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Orthogonal rational functions and quadrature on an interval

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Abstract

Rational functions with real poles and poles in the complex lower half-plane, orthogonal on the real line, are well known. Quadrature formulas similar to the Gauss formulas for orthogonal polynomials have been studied. We generalize to the case of arbitrary complex poles and study orthogonality on a finite interval. The zeros of the orthogonal rational functions are shown to satisfy a quadratic eigenvalue problem. In the case of real poles, these zeros are used as nodes in the quadrature formulas.
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1. Introduction

We consider linear vector spaces of rational functions with poles in a prescribed set of complex numbers. Let a sequence of poles $A = \{\alpha_1, \alpha_2, \alpha_3, \ldots\} \subset \hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$ be given (where $\mathbb{C}$ denotes the complex plane) and define

$$\pi_n(z) = \prod_{k=1}^{n} (z - \alpha_k).$$

If $\mathscr{P}_n$ denotes the space of polynomials of degree at most n over the complex field, then we can define the space of rational functions of degree n as $\mathscr{L}_n = \{p_n/\pi_n\colon\ p_n \in \mathscr{P}_n\}$.

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Since A is a countable subset of $\mathbb{C}$, it is always possible to find an $\alpha \in \mathbb{C}$ such that $\alpha_k \neq \alpha$ for all k. Without loss of generality we can take this value to be the origin. So in what follows we assume that $\alpha_k \neq 0$, $k = 0, 1, \ldots$. A basis for $\mathscr{L}_n$ is then given by

$$b_0 = 1, \quad b_n = \prod_{k=1}^{n} Z_k(z), \quad n \geqslant 1 \text{ with } Z_k(z) = \frac{z}{1 - z/\alpha_k}.$$

Take by convention $\alpha_0 = \infty$. The involution operation or substar conjugate of a function is defined as

$$f_*(z) = \overline{f(\bar{z})}$$

and the superstar transformation for $f \in \mathscr{L}_n$ as

$$f^*(z) = \frac{b_n(z)}{b_{n*}(z)} f_*(z).$$

Note that $\mathscr{L}_n^* = \mathscr{L}_n$.

Now let μ be a positive bounded measure on the extended real line $\hat{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$ normalized such that $\mu(\hat{\mathbb{R}}) = 1$ and whose support is an infinite set, then

$$\langle f, g \rangle = \int_{\hat{\mathbb{R}}} f(z)\overline{g(z)}\, \mathrm{d}\mu(z)$$

defines an inner product which turns $\mathscr{L}_n$ into a unitary space. By orthogonalization of the sequence $\{b_0, b_1, \ldots\}$, one obtains the orthonormal rational functions $\{\phi_0, \phi_1, \ldots\}$. Assume these functions are normalized such that the leading coefficient of their expansion in the basis $\{b_k\}$ is real and positive. Since the measure is normalized, it follows that $\phi_0 = 1$. The function ϕ_n will be called *exceptional* if its numerator p_n satisfies $p_n(\alpha_{n-1}) = 0$ and *degenerate* if $p_n^*(\alpha_{n-1}) = 0$. Note that if all $\alpha_k = \infty$, then the rational situation reduces to the polynomial case.

Furthermore, we define para-orthogonal functions as

$$Q_n(z, \tau) = \phi_n(z) + \tau\phi_n^*(z), \quad \tau \in \mathbb{T}, \ n \geqslant 1,$$

where $\mathbb{T}$ denotes the unit circle in the complex plane. They are called para-orthogonal because they are only orthogonal to a subspace of $\mathscr{L}_{n-1}$: it is easily checked that $Q_n \perp (Z_{n-1}/Z_{n*})\mathscr{L}_{n-2}$.

In [1] a distinction is made between real poles and complex poles in the lower half-plane $\mathbb{L}$. It is our present aim to minimize that distinction as much as possible, for it turns out that the case of real poles can mostly be treated as a special case of the general situation with arbitrary complex poles. This is the approach we will follow.

In the next section, we will formulate a recurrence relation for the ϕ_n which holds for arbitrary complex poles. Next we will look at certain Gauss-like quadrature formulas and limit our attention to the case of orthogonality on a finite interval. In the case of real poles, the nodes in the quadrature formulas are the zeros of $\phi_n(z)$. In the last section, we will show that they satisfy a quadratic eigenvalue problem.

2. A fundamental recurrence relation

In the case of real poles, it can be shown [1] that, under certain regularity conditions, the orthonormal functions ϕ_n satisfy the following three-term recurrence relation:

$$\phi_n = \left(A_n Z_n + B_n \frac{Z_n}{Z_{n-1}} \right) \phi_{n-1} + C_n \frac{Z_n}{Z_{n-2}} \phi_{n-2}.$$

The following theorem says that the same relation holds for functions with arbitrary complex poles, if we replace Z_{n-2} with its substar conjugate $Z_{(n-2)*}$ (or equivalently α_{n-2} with $\bar{\alpha}_{n-2}$). For the proof we refer to [5].

