Rational Krylov sequences and Orthogonal Rational Functions

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Abstract

In this paper we study the relationship between spectral decomposition, orthogonal rational functions and the rational Lanczos algorithm, based on a simple identity for rational Krylov sequences.

Keywords : Rational Krylov sequences, orthogonal rational functions, Lanczos algorithm, three-term recurrence relation.
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Rational Krylov sequences and Orthogonal Rational Functions.*

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Abstract

In this paper we study the relationship between spectral decomposition, orthogonal rational functions and the rational Lanczos algorithm, based on a simple identity for rational Krylov sequences.

Keywords: Rational Krylov sequences, orthogonal rational functions, Lanczos algorithm, three-term recurrence relation.

1 Introduction

If A is a linear operator on a Hilbert space H (e.g. a large $N \times N$ matrix operating on $\mathbb{C}^N$) and $v \in H$, then the space $K_{n+1}(A, v) = \text{span}\{v_0, \ldots, v_n\}$ with $v_k = A^k v$ is called a Krylov subspace. To solve a linear equation $Ax = b$ or an eigenvalue problem for A, the problem is projected onto a Krylov subspace of finite (i.e. low) dimension ($n \ll N$ in the matrix example) and this low dimensional problem is solved to give an approximation to the original problem. To compute the projection, an orthogonal basis is constructed for the Krylov subspace. Clearly, the $(k+1)^{th}$ orthogonal vector q_k has to be a combination of the first $k+1$ vectors in the Krylov sequence. Hence it is of the form $q_k = \phi_k(A)v$ with $\phi_k(z)$ a polynomial of degree k.

Suppose that A is hermitian. Orthonormality of $q_k^* q_l = \delta_{k,l}$ is then equivalent with the orthonormality of the polynomials $\langle \phi_k, \phi_l \rangle = \delta_{k,l}$ with respect to the inner product defined by $\langle \phi_k, \phi_l \rangle = M(\phi_k \overline{\phi_l})$, where the linear functional M is defined on the space of polynomials by its moments $m_k = M(z^k) = v^* A^k v$ (see [3]). Since the classical moment matrix has a Hankel structure, this theory will be related to orthogonality of polynomials on the real line. Thus, in the classical Lanczos method for hermitian matrices, the three-term recurrence relation for the orthogonal polynomials leads to a

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short recurrence between the successive vectors q_k, meaning that q_k can be computed from q_{k-1} and q_{k-2} without the need for a full Gram-Schmidt orthogonalisation.

Computing the v_k is like an application of the power method and therefore, the v_k will quickly converge to an eigenvector corresponding to a dominant eigenvalue. Thus, if we want an eigenvalue near μ, we should not iterate with A, but with $B = (A - \mu I)^{-1}$. The rational Krylov method (RKS) of A. Ruhe [4, 5, 6] allows for a different shift μ in every iteration step. Thus, $v_k = (A - \mu_k I)^{-1} v_{k-1}$, or even more generally $v_k = (A - \sigma_k I)(A - \mu_k I)^{-1} v_{k-1}$, where μ_k is used to enforce the influence of the eigenspaces of the eigenvalues in the proximity of μ_k, while σ_k is used to suppress the influence of the eigenspaces of the eigenvalues in the neighbourhood of σ_k. This construction of v_k means that we may write v_k as $v_k = r_k(A)v$ with r_k a rational function of the form $p_k(z)/[(z-\mu_1)\cdots(z-\mu_k)]$, where p_k is a polynomial of degree k at most, so that after orthogonalising v_k with respect to the previous vectors, we obtain a vector $q_k = \varphi_k(A)v$, where again $\varphi_k(z)$ is a rational function of the same form as r_k.

Orthogonal rational functions (ORFs) on the real line are a generalisation of orthogonal polynomials (OPs) on the real line in such a way that the OPs return if all the poles are at infinity. If A is hermitian again, it will be obvious that orthogonality of the q_k will lead to some orthogonality of the rational functions φ_k, so that a simple recurrence of the ORFs will lead to an efficient implementation of the RKS. Hence, the aim of this paper is to generalise the results in [3] for Krylov sequences and OPs on the real line to the case of RKS and ORFs.

The outline of this paper is as follows. After an overview of the necessary theoretical preliminaries in Section 2, Section 3 deals with reformulating those results in [3] that still hold for the rational case. Next, in Section 4 we derive, under certain conditions on the poles μ_k, a three-term recurrence relation for the orthonormal vectors q_k. In Section 5 we take a closer look at the conditions on the poles. We conclude this paper with some numerical examples in Section 6.

2 Preliminaries

The field of complex numbers will be denoted by $\mathbb{C}$. For the real line we use the symbol $\mathbb{R}$ and for the positive real line $\mathbb{R}^+ = \{z \in \mathbb{R} : z \geq 0\}$. If the number zero is omitted from the set X, this will be represented by X_0, e.g. $\mathbb{R}_0 = \mathbb{R} \setminus \{0\}$.

Suppose the sequence of $N+1 < \infty$ numbers $\mathcal{M} = \{\mu_0, \mu_1, \ldots, \mu_N\} \subset \mathbb{R}_0 \cup \{\infty\}$ is given, and define the factors

$$Z_k(z) = \frac{z}{1 - \mu_k^{-1} z}, \quad k = 1, 2, \ldots, N, \tag{1}$$

and the products

$$b_0(z) \equiv 1, \quad b_k(z) = Z_k(z) b_{k-1}(z), \quad k = 1, 2, \ldots, N. \tag{2}$$

Then the space of rational functions with poles in $\{\mu_1, \ldots, \mu_n\}$, $n \leq N$ is defined as

$$\mathcal{L}_n = \text{span}\{b_0(z), b_1(z), \ldots, b_n(z)\}.$$

In the special case of all $\mu_k = \infty$, the factor in (1) becomes z and the products in (2) become $b_k(z) = z^k$.

Orthonormalising the basis $\{b_0(z), \ldots, b_n(z)\}$ with respect to an inner product defined by a real positive definite linear functional M on a subset of the real line,

$$\langle f, g \rangle = M\{f\overline{g}\}, \quad f, g \in \mathcal{L}_n,$$

we obtain the orthonormal rational functions (ORFs) $\{\varphi_0(z), \ldots, \varphi_n(z)\}$.

Let $\mathcal{P}_k$ represents the space of polynomials of degree less than or equal to k. Suppose that $p_k \in \mathcal{P}_k$ and define $\pi_k \in \mathcal{P}_k$ by

$$\pi_0(z) \equiv 1, \quad \pi_k(z) = \prod_{j=1}^{k}(1 - \mu_j^{-1} z), \quad k = 1, 2, \ldots. \tag{3}$$

We then call φ_k singular when $\varphi_k(z) = \frac{p_k(z)}{\pi_k(z)}$ and $p_k(\mu_{k-1}) = 0$ for $k > 1$ ($p_0(z) \equiv 0$, respectively $p_1(z) \equiv c \in \mathbb{R}$, in case of $k = 0$, respectively $k = 1$), and regular in all other cases. A zero of p_k at ∞ then means that the degree of p_k is less than k. With this, the following recurrence relation has been proven in [1, Thm. 11.1.2 and Lem. 11.1.6].

Theorem 2.1. *Take by convention $\mu_{-1} = \infty$. Then the ORFs φ_{k-1}, φ_k and φ_{k+1} are regular, for $k = 0, \ldots, N-1$, iff they satisfy the following three-term recurrence relation:*

$$\begin{aligned} z\varphi_k(z) = \beta_{k-1}\left(1 - \mu_{k-1}^{-1} z\right)\varphi_{k-1}(z) + \alpha_k\left(1 - \mu_k^{-1} z\right)\varphi_k(z) \\ + \beta_k\left(1 - \mu_{k+1}^{-1} z\right)\varphi_{k+1}(z). \end{aligned}$$

The initial conditions are $\varphi_{-1}(z) \equiv 0$ and $\varphi_0(z) \equiv \{\langle 1, 1\rangle\}^{-1/2}$. The coefficients are finite and β_k is different from zero. Furthermore, β_k can be chosen positive real with $\beta_{-1} = 1$ so that the functions φ_k are uniquely determined.

The formulation used here for the theorem is based on the results in [2, Sec. 4], except that we do not necessarily take $\mu_0 = \infty$ by convention.

The zeros of φ_k can be computed from the recurrence coefficients by solving a generalised eigenvalue problem, as given in the following theorem from [2, Sec. 5].

Theorem 2.2. *Suppose that the ORFs φ_j, for $j = 0, \ldots, n$ and $1 \leq n \leq N$ are regular. Define the matrices*

$$J_n = \begin{bmatrix} \alpha_0 & \beta_0 & 0 & \cdots & 0 \\ \beta_0 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \beta_{n-2} \\ 0 & \cdots & 0 & \beta_{n-2} & \alpha_{n-1} \end{bmatrix}, \quad D_n = \begin{bmatrix} \mu_0^{-1} & 0 & \cdots & 0 \\ 0 & \mu_1^{-1} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \mu_{n-1}^{-1} \end{bmatrix}. \tag{4}$$

Then the eigenvalues λ_j, $j = 1, \ldots, n$ of the generalised eigenvalue problem

$$(I_n + J_n D_n)^{-1} J_n v^j = \lambda_j v^j,$$

where I_n is the $n-$dimensional unit matrix and $v^j \in \mathbb{C}^n$ (the superscript ^{j} here denotes an index), are equal to the nodes $z_{n,j}$ of $\varphi_n(z)$.

