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Rational Krylov matrices and *QR* steps on Hermitian diagonal-plus-semiseparable matrices

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SUMMARY

We prove that the unitary factor appearing in the *QR* factorization of a suitably defined rational Krylov matrix transforms a Hermitian matrix having pairwise distinct eigenvalues into a diagonal-plus-semiseparable form with prescribed diagonal term. This transformation is essentially uniquely defined by its first column. Furthermore, we prove that the set of Hermitian diagonal-plus-semiseparable matrices is invariant under *QR* iteration. These and other results are shown to be the rational counterpart of known facts involving structured matrices related to polynomial computations. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: eigenvalue problems; *QR* algorithm; rational Krylov matrices; diagonal-plus-semiseparable matrices

1. INTRODUCTION

In order to summarize the results to be presented in this paper, and to shed light on their relevance, we review shortly some well-known facts concerning structured matrices connected with polynomial computations, see References [1, 2].

Consider an $n \times n$ Hermitian matrix A having eigenvalues λ_i, and a complex n-vector v. Furthermore, let $K = \mathscr{K}(A, v)$ be the $n \times n$ Krylov matrix defined by A and v, that is, $K = [v, Av, \ldots, A^{n-1}v]$. If A has spectral factorization $A = U\Lambda U^{\mathrm{H}}$ and we let $U^{\mathrm{H}}v = w = (w_1, \ldots, w_n)^{\mathrm{T}}$, then $K = U[w, \Lambda w, \ldots, \Lambda^{n-1}w] = U\,\mathrm{diag}(w_1, \ldots, w_n)V$, where V is the Vandermonde

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matrix

$$V = \begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^{n-1} \\ \vdots & \vdots & \cdots & \vdots \\ 1 & \lambda_n & \cdots & \lambda_n^{n-1} \end{pmatrix}$$

Hence, K is non-singular if and only if the numbers λ_i are pairwise distinct and all the entries of w are non-zero. If this is the case, consider the unitary factorization $K = QR$. Then $T = Q^{\mathrm{H}}AQ$ is an irreducible tridiagonal matrix. The matrix T can also be computed without explicitly forming K by simply applying the Lanczos algorithm to A and the starting vector v. Using a short notation, we can write $T = \mathscr{L}(A, v)$. Actually, the unitary transformation Q that brings an Hermitian matrix A to tridiagonal form is uniquely defined in terms of the first column of Q: This is the essential content of the Implicit-Q theorem for tridiagonal matrices. Finally, it is well known that the set of Hermitian tridiagonal matrices is closed under QR iterations. Moreover, if the matrix $\tilde{T}$ is the result of a QR step from T,

$$T - \sigma I = Q_1 R_1, \quad \tilde{T} = R_1 Q_1 + \sigma I$$

then $\tilde{T}$ is the same matrix obtained by the Lanczos tridiagonalization process applied to A and the starting vector $(A - \sigma I)v$, that is, $\tilde{T} = \mathscr{L}(A, (A - \sigma I)v)$.

The plan of this paper is as follows: Firstly, in the next section we set some basic notations and introduce the two matrix structures that are exploited in this paper, namely, the class of diagonal-plus-semiseparable (dpss) matrices, and a rational variant of classical Krylov matrices. Section 3 is devoted to an analysis of algebraic properties of rational Krylov matrices. In particular, we prove that the conditions for non-singularity of rational Krylov matrices are the same as for classical Krylov matrices. Moreover, in Theorem 1 we prove that any Hermitian matrix is transformed into dpss form by the unitary factor of a suitably defined rational Krylov matrix, thus giving a rational counterpart of the classical Lanczos tridiagonalization algorithm. We show in Theorem 2 that the above-mentioned transformation is essentially identifiable by its first column. As a consequence, we solve in Theorem 3 a particular inverse eigenvalue problem for dpss matrices that generalizes [3, Theorem 4]. In the last section we prove our main results, showing that the set of Hermitian dpss matrices is closed under QR iterations. In particular, Theorem 4 shows that the relationship between a QR step on dpss matrices and the rational variant of the Lanczos algorithm is the same as in the classical case.

2. BASIC NOTATIONS

Throughout this paper, all matrices are assumed to have order n, and e_i will denote the ith column of the identity matrix I. Although our results are presented using (complex) Hermitian and unitary matrices, they have an obvious restatement with real symmetric and orthogonal matrices, respectively.

