist two orthogonal matrices $\tilde{U}$ and $\tilde{V}$ such that*

$$\tilde{S}_l = \tilde{U}\hat{S}_l\tilde{V}$$

is a lower triangular semiseparable matrix and $\tilde{V}e_1 = e_1$.

PROOF:
The theorem is proven by constructing an algorithm which transforms $\hat{S}_l$ into a lower triangular semiseparable matrix, in which the orthogonal transformations applied to the right have the £rst column equal to e_1. Without loss of generality we assume $\hat{S}_l \in \mathbb{R}^{5\times 5}$. Let

$$\hat{S}_l = \begin{pmatrix} \boxtimes & \otimes & 0 & 0 & 0 \\ \boxtimes & \boxtimes & 0 & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \end{pmatrix},$$

where $\otimes$ denotes the bulge to be chased. Moreover, the entries of the matrix satisfying the semiseparable structure are denoted by $\boxtimes$. At the £rst step a Givens transformation $\tilde{U}_1$ is applied to the left of $\hat{S}_l$ in order to annihilate the bulge,

$$\tilde{U}_1\hat{S}_l = \begin{pmatrix} \times & 0 & 0 & 0 & 0 \\ \times & \times & 0 & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \end{pmatrix}. \quad (13)$$

Although $\tilde{U}_1\hat{S}_l$ is lower triangular, the semiseparable structure is lost in its £rst two rows. In order to retrieve it, a Givens rotation $\tilde{V}_1$, constructed according to Theorem 4, and acting to the second and the third column of $\tilde{U}_1\hat{S}_l$ is applied to the right, in order to make the £rst two columns, in the lower triangular part, proportional.

$$\tilde{U}_1\hat{S}_l = \begin{pmatrix} \boxtimes & 0 & 0 & 0 & 0 \\ \times & \times & 0 & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \end{pmatrix} \xrightarrow{\tilde{U}_1\hat{S}_l\tilde{V}_1} \begin{pmatrix} \boxtimes & 0 & 0 & 0 & 0 \\ \boxtimes & \boxtimes & \times & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & \boxtimes \end{pmatrix}.$$

Hence, applying $\tilde{U}_1$ and $\tilde{V}_1$ to the right and to the left of $\hat{S}_l$, respectively, the bulge is moved one position downward the super diagonal (see £g. 1), retrieving the semiseparable structure in the lower triangular part. Recursively applying the latter procedure the matrix $\tilde{U}_4 \cdots \tilde{U}_1\hat{S}_l\tilde{V}_1 \cdots \tilde{V}_4$ is a lower triangular semiseparable matrix. Then the theorem holds choosing $\tilde{U} = \tilde{U}_4 \cdots \tilde{U}_1$ and $\tilde{V} = \tilde{V}_1 \cdots \tilde{V}_4$.

■

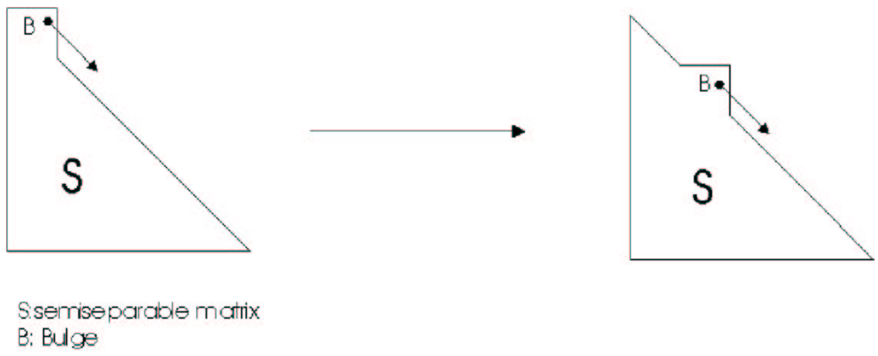

Figure 1: Graphical representation of the chasing

8 One iteration of the new method applied to upper triangular semiseparable matrices.

In this section we describe one iteration of the proposed algorithm for computing the singular values of an upper triangular semiseparable matrix. Morever we prove the equivalence between the latter iteration and one iteration of the implicit *QR*–method applied to UTSS matrices. One iteration of the proposed method consists of the following 4 steps.

Step 1. $n-1$ Givens transformations $G_1, \ldots, G_{n-1}$ are performed to the right of S_u swappping it into a lower triangular semiseparable matrix S_l.

