Structures preserved by the QR-algorithm

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Report TW 399, August 2004

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Abstract

In this paper we investigate some classes of structures that are preserved by applying a (shifted) QR-step on a matrix A. We will handle two classes of such structures: the first we call polynomial structures, for example a matrix being Hermitian or Hermitian up to a rank one correction, and the second we call rank structures, which are encountered for example in all kinds of what we could call Hessenberg-like and lower semiseparable-like matrices. An advantage of our approach is that we define a structure by decomposing it as a collection of 'building stones' which we call structure blocks. This allows us to state the results in their natural, most general context.

Keywords : (shifted) QR-algorithm, Hessenberg-like matrices, lower semiseparable-like matrices, rank structure, polynomial structure
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1 Introduction.

It is a classical result in numerical linear algebra that, when applying the QR-algorithm on an (unreduced) Hessenberg matrix, the resulting matrix is again of Hessenberg type. A similar statement can be made for Hermitian matrices, thus the property of being Hermitian is also preserved by the QR-algorithm. Combining these two properties, one is led to the classical $\mathcal{O}(n)$ algorithm for applying a QR-step on a Hermitian, tridiagonal matrix: see [7], p. 417 for the tridiagonal and p. 342 for the Hessenberg case.

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Besides the classical theory, recently several papers have appeared which study the QR-algorithm for specific classes of matrices, having certain structure which is preserved by applying a QR-step. In [1], several matrix shapes are studied which are invariant under the QR-algorithm. In [2], the preservation of a suitable structure is used to devise an efficient implementation of the QR-algorithm for Frobenius (i.e., companion) matrices. The QR algorithm is especially useful for this class of matrices, since it can be used here to yield an iterative solver for polynomial root location. In [5], the preservation of semiseparable plus diagonal structure by applying a QR-step is proved as a consequence of the theory of 'rational Krylov matrices'. In [3], an efficient implementation is devised for what the authors call 'generalized semiseparable matrices'. For both these examples, the structure includes the so-called arrowhead matrices, which just as Frobenius matrices are a useful class for polynomial root location. In [10], an efficient and implicit QR-solver is described for the case of semiseparable matrices, using the so-called Givens-vector representation to obtain stable computations. By using a preliminary similarity transformation into semiseparable form, the QR-algorithm can be used here to compute the eigenvalue decomposition of an arbitrary Hermitian matrix: see [9].

In this paper, we investigate from a theoretical point of view two general classes of structure which are preserved by applying the QR-algorithm. The structures we consider generalize the classical and well-known cases of Hessenberg and Hermitian structures, and they also generalize the structures which are considered in the papers mentioned above (except the structures of [1], which are of a different flavour).

We make a distinction between two types of structure: polynomial and rank structures. For the case of rank structures, the structure can be decomposed as a collection of so-called 'structure blocks'. One feature of these structure blocks is that they are an intrinsic generalization of the 'shifted' QR-algorithm, in the sense that every block is allowed to have its own shift element. Apart from the level of generality resulting from this approach, it will also have a benefit for the proofs, which can then be restricted to the more easy case of the QR-algorithm without shift.

For the case of rank structures, in general the preservation of structure will only hold in the *nonsingular* case. The solution of the singular case is deferred to [4]; this is because it requires the introduction of several concepts (effectively eliminating QR-decompositions, sparse Givens patterns) which have a more technical flavour than the exposition in this paper, and which allow a detailed, stand-alone treatment.

For further reference, let us recall here the two defining equations of the shifted QR-algorithm. These equations show how to obtain from the matrix $A^{(\nu)} \in \mathbb{C}^{n\times n}$ a new iterate $A^{(\nu+1)}$:

$$A^{(\nu)} - \lambda I = QR \tag{1}$$

$$A^{(\nu+1)} = RQ + \lambda I, \tag{2}$$

where $\lambda \in \mathbb{C}$ is called the *shift*, Q is unitary and R upper triangular. As it is known, by appropriately choosing shifts the matrices $A^{(\nu)}$ converge to (block) upper triangular form, or to diagonal form in the Hermitian case, and hence the QR-algorithm can be used to determine the eigenvalues of a given matrix $A = A^{(0)}$.

From the defining equations, one can easily deduce the following similarity relations

$$A^{(\nu+1)} = Q^H A^{(\nu)} Q \tag{3}$$

$$A^{(\nu+1)} = R A^{(\nu)} R^{-1}, \tag{4}$$

where (4) is of course only valid if R is nonsingular (equivalently, if $A^{(\nu)} - \lambda I$ is nonsingular). It turns out that Equations (3) and (4) are very useful for the preservation of structure: more precisely (3) will lead to the preservation of polynomial structures (Section 2), while (4) will lead to the preservation of rank structures (Section 3).