Let $a_1,\ldots,a_n$ and $b_1,\ldots,b_n$ be complex numbers such that $a_i b_i \in \mathbb{R}$, for $i=1,\ldots,n$. The Hermitian matrix

$$S=\begin{pmatrix} a_1b_1 & \overline{a_2b_1} & \cdots & \overline{a_nb_1} \\ a_2b_1 & a_2b_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \overline{a_nb_{n-1}} \\ a_nb_1 & \cdots & a_nb_{n-1} & a_nb_n \end{pmatrix}=S^{\mathrm{H}}$$

is a *semiseparable* matrix. According to this definition, a matrix is semiseparable if and only if its triangular parts, both lower and upper, are the same of a rank-one matrix. In fact, Hermitian semiseparable matrices are but a minor generalization of the real symmetric case, since for any Hermitian S there exists a unitary diagonal matrix Δ such that $\Delta S \Delta^{\mathrm{H}}$ is real and symmetric. We refer to References [4–7] for recent accounts on structural and computational properties of symmetric semiseparable matrices. Remark that Hermitian rank-one matrices are semiseparable.

In what follows, we are concerned with Hermitian matrices M that can be decomposed into the sum of a (real) diagonal matrix D and a semiseparable matrix S, $M=D+S$. Such matrices are henceforth called *diagonal-plus-semiseparable* [3, 8, 9] (dpss, for brevity). According to the above definition, this class includes the two main non-trivial examples of symmetric matrices having prescribed spectrum, namely, symmetric arrowhead matrices and diagonal-plus-rank-one matrices [10]. A great interest is arising recently around this structured matrix class. Indeed, the computational properties of these matrices appear to be analogous to that of tridiagonal matrices. Fast and stable algorithms for the computation of their inverses, characteristic polynomials, and the solution of associated linear systems and eigenproblems, have been published, e.g. in References [8, 11–13].

Let A be any Hermitian matrix, and let $d_1,\ldots,d_n$ be real numbers, not necessarily distinct, such that

$$\det(A-d_iI)\neq 0, \quad i=1,\ldots,n \tag{1}$$

This hypothesis will be tacitly assumed throughout this paper. We will use the notations $d=(d_1,\ldots,d_n)^{\mathrm{T}}$ and $D=\mathrm{diag}(d_1,\ldots,d_n)$ for the diagonal matrix whose entries are $d_1,\ldots,d_n$.

Define the rational functions

$$\phi_1(\lambda)=(\lambda-d_1)^{-1}, \quad \phi_i(\lambda)=(\lambda-d_i)^{-1}\phi_{i-1}(\lambda),\ \ i=2,\ldots,n \tag{2}$$

Furthermore, for any complex vector v, we define the matrix

$$\mathscr{K}_{\mathscr{R}}(A,v)=[\phi_1(A)v,\ldots,\phi_n(A)v] \tag{3}$$

as the *rational Krylov matrix* generated by A, the poles d_i and the vector v. We omit to indicate the dependence of $\mathscr{K}_{\mathscr{R}}(A,v)$ from $d_1,\ldots,d_n$, since they will not be considered as variables in what follows. Observe that the matrix $\mathscr{K}_{\mathscr{R}}(A,v)$ is well defined whenever conditions (1) are fulfilled. The above definition is basically the same as introduced in References [14, 15], where one sets $\phi_1(\lambda)=1$ and the matrix A is not assumed to be Hermitian. In the above-mentioned papers, a variant of the Lanczos algorithm is introduced to compute the QR factorization of rational Krylov matrices. In fact, this *rational Krylov iteration*, as it is called in Reference [15], starts with a vector q_1 having unit length and builds up an orthonormal basis $Q=[q_1,\dots,q_n]$, one column at a time, in each step multiplying q_i with the shifted and inverted matrix $(A-d_iI)^{-1}$, and orthogonalizing the resulting vector with respect to the previously computed part of the basis by means of the Gram–Schmidt procedure. When all the poles d_i are equal, this algorithm reduces to the well-known shifted and inverted Arnoldi algorithm. Further analysis and variants of this algorithm, and its applications to the computation of generalized eigenvalues also in the non-Hermitian case, are given e.g. in References [16–18], mainly in the context of model reduction problems.

Finally, for any matrix X, we will denote $\mathcal{Q}(X)$ the unitary factor in the factorization $X=QR$, that is, $\mathcal{Q}(X)=Q$, such that the diagonal entries of R are non-negative. We recall that, while the function $\mathcal{Q}$ is not uniquely defined when its argument is a singular matrix, the restriction of the map $\mathcal{Q}$ to the set of invertible matrices is not only continuous but also differentiable, see e.g. Reference [19].

3. PROPERTIES OF RATIONAL KRYLOV MATRICES

In what follows, we need to assess the non-singularity of rational Krylov matrices. In the next result we state the necessary and sufficient conditions ensuring this case.

Lemma 1

Let $A=U\Lambda U^{\mathrm{H}}$ be the spectral decomposition of the Hermitian matrix A, where $\Lambda=\mathrm{diag}(\lambda_1,\dots,\lambda_n)$, and let $U^{\mathrm{H}}v=w=(w_1,\dots,w_n)^{\mathrm{T}}$. The matrix $K=\mathscr{K}_{\mathscr{R}}(A,v)$ is non-singular if and only if $\lambda_i\neq\lambda_j$ for $i\neq j$ and all entries of w are non-zero.