Step 2. One more Givens transformation G_n is computed in order to introduce the shift. As seen in § 7, the application of this Givens transformation to the right of the lower triangular semiseparable matrix creates a bulge.

Step 3. The bulge is chased by $n-2$ Givens transformations, $G_{n+1}, \ldots, G_{2n-2}$ retrieving the lower triangular semiseparable structure.

Step 4. The latter matrix is swapped back to upper triangular form. This is done by applying $n-1$ more Givens transformations to the left, without destroying the semiseparable structure.

Remark 1 *Actually, the Givens rotations of Step 1 and Step 4 are not explicitely applied to the matrix, the semiseparable structure allows us to calculate the resulting semiseparable matrix (the representation of this matrix) in a very cheap way with $O(n)$ ¤ops.*

Remark 2 *The Givens rotations involved in Step 1, Step 2 and Step 3, are those described in § 6, needed to compute the Q factor of the QR factorization of $S_u^T S_u - \kappa I$.*

Remark 3 *If the shift is not considered, only step 1 and step 4 are performed at each iteration of the method.*

It remains to prove that one iteration of the latter method is equivalent to one iteration of the implicit QR–method applied to an upper triangular semiseparable matrix S_u , i.e., if Q_1 is the orthogonal factor of the QR factorization of $S_u^T S_u - \kappa I = S - \kappa I$, and Q_2 is the matrix of the product of the orthogonal matrices applied to the right of S_u during one iteration of the proposed method, then Q_1 and Q_2 are essentially the same, i.e.,

$$Q_1 = Q_2 diag(\pm 1, \ldots, \pm 1).$$

Assume an implicit QR–iteration is performed on the matrix S. This can be written in the following form:

$$Q_1^T S Q_1 = S_1. \tag{14}$$

Now we show how one iteration of the new method performed on the matrix S_u can also be rewritten in terms of the matrix $S = S_u^T S_u$. This is achieved in the following way. (All the steps mentioned in the beginning of the section are now applied to the matrix S_u.) First the $n-1$ Givens transformations are performed on the matrix S_u, transforming the matrix into lower triangular semiseparable form. In the following equations, all the transformations performed on the matrix S_u are £tted in the equation $S = S_u^T S_u$ to see what happens to the matrix S.

$$G_{n-1}^T \cdots G_1^T S G_1 \cdots G_{n-1} = \left(G_{n-1}^T \cdots G_1^T S_u^T\right)(S_u G_1 \cdots G_{n-1}) = ({S_l}^{(0)})^T {S_l}^{(0)}.$$

One more Givens transformation G_n is now applied, introducing a bulge in the matrix S_l.

$$G_n^T G_{n-1}^T \cdots G_1^T S G_1 \cdots G_{n-1} G_n = G_n^T ({S_l}^{(0)})^T {S_l}^{(0)} G_n.$$

Taking Theorem 4 into account, there exist two orthogonal matrices U and V, with $Ve_1 = e_1$, such that $U{S_l}^{(0)} G_n V$ is again a lower triangular semiseparable matrix. This leads to the equation:

$$V^T G_n^T G_{n-1}^T \cdots G_1^T S G_1 \cdots G_{n-1} G_n V = V^T G_n^T ({S_l}^{(0)})^T U^T U {S_l}^{(0)} G_n V.$$

The £nal step consists of swapping the lower triangular matrix $U{S_l}^{(0)} G_n V^T$ back into upper triangular semiseparable form. This is accomplished by applying $n-1$ more Givens rotations to the left of $U{S_l}^{(0)} G_n V$. Thus, denoted by $Q_2 = G_1 \cdots G_{n-1} G_n V$ and taking (8) into account, we have

$$Q_2^T S_u^T S_u Q_2 = S_2 \tag{15}$$

with Q_2 orthogonal and S_2 a semiseparable matrix.

We observe that $Q_1 e_1 = Q_2 e_1$. This holds because the £rst n Givens transformations are the same Givens transformations as performed in a QR step on S, and the fact that $Ve_1 = e_1$.

To prove that the orthogonal matrices Q_1 and Q_2 are essentially the same we need the following results

Proposition 1 *Suppose S_u is an upper triangular semiseparable matrix, with nonzero elements on the diagonal. Then the matrix $S = S_u^T S_u$ is nonsingular.*

PROOF:
Obvious. ■

In case $rank(A) = l \leq n \leq m$, the last $m-l$ rows and the last $n-l$ columns of the UTSS matrix, computed by the proposed reduction algorithm, are zero. Hence, the problem is reduced to apply the method to a UTSS matrix of order $n-l$.