The elements of $\mathbb{C}^N$ will be represented by column vectors of length N with the indices running from 0 to $N-1$. These vectors may also be interpreted as rational functions. If $c = (c_0, \ldots, c_{N-1})^T$ is a vector, we assign to it the rational function

$$\hat{c}(z) = c_0 b_0(z) + c_1 b_1(z) + \ldots + c_{N-1} b_{N-1}(z) = b(z) \cdot c \in \mathcal{L}_{N-1},$$

where $b(z)$ represents the vector $b(z) = (b_0(z), b_1(z), \ldots, b_{N-1}(z))$. A row of vectors in $\mathbb{C}^N$

$$C_{N\times m} = \left(c^0, c^1, \ldots, c^{m-1}\right)$$

will also frequently be interpreted as an N by m matrix

$$(C_{N\times m})_{i,j+1} = \left(c^j\right)_i, \quad i = 1, 2, \ldots, N, \quad j = 0, 1, \ldots, m-1,$$

where $\left(c^j\right)_i$ denotes the i^{th} coordinate of the vector c^j. In the remainder of this paper a superscript ^{j} represents an index in the case of a vector, while for constants and matrices it denotes a power. Furthermore, the superscript ^{T} and * denote respectively the transpose and the complex conjugate transpose. Finally, in the special case of an n by n matrix, we shall use the notation $C_n = C_{n\times n}$ for $n < N$, and $C = C_{N\times N}$ for $n = N$.

Given a vector $c = (c_0, \ldots, c_{N-1})^T$ we denote by $D(c)$ the diagonal matrix with $c_0, \ldots, c_{N-1}$ on the diagonal.

3 Extension of the polynomial case to the rational case

The results from Section 3 up to Section 6 of [3] for the polynomial case remain valid for the case of rational functions. Therefore, in this section we reformulate those results for the case of rational functions. For the proof of the theorems, we refer to [3, Sec. 3–6].

Spectral decompositions. A matrix P is said to be a projector if $P^2 = P$. A projector P is an orthogonal projector if P is hermitian. If p is a vector with $\|p\|_2 = 1$, then pp^* is the orthogonal projector onto the line generated by p. In a similar way, given an orthonormal set of vectors $p^0, \ldots, p^k$, the sum $\sum_{j=0}^{k} p^j (p^j)^*$ is the orthogonal projection onto the linear span of the vectors $p^0, \ldots, p^k$.

Given a hermitian N by N matrix A, we assign to it an operator valued function $E(\lambda)$ on the real line with the following properties:

1. For each λ the operator $E(\lambda)$ is either zero or an orthogonal projector;

2. $E(\lambda_1)E(\lambda_2) = 0$ if $\lambda_1 \neq \lambda_2$;

3. $\sum E(\lambda) = 1$;

4. $A = \sum \lambda E(\lambda)$.

This way, the matrix A is represented as a weighed sum of projectors, where λ ranges over the whole real line, but the cardinality of the set of those λ for which $E(\lambda) \neq 0$ does not exceed the size of the matrix A.

It is well known that a hermitian matrix A is unitarily diagonalisable and that its eigenvalues are real. Hence, let A be of size N by N, then there exist N real numbers $\lambda_1, \ldots, \lambda_N$ and an orthonormal set of vectors $u^1, \ldots, u^N$ so that

$$Au^j = \lambda_j u^j, \quad j = 1, 2, \ldots, N.$$

If U is the matrix $(u^1, \ldots, u^N)$ and $\Lambda = D((\lambda_1, \ldots, \lambda_N)^T)$, this set of equations may be rewritten in the form

$$AU = U\Lambda.$$

It is obvious that

$$A = \sum_{j=1}^{N} \lambda_j u^j (u^j)^*,$$

where the operators $u^j(u^j)^*$ are rank one projectors onto a one-dimensional space. So, to define the function $E(.)$, we set $E(\alpha) = 0$ if α does not belong to the spectrum of A. If α is one of the eigenvalues, we define $E(\alpha)$ as the sum $\sum u^j(u^j)^*$ for those j satisfying $\lambda_j = \alpha$.

Suppose the sequence $\mathcal{M}$, as defined before, satisfies the condition that $\mathcal{M} \cap \{\lambda_1, \ldots, \lambda_N\} = \emptyset$. Then we define the factors

$$\begin{aligned} Z_k(A) &= (I - \mu_k^{-1}A)^{-1}A = A(I - \mu_k^{-1}A)^{-1} \\ &= \frac{A}{I - \mu_k^{-1}A}, \quad k = 1, 2, \ldots, N, \end{aligned}$$

and products

$$b_0(A) \equiv I, \quad b_k(A) = Z_k(A)b_{k-1}(A) = b_{k-1}(A)Z_k(A), \quad k = 1, 2, \ldots, N.$$

Note that the order of multiplication does not matter, and hence the factors and products are well defined. If $r = (r_0, \ldots, r_{N-1})^T$ is a vector so that $\hat{r}(z) \in \mathcal{L}_{N-1}$, we assign to it the rational matrix-valued function

$$\hat{r}(A) = r_0 b_0(A) + r_1 b_1(A) + \ldots + r_{N-1} b_{N-1}(A).$$

Using the representation $A = \sum \lambda E(\lambda)$, it is easy to see that

$$\hat{r}(A) = \sum \hat{r}(\lambda)E(\lambda) = \sum \left[b(\lambda) \cdot r\right] E(\lambda).$$

Scalar products on $\mathbb{C}^N$. The standard scalar product on $\mathbb{C}^N$ will be denoted by

$$(c,d) = d^*c = \sum_{j=0}^{N-1} c_j d_j^*.$$

Every positive definite scalar product on $\mathbb{C}^N$ is given by the expression $(Bc,d) = d^*Bc$, where B is a suitable positive definite N by N matrix.

Suppose m is a nonnegative discrete measure on the real line so that the set of those λ where $m(\lambda) > 0$ is finite. To define a semi-definite scalar product $(c,d)_m$ on $\mathbb{C}^N$, we consider the rational functions $\hat{c}(\lambda)$ and $\hat{d}(\lambda)$ corresponding to the vectors c and d and set

$$(c,d)_m = \sum \hat{c}(\lambda)\hat{d}(\lambda)^* m(\lambda).$$

If A is a hermitian N by N matrix and q is a nonzero vector in $\mathbb{C}^N$, it is easy to see that we can choose for example

$$0 \leq m(\lambda) = \|E(\lambda)q\|_2^2.$$

Observe that $\sum m(\lambda) = \|q\|_2^2$. If c and d are two vectors in $\mathbb{C}^N$, we have that

$$\begin{aligned}(\hat{c}(A)q, \hat{d}(A)q) &= \left(\sum \hat{c}(\lambda)E(\lambda)q, \sum \hat{d}(\lambda)E(\lambda)q\right) \\ &= \sum \hat{c}(\lambda)\hat{d}(\lambda)^* \|E(\lambda)q\|_2^2 = (c,d)_m.\end{aligned}$$

Now, let us make the additional assumption that the spectrum of A has no multiplicities. With $Au^j = \lambda_j u^j$ for $j = 1, \ldots, N$ and $(u^i, u^j) = \delta_{i,j}$, where $\delta_{i,j}$ denotes the Kronecker delta, we have that $E(\lambda_j) = u^j(u^j)^*$, so that

$$m(\lambda_j) = \|E(\lambda_j)q\|_2^2 = |(q,u^j)|^2, \quad j = 1, 2, \ldots, N,$$

and the corresponding scalar product is then

$$(c,d)_m = \sum_{j=1}^{N} \hat{c}(\lambda_j)\hat{d}(\lambda_j)^* m(\lambda_j).$$

Next, consider the matrix

$$V = \begin{bmatrix} b(\lambda_1) \\ \vdots \\ b(\lambda_N) \end{bmatrix}. \tag{5}$$

Given a vector $c \in \mathbb{C}^N$, it holds that

$$Vc = (\hat{c}(\lambda_1), \ldots, \hat{c}(\lambda_N))^T$$

is a set of values of the rational function corresponding to c at the points $\lambda_1, \ldots, \lambda_N$. If $B = V^*MV$, where $M = D((m(\lambda_1), \ldots, m(\lambda_N))^T)$, then

$$(Bc,d) = (Vd)^*M(Vc) = \sum_{j=1}^{N} \hat{c}(\lambda_j)\hat{d}(\lambda_j)^* m(\lambda_j) = (c,d)_m.$$

Hence, it follows that the scalar product $(\cdot,\cdot)_m$ is positive definite iff the hermitian matrix A has N distinct eigenvalues λ_j and q is chosen in such a way that $m(\lambda_j) = |(q,u^j)|^2 > 0$ for $j = 1,\ldots,N$.