Proof

By hypothesis (1), for $i,j=1,\dots,n$ all the numbers $d_j-\lambda_i$ are different from zero, hence the matrix

$$F\equiv(\phi_j(\lambda_i))_{i,j=1\dots n}$$

is well defined. Introduce the monic polynomials

$$\pi_0(\lambda)=1,\quad \pi_j(\lambda)=\prod_{i=1}^{j}(\lambda-d_{n-i+1}),\;\; j=1,\dots,n-1$$

We have formally

$$\phi_j(\lambda)=\phi_n(\lambda)\pi_{n-j}(\lambda),\quad j=1,\dots,n$$

As a consequence, we can factor the matrix F as

$$F = \begin{pmatrix} \phi_n(\lambda_1) & & O \\ & \ddots & \\ O & & \phi_n(\lambda_n) \end{pmatrix} \begin{pmatrix} \pi_{n-1}(\lambda_1) & \cdots & \pi_0(\lambda_1) \\ \vdots & \cdots & \vdots \\ \pi_{n-1}(\lambda_n) & \cdots & \pi_0(\lambda_n) \end{pmatrix}$$
$$= \begin{pmatrix} \phi_n(\lambda_1) & & O \\ & \ddots & \\ O & & \phi_n(\lambda_n) \end{pmatrix} \begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^{n-1} \\ \vdots & \vdots & \cdots & \vdots \\ 1 & \lambda_n & \cdots & \lambda_n^{n-1} \end{pmatrix} JC$$

where J is the reversal permutation matrix and C is an upper triangular matrix having unit diagonal, built from the coefficients of the polynomials $\pi_i(\lambda)$ in the monomial basis. Since $\phi_n(\lambda_i) \neq 0$, the matrix F is non-singular if and only if the Vandermonde matrix with nodes $\lambda_1, \ldots, \lambda_n$ is non-singular, that is, when $\lambda_i \neq \lambda_j$ for $i \neq j$. The ith column of K is

$$Ke_i = \phi_i(A)v = U\phi_i(\Lambda)w = U \operatorname{diag}(w_1, \ldots, w_n)Fe_i$$

Hence we have $K = U \operatorname{diag}(w_1, \ldots, w_n)F$. From the preceding factorization we obtain the claim. □

Next, we prove that non-singular rational Krylov matrices are dense in the set of all rational Krylov matrices:

Corollary 1
Given a rational Krylov matrix $K = \mathscr{K}_{\mathscr{R}}(A, v)$, for any matrix norm $\|\cdot\|$ and any $\varepsilon > 0$ there exists a non-singular rational Krylov matrix $\tilde{K} = \mathscr{K}_{\mathscr{R}}(\tilde{A}, \tilde{v})$ such that $\|K - \tilde{K}\| \leqslant \varepsilon$.

Proof
If K is non-singular then simply choose $K = \tilde{K}$. In the other case, consider the spectral factorization $A = U\Lambda U^{\mathrm{H}}$. We can perform an arbitrarily small perturbation on the matrix Λ so that the perturbed matrix $\tilde{\Lambda}$ has pairwise distinct eigenvalues. Analogously, an arbitrarily small perturbation on the vector v will make all entries of $U^{\mathrm{H}}\tilde{v}$ different from zero. By the preceding lemma, the matrix $\tilde{K} = \mathscr{K}_{\mathscr{R}}(\tilde{A}, \tilde{v})$, with $\tilde{A} = U\tilde{\Lambda}U^{\mathrm{H}}$, is non-singular. The claim thus follows since all norms in a finite-dimensional vector space are equivalent, and the map $(A, v) \mapsto \mathscr{K}_{\mathscr{R}}(A, v)$ is continuous. □

Rational Krylov matrices have a kind of *displacement structure* as defined in Reference [20], since they are usefully characterized as solution of a particular matrix equation:

Lemma 2
If the matrix $K = \mathscr{K}_{\mathscr{R}}(A, v)$ is well defined, that is, conditions (1) are fulfilled, then K is the unique solution of the matrix equation

$$AK - KB = ve_1^{\mathrm{T}} \tag{4}$$

where B is the upper bidiagonal matrix

$$B = \begin{pmatrix} d_1 & 1 & & \\ & d_2 & \ddots & \\ & & \ddots & 1 \\ & & & d_n \end{pmatrix} \tag{5}$$

Proof
By the hypothesis (1), the spectra of the matrices A and B are disjoint. Hence, the operator $X \mapsto AX - XB$ is invertible, see e.g. Reference [21, Chapter 5]. As a consequence, the solution of the matrix equation $AX - XB = ve_1^{\mathrm{T}}$ exists and is unique. We show that the matrix K is such a solution by considering the matrix equation (4) column by column. For the first column we have:

$$(AK - KB)e_1 = A\phi_1(A)v - d_1\phi_1(A)v = (A - d_1 I)\phi_1(A)v = v$$

For the ith column, with $i = 2, \ldots, n$, we have

$$(AK - KB)e_i = A\phi_i(A)v - d_i\phi_i(A)v - \phi_{i-1}(A)v = (A - d_i I)\phi_i(A)v - \phi_{i-1}(A)v = 0$$

owing to the definition (2). Hence the matrices $AK - KB$ and ve_1^{T} have the same columns and Equation (4) is proved. □

There is a link between rational Krylov matrices and dpss matrices, that mirrors the one existing between classical Krylov matrices and tridiagonals.