Proposition 2 *Suppose S is a nonsingular symmetric semiseparable matrix. Then S can be written as the sum of a rank 1 matrix and a strictly upper triangular matrix, where the supdiagonal elements of this matrix are different from zero.*

PROOF:
This fact will be proven by contradiction. Assuming that there exist supdiagonal elements equal to zero. It will be proven that the matrix S has to be singular.

Assume the symmetric semiseparable matrix S has generators $u = [u_1, \ldots, u_n]^T$ and $v = [v_1, \ldots, v_n]^T$. One can write S as the sum of a rank 1 matrix and a strictly upper triangular matrix [2] $R = triu(vu^T - uv^T, 1)$.

$$S = uv^T + R.$$

Assume that there exists a certain $k \in \mathbb{N}$ such that $v_k u_{k-1} - u_k v_{k-1} = 0$, this will lead to a contradiction.

- Assume $u_k, u_{k-1}, v_k, v_{k-1}$ to be different from zero. Rows k and $k-1$ of the semiseparable matrix S will look like:

$$\begin{pmatrix} u_{k-1}v_1 & u_{k-1}v_2 & \cdots & u_{k-1}v_{k-2} & u_{k-1}v_{k-1} & u_k v_{k-1} & u_{k+1}v_{k-1} & \cdots & u_n v_{k-1} \\ u_k v_1 & u_k v_2 & \cdots & u_k v_{k-2} & u_k v_{k-1} & u_k v_k & u_{k+1}v_k & \cdots & u_n v_k \end{pmatrix}.$$

  Because of the semiseparable structure of S, row k and $k-1$ are dependent from element 1 up to element $k-1$, and both rows have dependency from element k up to element n. Because now $v_k u_{k-1} = u_k v_{k-1}$, the following equation holds (these are the columns $k-1$ and k):

$$\begin{pmatrix} u_{k-1}v_{k-1} & u_k v_{k-1} \\ u_k v_{k-1} & u_k v_k \end{pmatrix} = \begin{pmatrix} u_{k-1}v_{k-1} & u_k v_{k-1} \\ u_{k-1}v_k & u_k v_k \end{pmatrix}$$

  This means that row $k-1$ and row k in the semiseparable matrix S are dependent. This is in con¤ict with the nonsingularity of the matrix S.

- Assume $u_k = 0$ (the other cases can be dealt with in the same way). This means that either v_k or u_{k-1} has to be zero. Substituting these values in the rows $k-1$ and k immediately reveals the dependency between these rows which is in contradiction with the nonsingularity of the semiseparable matrix S.

[2] We denote the strictly upper triangular part using Matlab-style notation: $triu(\cdot, 1)$).

■

Now we are able to prove that an analogue of the Q-implicit theorem for symmetric tridiagonal matrices holds also for symmetric semiseparable matrices.

Theorem 6 (Q-implicit theorem for semiseparable matrices) *Suppose A is a nonsingular symmetric matrix and we have the following two equations:*

$$\begin{aligned} Q_1^T A Q_1 &= S_1 \quad (16) \\ Q_2^T A Q_2 &= S_2 \quad (17) \end{aligned}$$

with $Q_1 e_1 = Q_2 e_1$, where S_1 and S_2 are two semiseparable matrices and Q_1 and Q_2 are orthogonal matrices. Then the matrices S_1 and S_2 are essentially the same (see equation 1). Moreover, Q_1 and Q_2 are essentially the same.

PROOF:
Denoting $W = Q_1^T Q_2$ and using the equations (16) and (17) the following equality holds:

$$S_1 W = W S_2 \quad (18)$$

According to Proposition 2 we can write the matrices S_1 and S_2 in the following form:

$$\begin{aligned} S_1 &= u^{(1)} {v^{(1)}}^T + R^{(1)} \\ S_2 &= u^{(2)} {v^{(2)}}^T + R^{(2)} \end{aligned}$$

with $R^{(1)}$ and $R^{(2)}$ strictly upper triangular matrices with nonzero elements on the supdiagonals. The vectors $u^{(1)}, v^{(1)}, u^{(2)}$ and $v^{(2)}$ are the generators of the semiseparable matrices S_1 and S_2, respectively. They are normalized in such a way that $v_1^{(1)} = v_1^{(2)} = 1$. Together with equation (18) one gets:

$$\left(u^{(1)} {v^{(1)}}^T + R^{(1)}\right) W = W \left(u^{(2)} {v^{(2)}}^T + R^{(2)}\right). \quad (19)$$