Rational Krylov sequences. Given a hermitian N by N matrix A and a nonzero vector $q \in \mathbb{C}^N$, we define the rational Krylov sequence $K(A,q,\mathcal{M})$ as the columns of the Krylov matrix

$$K = (b_0(A)q, b_1(A)q, \ldots, b_{N-1}(A)q).$$

Theorem 3.1. *Suppose A is self-adjoint and of the form $A = U\Lambda U^*$ with $U = (u^1,\ldots,u^N)$ unitary and $\Lambda = D((\lambda_1,\ldots,\lambda_N)^T)$. If q is an arbitrary nonzero vector in $\mathbb{C}^N$, then*

$$K = UD(\tilde{q})V,$$

where V is given by (5) *and $\tilde{q} = U^*q$, i.e. the coordinate vector of q in the basis $u^1,\ldots,u^N$.*

The rational Lanczos process and ORFs. The application of the orthonormalisation process to the rational Krylov sequence is equivalent to the construction of an upper triangular matrix G so that the resulting sequence $Q = KG$ satisfies $Q^*Q = I$. By q^k and g^k we denote the $(k+1)^{th}$ column of respectively Q and G. Furthermore, let $\check{\varphi}_k = g^k$ and $\varphi_k(\cdot) = \hat{g}^k(\cdot)$.

Since $(\check{\varphi}_k, \check{\varphi}_l)_m = (\varphi_k(A)q, \varphi_l(A)q) = (K\check{\varphi}_k, K\check{\varphi}_l) = (q^k, q^l)$, the rational functions φ_k constitute an orthonormal system with respect to the measure m. We shall make the assumption that the scalar product $(.,.)_m$ is positive definite, and consequently, that the spectrum of A is simple. Therefore, we have the following theorem.

Theorem 3.2. *Let $\varphi_0,\ldots,\varphi_{N-1}$ be a sequence of rational functions.*

1. *Suppose $A = UD((\lambda_1,\ldots,\lambda_N)^T)U^*$, with $U = (u^1,\ldots,u^N)$ and $U^*U = I$, is a hermitian N by N matrix and q is a nonzero vector in $\mathbb{C}^N$. If the vectors $q^k = \varphi_k(A)q$ form an orthonormal set (or equivalently, if the matrix Q is the result of the rational Lanczos process applied to the pair (A,q)), then $\varphi_0,\ldots,\varphi_{N-1}$ is an orthonormal set of rational functions with respect to the discrete measure m so that*

$$m(z) = \begin{cases} |(q,u^j)|^2 & , \quad z = \lambda_j \\ 0 & , \quad z \notin \{\lambda_1,\ldots,\lambda_N\} \end{cases}.$$

2. *If m is a discrete measure with mass points $\lambda_1,\ldots,\lambda_N$, and if $\varphi_0,\ldots,\varphi_{N-1}$ is an orthonormal set of rational functions with respect to the measure m, then the vectors $q^k = \varphi_k(A)q$ form an orthonormal set for the standard scalar product $(\cdot,\cdot)$ in $\mathbb{C}^N$ for every pair (A,q) of the form*

$$A = UD((\lambda_1,\ldots,\lambda_n)^T)U^*, \quad q = \sum_{j=1}^{n} m(\lambda_j)^{1/2}u^j,$$

where $U = (u^1,\ldots,u^N)$ is an arbitrary unitary matrix.

The following theorem shows how to recover m if G is given.

Theorem 3.3. *Let m be a measure concentrated in N distinct points $\lambda_1, \ldots, \lambda_N$ with $m(\lambda_j) > 0$. Let $\varphi_0, \ldots, \varphi_{N-1}$ be the system of ORFs corresponding to m. Then*

$$m(\lambda_j) = \left(\sum_{k=0}^{N-1} |\varphi_k(\lambda_j)|^2 \right)^{-1}.$$

4 The three-term recurrence relation

Consider a hermitian N by N matrix A with simple spectrum and a nonzero vector $q \in \mathbb{C}^N$ chosen in such a way that the scalar product $(\cdot, \cdot)_m$ is positive definite. Then we have the following lemma.

Lemma 4.1. *Assume the discrete measure m and the scalar product $(\cdot, \cdot)_m$ as defined before. Then the Krylov matrix K is nonsingular ($K_{N\times n}$ is of full rank for $1 \leq n \leq N$) for every sequence of poles outside the spectrum of $A = UD\left((\lambda_1, \ldots, \lambda_N)^T\right) U^*$ with $U^*U = I$ and $U = (u^1, \ldots, u^N)$, if the scalar product $(\cdot, \cdot)_m$ is positive definite.*

Proof. Suppose that for a certain sequence of poles it holds with $b_n(z) \in \mathcal{L}_n \setminus \mathcal{L}_{n-1}$ that $b_n(A)q \in K_{N\times n}$ for an arbitrary $n \in \{1, \ldots, N-1\}$. It follows then that there exists a function $\frac{p_{n-1}(z)}{\pi_{n-1}(z)} \in \mathcal{L}_{n-1}$ so that

$$\left(b_n(A) - \frac{p_{n-1}(A)}{\pi_{n-1}(A)} \right) q = \mathbf{0},$$

where **0** denotes the zero-vector in $\mathbb{C}^N$. Hence,

$$\sum_{j=1}^{N} \frac{\lambda_j^n - (1 - \mu_n^{-1}\lambda_j) p_{n-1}(\lambda_j)}{\pi_n(\lambda_j)} \epsilon_j m(\lambda_j)^{1/2} u^j = \mathbf{0}, \quad |\epsilon_j| = 1 \text{ for } j = 1, \ldots, N.$$

Because $m(\lambda_j) > 0$ for $j = 1, \ldots, N$ and the sequence $u^1, \ldots, u^N$ is an orthonormal set, this can only be true if for every $j \in \{1, \ldots, N\}$

$$\frac{\lambda_j^n - (1 - \mu_n^{-1}\lambda_j) p_{n-1}(\lambda_j)}{\pi_n(\lambda_j)} = 0.$$

But this implies that $b_n(z) = \frac{p_{n-1}(z)}{\pi_{n-1}(z)} \in \mathcal{L}_{n-1}$ due to the fact that $n < N$. Hence, we get a contradiction. $\square$

The rational Lanczos process applied to the pair (A, q) produces the unitary matrix $Q = (q^0, \ldots, q^{N-1})$. Denote by T the matrix $T = Q^*AQ$. Thus, $AQ = QT$ so that T is the matrix of A taken in the basis Q. In the polynomial case (i.e. $\mu_k = \infty$ for $k = 0, \ldots, N$) it has been proven that T is real symmetric tridiagonal. In the rational case, however, this will not be so. Nevertheless, it is possible to prove that, under certain conditions on the poles, there exists a matrix J so that J is real symmetric tridiagonal with positive subdiagonal and

$$T = (I + JD)^{-1} J = J(I + DJ)^{-1}, \quad D = D((\mu_0^{-1}, \mu_1^{-1}, \ldots, \mu_{N-1}^{-1})^T),$$

and conversely

$$J = (I - TD)^{-1} T = T(I - DT)^{-1}.$$

We shall call $q^k = \varphi_k(A)q$, for $k = 0, 1, \ldots, N$ singular iff φ_k is singular, and regular in all other cases. In the special case of $k = N$, we define φ_N by

$$\varphi_N(z) = c_N \frac{\prod_{j=1}^{N}(z - \lambda_j)}{\pi_N(z)}, \tag{6}$$

where $\pi_N(z)$ is given by (3) and $c_N \neq 0$. This way we have that

1. $\varphi_N \in \mathcal{L}_N \setminus \mathcal{L}_{N-1}$,
2. φ_N is orthogonal to $\mathcal{L}_{N-1}$ with respect to the measure m,
3. φ_N is regular,
4. $q^N \triangleq \varphi_N(A)q = \mathbf{0}$, where **0** denotes the zero-vector in $\mathbb{C}^N$.

The following theorem follows directly from Theorem 2.1.

Theorem 4.2. *Take by convention $\mu_{-1} = \infty$ and $q^N = \mathbf{0}$. Suppose that the matrix K is nonsingular. Then the orthonormal vectors q^{k-1}, q^k and q^{k+1} are regular, for $k = 0, 1, \ldots, N-1$, iff they satisfy the following three-term recurrence relation:*

$$Aq^k = \beta_{k-1}\left(I - \mu_{k-1}^{-1}A\right) q^{k-1} + \alpha_k \left(I - \mu_k^{-1}A\right) q^k + \beta_k \left(I - \mu_{k+1}^{-1}A\right) q^{k+1}. \tag{7}$$

The initial conditions are $q^{-1} \equiv 0$ and $q^0 \equiv \frac{q}{\|q\|}$. The coefficients are finite and β_k is different from zero.