Theorem 1
If the matrix $K = \mathscr{K}_{\mathscr{R}}(A, v)$ is non-singular, and $\mathscr{Q}(K) = Q$, then $Q^{\mathrm{H}}AQ$ is an Hermitian dpss matrix, $Q^{\mathrm{H}}AQ = D + S$, with the diagonal matrix $D = \mathrm{diag}(d_1, \ldots, d_n)$.

Proof
For any matrix $X \equiv (x_{i,j})$ let $\mathrm{triu}(X)$ be the strictly upper triangular matrix whose (i,j)-entry is zero if $i \geqslant j$ and $x_{i,j}$ otherwise. Let $K = QR$ be the unitary factorization of K. In the notations of the preceding lemma, from $AQR - QRB = ve_1^{\mathrm{T}}$ and owing to the non-singularity of the factor R, we have

$$\begin{aligned} Q^{\mathrm{H}}AQ &= RBR^{-1} + Q^{\mathrm{H}}ve_1^{\mathrm{T}}R^{-1} \\ &= R\left[D + \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ O & & & 0 \end{pmatrix}\right]R^{-1} + Q^{\mathrm{H}}ve_1^{\mathrm{T}}R^{-1} \\ &= D + \mathrm{triu}(RBR^{-1}) + Q^{\mathrm{H}}ve_1^{\mathrm{T}}R^{-1} \end{aligned}$$

Hence, $Q^{\mathrm{H}}AQ - D$ is the sum of a strictly upper triangular matrix and a rank-one matrix; furthermore, it is Hermitian, so it must be semiseparable. □

The following example shows that the hypothesis of non-singularity of the matrix K in the above theorem is essential: consider

$$D = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad v = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Then we have

$$K = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} = R, \quad Q = I, \quad M = S = A$$

hence, S is not semiseparable, according to our definition.

Apart of the special cases leading to a singular K, Theorem 1 introduces a unitary transformation of the matrix A into dpss form, whose diagonal term is related to the poles of the rational functions (2). In the sequel, we denote this transformation by $\mathscr{L}_{\mathscr{R}}(A, v)$:

$$\mathscr{L}_{\mathscr{R}}(A, v) = M \iff \begin{cases} M = Q^{\mathrm{H}}AQ \\ Q = \mathscr{Q}(\mathscr{K}_{\mathscr{R}}(A, v)) \end{cases}$$

The map $\mathscr{L}_{\mathscr{R}}$ is obviously continuous, being the composition of continuous functions, but not one-to-one, apart of trivial cases, as it should be made clear by considering the number of parameters describing its arguments and result. For example, for any positive scalar α we have $\mathscr{L}_{\mathscr{R}}(A, \alpha v) = \mathscr{L}_{\mathscr{R}}(A, v)$. In the next lemma we examine a particular transformation of its arguments leaving the result unchanged.

Lemma 3
Let $M = \mathscr{L}_{\mathscr{R}}(A, v)$, and $\tilde{A} = V^{\mathrm{H}}AV$, for some unitary matrix V. Then for $w = V^{\mathrm{H}}v$ we have $M = \mathscr{L}_{\mathscr{R}}(\tilde{A}, w)$.

Proof
Let $K = \mathscr{K}_{\mathscr{R}}(A, v)$ and $\tilde{K} = \mathscr{K}_{\mathscr{R}}(\tilde{A}, w)$. The ith columns of K and $\tilde{K}$ are, respectively,

$$Ke_i = \phi_i(A)v, \qquad \tilde{K}e_i = \phi_i(V^{\mathrm{H}}AV)w = V^{\mathrm{H}}\phi_i(A)Vw = V^{\mathrm{H}}\phi_i(A)v$$

Hence, $\tilde{K} = V^{\mathrm{H}}K$, and we obtain $\mathscr{Q}(\tilde{K}) = V^{\mathrm{H}}Q$ where $Q = \mathscr{Q}(K)$. Finally, we have

$$\mathscr{L}_{\mathscr{R}}(\tilde{A}, w) = (V^{\mathrm{H}}Q)^{\mathrm{H}}\tilde{A}(V^{\mathrm{H}}Q) = Q^{\mathrm{H}}V\tilde{A}V^{\mathrm{H}}Q = Q^{\mathrm{H}}AQ = \mathscr{L}_{\mathscr{R}}(A, v)$$

and the proof is complete. □

Observe that, for any vector v, the matrices A and $M = \mathscr{L}_{\mathscr{R}}(A, v)$ are similar. Hence, under assumption (1), all matrices $M - d_iI$ are non-singular.