Denoting the columns of W as $(w_1, w_2, \ldots, w_n)$, the fact that $Q_1 e_1 = Q_2 e_1$ leads to the fact that $w_1 = e_1$. Multiplying (19) to the right by e_1, gives

$$u^{(1)} = W u^{(2)}. \quad (20)$$

Using this equation, we prove now by induction that

$$\begin{aligned} W &= diag(\pm 1, \pm 1, \ldots, \pm 1) \quad (21) \\ {v^{(1)}}^T W &= {v^{(2)}}^T. \quad (22) \end{aligned}$$

$k = 1$. This is a trivial step, because $v_1^{(1)} = v_1^{(2)} = 1$ and $w_1 = e_1$.

$k > 1$. Suppose the equations (21) and (22) hold up to the $(k-1)$–th element of $v^{(1)}$ and $v^{(2)}$ and $(k-1)$–th column of W. Taking (20) into account, (19) becomes

$$u^{(1)} \left({v^{(1)}}^T W - {v^{(2)}}^T\right) = \left(W R^{(2)} - R^{(1)} W\right). \quad (23)$$

Multiplying (23) to the right by e_k, we have

$$u^{(1)}\left(v^{(1)^T}W - v^{(2)^T}\right)e_k = \left(WR^{(2)} - R^{(1)}W\right)e_k. \tag{24}$$

Because of the special structure of $W, R^{(1)}$ and $R^{(2)}$ the element in the £nal position in the vector on the right–hand–side of (24) is equal to zero. Because $u_n^{(1)}$ is different from zero, (otherwise A would have been singular) the following equation holds:

$$u_n^{(1)}\left(v^{(1)^T}W - v^{(2)^T}\right)e_k = 0 \tag{25}$$

This means that

$$v^{(1)^T}w_k - v_k^{(2)} = 0 \tag{26}$$

holds. Therefore equation (22) is already satis£ed up to element k:

$$v^{(1)^T}(w_1, w_2, \ldots, w_k) = \left(v_1^{(2)}, v_2^{(2)}, \ldots, v_k^{(2)}\right) \tag{27}$$

Using equation (27) together with equation (24) leads to the fact that the complete right–hand–side of equation (24) has to be zero. This gives the following equation:

$$R^{(1)}We_k = WR^{(2)}e_k \tag{28}$$

leading to

$$R^{(1)}We_k = W\left(\sum_{j=1}^{k-1}\alpha_j e_j\right) \tag{29}$$

with the α_j as nonzero factors apearing in $R^{(2)}$. Because of the structure of W and the fact that $R^{(1)}$ is strictly upper triangular with nonzero supdiagonal elements, w_k can only have his £rst k elements different from zero. This together with the fact that W is orthogonal means that $w_k = \pm e_k$.

Using the equations (20), (21) and (22), states the fact that S_1 and S_2, and Q_1 and Q_2 are essentially the same. ■

As a consequence, one iteration of the proposed method is equivalent to one iteration of the implicit QR-method applied to UTSS matrices.

Moreover, we have "implicitly" proven that the semiseparable structure is preserved by the QR–method. In fact, the following theorem holds.

Theorem 7 *Let $S^{(1)}$ be a symmetric semiseparable matrix. Consider the QR–method*

$$\begin{cases} [Q^{(i)}, R^{(i)}] = qr(S^{(i)} - \kappa_i I) \\ S^{(i)} = R^{(i)}Q^{(i)} + \kappa_i I \end{cases} \quad i = 1, 2, \ldots,$$

where κ_i, $i = 1, 2, \ldots,$ are suitable shifts. Then $\{S^{(i)}\}$ is a sequence of symmetric semiseparable matrices.

PROOF:The proof follows directy form Th. 6. ■

9 The numerical method

Only a brief description of the numerical method is given.

Suppose we have an m by n matrix A, whose singular values we would like to compute (with $m \geq n$).

- step 1: The £rst step consists of transforming the matrix A into the UTSS form for applying the implicit QR–method to UTSS matrices. This means that A is transformed, via orthogonal transformations to the left and the right, into a UTSS matrix. It turns out that if $rank(A) = l \leq n \leq m$, then the last $m-l$ rows and the last $n-l$ columns of the computed UTSS matrix are zero. In this case the problem is reduced to apply the method to compute the singular value of a UTSS matrix of order $n-l$.

- step 2: In this step an implicit QR-iteration is performed to an upper triangular semiseparable matrix. A complete explanation of this step can be found in the previous sections.