2 Polynomial structures.

The first type of preserved structure is rather straightforward.

Definition 1 *We define a polynomial structure on $\mathbb{C}^{n\times n}$ as a collection $\mathcal{P} = \{p_k\}_k$ where each p_k is a polynomial in 7 variables. We say a matrix $A \in \mathbb{C}^{n\times n}$ to satisfy the polynomial structure if for every k, there exist a Hermitian matrix* Herm_k*, a unitary matrix* Uni_k *and a rank at most r matrix* $(\mathrm{Rk}\ r)_k$ *such that*

$$p_k(A, A^H, A^{-1}, A^{-H}, \mathrm{Herm}_k, \mathrm{Uni}_k, (\mathrm{Rk}\ r)_k) = 0.$$

Given some polynomial structure $\mathcal{P}$, we denote by $\mathcal{M}_{\mathcal{P}}$, or shortly $\mathcal{M}$ the set of matrices in $\mathbb{C}^{n\times n}$ which satisfy this polynomial structure.

Theorem 2 *Polynomial structure is preserved by the QR-algorithm, i.e. $A^{(\nu)} \in \mathcal{M}$ implies also the new QR-iterate $A^{(\nu+1)} \in \mathcal{M}$ for every polynomial structure $\mathcal{P}$. And conversely, so no extra structure can be introduced.*

PROOF. Obviously, any unitary matrix Q can be 'pulled through' such a polynomial relation, in the sense that

$$Q^H p(A, A^H, A^{-1}, A^{-H}, \mathrm{Herm}, \mathrm{Uni}, \mathrm{Rk}\ r)Q = p(A_Q, A_Q^H, A_Q^{-1}, A_Q^{-H}, \mathrm{Herm}_Q, \mathrm{Uni}_Q, (\mathrm{Rk}\ r)_Q),$$

where

$$A_Q := Q^H A Q, \quad \mathrm{Herm}_Q := Q^H (\mathrm{Herm}) Q, \quad \mathrm{Uni}_Q := Q^H (\mathrm{Uni}) Q, \quad (\mathrm{Rk}\ r)_Q := Q^H (\mathrm{Rk}\ r) Q.$$

Note that Herm_Q, Uni_Q and $(\mathrm{Rk}\ r)_Q$ are again Hermitian, unitary and of rank at most r, respectively. It follows that all polynomial structures that are satisfied by A, must carry over to the matrix $A_Q = Q^H AQ$. By (3), in particular this must hold for the matrices $A^{(\nu)}$ and $A^{(\nu+1)} = Q^H A^{(\nu)} Q$ which are obtained by applying the QR-algorithm.

For the converse statement we can use the same argument, but this time switching the roles of Q and Q^H by using the equation $A^{(\nu)} = QA^{(\nu+1)}Q^H$.

□

Let us give some applications of Theorem 2. The theorem can be applied to the polynomial structures $\mathcal{P}$ which yield the classes $\mathcal{M}$ of Hermitian matrices: $A - A^H = 0$, or alternatively $A - \mathrm{Herm} = 0$; normal matrices: $AA^H - A^H A = 0$, or alternatively $A^H = p(A)$ for a certain polynomial p; unitary matrices: $A^H - A^{-1} = 0$, or alternatively $A - \mathrm{Uni} = 0$ (see [8, 6] for an implementation of the QR-algorithm for unitary Hessenberg matrices); unitary plus rank at most r matrices: $A - \mathrm{Uni} - \mathrm{Rk}\ r = 0$; matrices having some prescribed spectrum: $p_\chi(A) = 0$ where p_χ is the characteristic polynomial of A, and so on. Thus all these structures are preserved by applying the QR-algorithm.

Also Frobenius (i.e., companion) matrices can be considered. In [2], it is shown that these matrices satisfy the polynomial structure $A - A^{-H} - \mathrm{Rk}\ 2 = 0$, and furthermore this observation was used to devise an efficient implementation of the QR-algorithm for this class of matrices.

In [3], an efficient QR-solver is devised for a class of matrices which satisfy the polynomial relation $A - \mathrm{Herm} - \mathrm{Rk}\ 1 = 0$. Thus these matrices are Hermitian up to a rank 1 correction. (In fact they were assumed to satisfy also some other kind of structure; see further).