The following theorem is almost the counterpart for dpss matrices of the classical Implicit-Q theorem for tridiagonal matrices, see Reference [2, Theorem 7.4.2]. Basically, it states that the similarity transformation bringing an Hermitian matrix A to a dpss form with prescribed diagonal term is essentially determined by the first column of the transforming matrix. Before stating it we need one further preliminary result.

Lemma 4
In the preceding notations and under the assumption (1), if $Q^{\mathrm{H}}AQ = D + S$ for some unitary matrix Q, then S has no zero columns or rows.

Proof
Since $\det(A - d_i I) \neq 0$ we have $\det(D + S - d_i I) \neq 0$. Hence $0 \neq (D + S - d_i I)e_i = Se_i$. The claim follows since S is Hermitian. □

Theorem 2
Suppose that Q_1 and Q_2 are unitary matrices such that $Q_1^{\mathrm{H}}AQ_1 = M_1$ and $Q_2^{\mathrm{H}}AQ_2 = M_2$ are Hermitian dpss matrices having the same diagonal term, that is, $M_1 = D + S_1$ and $M_2 = D + S_2$, with S_1 and S_2 semiseparable. Furthermore, suppose that $Q_1 e_1 = Q_2 e_1$. Then, for $i = 1, \ldots, n$, there exists a unitary diagonal matrix Δ such that $Q_2 = Q_1 \Delta$ and $M_1 = \Delta M_2 \Delta^{\mathrm{H}}$.

Proof
Introduce the matrix $W = Q_1^{\mathrm{H}} Q_2$. We obtain $We_1 = e_1$ and $M_1 W = WM_2$. Let $a^{(1)}, a^{(2)} \in \mathbb{C}^n$ be the first column of S_1 and S_2, respectively. We know from Lemma 4 that $a^{(1)}, a^{(2)}$ are non-zero. Then

$$d_1 e_1 + a^{(1)} = M_1 e_1 = M_1 W e_1 = WM_2 e_1 = W(d_1 e_1 + a^{(2)}) = d_1 e_1 + Wa^{(2)}$$

Hence $a^{(1)} = Wa^{(2)}$. Moreover, for some scalars α_1, α_2 we have

$$M_1 W e_2 = WM_2 e_2 = W(d_2 e_2 + \alpha_1 a^{(2)} + \alpha_2 e_1) = d_2 W e_2 + \alpha_1 a^{(1)} + \alpha_2 e_1$$

We obtain $(M_1 - d_2 I)We_2 = \alpha_1 a^{(1)} + \alpha_2 e_1$. The right-hand side of the last equation belongs to the space generated by the first two columns of $M_1 - d_2 I$. Since $M_1 - d_2 I$ is non-singular by assumption (1), the second column of W has non-zero entries only in the first two positions. On the basis of the preceding result we can start a finite induction argument: For $i = 2, \ldots, n$, given that the first $i - 1$ columns of W are in upper triangular form, there exist some scalar α_i and two vectors f_i and g_i belonging to the linear span of $e_1, \ldots, e_{i-1}$, such that

$$M_1 W e_i = WM_2 e_i = W(d_i e_i + \alpha_i a^{(2)} + f_i) = d_i W e_i + \alpha_i a^{(1)} + g_i$$

so that we obtain $(M_1 - d_i I)We_i = \alpha_i a^{(1)} + g_i$. The right-hand side of the preceding equation belongs to the space generated by the first i columns of $M_1 - d_i I$. In fact, for $1 \leqslant j \leqslant i$, we have $(M_1 - d_i I)e_j \in \mathrm{Span}\{a^{(1)}, e_1, \ldots, e_{i-1}\}$ because of the semiseparable structure of M_1. Since $M_1 - d_i I$ is invertible, the associated map is one-to-one from $\mathrm{Span}\{e_1, \ldots, e_i\}$ to $\mathrm{Span}\{a^{(1)}, e_1, \ldots, e_{i-1}\}$. Observe that $\alpha_i a^{(1)} + g_i$ belongs to the latter subspace by hypothesis. Hence, $We_i \in \mathrm{Span}\{e_1, \ldots, e_i\}$, that is, the ith column of W has zeros below the ith entry. Finally, we conclude that W is upper triangular. Since W is also unitary, it must be diagonal, so we have the claim with $W = \Delta$. □

On the basis of the preceding theorem, we can state a converse result of Theorem 1.