- step 3: Check if the output from step 2 has converged to a singular value. If so, cut off this singular value and go back to step 2, keep doing so until all the singular values are found. For details on the cutting criterion, we refer the interested reader to [12].

A little more has to be said about the implementation, the complete paper is written in terms of the generators u and v of the semiseparable matrix. Although the representation of a semiseparable matrix in terms of its generators u and v is usefull from a theoretical point of view, it is unstable. Especially when applying the QR algorithm, the vectors u and v tend to loose very quick a lot of digits. Therefore we choose to use another way to represent the semiseparable matrices, by means of sequence of Givens transformations and a vector. More information about this representation can for example be found in [10].

10 Numerical experiments

10.1 Approximating the singular values via the UTSS reduction

As mentioned in § 2, the proposed algorithm for reducing real matrices into UTSS ones gives good approximations of the largest singular values after few steps. In these £rst experiments we show that the proposed reduction can be used as a Rank–revealing factorization [1, 8, 2], too. In particular, it is compared with the QLP decomposition [8] in the next three examples. In the pictures, the solid lines indicate the singular values and the dashed lines indicate the absolute value of the entries in the main diagonal of L_{QLP} (left) and $UTSS$ (right), respectively. L_{QLP} denotes the lower triangular factor of the QLP factorization [8].

Example 1 *In this example we reconstruct the matrix considered in [8, p. 1341]. A* *square matrix* $\hat{A} \in \mathbb{R}^{100 \times 100}$ *is considered, whose £rst* $j = 50$ *singular values are*

$$\begin{cases} \hat{\sigma}_i = 10^{-\alpha(i-1)/(j-1)}, & i = 1, \dots, j \\ \hat{\sigma}_i = 0 & i = j+1, \dots, 100. \end{cases} \tag{30}$$

where $\alpha = 1.5$. *The matrix* A *is obtained perturbing* $\hat{A}$,

$$A = \hat{A} + \hat{\sigma}_j 10^{-\beta} \Gamma, \tag{31}$$

where $\beta = 2.5$ *and* $\Gamma \in \mathbb{R}^{100 \times 100}$, *with random entries, chosen from a normal distribution with mean zero and variance one.*

In £g. 2 the performance of the QLP and the upper triangular semiseparable decompositions (UTSS) are compared. It can be seen that the curve of the approximation of the singular values given by UTSS decomposition tracks the singular values with remarkable £delity. In Table 1 we report the maxima of the absolute and relative errors

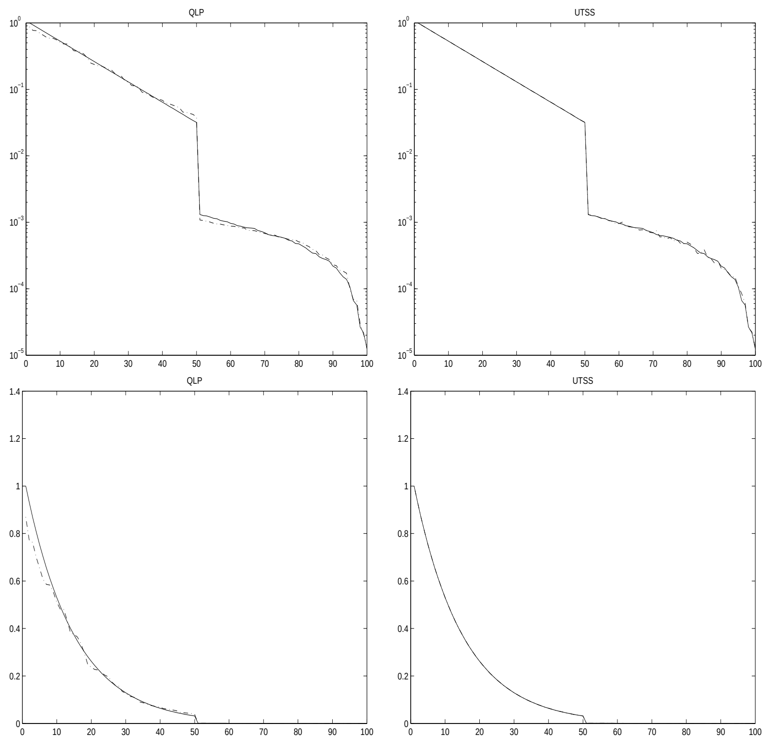

Figure 2: QLP (left) and UTSS (right) decompositions compared. Top: log scale, bottom: real scale

of the approximations of the £rst 50 *singular values obtained by the two considered decompositions.*