Remark 3 *Some generalizations of polynomial structure:*

1. *The variable* Rk r *denotes a matrix of rank at most r, or equivalently a matrix with $\lambda = 0$ being at least an $(n-r)-$fold eigenvalue. This can be generalized by requiring a matrix to have a fixed eigenvalue spectrum and/or singular spectrum (in particular, a fixed 2-norm of the matrix), since both these spectra are preserved by a similarity transformation $A \mapsto Q^H AQ$.*

2. *Apart from* Herm*,* Uni *and* Rk r*, we can in fact introduce an extra variable for any kind of polynomial structure, and in this way obtain several new structures. For example, we can consider the structure $A = \mathrm{Herm} + C$, where the variable C denotes a correction matrix having rank at most r and 2-norm not exceeding some given value $c > 0$. Another example is the structure $i(A - A^H) = C$ where $i := \sqrt{-1}$ and C denotes a Hermitian matrix having rank equal to 2 and inertia given by $(1, 1, n-2)$. We could even allow a set of several variables $\{(\mathrm{Herm})_i\}_i$, $\{(\mathrm{Uni})_i\}_i$, $\{(\mathrm{Rk}\ r_i)_j\}_{i,j}$, ... to appear in the polynomial relations p_k.*

3. *Apart from A^{-1} and A^{-H}, the polynomial relations may also contain subexpressions of the form $(A^2 + A)^{-1}$, $(A + \mathrm{Herm})^{-1}$, and so on. Thus the polynomial structures could be generalized to 'rational structures'.*

For several of the mentioned examples, the matrices under consideration do not only satisfy a *polynomial* structure, but also what we could call a *rank structure* in their lower triangular part; for example Frobenius matrices satisfy a Hessenberg type of structure and the matrices in [3] were assumed to be lower semiseparable plus diagonal. We will handle these structures now from a general point of view.

3 Rank structures.

We start with the definition of rank structure.

Definition 4 *We define a rank structure on $\mathbb{C}^{n\times n}$ as a collection of so-called structure blocks $\mathcal{R} = \{\mathcal{B}_k\}_k$. Each structure block $\mathcal{B}_k$ is characterized as a 4-tuple*

$$\mathcal{B}_k = (i_k, j_k, r_k, \lambda_k),$$

where i_k is the row index, j_k the column index, r_k the rank upper bound and $\lambda_k \in \mathbb{C}$ is called the shift element of $\mathcal{B}_k$. We say a matrix $A \in \mathbb{C}^{n\times n}$ to satisfy the rank structure if for each k,

$$\text{Rank } A_k(i_k : n, 1 : j_k) \leq r_k, \quad \textit{where } A_k = A - \lambda_k I.$$

Thus after subtracting the shift element, we must get a low rank block. Given some rank structure $\mathcal{R}$, we denote by $\mathcal{M}_{\mathcal{R}}$, or shortly $\mathcal{M}$ the set of matrices in $\mathbb{C}^{n\times n}$ which satisfy the structure. As a special case, when all structure blocks $\mathcal{B}_k$ have shift λ_k equal to zero, then we speak about a pure rank structure on $\mathbb{C}^{n\times n}$. We denote such a structure by $\mathcal{R}_{\text{pure}}$, and we use the notation $\mathcal{M}_{\mathcal{R}_{\text{pure}}}$, or shortly $\mathcal{M}_{\text{pure}}$ to denote the class of matrices which satisfy this pure rank structure.

Convention 5 *When the structure block $\mathcal{B}_k$ does not intersect the diagonal, then the shift element λ_k has no meaning and we agree to set it equal to zero. When some of the indices i_k or j_k fall out of the allowed range $\{1, \ldots, n\}$, we agree to consider the structure block $\mathcal{B}_k$ as meaningless. Also structure blocks which are identically satisfied (for example the matrix element $a_{n,1}$ being of rank at most 2), or which are implied by other structure blocks, are considered meaningless. Structures $\mathcal{R}$, $\tilde{\mathcal{R}}$ which are obtained from each other by adding or removing a number of meaningless structure blocks, can be considered as equivalent. Indeed, the corresponding classes of matrices satisfy $\mathcal{M}_{\mathcal{R}} = \mathcal{M}_{\tilde{\mathcal{R}}}$.*

Figure 1 shows an example with two structure blocks.

A general and useful example of pure structure is the class $\mathcal{M}_{\text{pure}} = \mathcal{S}_{(s,r)}$ of (s, r)-*lower semiseparable matrices*, where $-(n-1) \leq s \leq n-1$ is the *subdiagonal index* and $r \geq 0$ is the *semiseparability rank*. We can define this class by using the structure blocks $\mathcal{B}_k = (i_k, j_k, r_k, \lambda_k) = (k - s, k, r, 0)$, $k = 1, \ldots, n$. Stated otherwise, we have that $A \in \mathcal{S}_{(s,r)}$ if and only if every rectangular submatrix that

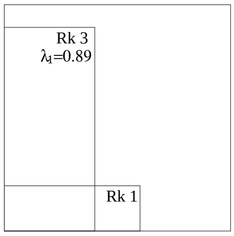

Figure 1: Example of a rank structure with two structure blocks. The left structure block $\mathcal{B}_1$ intersects the diagonal and has shift $\lambda_1 = 0.89$, while the second structure block $\mathcal{B}_2$ is 'pure'.

can be taken out of the part that is lying on and beneath the sth subdiagonal of A, is of rank at most r. Figure 2 illustrates the class $\mathcal{S}_{(s,r)}$ with s negative.