Corollary 2
Let $M = D + S$ be a dpss matrix having pairwise distinct eigenvalues, such that all matrices $M - d_i I$ are non-singular, and let $M = U\Lambda U^{\mathrm{H}}$ be its spectral factorization. If all entries of $U^{\mathrm{H}} e_1$ are non-zero then there exists a unitary diagonal matrix Δ and a vector v such that $K = \mathscr{K}_{\mathscr{R}}(\Lambda, v)$ is non-singular and $\Delta M \Delta^{\mathrm{H}} = \mathscr{L}_{\mathscr{R}}(\Lambda, v)$.

Proof
Firstly, let $v = (\Lambda - d_1 I)U^{\mathrm{H}} e_1$ and $K = \mathscr{K}_{\mathscr{R}}(\Lambda, v)$. The matrix K is non-singular by Lemma 1, since $\Lambda - d_1 I$ is non-singular. The first column of K is $Ke_1 = (\Lambda - d_1 I)^{-1} v = U^{\mathrm{H}} e_1$, hence it is a unit length vector. Let $Q = \mathscr{Q}(K)$. From Theorem 1 we have that $Q^{\mathrm{H}} \Lambda Q$ is a dpss matrix with diagonal term equal to D. Since $Qe_1 = Ke_1 = U^{\mathrm{H}} e_1$, and both Q and U^{H} bring Λ into dpss form with the same diagonal term D, by Theorem 2 there exists a unitary diagonal matrix Δ such that $U^{\mathrm{H}} = Q\Delta$. Moreover,

$$\mathscr{L}_{\mathscr{R}}(\Lambda, v) = Q^{\mathrm{H}} \Lambda Q = \Delta U \Lambda U^{\mathrm{H}} \Delta^{\mathrm{H}} = \Delta M \Delta^{\mathrm{H}}$$

and the proof is complete. □

As a minor by-product of the preceding analysis, we address the problem of reconstructing a dpss matrix from its eigenvalues, the diagonal term, and some additional information. The following theorem generalizes Theorem 4 in Reference [3] to the case where the diagonal entries of D are arbitrary, and proves that the reconstructed matrix M is substantially unique.

Theorem 3
Given two real diagonal matrices $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ and $D = \mathrm{diag}(d_1, \ldots, d_n)$, and a unit vector v, if the matrix $K = \mathscr{K}_{\mathscr{R}}(\Lambda, v)$ is well defined and non-singular, there exists a unitary matrix Q, which is unique apart of a unitary scaling of its columns, such that $Q^{\mathrm{H}} \Lambda Q - D$ is semiseparable and $Qe_1 = v$.

Proof
Let $w = (\Lambda - d_1 I)v$ and $\hat{K} = \mathscr{K}_{\mathscr{R}}(\Lambda, w)$. The matrix $\hat{K}$ is non-singular, due to Lemma 1. Indeed, all diagonal entries of $\Lambda - d_1 I$ are non-zero, hence the same must be true for the entries of w. Let $Q = \mathscr{Q}(\hat{K})$. Observe that the first column of $\hat{K}$ is v, so we have $Qe_1 = v$. Hence the matrix $M = \mathscr{L}_{\mathscr{R}}(\Lambda, w)$ is a dpss matrix with diagonal term D by Theorem 1. The claim follows from Theorem 2. □

4. ANALYSIS OF *QR* STEPS ON HERMITIAN DPSS MATRICES

This last section contains the main results of this paper, proving that the Hermitian dpss structure is invariant under QR iterations.

Theorem 4
Let $M_1 = \mathscr{L}_{\mathscr{R}}(A, v)$, for some Hermitian matrix A and a complex vector v. Let M_2 be the matrix obtained after performing a QR step with shift $\sigma \in \mathbb{R}$:

$$M_1 - \sigma I = Q_1 R_1, \quad M_2 = R_1 Q_1 + \sigma I$$

If the matrix $M_1 - \sigma I$ is non-singular, then $M_2 = \mathscr{L}_{\mathscr{R}}(A, w)$ where $w = (A - \sigma I)v$.

Proof
By assumptions we have $M_1 = Q^{\mathrm{H}}AQ$, where Q is the unitary factor in $K = QR$ and $K = \mathscr{K}_{\mathscr{R}}(A, v)$. By Lemma 2 we have $AK = KB + ve_1^{\mathrm{T}}$, where B is as in (5). Firstly, suppose K be invertible. Let $F = B + K^{-1}ve_1^{\mathrm{T}}$. From $AK = KF$ we have

$$RF = Q^{\mathrm{H}}KF = Q^{\mathrm{H}}AK = Q^{\mathrm{H}}AQQ^{\mathrm{H}}K = M_1R$$

Moreover,

$$(A - \sigma I)QR = QR(F - \sigma I) = Q(M_1 - \sigma I)R = QQ_1R_1R$$

As a consequence, QQ_1 is the unitary factor of a rational Krylov matrix:

$$\tilde{K} = (A - \sigma I)K = \mathscr{K}_{\mathscr{R}}(A, (A - \sigma I)v) = \mathscr{K}_{\mathscr{R}}(A, w)$$