M	$\max_{i\in 1,\ldots,50} \lvert\sigma_i - \lvert diag(M(i,i))\rvert\rvert$	$\max_{i\in 1,\ldots,50} \frac{\lvert\sigma_i - \lvert diag(M(i,i))\rvert\rvert}{\sigma_i}$
QLP	$1.6006e-001$	$1.7175e-001$
UTSS	$1.2094e-06$	$3.3261e-05$

Table 1: Absolute and relative errors of the singular value approximation by QLP and UTSS

In the next two examples the matrices are constructed in a way similar to the one considered in Example 1, with different values of j,α and β.

Example 2 *In this second example the parameters* j,α *and* β *in (30) and (31) are chosen equal to* $2, 0.5$ *and* 2.0, *with a clear gap between the second and the third singular value (see £g. 3). Also in this case the UTSS decomposition behaves better than QLP. As mentioned before, information on the largest singular values can be*

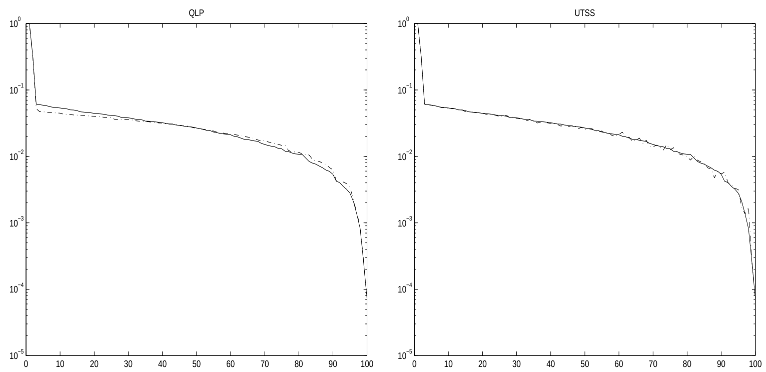

Figure 3: QLP (left) and UTSS (right) decompositions compared. (log scale)

gained after few steps of the UTSS reduction. In Table 2 the two largest singular values of the matrix together with the values $|SS^{(i)}((k,k))|$, $k = 1,2$, $i = 1,\ldots,7$, *i.e., the absolute values of the £rst two entries in the main diagonal of the matrix obtained after i steps of the UTSS reduction. Moreover, the two £rst entries in the main diagonal of the triangular factor* L_{QLP} *of the QLP decompsition are reported. It can be seen that after few steps of the URSS reduction the two largest singular values are accurately computed.*

Example 3 *In this third example the parameters* j,α *and* β *in (30) and (31) are chosen equal to* $3, 1.5$ *and* 4.0, *There is a large gap between the third and the fourth singular value (see £g. 4). In table 3 the three largest singular values of the matrix together with the values* $|SS^{(i)}((k,k))|$, $k = 1,2,3$, $i = 1,\ldots,8$, *i.e., the absolute values of the £rst three entries in the main diagonal of the matrix obtained after i steps of the UTSS reduction.*

	σ_1	σ_2
	$1.004007749617077e+00$	$3.171647946462712e-01$
i	$\lvert SS^{(i)}((1,1))\rvert$	$\lvert SS^{(i)}((2,2))\rvert$
1	$9.003431675028809e-01$	$6.923270811147938e-03$
2	$1.002984885934289e+00$	$2.858623233957385e-01$
3	$1.003997546826368e+00$	$3.171502340311552e-01$
4	$1.004007648011370e+00$	$3.171648133219319e-01$
5	$1.004007748605242e+00$	$3.171647949543492e-01$
6	$1.004007749607001e+00$	$3.171647946494437e-01$
7	$1.004007749616977e+00$	$3.171647946463032e-01$
8	$1.004007749617077e+00$	$3.171647946462718e-01$
	$\lvert L_{QLP}(1,1)\rvert$	$\lvert L_{QLP}(2,2)\rvert$
	$9.871546358974473e-01$	$3.087229505180081e-01$

Table 2: Approximation of the two largest singular values after *i* steps of the UTSS reduction

10.2 Accuracy and ef£ciency of the implicit *QR*–method

Numerical tests are performed comparing the behavior of the classical and the proposed algorithm for computing the singular values of several matrices. Special attention is paid to the accuracy of both the algorithms for different sets of the singular values and to the number of *QR* steps needed to compute all the singular values of the matrices. The £rst £gure shows a comparison in number of implicit *QR* iterations performed. It shows that the semiseparable approach needs less steps in order to £nd the singular values but one should not forget that a semiseparable implicit *QR* step costs a little more than a corresponding step on the bidiagonal.