Suppose that the orthonormal vectors q^k, for $k = 0, \ldots, n$ with $n \leq N$ are regular, and let $Q_{N\times n}$ denote the matrix containing the first n columns of Q. With I_n, D_n and J_n as defined before in Theorem 2.2 and $e_n = (0, \ldots, 0, 1)^T \in \mathbb{C}^n$, it follows from Theorem 4.2 that

$$\begin{aligned} AQ_{N\times n} &= \begin{bmatrix} Q_{N\times n} & q^n \end{bmatrix} \cdot \begin{bmatrix} J_n \\ \beta_{n-1} e_n^T \end{bmatrix} - A \begin{bmatrix} Q_{N\times n} & q^n \end{bmatrix} \cdot \begin{bmatrix} D_n J_n \\ \mu_n^{-1} \beta_{n-1} e_n^T \end{bmatrix} \\ &= Q_{N\times n} J_n - AQ_{N\times n} D_n J_n + \beta_{n-1}(I - \mu_n^{-1}A) q^n e_n^T, \end{aligned}$$

or equivalently

$$AQ_{N\times n}(I_n + D_n J_n) = Q_{N\times n} J_n + \beta_{n-1}(I - \mu_n^{-1}A) q^n e_n^T. \tag{8}$$

Let $T_n = Q_{N\times n}^* A Q_{N\times n}$ with $n \leq N$. Multiplying from the left on both sides of (8) with $Q_{N\times n}^*$ then gives

$$T_n(I_n + D_n J_n) = J_n - \beta_{n-1}\mu_n^{-1} Q_{N\times n}^* A q^n e_n^T.$$

Furthermore, because $J_n(I_n + D_n J_n)^{-1} = (I_n + J_n D_n)^{-1} J_n$, it follows that

$$(I_n + J_n D_n)^{-1} J_n - T_n = R_n,$$

where R_n is an n by n hermitian matrix with rank$(R_n) \leq 1$ given by

$$\begin{aligned} R_n &= \beta_{n-1} \mu_n^{-1} g_n h_n^* \\ g_n &= Q_{N\times n}^* A q^n \\ h_n &= (I_n + J_n D_n)^{-1} e_n. \end{aligned}$$

In the polynomial case ($\mu_k = \infty$ for $k = 0, \ldots, N$), it holds that rank$(R_n) = 0$ for $n = 1, \ldots, N$. In this case we have that $T_n = J_n$ so that the eigenvalues of T_n are the zeros (i.e. the eigenvalues of J_n) of the orthonormal polynomial (OP) of degree n. These eigenvalues of T_n are called Arnoldi eigenvalue estimates (or Ritz values) with respect to the Krylov matrix $K_{N\times n}$ since some of these eigenvalues may be extraordinarily accurate approximations to some of the eigenvalues of A. It is well known that the approximation is better for the in absolute value largest eigenvalues of A. For the rational case, one might expect that some of the eigenvalues of T_n still are accurate approximations to some of the eigenvalues of A. In the more general rational case, however, the eigenvalues of T_n are not necessarily the zeros of the ORF φ_n, unless either $n = N$, $\mu_n = \infty$ or $q^n = \mathbf{0}$ (which for $n < N$ means that the Lanczos process breaks down at step n). Nevertheless, many observations strongly indicate that most of the zeros of φ_n do not differ much from the eigenvalues of T_n. Therefore, we believe that some of the zeros of φ_n are accurate approximations to some of the eigenvalues of A too. Consider for instance the case of one multiple pole $\mu_k = \mu \neq \infty$ for $k = 0, \ldots, N$. Then the ORFs $\varphi_n(z)$ can be mapped onto the OPs $\phi_n(t)$ by the transformation

$$\tau : z \to t : t = \tau(z) = \frac{z}{1 - \mu^{-1} z},$$

so that $\phi_n(t) = \phi_n(\tau(z)) = \varphi_n(z)$ and $\phi_n(B) = \phi_n(\tau(A)) = \varphi_n(A)$, where

$$B = \frac{A}{I - \mu^{-1} A}.$$

And vice versa, the OPs $\phi_n(t)$ can be mapped onto the ORFs $\phi_n(z)$ by the inverse transformation

$$\tau^{-} : t \to z : z = \tau^{-}(t) = \frac{t}{1 + \mu^{-1} t},$$

so that $\varphi_n(z) = \varphi_n(\tau^{-}(t)) = \phi_n(t)$ and $\varphi_n(A) = \varphi_n(\tau^{-}(B)) = \phi_n(B)$, where

$$A = \frac{B}{I + \mu^{-1} B}.$$

It is not difficult to see that

$$Q^* B Q = J \Leftrightarrow Q^* A Q = (I + JD)^{-1} J.$$

Furthermore we then have that $Q^*_{N\times n}BQ_{N\times n} = J_n$, but $Q^*_{N\times n}AQ_{N\times n} \neq (I_n + J_nD_n)^{-1}J_n$. Clearly, the eigenvalues $\tilde{\lambda}_j$, for $j = 1, \ldots, n$, of J_n are Arnoldi eigenvalue estimates for the matrix B, while the zeros $z_{n,j}$, for $j = 1, \ldots, n$, of φ_n are the eigenvalues of J_n transformed by the mapping τ^-, i.e.

$$z_{n,j} = \tau^- \left(\tilde{\lambda}_j\right), \quad j = 1, \ldots, n.$$

Consequently, although $(I_n + J_nD_n)^{-1}J_n \neq T_n$, the zeros of φ_n can be seen as Ritz values for the matrix A with respect to the Krylov matrix $K_{N\times n}$ as well.

To compute J, we define the vectors $x^{n-1}, y^{n-1} \in \mathbb{C}^N$ with $n = 1, \ldots, N$ by

$$\begin{aligned} x^{n-1} &= Z_n(A)\left\{\beta_{n-2}\left(\mu_{n-2}^{-1} - \mu_n^{-1}\right)q^{n-2} + q^{n-1}\right\} - \beta_{n-2}q^{n-2} \\ y^{n-1} &= \left[I + \left(\mu_n^{-1} - \mu_{n-1}^{-1}\right)Z_n(A)\right]q^{n-1}, \end{aligned} \tag{9}$$

where we set $\mu_N = \mu_{N-1}$ for the special case of $n = N$. Then it follows from (7) that

$$\beta_{n-1}q^n = x^{n-1} - \alpha_{n-1}y^{n-1}, \quad n = 1, \ldots, N. \tag{10}$$

Multiplying with $(q^l)^*$, for $l \in \{0, \ldots, n-1\}$, from the left on both sides of (10) and solving for α_{n-1} gives

$$\alpha_{n-1} = \frac{(q^l)^*x^{n-1}}{(q^l)^*y^{n-1}}. \tag{11}$$

Next, taking the 2-norm on both sides of Equation (10) we find that

$$\beta_{n-1} = \|x^{n-1} - \alpha_{n-1}y^{n-1}\|_2,$$

so that q^n is then given by

$$q^n = \beta_{n-1}^{-1}\left(x^{n-1} - \alpha_{n-1}y^{n-1}\right).$$

Finally, with the initial conditions $q^{-1} = \mathbf{0}$ and $q^0 = q/\|q\|_2$, it holds for $n = 1$ that

$$\begin{aligned} \alpha_0 &= \frac{(q^0)^*Z_1(A)q^0}{1 + \left(\mu_1^{-1} - \mu_0^{-1}\right)(q^0)^*Z_1(A)q^0} \\ \beta_0 &= \|\left[\{1 - \alpha_0(\mu_1^{-1} - \mu_0^{-1})\}Z_1(A) - \alpha_0 I\right]q^0\|_2 \\ &= (q^0)^*\left[\{1 - \alpha_0(\mu_1^{-1} - \mu_0^{-1})\}Z_1(A) - \alpha_0 I\right]^2 q^0 \\ q^1 &= \beta_0^{-1}\left[\{1 - \alpha_0(\mu_1^{-1} - \mu_0^{-1})\}Z_1(A) - \alpha_0 I\right]q^0. \end{aligned}$$

5 Forbidden poles

Suppose that the set $\mu_0, \ldots, \mu_{n-1}$ is fixed for $1 \leq n \leq N$, so that the orthonormal vectors $q^0, \ldots, q^{n-1}$ are regular. Note that for $n \geq 2$, this implies that we assume that the recurrence coefficients $\alpha_0, \beta_0, \ldots, \alpha_{n-2}, \beta_{n-2}$ are fixed. Furthermore, we will again assume that the spectrum of A is simple, and that the vector $q \in \mathbb{C}^N$ has been chosen in such a way that the corresponding Krylov matrices $K_{N\times n}$ for $n =$

$1, \ldots, N$ are of full rank. When choosing a pole $\mu_n = \mu$, we have to make sure that the resulting orthonormal vector q^n is regular so that the three-term recurrence relation holds true. Hence, the question is how we can determine whether the vector q^n is regular. Therefore, we will again prove the three-term recurrence relation of the orthonormal vectors, but now in a different way. First we will give a temporary definition of *forbidden poles*.

Definition 5.1. *Suppose that the sequence of poles $\mathcal{M}_{n-1} = \{\mu_0, \ldots, \mu_{n-1}\} \subset \mathbb{R}_0 \cup \{\infty\}$ is fixed for $1 \leq n \leq N-1$. Then we say that μ_n is a* forbidden pole *iff μ_n satisfies at least one of the following three conditions:*

1. *μ_n is an eigenvalue of A;*
2. *$\left(y^{n-1}, q^{n-1}\right) = 0$, where y^{n-1} is given by* (9)*;*
3. *for $n > 1$, μ_n is an eigenvalue of $\left(I_{n-1} + J_{n-1} D_{n-1}\right)^{-1} J_{n-1}$, with I, D and J as defined before in Theorem 2.2.*

Note that μ_0 and μ_N can never be *forbidden poles* due to the fact that respectively q^0 and q^N do not depend on them. Nevertheless, we will assume that they are outside the spectrum of A.