The matrix $\tilde{K}$ is non-singular. Indeed, by Lemma 1, if $A = U\Lambda U^{\mathrm{H}}$, the non-singularity of K implies that all entries of $U^{\mathrm{H}}v$ are non-zero. Observe that $U^{\mathrm{H}}w = U^{\mathrm{H}}(A - \sigma I)v = (\Lambda - \sigma I)U^{\mathrm{H}}v$. Since $\Lambda - \sigma I$ is a non-singular diagonal matrix, also the entries of $U^{\mathrm{H}}w$ are non-zero. Since $M_2 = (QQ_1)^{\mathrm{H}}A(QQ_1)$ we obtain the claim from Theorem 1. The general case follows from a continuity argument. Indeed, with the help of Corollary 1, for any matrix norm $\|\cdot\|$ we can find a sequence of matrices $\{A_n\}$ and vectors $\{v_n\}$, converging to A and v, respectively, such that all matrices $K_n = \mathscr{K}_{\mathscr{R}}(A_n, v_n)$ are invertible. Clearly, we have $K_n \to K$ as $n \to \infty$. Since the set of unitary matrices is compact, we can extract from $\{A_n\}$ and $\{v_n\}$ subsequences $\{A_m\}$ and $\{v_m\}$, such that the sequence $\{\mathscr{Q}(K_m)\}$ converges to a unitary matrix Q. Since $Q_m^{\mathrm{H}}K_m$ is upper triangular, the same must be true for $Q^{\mathrm{H}}K$. By applying the preceding discussion, a QR step with shift σ from $M_{m,1} = \mathscr{L}_{\mathscr{R}}(A_m, v_m)$ leads to $M_{m,2} = \mathscr{L}_{\mathscr{R}}(A_m, (A_m - \sigma I)v_m)$. Letting m go to infinity, from the continuity of the map $\mathscr{L}_{\mathscr{R}}$ we obtain the claim. □

The special case $D = O$ of the preceding theorem was also shown in Reference [4], by exploiting the low-rank structure of the triangular parts of a semiseparable matrix. Details on the implementation of QR steps on matrix classes including dpss matrices, also in the non-symmetric case, are given in References [6, 22, 23]. We observe that, with the help of Corollary 2, the proof of the preceding theorem leads also to a further result:

Corollary 3
Let M_1 be an Hermitian dpss matrix, $M_1 = D + S_1$, with $D = \mathrm{diag}(d_1, \ldots, d_n)$, such that all eigenvalues of M_1 are different from the numbers d_i. Let M_2 be the matrix obtained after performing a QR step with shift $\sigma \in \mathbb{R}$, as in the preceding theorem. If $M_1 - \sigma I$ is non-singular, then M_2 is an Hermitian dpss matrix that can be decomposed as $M_2 = D + S_2$, for some semiseparable matrix S_2.

The hypothesis of non-singularity of $M_1 - \sigma I$ appearing in the preceding theorem and corollary cannot be dropped out, as shown in the following counterexample: consider the matrices

$$S_1 = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}, \quad M_1 = D + S_1 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

Clearly, M_1 is singular, and for $\sigma = 0$ we have the unitary factorization $M_1 = QR$ with

$$Q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad R = \begin{pmatrix} \sqrt{2} & \sqrt{2} \\ 0 & 0 \end{pmatrix}$$

Thus the QR step from M_1 leads to

$$M_2 = RQ = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}, \quad S_2 = M_2 - D = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$$

and the matrix S_2 is not semiseparable.

5. CONCLUSIONS

The main aim of this paper is to show that the set of Hermitian dpss matrices is invariant under shifted QR steps. Incidentally, our discussion shows that there is a close relationship between matrices arising from polynomial computations and matrices arising from computations with rational functions: In some sense, dpss matrices are a rational counterpart of irreducible tridiagonal matrices, exactly as rational Krylov matrices are of classical Krylov matrices. The development of this analogy will be continued elsewhere, in particular, with regard to the study of sequences of rational orthogonal functions. Preliminary results in this direction are given in Reference [24].

The preceding results were sometimes obtained under minor hypotheses, e.g. the non-singularity of rational Krylov matrices appearing in our arguments, as in Theorem 1, and the assumption that the eigenvalues of A are all distinct. Furthermore, one major limit of this paper is the assumption that all matrices $A - d_i I$ are non-singular. As a consequence, Theorem 2 is not the exact counterpart of the well-known Implicit-Q theorem for tridiagonal matrices [2, Theorem 7.4.2], due to the hypothesis on non-singularity of the matrices $M_1 - d_i I$.

The generalization of these results under weaker hypotheses, for example, with the help of structural properties of semiseparable matrices analysed in References [4, 7], is also a possible direction of further research.