As a special case, if $(s, r) = (0, 1)$ then the class $\mathcal{S}_{(s,r)}$ will yield us what we could call the class of (usual) lower semiseparable matrices. Other examples of classes $\mathcal{S}_{(s,r)}$ are Hessenberg matrices with k subdiagonals: $(s, r) = (-k - 1, 0)$, $k \geq 0$, with $k = 1$ corresponding to the usual Hessenberg matrices, and $k = 0$ for upper triangular matrices.

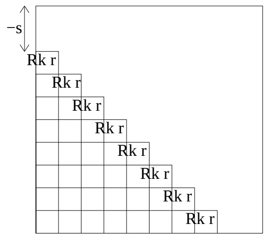

Figure 2: Example of a class $\mathcal{S}_{(s,r)}$, with negative subdiagonal index s. Because $s < 0$ in this case, the structure does not reach the diagonal.

As an example of rank structures which are not pure, a general example is the class $\mathcal{M}$ of $(0, r)$-*lower semiseparable plus diagonal matrices.* We can define this class by using the structure blocks $\mathcal{B}_k = (i_k, j_k, r_k, \lambda_k) = (k, k, r, \lambda_k)$, $k = 1, \ldots, n$, where the λ_k are the so-called *diagonal elements.* The meaning of this is that by subtracting the λ_k from the diagonal, every matrix that can be taken out of the lower triangular part of the matrix (including the diagonal) must have rank at most r. For $r = 0$ this yields the usual upper triangular matrices, including the information about their diagonal, and for $r = 1$ these matrices can be called (usual) lower semiseparable plus diagonal matrices.

Remark 6 *1. Every rank structure induces a pure structure. Thus for every class $\mathcal{M}$ we have $\mathcal{M} \subseteq \mathcal{M}_{\text{pure}}$, where $\mathcal{M}_{\text{pure}}$ is obtained by restricting to the induced, lower triangular rank structure (Including, if there were, the* *structure blocks which intersect the diagonal and additionally have $\lambda_k = 0$). Remark that a single structure block $\mathcal{B}_k$ will in general induce several pure blocks below the diagonal: see Figure 3. In the sequel, we will be mainly interested in one of them: setting $l_k = \min\{j_k, i_k - 1\}$, then we define the induced left pure structure block of $\mathcal{B}_k$ as the 4-tuple $\mathcal{B}_{\text{left},k} = (i_k, l_k, r_k, 0)$ if $\lambda_k \neq 0$, and $\mathcal{B}_{\text{left},k} = \mathcal{B}_k$ if $\lambda_k = 0$.*

2. *An important observation is that, if A is a matrix having some general rank structure, then the shifted matrix $A - \lambda I$ will again have rank structure, with shift elements of the structure blocks equal to $\lambda_k - \lambda$. As a consequence, to investigate the preservation of rank structures, it follows obviously from the QR-equations (1) and (2) that we are allowed to forget about the shift λ which is built in in the QR-algorithm, and instead just absorb it into the structure! Hence in the sequel, all our theorems will be stated for the QR-algorithm without shift.*

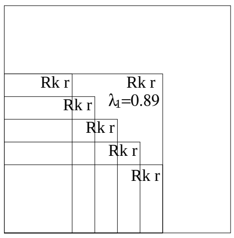

Figure 3: Example of induced pure structure: the huge structure block $\mathcal{B}_1$ with shift $\lambda_1 = 0.89$ induces 5 pure structure blocks just below the diagonal, following a kind of staircase form. The leftmost of them is called the induced left pure structure block of $\mathcal{B}_1$.

Now we prove:

Theorem 7 *(The nonsingular case:) If $A \in \mathcal{M}$ is nonsingular then*

1. *the rank structure is preserved by applying a QR-step without shift on A, and conversely, so no extra structure can be introduced;*

2. *moreover, for each QR-decomposition $A = QR$, we have that $Q \in \mathcal{M}_{\text{pure}}$, the induced pure class of $\mathcal{M}$.*

PROOF.

1. Note that, for the proof, it will be sufficient to consider a single structure block $\mathcal{B}_k$, corresponding to a certain shift λ_k. By (4), the QR-algorithm transforms A into

$$RAR^{-1} =: R(A_{\text{pure},k} + \lambda_k I)R^{-1} = RA_{\text{pure},k}R^{-1} + \lambda_k I, \qquad (5)$$

where $A_{\text{pure},k} := A - \lambda_k I$ satisfies the structure block $\mathcal{B}_{\text{pure},k}$ which is defined from $\mathcal{B}_k$ by putting the shift element λ_k equal to zero. It is then sufficient if we can prove that in (5), the term $RA_{\text{pure},k}R^{-1}$ will still satisfy $\mathcal{B}_{\text{pure},k}$.