Theorem 5.2. *Take by convention $q^N = \mathbf{0}$. Furthermore, for the sake of simplicity in notation we will assume that $\mu_N = \mu_{N-1}$. Suppose that the sequence $\mathcal{M}_n$ for $1 \leq n \leq N$ does not contain any* forbidden poles*. Then there exists a set of finite constants $\{f_{n-1,0}, f_{n-1,1}, \ldots, f_{n-1,n}\}$, with $f_{n-1,n} \neq 0$ for $n < N$, so that*

$$A q^{n-1} = \sum_{j=0}^{n} f_{n-1,n} (I - \mu_j^{-1} A) q^j. \tag{12}$$

Proof. If μ_n is not a *forbidden pole*, it follows from the first condition in Definition 5.1 that μ_n is outside the spectrum of A, and hence, $Z_n(A)$ is well defined. Because $Z_n(A) q^{n-1} \in \text{span}\{q^0, \ldots, q^n\}$, there exist finite constants $h_{n-1,j}$, with $j = 0, \ldots, n$, so that

$$Z_n(A) q^{n-1} = \sum_{j=0}^{n} h_{n-1,j} q^j, \quad h_{n-1,j} = \left(Z_n(A) q^{n-1}, q^j\right). \tag{13}$$

It also holds that

$$Z_n(A) q^{n-1} = Z_n(A) \varphi_{n-1}(A) q = \frac{A p_{n-1}(A)}{\pi_n(A)} q.$$

Therefore, under the assumption that the scalar product $(\cdot, \cdot)_m$ is positive definite, we have for $1 < n < N$ that $h_{n-1,n} = 0$ iff $p_{n-1}(\mu_n) = 0$. The third condition in Definition 5.1 implies that $p_{n-1}(\mu_n) \neq 0$ if μ_n is not a *forbidden pole*.

From (13) it follows for $n = 1, \ldots, N$ that

$$\begin{aligned} A q^{n-1} &= (I - \mu_n^{-1} A) \sum_{j=0}^{n} h_{n-1,j} q^j \\ &= \sum_{j=0}^{n} h_{n-1,j} (I - \mu_j^{-1} A) q^j + \sum_{j=0}^{n} h_{n-1,j} \eta_{n-1,j} A q^j, \end{aligned}$$

where

$$\eta_{n-1,j} = \mu_j^{-1} - \mu_n^{-1}.$$

Or equivalently,

$$v_{n-1} A q^{n-1} = \sum_{j=0}^{n} h_{n-1,j} (I - \mu_j^{-1} A) q^j + \sum_{j=0}^{n-2} h_{n-1,j} \eta_{n-1,j} A q^j,$$

with $v_{n-1} = 1 - h_{n-1,n-1}\eta_{n-1,n-1} = \left(y^{n-1}, q^{n-1}\right)$. Because μ_n is not a *forbidden pole*, the second condition in Definition 5.1 is not satisfied, so that $v_{n-1} \neq 0$. Consequently, we have that

$$A q^{n-1} = \sum_{j=0}^{n} \frac{h_{n-1,j}}{v_{n-1}} (I - \mu_j^{-1} A) q^j + \sum_{j=0}^{n-2} \frac{h_{n-1,j}\eta_{n-1,j}}{v_{n-1}} A q^j. \tag{14}$$

For $i = n-1 = 0$, this becomes

$$\begin{aligned} A q^0 &= \frac{h_{0,0}}{v_0} (I - \mu_0^{-1} A) q^0 + \frac{h_{0,1}}{v_0} (I - \mu_1^{-1} A) q^1 \\ &= f_{0,0} (I - \mu_0^{-1} A) q^0 + f_{0,1} (I - \mu_1^{-1} A) q^1, \end{aligned}$$

where $f_{0,0}$ and $f_{0,1}$ are finite and $f_{0,1} \neq 0$ if μ_1 is not a *forbidden pole*. So the statement holds for $i = 0$.

Let us now suppose that the statement is true for $i = 0, \ldots, n-2$ under the condition that $\mathcal{M}_{i+1}$ does not contain any *forbidden poles*. Then under the same condition for $i = n-1$ we have that

$$\begin{aligned} A q^{n-1} &= \sum_{j=0}^{n} \frac{h_{n-1,j}}{v_{n-1}} (I - \mu_j^{-1} A) q^j \\ &\qquad + \sum_{j=0}^{n-2} \left[\frac{h_{n-1,j}\eta_{n-1,j}}{v_{n-1}} \sum_{l=0}^{j+1} f_{j,l} (I - \mu_l^{-1} A) q^l \right] \\ &= \sum_{j=0}^{n} f_{n-1,j} (I - \mu_j^{-1} A) q^j. \end{aligned} \tag{15}$$

Because every $f_{n-1,j}$ is the result of a finite sum of finite numbers, the result itself is finite as well. Furthermore, it holds that $f_{n-1,n} = \frac{h_{n-1,n}}{v_{n-1}}$, so that $f_{n-1,n} \neq 0$ for $n < N$. $\square$

Assume that the sequence $\mathcal{M} = \mathcal{M}_N$ does not contain any *forbidden poles*, and define the matrix F by

$$F = \begin{bmatrix} f_{0,0} & \cdots & \cdots & \cdots & f_{N-1,0} \\ f_{0,1} & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & f_{N-2,N-1} & f_{N-1,N-1} \end{bmatrix}. \tag{16}$$

Then it follows from the previous theorem that

$$AQ = QF - AQDF,$$

or equivalently,

$$AQ(I + DF) = QF.$$

Note that we get the same kind of formula as before, in Section 4, except that J is tridiagonal while F is a Hessenberg matrix. Assuming that the vectors q^n, for $n = 1, \ldots, N-1,$ are determined in such a way that F has a positive real subdiagonal, we have the following two lemmas.

Lemma 5.3. *Suppose that the sequence $\mathcal{M}$ does not contain any* forbidden poles*. Then, with F given by* (16) *and $D = D((\mu_0^{-1}, \mu_1^{-1}, \ldots, \mu_{N-1}^{-1})^T)$, it holds that the inverse of $(I + DF)$ exists.*

Proof. Suppose that $\det(I + DF) = 0$. Then there exists a nonzero vector $c \in \mathbb{C}^N$ so that $(I + DF)c = \mathbf{0}$. Hence

$$\begin{aligned} Q^*AQ(I + DF)c = \mathbf{0} \quad &\Rightarrow \quad Fc = \mathbf{0} \Rightarrow DFc = \mathbf{0} \\ &\Rightarrow \quad (I + DF - I)c = \mathbf{0} \Rightarrow c = \mathbf{0}. \end{aligned}$$

But this is in contradiction with our assumption that c is a nonzero vector. Thus it holds that $\det(I + DF) \neq 0$. □

Lemma 5.4. *Suppose that the sequence $\mathcal{M}$ does not contain any* forbidden poles*. Then the matrix F, given by* (16)*, is real symmetric tridiagonal.*

Proof. Because the matrix A is hermitian, we have that

$$\begin{aligned} F(I + DF)^{-1} &= T = T^* \\ &= (I + DF)^{-*}F^*, \end{aligned}$$

so that

$$(I + DF)^*F = F^*(I + DF).$$

Due to the fact that D is a real diagonal matrix, and hence $D = D^*$, it follows that

$$F + F^*DF = F^* + F^*DF \Rightarrow F = F^*.$$

Thus it holds that the matrix F is hermitian. Finally, because the matrix F is a Hessenberg matrix with positive real subdiagonal, it follows that F is real symmetric tridiagonal. □

From the previous lemma we can conclude that $F = J$. Hence, we have proven that the orthonormal vectors $q^0, \ldots, q^n$ are regular if $\mathcal{M}_n$ does not contain any *forbidden poles*.

Remark 5.5. *With our temporary definition of* forbidden poles*, the opposite is not necessarily true, i.e. if the orthonormal vectors $q^0, \ldots, q^n$ are regular, $\mathcal{M}_n$ may contain* forbidden poles*. Consider the case of one* forbidden pole *μ_n satisfying the second and third condition, but not the first. Equation* (15) *then becomes*

$$\begin{aligned} 0 &= v_{n-1} A q^{n-1} \\ &= \sum_{j=0}^{n-1} h_{n-1,j}(I - \mu_j^{-1} A) q^j + \sum_{j=0}^{n-2} \left[h_{n-1,j} \eta_{n-1,j} \sum_{l=0}^{j+1} f_{j,l} (I - \mu_l^{-1} A) q^l \right] \\ &= \sum_{j=0}^{n-1} \ddot{h}_{n-1,j} (I - \mu_j^{-1} A) q^j. \end{aligned}$$

Thus, if $\ddot{h}_{n-1,j} = 0$ for $j = 0, \ldots, n-1$, we cannot conclude that q^n is singular.