REFERENCES

1. Bai Z, Demmel J, Dongarra J, Ruhe A, Van der Vorst H. *Templates for the Solution of Algebraic Eigenvalue Problems*. Society for Industrial and Applied Mathematics: Philadelphia, PA, 2000.
2. Golub GH, Van Loan CF. *Matrix Computations*. The Johns Hopkins University Press: Baltimore, MD, 1996.
3. Fasino D, Gemignani L. Direct and inverse eigenvalue problems for diagonal-plus-semiseparable matrices. *Numerical Algorithms* 2003; **34**:313–324.
4. Bevilacqua R, Del Corso GM. Existence, uniqueness and algorithms for matrix unitary reduction to semiseparable form. *Technical Report TR-03-12*, Università di Pisa, Dipartimento di Informatica, 2003.
5. Van Barel M, Vandebril R, Mastronardi N. The Lanczos-Ritz values appearing in an orthogonal similarity reduction of a matrix into semiseparable form. *Report TW360*, Department of Computer Science, K. U. Leuven, Leuven, Belgium, May 2003.
6. Vandebril R, Van Barel M, Mastronardi N. An implicit *QR* algorithm for semiseparable matrices, to compute the eigendecomposition of symmetric matrices. *Report TW367*, Department of Computer Science, K. U. Leuven, Leuven, Belgium, August 2003.
7. Vandebril R, Van Barel M, Mastronardi N. A note on the representation and definition of semiseparable matrices. *Report TW368*, Department of Computer Science, K. U. Leuven, Leuven, Belgium, October 2003.

8. Eidelman Y, Gohberg I. Fast inversion algorithms for diagonal plus semiseparable matrices. *Integral Equations and Operator Theory* 1997; **27**:165–183.
9. Fasino D, Mastronardi N, Van Barel M. Fast and stable algorithms for reducing diagonal-plus-semiseparable matrices to tridiagonal and bidiagonal form. *Contemporary Mathematics* 2003; **323**:105–118.
10. Fiedler M. Expressing a polynomial as the characteristic polynomial of a symmetric matrix. *Linear Algebra and its Applications* 1990; **141**:265–270.
11. Fasino D, Gemignani L. Fast and stable solution of banded-plus-semiseparable linear systems. *Calcolo* 2002; **39**:201–217.
12. Mastronardi N, Chandrasekaran S, Van Huffel S. Fast and stable reduction of diagonal plus semi-separable matrices to tridiagonal and bidiagonal form. *BIT* 2001; **41**:149–157.
13. Mastronardi N, Chandrasekaran S, Van Huffel S. Fast and stable two-way algorithm for diagonal plus semi-separable systems of linear equations. *Numerical Linear Algebra with Applications* 2001; **8**:7–12.
14. Ruhe A. Rational Krylov sequence methods for eigenvalue computation. *Linear Algebra and its Applications* 1984; **58**:391–405.
15. Ruhe A. Rational Krylov, a practical algorithm for large sparse nonsymmetric matrix pencils. *SIAM Journal on Scientific and Statistical Computation* 1998; **19**:1535–1551.
16. Gallivan K, Grimme E, Van Dooren P. A rational Lanczos algorithm for model reduction. *Numerical Algorithms* 1996; **12**:33–63.
17. Ruhe A, Skoogh D. Rational Krylov algorithms for eigenvalue computation and model reduction. *Applied Parallel Computing* (Umeaa, 1998), Lecture Notes in Computer Science, vol. 1541. 1998; 491–502.
18. Sorensen DC. Implicit application of polynomial filters in a k-step Arnoldi method. *SIAM Journal on Matrix Analysis and Applications* 1992; **13**:357–385.
19. Bhatia R. Matrix factorizations and their perturbations. *Linear Algebra and its Applications* 1994; **197**:245–276.
20. Kailath T, Sayed AH. Displacement structure: theory and applications. *SIAM Review* 1995; **37**:297–386.
21. Stewart GW, Sun J-G. *Matrix Perturbation Analysis*. Academic Press: San Diego, CA, 1990.
22. Bini D, Gemignani L, Pan VY. *QR-like Algorithms for Generalized Semiseparable Matrices*, 2003, submitted.
23. Vandebril R, Van Barel M, Mastronardi N. A *QR*-method for computing the singular values via semiseparable matrices. *Report TW366*, Department of Computer Science, K. U. Leuven, Leuven, Belgium, August 2003.
24. Van Barel M, Fasino D, Gemignani L, Mastronardi N. Orthogonal rational functions and structured matrices. *Report TW350*, Department of Computer Science, K. U. Leuven, Leuven, Belgium, November 2002, *SIAM Journal on Matrix Analysis and Applications*, in press.
25. Fasino D, Gemignani L. A Lanczos-type algorithm for the *QR* factorization of regular Cauchy matrices. *Numerical Linear Algebra with Applications* 2002; **9**:305–319.