To prove this remaining problem, remark that the factor R^{-1} makes linear combinations of the columns of $A_{\text{pure},k}$, and because R^{-1} is upper triangular, these linear combinations only involve 'previous' columns and hence will not destroy the pure structure blocks in the lower left corner of $A_{\text{pure},k}$. A similar reasoning can be applied for the factor R. This proves the theorem.

For the converse statement we can use the same argument, but this time switching the roles of R and R^{-1} by using the equation $A^{(\nu)} = R^{-1}A^{(\nu+1)}R$.

2. This follows from the equation $Q = AR^{-1}$, where the factor R^{-1} takes linear combinations of the columns of A, only involving 'previous' columns, and hence this operation can not destroy the pure structure of A. □

Our next objective is to investigate whether structure is also preserved in case A is *singular*. It turns out that we have to be more careful for answering this question.

Let us first give an example to illustrate this. Consider the matrix

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix} \in \mathcal{M}, \tag{6}$$

where $\mathcal{M}$ is the class of matrices with left bottom element equal to zero. We claim that A has essentially infinitely many QR-decompositions. Indeed: this follows since the first column of A is zero, implying that *every* unitary matrix $Q \in \mathbb{C}^{2\times 2}$ can be used to solve the QR-equation $Q^H A = R$. However, it is easy to check that essentially only two of these QR-factorizations exist for which the new QR-iterate $Q^H AQ$ belongs to $\mathcal{M}$: the ones with the identity matrix $Q_1 := I_2$, and with the matrix $Q_2 := \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$.

This example shows that we should be careful in the singular case. Let us first give an auxiliary definition.

Definition 8 *Let A be an arbitrary matrix, possibly singular. We define $\mathcal{I} = \{1, \dots, n\}$. We define $\mathcal{I}_{\text{dep},A}$ to be the subset of $\mathcal{I}$ consisting of the indices of all columns of A which can be written as a linear combination of the previous columns. Then let $\mathcal{B}_k$ be an arbitrary structure block, with $\lambda_k \neq 0$. We define a partition*

$$\mathcal{I} = \mathcal{I}_{\text{left},k} \cup \mathcal{I}_{\text{middle},k} \cup \mathcal{I}_{\text{right},k}, \tag{7}$$

where $\mathcal{I}_{\text{left},k} = \mathcal{I} \cap \{1, \dots, l_k\}$, the indices of the columns appearing in the induced left pure structure block (see Remark 6.1), $\mathcal{I}_{\text{middle},k} = \mathcal{I} \cap \{l_k + 1, \dots, j_k\}$, the indices of the columns appearing in the non-pure part of the structure block, and

$\mathcal{I}_{\text{right},k} = \mathcal{I} \cap \{j_k+1,\ldots,n\}$, *the remaining column indices. If* $\mathcal{B}_k$ *is a pure structure block* ($\lambda_k = 0$)*, then we use the partition* $\mathcal{I} = \mathcal{I}_{\text{left},k} \cup \mathcal{I}_{\text{right},k}$ *which is defined as (7) except that the set* $\mathcal{I}_{\text{middle},k}$ *has been absorbed into the set* $\mathcal{I}_{\text{left},k}$ *(Remark 6.1).*

For example, in Figure 3 above we have $\mathcal{I}_{\text{left},k} = \{1,2,3\}$, $\mathcal{I}_{\text{middle},k} = \{4,5,6,7\}$ and $\mathcal{I}_{\text{right},k} = \{8,9,10\}$. If instead the structure block would have been pure, i.e. $\lambda_1 = 0$, then we would have had $\mathcal{I}_{\text{left},k} = \{1,2,3,4,5,6,7\}$ and $\mathcal{I}_{\text{right},k} = \{8,9,10\}$.

Now we prove:

Theorem 9 *(The singular case:) Let* $\mathcal{B}_k$ *be a structure block and let* $A \in \mathcal{M}_{\mathcal{B}_k}$ *be an arbitrary matrix, possibly singular. Then for each QR-decomposition* $A = QR$*, the new QR-iterate (without shift) will satisfy*

1. *if* $\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{left},k} = \emptyset$*, then it satisfies* $\mathcal{B}_k$*;*
2. *more generally, it satisfies* $\tilde{\mathcal{B}}_k$*, where the structure block* $\tilde{\mathcal{B}}_k$ *is obtained from* $\mathcal{B}_k$ *by working with the new rank upper bound* $\tilde{r}_k := r_k + \#(\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{left},k})$.