In practice, α_{n-1}, given by (11)*, will most of the time be computed with q^{n-1}. Therefore, if μ_n only satisfies the second condition, the denominator in* (11) *equals zero, so that $\alpha_{n-1} = \infty$. However, if μ_n also satisfies the third condition, many observations strongly indicate that*

- *the denominator in* (11) *tends to zero as well;*
- *q^n is regular;*
- *α_{n-1} can be computed more accurately with the aid of another orthonormal vector q^j with $j < n-1$.*

However, at the moment of writing we did not found a proof for these observations. Therefore, we will still consider μ_n a forbidden pole*, even when it simultaneously satisfies the second and third condition. The least we can say for sure, is that*

1. *the first condition in Definition 5.1 is essential. Otherwise, we can never have that $q^N = \mathbf{0}$ (see Equation* (6)*);*
2. *if μ_n satisfies either the second or third condition, q^n is singular;*
3. *if $\mathcal{M}_n$ does not contain any* forbidden poles*, then the rational Lanczos process breaks down at step n iff the matrix A has just $n-1$ distinct eigenvalues or the vector q is a combination of just $n-1$ eigenvectors of A.*

Suppose that $\mathcal{M}_{n-1}$, for $n > 0$, does not contain any *forbidden poles*. With $A = UD\left((\lambda_1, \ldots, \lambda_N)^T\right) U^*$ and $U^*U = I$, the second condition in Definition 5.1, for $\mu_n = \mu$, can be rewritten as

$$\begin{aligned} 0 &= (q^{n-1})^* \left[I + \frac{(\mu^{-1} - \mu_{n-1}^{-1})A}{I - \mu^{-1}A} \right] q^{n-1} \\ &= (q^{n-1})^* \left[\frac{I - \mu_{n-1}^{-1} A}{I - \mu^{-1} A} \right] q^{n-1} \\ &= (\tilde{q}^{n-1})^* D \left(\left(\frac{1 - \mu_{n-1}^{-1}\lambda_1}{1 - \mu^{-1}\lambda_1}, \ldots, \frac{1 - \mu_{n-1}^{-1}\lambda_n}{1 - \mu^{-1}\lambda_n} \right)^T \right) \tilde{q}^{n-1}, \end{aligned}$$

where $\tilde{q}^{n-1} = U^* q^{n-1} = (w_0, \ldots, w_{N-1})^T$ and $\sum_{j=1}^{N} |w_{j-1}|^2 = 1$. So, let us define $h_n(\breve{\mu})$ by

$$h_n(\breve{\mu}) = \sum_{j=1}^{N} |w_{j-1}|^2 \frac{1 - \breve{\mu}_{n-1}\lambda_j}{1 - \breve{\mu}\lambda_j} = \frac{g_{N-1}(\breve{\mu})}{\rho_N(\breve{\mu})}, \tag{17}$$

with $\breve{\mu}_{n-1} = \mu_{n-1}^{-1}$ and $\breve{\mu} = \mu^{-1} \in \mathbb{R}$, $g_{N-1} \in \mathcal{P}_{N-1}$ and $\rho_N(\breve{\mu}) = \prod_{j=1}^{N}(1 - \breve{\mu}\lambda_j)$. Then the second condition in Definition 5.1 is satisfied iff $\breve{\mu}$ is a zero of $h_n(\breve{\mu})$. Moreover, if $\breve{\mu}$ is a pole of $h_n(\breve{\mu})$, the first condition in Definition 5.1 is satisfied. Hence, we have proven the following theorem.

Theorem 5.6. *Let $h_n(\breve{\mu})$, with $\breve{\mu} \in \mathbb{R}$ and $n > 0$, be given by* (17)*. Suppose $\mu_0, \ldots, \mu_{n-1}$ are not* forbidden poles*. Then $\mu_n = \breve{\mu}^{-1}$ is a* forbidden pole *if $\breve{\mu}$ is a zero or pole of $h_n(\breve{\mu})$.*

Note that $\mu = \mu_{n-1}$ can never be a *forbidden pole*, due to the fact that μ_{n-1} is not an eigenvalue of A, $p_{n-1}(\mu_{n-1}) \neq 0$ (because $\varphi_{n-1} \in \mathcal{L}_{n-1} \setminus \mathcal{L}_{n-2}$) and $h_n(\breve{\mu}_{n-1}) = 1 \neq 0$. Furthermore, it follows from the previous theorem that there can be no more than $2(N-1)+n$ *forbidden poles*. The upper bound for this maximum number of *forbidden poles* can be reduced even more. Therefore, we first need the following lemma.

Lemma 5.7. *Suppose that $\lambda_s \neq 0$ is an eigenvalue of A and assume that the sequence $\mathcal{M}_{n-1}$ for $n > 1$ does not contain any* forbidden poles*. Then $h_n(\lambda_s^{-1}) \in \mathbb{R}$ iff $p_{n-1}(\lambda_s) = 0$. Furthermore, $\lim_{\breve{\mu}\to\infty} h_n(\breve{\mu}) \neq 0$ iff $\det A = 0$ and $p_{n-1}(0) \neq 0$.*

Proof. First, note that

$$\tilde{q}^{n-1} = U^* q^{n-1} = U^* \varphi_{n-1}(A) q = D\left((\varphi_{n-1}(\lambda_1), \ldots, \varphi_{n-1}(\lambda_N))^T\right)\tilde{q},$$

where $\tilde{q} = U^* q$, so that $|w_{s-1}|^2 = |\varphi_{n-1}(\lambda_s)|^2 m(\lambda_s) = \left|\frac{p_{n-1}(\lambda_s)}{\pi_{n-1}(\lambda_s)}\right|^2 m(\lambda_s)$, with $m(\lambda_s) > 0$. Hence, $w_{s-1} = 0$ iff $p_{n-1}(\lambda_s) = 0$. For $\lambda_s \neq 0$ it now holds that

$$\begin{aligned}
\lim_{\breve{\mu}\to\lambda_s^{-1}} h_n(\breve{\mu}) &= \left[\sum_{j=1, j\neq s}^{N} |w_{j-1}|^2 \frac{1 - \breve{\mu}_{n-1}\lambda_j}{1 - \lambda_s^{-1}\lambda_j}\right] + |w_{s-1}|^2 \lim_{\breve{\mu}\to\lambda_s^{-1}} \frac{1 - \breve{\mu}_{n-1}\lambda_s}{1 - \breve{\mu}\lambda_s} \\
&= \tilde{h}_n(\lambda_s^{-1}) + |w_{s-1}|^2 (1 - \breve{\mu}_{n-1}\lambda_s) \lim_{\breve{\mu}\to\lambda_s^{-1}} \frac{1}{1 - \breve{\mu}\lambda_s},
\end{aligned}$$

with $\tilde{h}_n(\lambda_s^{-1}) \in \mathbb{R}$ and $(1 - \breve{\mu}_{n-1}\lambda_s) \neq 0$. So, we have that $\lim_{\breve{\mu}\to\lambda_s^{-1}} h_n(\breve{\mu}) \in \mathbb{R}$ iff $w_{s-1} = 0$.

Finally, for $\breve{\mu}$ tending to infinity, we have that

$$\begin{aligned}
\lim_{\breve{\mu}\to\infty} h_n(\breve{\mu}) &= \sum_{j=1}^{N} |w_{j-1}|^2 (1 - \breve{\mu}_{n-1}\lambda_j) \lim_{\breve{\mu}\to\infty} \frac{1}{1 - \breve{\mu}\lambda_j} \\
&= \begin{cases} 0 & \text{if} \quad \det A \neq 0 \\ |\varphi_{n-1}(0)|^2 m(0) & \text{if} \quad \det A = 0 \end{cases}.
\end{aligned}$$

∎

Because $\mu \in \mathbb{R}_0 \cup \{\infty\}$ (or equivalently $\breve{\mu} \in \mathbb{R}$), we only have to consider the eigenvalues of A different from zero in the first condition of Definition 5.1. This way, it follows from the previous lemma that Definition 5.1 is equivalent with the following final definition for *forbidden poles*.

Definition 5.8. *Suppose that the sequence of poles $\mathcal{M}_{n-1} = \{\mu_0, \ldots, \mu_{n-1}\} \subset \mathbb{R}_0 \cup \{\infty\}$ is fixed for $1 \leq n \leq N-1$. Then we say that μ_n is a* forbidden pole *iff μ_n satisfies at least one of the following two conditions:*

1. *$\breve{\mu} = \mu_n^{-1}$ is a pole or zero of $h_n(\breve{\mu})$ given by* (17),
2. *for $n > 1$, $\mu = \mu_n$ is an eigenvalue of $(I_{n-1} + J_{n-1}D_{n-1})^{-1} J_{n-1}$, with I, D and J as defined before in Theorem 2.2.*

Theorem 5.9. *Suppose that $\varphi_{n-1}(\lambda_s) = 0$ for $1 < n < N$ and $s = 1, \ldots, m \leq n-1$, with $L_m = \{\lambda_s\}_{s=1}^m \subset \{\lambda_1, \ldots, \lambda_N\} = L_N$. Then there can be no more than $2(N-1-m)+n$* forbidden poles.

Proof. If $0 \notin L_m$, it follows directly from Lemma 5.7 that m finite poles vanish with m finite zeros. If, on the other hand, it holds that $\lambda_s = 0 \in L_m$, then we have that

$$h_n(\breve{\mu}) = \sum_{j=1, j\neq s}^{N} |w_{j-1}|^2 \frac{1 - \breve{\mu}_{n-1}\lambda_j}{1 - \breve{\mu}\lambda_j} = \frac{g_{N-2}(\breve{\mu})}{\rho_{N-1}(\breve{\mu})},$$

with $g_{N-2} \in \mathcal{P}_{N-2}$ and $\rho_{N-1}(\breve{\mu}) = \prod_{j=1, j\neq s}^{N}(1 - \breve{\mu}\lambda_j)$. Furthermore, it follows from the previous lemma that $m-1$ of the remaining finite poles vanish with $m-1$ finite zeros. $\square$

6 Numerical examples

In every example that follows, we have taken $q = (1, 1, \ldots, 1)^T$.