Figure 6 and Figure 7 show comparisons in accuracy of the two approaches. In the £rst £gure the singular values were chosen equal spaced, in the second approach the singular values ranged from 1 to *n*. Both £gures show that the two approaches are equally accurate.

11 Conclusion and future work.

In this paper an iterative method to compute the singular values of a real matrix is presented. The matrix is £rst reduced into an upper triangular semiseparable one by means of orthogonal transformations. We have proved that the latter reduction can be considered as a kind of nested subspace iteration, where the size of the subspace is increased by one dimension at each step of the reduction. As a consequence the largest singular values, are already computed with high precision after few steps of the algorithm. Hence this algorithm can be used for solving problems where only the knowledge of the largest singular values, and the corresponding vectors, is needed [6, 14, 13, 17, 18].

Once the upper triangular semiseparable matrix has been computed, its singular val-

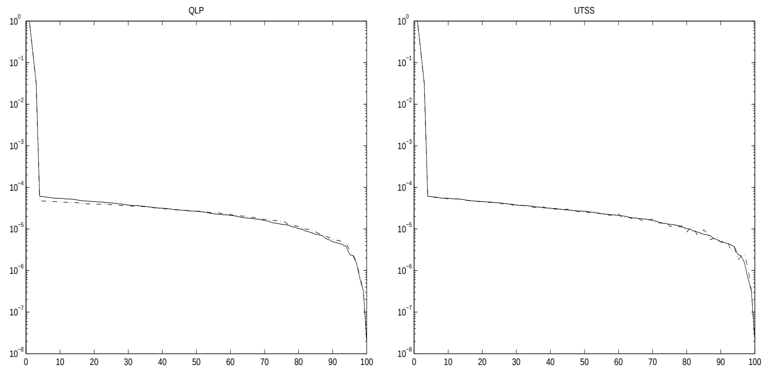

Figure 4: Rank determination: low rank. QLP decomposition (left), UTSS decomposition (right)

ues can be computed reapplying the proposed algorithm to the semiseparable matrix in an iterative fashion (in this case the sequence of the generated semiseparable matrices converges to a block upper triangular semiseparable matrix, where the singular values of each block are equal).

However, to compute the singular value of an upper triangular semiseparable matrix we have developed an iterative method. We have proved that each iteration of the latter method is equivalent to an iteration of the implicit *QR*–method applied to an upper triangular semiseparable matrix.

Future work will be concerned with a detailed study on an accurate criterion of splitting the semiseparable matrix generated by the algorithm into a block diagonal matrix, whose blocks are upper triangular semiseparable matrices, i.e. a criterion that allows to divide when a nondiagonal block of the matrix can be considered *"negligible"*.

	σ_1	σ_2	σ_3
	$1.000004042684463e+00$	$1.778201642674659e-01$	$3.161972544018923e-02$
i	$\lvert SS^{(i)}((1,1))\rvert$	$\lvert SS^{(i)}((2,2))\rvert$	$\lvert SS^{(i)}((3,3))\rvert$
1	$9.967626749215344e-01$	$1.035601411890967e-03$	$2.608369559115160e-04$
2	$1.000000999222685e+00$	$1.718996786146044e-01$	$5.201067496428890e-04$
3	$1.000004039641782e+00$	$1.778139224768302e-01$	$3.161900862253057e-02$
4	$1.000004042681421e+00$	$1.778201580266497e-01$	$3.161972655001837e-02$
5	$1.000004042684460e+00$	$1.778201642612264e-01$	$3.161972544129883e-02$
6	$1.000004042684463e+00$	$1.778201642674597e-01$	$3.161972544019034e-02$
7	$1.000004042684463e+00$	$1.778201642674659e-01$	$3.161972544018923e-02$
	$\lvert L_{QLP}(1,1)\rvert$	$\lvert L_{QLP}(2,2)\rvert$	$\lvert L_{QLP}(3,3)\rvert$
	$9.968820908796829e-01$	$1.782046218248874e-01$	$3.164898941938965e-02$

Table 3: Approximation of the three largest singular values after i steps of the UTSS reduction