Remark. a. The strength of this theorem is that it works for an *arbitrary* QR-decomposition $A = QR$, of which there can be a lot since A is allowed to be singular.

b. In the proof of part 1 we will only handle the more 'difficult' case where $\lambda_k \neq 0$. The statement for $\lambda_k = 0$ is much weaker (since there is no set $\mathcal{I}_{k,\text{middle}}$ to take care of); its proof can be obtained from the following proof by just skipping all arguments involving $\mathcal{I}_{k,\text{middle}}$ (where we will effectively need the condition $\lambda_k \neq 0$ several times).

PROOF.

1. Let $A = QR$ be an arbitrary QR-decomposition. Denoting with $c_1 < \ldots < c_m$ the elements of $\mathcal{I}_{\text{dep},A}$, then the $(1,1),\ldots,(c_1-1,c_1-1)$ elements of the upper triangular matrix R must be necessarily non-zero, while the (c_1,c_1) element must be zero. If follows that, denoting with $G_{k,l}$ a Givens transformation acting on rows k and l, then we can subsequently find Givens transformations $G_{c_1,l}$, $l = c_1+1,\ldots,n$ such that $G_{c_1,n}\ldots G_{c_1,c_1+1}R$ has its c_1th row entirely zero. (The reader should make a picture of the situation to see this!) Having done this, again the $(c_1+1,c_1+1),\ldots,(c_2-1,c_2-1)$ elements of this (updated) upper triangular matrix must be non-zero, while the (c_2,c_2) element must be zero. We can then repeat the above argument, and proceeding in this way yields us a unitary row transformation

$$G = (G_{c_m,n}\ldots G_{c_m,c_m+1})\ldots(G_{c_1,n}\ldots G_{c_1,c_1+1}), \tag{8}$$

such that $GR = \tilde{J}\tilde{R}$, where $\tilde{J} = \text{diag}\{0,1\}$ is a diagonal matrix with zeros standing precisely on the diagonal positions with index in $\mathcal{I}_{\text{dep},A}$, and where $\tilde{R}$ can be chosen to be a *nonsingular* upper triangular matrix. Moreover, rewriting the above as $G(Q^H A) = \tilde{J}\tilde{R}$, then we obtain a kind of 'canonical' QR-decomposition

$$A = \tilde{Q}\tilde{J}\tilde{R}, \tag{9}$$

with $\tilde{Q} := QG^H$.

Next, note that $Q^H AQ = (G^H \tilde{Q}^H)A(\tilde{Q}G)$, showing that the new QR-iterates of the 'original' and 'canonical' QR-decompositions are related by

$$RQ = G^H(\tilde{J}\tilde{R}\tilde{Q})G, \tag{10}$$

showing that it is sufficient to prove that (i) $\tilde{J}\tilde{R}\tilde{Q} \in \mathcal{M}_{\mathcal{B}_k}$, i.e. the theorem holds for the new QR-iterate of the *canonical* QR-decomposition (9), and (ii) the similarity transformation $\tilde{J}\tilde{R}\tilde{Q} \mapsto G^H(\tilde{J}\tilde{R}\tilde{Q})G$ can not destroy the structure block $\mathcal{B}_k$ anymore.

First we prove (ii). Defining $\mathcal{B}_{\text{pure},k}$ from $\mathcal{B}_k$ by putting the shift equal to zero, we will actually prove that $\mathcal{B}_{\text{pure},k}$ can not be destroyed by the similarity transformation $\tilde{J}\tilde{R}\tilde{Q} - \lambda_k I \mapsto G^H(\tilde{J}\tilde{R}\tilde{Q} - \lambda_k I)G$.