Example 6.1. *First, let us consider the case that*

$$\begin{aligned} A = D((&1, 2, \ldots, 20, 101, 102, \ldots, 120, 201, 202, \ldots, 220, 301, 302, \ldots, 320, \\ &401, 402, \ldots, 420, 501, 502, \ldots, 520, 601, 602, \ldots, 620, \\ &701, 702, \ldots, 720, 801, 802, \ldots, 820, 901, 902, \ldots, 920)^T) \end{aligned} \tag{18}$$

and

$$\begin{aligned} \mathcal{M} = \{&\mu_0 = \mu_1 = \mu_2 = \ldots = \mu_9 = 425, \mu_{10} = \mu_{12} = \ldots = \mu_{19} = 895, \\ &\mu_{20} = \mu_{22} = \ldots = \mu_{29} = 25, \mu_{30} = \mu_{32} = \ldots = \mu_{39} = 125\}. \end{aligned} \tag{19}$$

Figure 1 then graphically shows the zeros of $\varphi_k(z)$ for $k = 1, \ldots, 39$. Starting with a pole in 425, this graph clearly illustrates the convergence of one or more zeros of $\varphi_k(z)$ to the eigenvalues of A the closest to 425. When, for instance at $k = 10$, the pole in

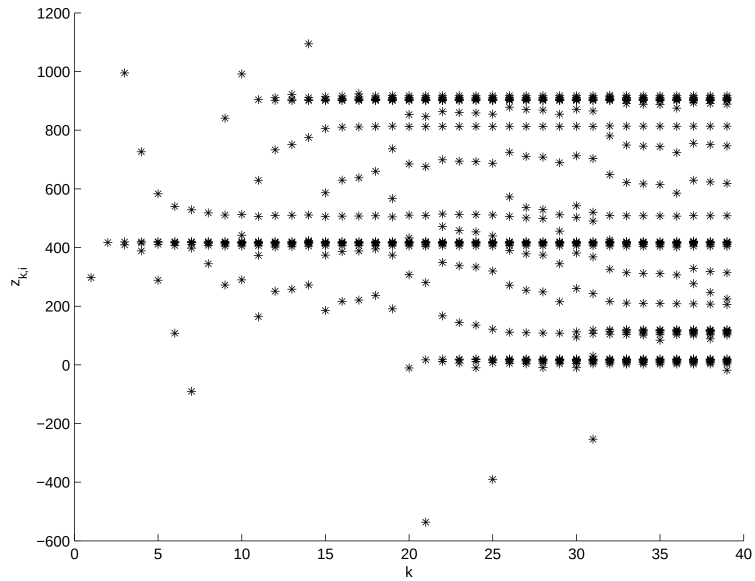

Figure 1: The zeros $z_{k,i}$ of $\varphi_k(z)$ for $k = 1, \dots, 39$ and $i = 1, \dots, k$ when A is given by (18) and the poles are given by (19).

425 *is changed into a pole in* 895*, a few steps later the graph shows the introduction of zeros in the proximity of the eigenvalues of* A *the closest to* 895*. Similarly, the graph shows the introduction of zeros in the proximity of the eigenvalues of* A *the closest to* 25 *and* 125 *a few steps after the pole is changed into respectively* 25 *at* $k = 20$ *and* 125 *at* $k = 30$*.*

Example 6.2. *Next, consider the case that*

$$A = D((5, 5.3, 5.7, 6.2, 6.7, 7.3, 8, 8.9, 10, 11.4, 13.3, 16, 20, 26.7, 40, 80)^T) \quad (20)$$

and

$$\mathcal{M} = \{\mu_k = 13, k = 0, \dots, 15\}. \quad (21)$$

Table 1 then gives the zeros of $\varphi_4(z)$ *and* $\varphi_8(z)$ *as well as their inverse values. The values in bold are approximately equal to one of the eigenvalues of* A*. For instance, for* $k = 4$*, we can deduce from this table that* $\varphi_4(z)$ *has a node* $z_{4,3} \approx 13.3$*, which is indeed the eigenvalue of* A *the closest to the pole* 13*. Hence, when determining* q^5*, we could have decided to choose another pole* $\tilde{\mu}_5$*. Or we could have waited until the determination of* q^9 *to choose another pole* $\tilde{\mu}_9$*. Let* $\breve{\mu} = \tilde{\mu}^{-1}$*, then Figure 2 above shows the graph of* $h_5(\breve{\mu})$*, given by* (17)*, while Figure 2 beneath shows the graph of* $h_9(\breve{\mu})$*. Comparing both graphs, they clearly show that the poles of* $h_9(\breve{\mu})$ *in the inverse eigenvalues of* A *vanish with the same zeros of* $\varphi_8(z)$ *(see also the values in bold in Table 1).*

		$z_{k,i}$		$z_{k,i}^{-1}$	
i	k	4	8	4	8
1		5.8332	5.7289	0.171	0.175
2		11.2957	8.3603	0.089	0.119
3		**13.3000**	9.9859	**0.075**	0.100
4		17.1800	**11.4000**	0.058	**0.088**
5			**13.3000**		**0.075**
6			**16.0001**		**0.063**
7			20.2251		0.049
8			38.4973		0.026

Table 1: The zeros $z_{k,i}$ of $\varphi_k(z)$ for $k = 4, 8$ and $i = 1, \ldots, k$ when A is given by (20) and the poles are given by (21). The values in bold are approximately equal to one of the eigenvalues of A. The inverse $z_{k,i}^{-1}$ of these values is given as well.

i	eig(A)	$z_{16,i}$	$\tilde{z}_{16,i}$
1	5	4.9953	5.0000
2	5.3	5.2986	5.3000
3	5.7	5.7000	5.7000
4	6.2	5.7008	6.2000
5	6.7	5.7024	6.7000
6	7.3	5.7039	7.3000
7	8	6.2004	8.0000
8	8.9	6.2022	8.9000
9	10	6.6939	10.0000
10	11.4	7.3579	11.4000
11	13.3	8.9032	13.3000
12	16	11.3691	16.0000
13	20	13.3000	20.0004
14	26.7	14.5657	26.7069
15	40	16.9531	40.0207
16	80	36.9986	80.0125

Table 2: The eigenvalues 'eig(A)' of A, given by (20), and the zeros $z_{16,i}$ and $\tilde{z}_{16,i}$ of $\varphi_{16}(z)$ when α_4 has been computed respectively with q^4 and q^3. The poles are given by $\{\mu_0 = \ldots = \mu_4 = 13, \mu_5 = \ldots = \mu_{15} = 5.8332\}$, where 5.8332 is a zero of $\varphi_4(z)$.

Finally, note that the inverse values of those zeros of $\varphi_{k-1}(z)$ that do not approximate an eigenvalue of A, seem to be zeros of $h_k(\breve{\mu})$. Consider for instance the case that $\tilde{\mu}_5 = \ldots = \tilde{\mu}_{15} = z_{4,1} = 5.8332$. Table 2 then gives the nodes of $\varphi_{16}(z)$, first when α_4 has been computed with q^4, and afterwards when α_4 has been computed with q^3.