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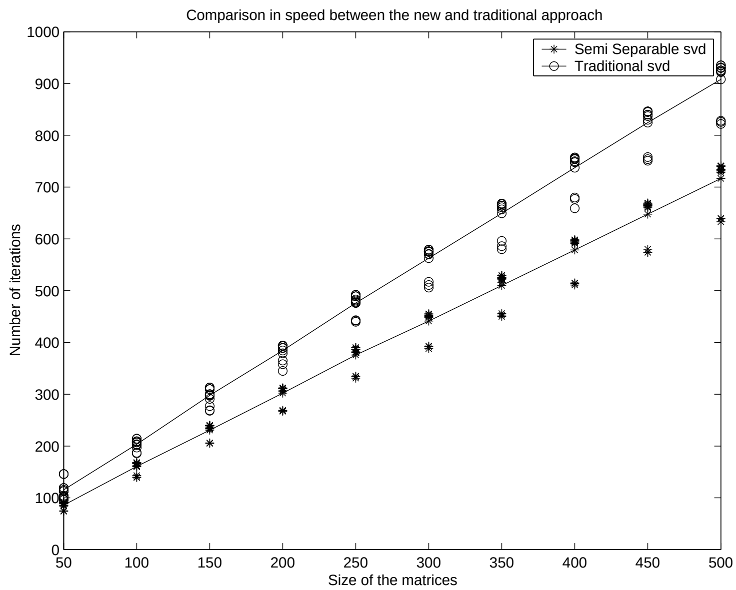

Figure 5: **Number of implicit *QR* steps**

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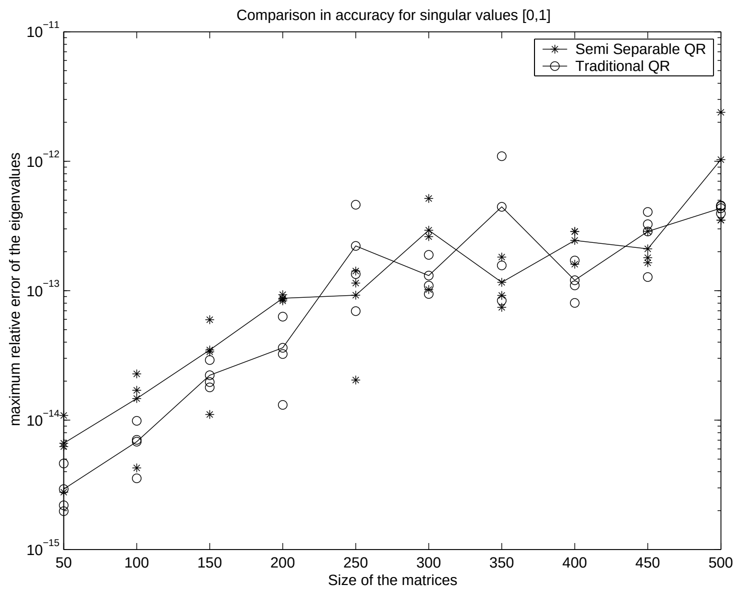

Figure 6: **Equal spaced singular values in** $(0, 1]$

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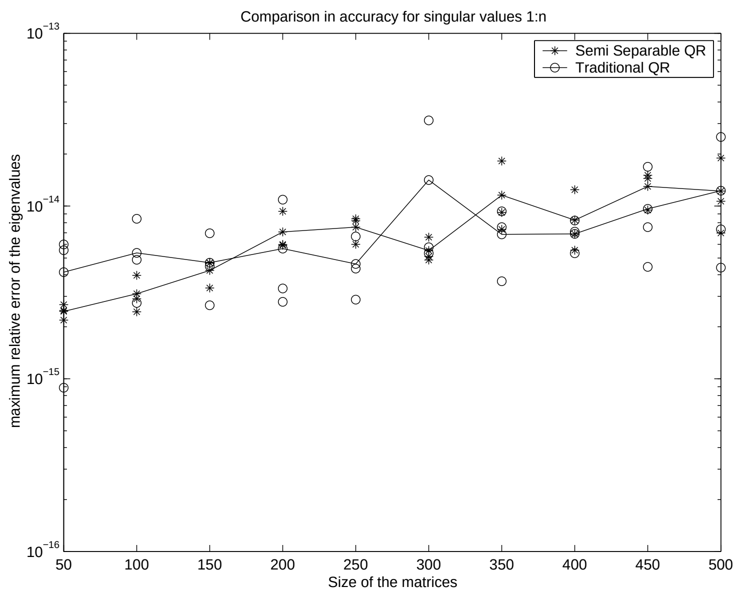

Figure 7: **Eigenvalues in** $1 : n$