Let us first multiply $\tilde{J}\tilde{R}\tilde{Q} - \lambda_k I$ on the right with the factor G. We distinguish between $c_i \in \mathcal{I}_{\text{right},k}$ and $c_i \in \mathcal{I}_{\text{middle},k}$ in (8). For $c_i \in \mathcal{I}_{\text{right},k}$, the $G_{c_i,l}$ act only on $\mathcal{I}_{\text{right},k}$, and hence can not influence $\mathcal{B}_{\text{pure},k}$. For $c_i \in \mathcal{I}_{\text{middle},k}$, let us suppose that we just applied all the $G_{c_{\tilde{i}},l}$, $\tilde{i} > i$ in (8). We claim that at this point, the c_ith row will be completely zero, except for its diagonal entry which is $-\lambda_k \neq 0$. Indeed: this follows since the original matrix $\tilde{J}\tilde{R}\tilde{Q} - \lambda_k I$ satisfied this property (by definition of $\tilde{J}$), and since it can not have been lost by applying the $G_{c_{\tilde{i}},l}$ with $\tilde{i} > i$. As a consequence, the j_ith column can not be written as a linear combination of the other columns. Then applying the $G_{c_i,l}$ with $l = n, n-1, \ldots, j_k + 1$, each such transformation can change column l, lying outside $\mathcal{B}_{\text{pure},k}$, and column c_i itself; but by what we just told, the latter can then never increase the rank of $\mathcal{B}_{\text{pure},k}$! Next we apply the $G_{c_i,l}$ with $l = j_k, j_k - 1, \ldots, 1$, and then $G_{c_i,l}$ is acting completely inside $\mathcal{B}_{\text{pure},k}$, hence not changing its rank anymore. Thus we showed that the factor G can not destroy $\mathcal{B}_{\text{pure},k}$; also the factor G^H can not, since it is acting on rows in $\mathcal{I}_{\text{middle},k} \cup \mathcal{I}_{\text{right},k}$, all belonging to $\mathcal{B}_{\text{pure},k}$. This proves (ii).

To prove (i), let us suppose that $A = \tilde{Q}\tilde{J}\tilde{R} \in \mathcal{M}_{\mathcal{B}_k}$. We will show that

$$\tilde{Q}\tilde{J}\tilde{R} \in \mathcal{M}_{\mathcal{B}_k} \;\Rightarrow\; \tilde{R}\tilde{Q}\tilde{J} \in \mathcal{M}_{\mathcal{B}_k} \;\Rightarrow\; \tilde{J}\tilde{R}\tilde{Q} \in \mathcal{M}_{\mathcal{B}_k}. \tag{11}$$

For the first implication, we can just take over the proof of Theorem 7.1, using the fact that $\tilde{R}$ is nonsingular. For the second implication, let us denote $m_1 = \#(\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{middle},k})$, and let the matrix $\tilde{J}_1 = \text{diag}\{0,1\}$ have zero diagonal elements precisely on the positions of $\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{middle},k}$. Then we claim that

$$\begin{aligned} \text{Rank } (\tilde{J}\tilde{R}\tilde{Q} - \lambda_k I)|_{\mathcal{B}_k} &= m_1 + \text{Rank } (\tilde{J}\tilde{R}\tilde{Q}\tilde{J}_1)|_{\mathcal{B}_k} && (12) \\ &\leq m_1 + \text{Rank } (\tilde{J}_1\tilde{R}\tilde{Q}\tilde{J}_1)|_{\mathcal{B}_k} && (13) \\ &= \text{Rank } (\tilde{R}\tilde{Q}\tilde{J} - \lambda_k I)|_{\mathcal{B}_k}. && (14) \end{aligned}$$

Indeed: for (12), note that $\tilde{J}\tilde{R}\tilde{Q} - \lambda_k I$ has its m_1 rows with index in $\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{middle},k}$ entirely zero, except for the diagonal entries which are $-\lambda_k \neq 0$; hence there can be no non-zero linear combination of the m_1 columns in $\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{middle},k}$ which is equal to a linear combination of the columns of the 'complementary' matrix $(\tilde{J}\tilde{R}\tilde{Q}\tilde{J}_1)|_{\mathcal{B}_k}$, obtained by 'skipping' these m_1 columns in $\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{middle},k}$, and this is precisely what (12) states. The transition from (13) to (14) is proved in a similar way, with the roles of rows and columns reversed. Finally, the transition from (12) to (13) is obvious. Together, these relations show that also the second implication of (11) is valid, hence proving (i).

2. Suppose that $\#(\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{left},k}) = c \neq 0$. Let $A = QR$ be an arbitrary QR-decomposition. We define a family of upper triangular matrices R_ϵ by replacing every zero diagonal element of R, with index in $\mathcal{I}_{\text{left},k}$, by the parameter ϵ. Defining a family of matrices $A_\epsilon := QR_\epsilon$, $\epsilon \in \mathbb{C}$, we claim that

   F1 A_ϵ can have no column dependencies inside $\mathcal{I}_{\text{left},k}$, except for $\epsilon = 0$;

   F2 $A_\epsilon \in \mathcal{M}_{\tilde{\mathcal{B}}_k}$ for all ϵ;

   F3 $\lim_{\epsilon \to 0} R_\epsilon = R$.