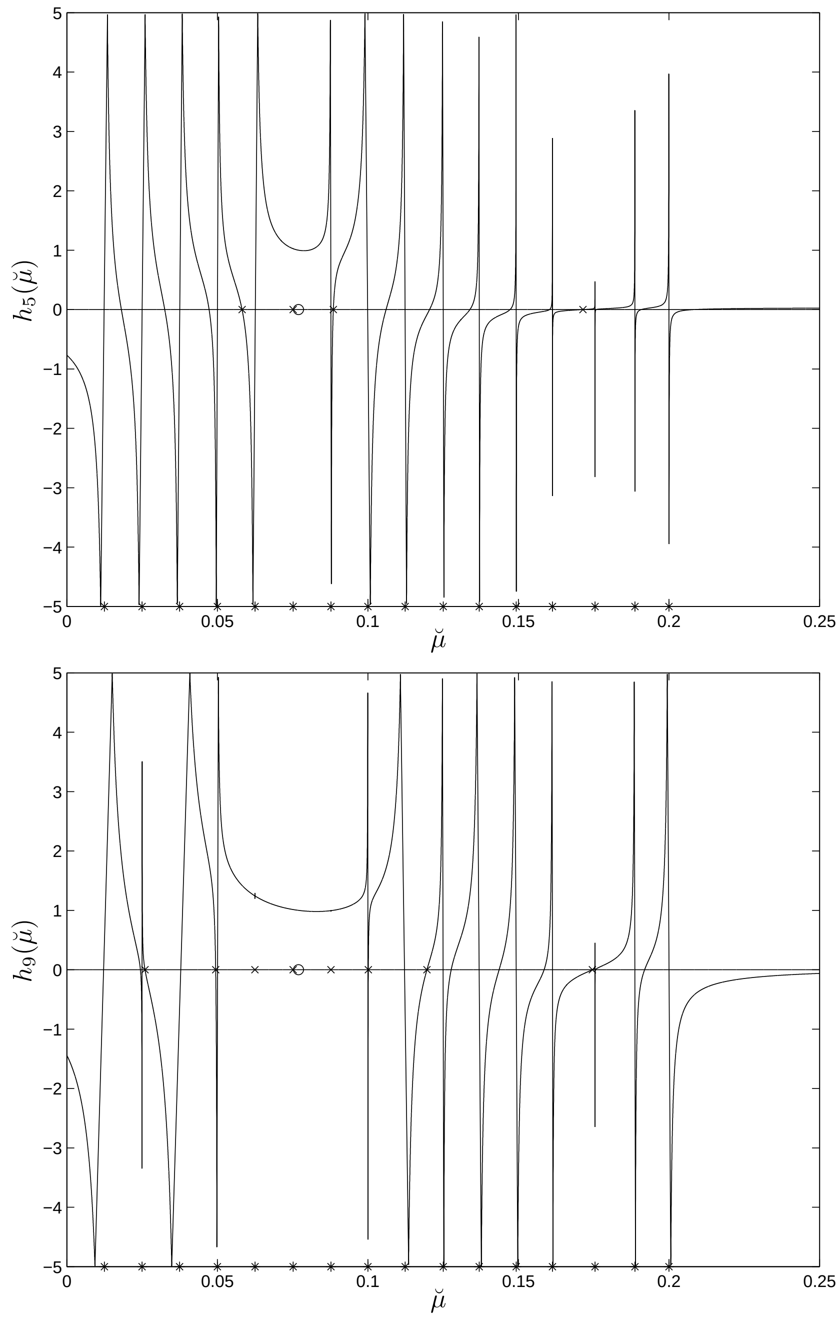

Figure 2: The graph of $h_k(\breve{\mu})$, given by (17), when A is given by (20) and $\breve{\mu}_{k-1} = 1/13$ (marked with an 'o'), for $k = 5$ (above) and $k = 9$ (beneath). The positions of the inverse eigenvalues of A are marked with a '$*$', while the positions of the inverse zeros of $\varphi_{k-1}(z)$ are marked with an '$\times$'.

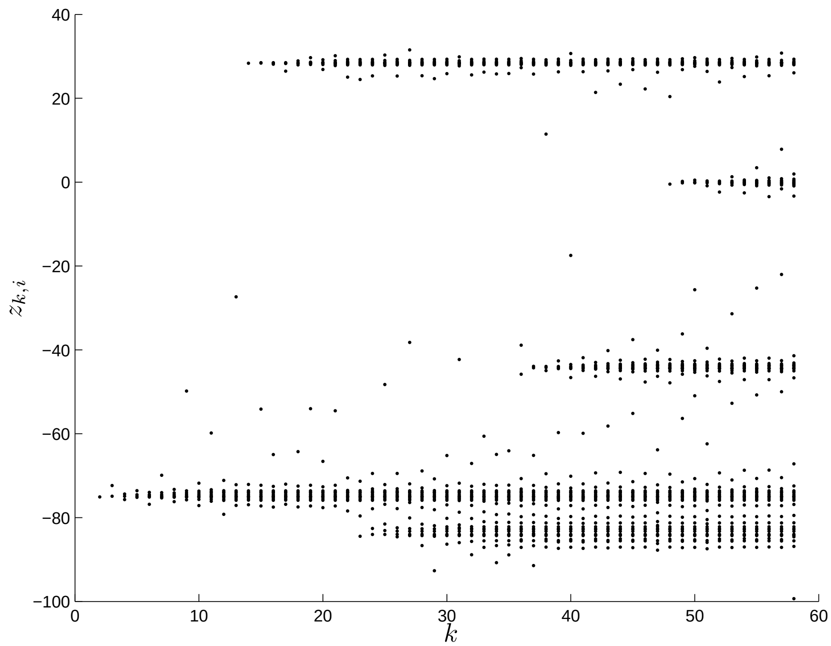

Figure 3: The zeros $z_{k,i}$ of $\varphi_k(z)$ for $k = 1, \ldots, 58$ and $i = 1, \ldots, k$ when A is given by (22) and the poles are given by (23).

Example 6.3. *Finally, consider the case that*

$$A = B + B^H \tag{22}$$

and

$$\begin{aligned}\mathcal{M} \quad = \quad & \{\mu_0 = \ldots = \mu_{12} = -74.70665262792586, \\ & \mu_{13} = \ldots = \mu_{21} = 28.43493168481659, \\ & \mu_{22} = \ldots = \mu_{34} = -83.62041912422748, \\ & \mu_{35} = \ldots = \mu_{46} = -44.09278169786580, \\ & \mu_{47} = \ldots = \mu_{58} = -0.07633138941779551\},\end{aligned} \tag{23}$$

where B is a random matrix of size 1000 by 1000. To generate this random matrix B, we used the matlab command RANDOM with exponential distribution and parameter equals one, i.e.

$$B = \text{random}('\text{exp}', 1, 1000, 1000).$$

Figure 3 then graphically shows the zeros of $\varphi_k(z)$ for $k = 1, \ldots, 58$, while Tables 3–7 illustrate the convergence of these zeros to the eigenvalues of A in the neighbourhood of the chosen poles.

k		
2	-75.07138158649700	
3	-74.90415598532118	-72.33545848125323
4	-74.88722821487410	-74.35442689734335
5	-74.88293719212363	-74.52247064066461
6	-74.88257941910386	-74.53039687584757
7	-74.88255314969979	-74.53073528541057
8	-74.88254936102433	-74.53075558708387
9	-74.88254921469675	-74.53075603831439
10	-74.88254921310352	-74.53075604269772
11	-74.88254921307571	-74.53075604277467
12	-74.88254921307535	-74.53075604277581
eig(A)	-74.88254921307539	-74.53075604277633

Table 3: Selection of zeros of $\varphi_k(z)$ for $k = 2, \ldots, 12$ together with two eigenvalues 'eig(A)' of A, given by (22), in the neighbourhood of the pole $\mu_k = -74.70665262792586$.

k		
14	28.34912717573689	
15	28.38206678607947	28.48889591607436
16	28.38260053019498	28.48727120290261
17	28.38262104605347	28.48724226540813
18	28.38262175296683	28.48724162263257
19	28.38262176941285	28.48724160040398
20	28.38262176957222	28.48724160006213
21	28.38262176957326	28.48724160005994
eig(A)	28.38262176957325	28.48724160005994

Table 4: Selection of zeros of $\varphi_k(z)$ for $k = 14, \ldots, 21$ together with two eigenvalues 'eig(A)' of A, given by (22), in the neighbourhood of the pole $\mu_k = 28.43493168481659$.

k		
23	-84.45655848650057	
24	-84.01378336701816	-82.58622618669277
25	-83.99882748400724	-83.08343357327384
26	-83.99444372863825	-83.23161100812494
27	-83.99347127968137	-83.24679334108409
28	-83.99342336103068	-83.24738972709405
29	-83.99341815210235	-83.24741918943062
30	-83.99341614761853	-83.24742209304441
31	-83.99341606464419	-83.24742218057737
32	-83.99341606102384	-83.24742218731915
33	-83.99341606096259	-83.24742218749245
34	-83.99341606096212	-83.24742218749395
eig(A)	-83.99341606096128	-83.24742218749370

Table 5: Selection of zeros of $\varphi_k(z)$ for $k = 23, \ldots, 34$ together with two eigenvalues 'eig(A)' of A, given by (22), in the neighbourhood of the pole $\mu_k = -83.62041912422748$.

k		
36	-45.81012402440861	
37	-44.28756728280433	-43.92468126641263
38	-44.22848506443002	-43.96007168770122
39	-44.22395584485643	-43.96172849534423
40	-44.22378193048641	-43.96178549173455
41	-44.22377594338028	-43.96178764163637
42	-44.22377568240039	-43.96178771998225
43	-44.22377567384875	-43.96178772201143
44	-44.22377567369579	-43.96178772204942
45	-44.22377567368481	-43.96178772204691
46	-44.22377567368464	-43.96178772204685
eig(A)	-44.22377567368397	-43.96178772204763

Table 6: Selection of zeros of $\varphi_k(z)$ for $k = 36, \ldots, 46$ together with two eigenvalues 'eig(A)' of A, given by (22), in the neighbourhood of the pole $\mu_k = -44.09278169786580$.

k		
48	-0.4838570877860278	
49	-0.1863101036041319	0.1837911717117914
50	-0.1776579965610296	0.03687735307379819
51	-0.1769717619800633	0.02453950362899089
52	-0.1769482165993965	0.02429560467638048
53	-0.1769432429686140	0.02428058031246304
54	-0.1769427918398407	0.02428001287400376
55	-0.1769427796416630	0.02428000080026274
56	-0.1769427794038496	0.02428000059346411
57	-0.1769427794022227	0.02428000059212321
58	-0.1769427794022236	0.02428000059210279
eig(A)	-0.1769427793333267	0.02428000049773565

Table 7: Selection of zeros of $\varphi_k(z)$ for $k = 48, \ldots, 58$ together with two eigenvalues 'eig(A)' of A, given by (22), in the neighbourhood of the pole $\mu_k = -0.07633138941779551$.

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