   Indeed: condition F1 is surely satisfied by the family R_ϵ, by construction, and hence also by the family $A_\epsilon = QR_\epsilon$ since

$$\text{span}\{\vec{A}_{\epsilon,1}, \ldots, \vec{A}_{\epsilon,l_k}\} = Q \times \text{span}\{\vec{R}_{\epsilon,1}, \ldots, \vec{R}_{\epsilon,l_k}\}, \tag{15}$$

   with Q nonsingular. To prove F2, we may note that at least the inclusion $\text{span}\{\vec{R}_1, \ldots, \vec{R}_{l_k}\} \subseteq \text{span}\{\vec{R}_{\epsilon,1}, \ldots, \vec{R}_{\epsilon,l_k}\} = \text{span}\{\vec{e}_1, \ldots, \vec{e}_{l_k}\}$ is satisfied for all $\epsilon \in \mathbb{C}$, by construction. Using (15), it follows that the same conclusion must hold when R is replaced by A, i.e.

$$\text{span}\{\vec{A}_1, \ldots, \vec{A}_{l_k}\} \subseteq \text{span}\{\vec{A}_{\epsilon,1}, \ldots, \vec{A}_{\epsilon,l_k}\}. \tag{16}$$

   Then taking into account the ranks, we see that the transition from the left to the right hand side of (16) can be obtained by adding (at most) c extra linearly independent column vectors; thus in particular, we have $A_\epsilon \in \mathcal{M}_{\tilde{\mathcal{B}}_k}$, hence proving condition F2. Finally, condition F3 follows by construction.

   Now using F1, F2 and F3, we can easily finish the proof: let $\epsilon \in \mathbb{C} \setminus \{0\}$, then F2 induces $A_\epsilon \in \mathcal{M}_{\tilde{\mathcal{B}}_k}$, and thus F1 allows us to apply part 1 of this theorem, stating that also the new QR-iterate $R_\epsilon Q \in \mathcal{M}_{\tilde{\mathcal{B}}_k}$. Clearly the same must then be true for the limit $RQ = (\lim_{\epsilon\to 0} R_\epsilon)Q = \lim_{\epsilon\to 0}(R_\epsilon Q)$. $\square$

As an illustrative example, let

$$A = \begin{bmatrix} 0.95 & 0.68 & 0.01 \\ 0.41 & 0.31 & 0.14 \\ 0 & 0 & 0.21 \end{bmatrix} \in \mathcal{M}_d, \tag{17}$$

where column 2 is a multiple of column 1 (only two decimal digits are shown), and where the class $\mathcal{M}_d$ is defined by the intersection of rows 2, 3 and columns 1, 2 being of rank at most 1, at least after subtracting the shift element d; obviously we have $A \in \mathcal{M}_d$ for *any* value of $d \in \mathbb{C}$. Now the intention is to apply the QR-algorithm by sampling a *completely random* QR-factorization $A = QR$. Following Theorem 9.1, the property $A \in \mathcal{M}_d$ must carry over to the new QR-iterate $Q^H AQ$ (at least for all non-zero choices of d). Indeed: to solve the equation $Q^H A = R$, we can do this by putting

$$Q^H = G_{2,3}G_{1,2}, \tag{18}$$

where $G_{1,2}$ eliminates the (2,1) and (2,2) elements of A, and where $G_{2,3}$ is arbitrary. Making a random choice for $G_{2,3}$, we obtained as a new QR-iterate

$$Q^H AQ = \begin{bmatrix} 1.22 & -0.18 & -0.22 \\ 0 & 0.21 & -0.10 \\ 0 & 0.02 & -0.01 \end{bmatrix}, \tag{19}$$

which obviously belongs to each of the $\mathcal{M}_d$. Note however that the place of the zeros of $Q^H AQ$ has been changed with respect to A.

For this same example (17), we can also consider $A \in \mathcal{M}_{\text{pure}}$ with $\mathcal{M}_{\text{pure}}$ defined by the intersection of row 3 and columns 1, 2 being of rank zero. Then choosing again a completely random QR-factorization of A, we see that the (3,1) element will still be zero in the new QR-iterate (19) (as predicted by Theorem 9.1), but the zero on the right of it has disappeared (maybe not surprisingly, since $\mathcal{I}_{\text{dep},A} \cap \mathcal{I}_{\text{left},k} = \{2\} \cap \{1,2\} \neq \emptyset$ in this case.)

If we want instead to preserve also the second zero element of $\mathcal{M}_{\text{pure}}$, all we have to do is being more careful for choosing a suitable, *non-random* QR-factorization $A = QR$. It is easy to check that we can realize this here by choosing $G_{2,3} = I_2$ in (18). A generalization of this idea to work in the general case, will be the subject of [4].

4 Conclusion.

In this paper we introduced in a theoretical way two general classes of structure which are preserved by the shifted QR-algorithm: polynomial and rank structures. Rank structures were defined as a collection of so-called structure blocks, with every structure block containing its own shift element. We proved that preservation of rank structure requires the given matrix to be nonsingular; the singular case will be handled in [4], by using the concepts of sparse Givens patterns and effectively eliminating QR-decompositions, both of them being concepts of independent interest.

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