Theorem 2.1. *For $n=2,3,\dots$, let $\phi_k \in \mathscr{L}_k$, $k=n-2,n-1,n$ be three successive orthonormal rational functions associated with the pole sequence $\{\alpha_1,\alpha_2,\dots,\} \subset \mathbb{C} \setminus \{0\}$. Then ϕ_{n-1} is nondegenerate and ϕ_n is nonexceptional if and only if there exists a recurrence relation of the form*

$$\phi_n = \left(A_n Z_n + B_n \frac{Z_n}{Z_{n-1}} \right) \phi_{n-1} + C_n \frac{Z_n}{Z_{(n-2)*}} \phi_{n-2}, \quad n \geqslant 2, \tag{2.1}$$

where the constant A_n is nonzero.

If we define $\phi_{-1} = 0$ the recursion holds for $n \geqslant 1$. Again if all poles are at infinity, we recover the well-known three-term recurrence relation for orthogonal polynomials.

3. Quadrature formulas

The use of the para-orthogonal functions $Q_n(z,\tau)$ as defined above lies in the fact that their zeros are simple and real and can be used as nodes in quadrature formulas which are exact in certain spaces of rational functions, analogous to the Gauss quadrature formulas for polynomials. This has been shown for the case of complex poles in the lower half-plane [1], but the proof remains valid for arbitrary complex poles. We need the following lemma. We omit the proof, which is very similar to the one for the case of complex poles in $\mathbb{L}$.

Lemma 3.1. *Let $\phi_n(z)$ be an orthonormal rational function with arbitrary complex poles $\{\alpha_1,\alpha_2,\dots,\alpha_n\} \subset \mathbb{C} \setminus \{0\}$. Let $\mathbb{L}$ and $\mathbb{U}$ denote the lower and upper half-plane, respectively. If $\alpha_n \in \mathbb{U}$ $(\mathbb{L},\mathbb{R})$, then the zeros of $\phi_n(z)$ are in $\mathbb{L}$ $(\mathbb{U},\mathbb{R})$. In particular, if α_n is real, the zeros of ϕ_n are real as well.*

It follows that ϕ_n equals ϕ_n^* (up to a constant of modulus one) if α_n is real. In this case the zeros of $Q_n(z,\tau)$ are independent of τ and are just the (real) zeros of $\phi_n(z)$. Fix τ and put $Q_n(z,\tau) = q_n(z,\tau)/\pi_n(z)$ then $Q_n(z,\tau)$ is called *regular* if none of the zeros of $q_n(z,\tau)$ coincides with any of the poles $\{\alpha_1,\dots,\alpha_n\}$. In that case we have the following lemma. Again the proof is very similar to the one for the case of complex poles in $\mathbb{L}$.

Lemma 3.2. *Let $\phi_n(z)$ be an orthonormal rational function with arbitrary complex poles $\{\alpha_1, \alpha_2, \ldots, \alpha_n\} \subset \mathbb{C} \setminus \{0\}$ and $Q_n(z,\tau) = \phi_n(z) + \tau\phi_n^*(z)$, $\tau \in \mathbb{T}$ the associated para-orthogonal function. If $Q_n(z,\tau)$ is regular, then $Q_n(z,\tau)$ has n simple zeros on $\hat{\mathbb{R}}$.*

If the numerator q_n of Q_n has degree $n-1$ we say that there is a zero at infinity. It always holds that the zeros of q_n are real and simple, but if Q_n is not regular, some of these zeros may cancel against some of the poles. Now define the space $\mathscr{R}_n$ as

$$\mathscr{R}_n = \mathscr{L}_n \cdot \mathscr{L}_{n*} = \left\{ \frac{p_n(z)}{\pi_n(z)\pi_{n*}(z)} : p_n \in \mathscr{P}_{2n} \right\}$$

and the weights λ_{nk} as

$$\lambda_{nk} = \left[\sum_{j=0}^{n-1} |\phi_j(\xi_k)|^2 \right]^{-1}$$

with $\xi_k = \xi_{nk}(\tau)$, $k = 1, \ldots, n$ the zeros of the quasi-orthogonal function $Q_n(z,\tau)$. Then the following theorem holds. It has been proved in [1] for poles in the lower half-plane, but since the proof depends mainly on Lemma 3.2 and the fact that $Q_n \perp (Z_{n-1}/Z_{n*})\mathscr{L}_{n-2}$, it holds for arbitrary complex poles as well.

Theorem 3.3. *Assume $Q_n(z,\tau)$ is regular. Then the quadrature formula*

$$\int_{\hat{\mathbb{R}}} f(z)\,\mathrm{d}\mu(z) \approx \sum_{k=1}^{n} \lambda_{nk} f(\xi_k)$$

with nodes and weights as defined above, is exact on $\mathscr{R}_{n-1}$, i.e. $\int_{\hat{\mathbb{R}}} f\,\mathrm{d}\mu = \sum_{k=1}^{n} \lambda_{nk} f(\xi_k)$ if $f \in \mathscr{R}_{n-1}$.

4. Finite interval

In this section, assume that μ has compact support $[a,b]$ and is absolutely continuous with respect to the Lebesgue measure on $[a,b]$. Without loss of generality we may take this interval to be $[-1,1]$. This means we can write $\mathrm{d}\mu(z) = w(z)\,\mathrm{d}z$ where $w(z)$ is a weight function which is nonnegative almost everywhere (with respect to the Lebesgue measure) and vanishes outside $[-1,1]$. Furthermore, assume that none of the poles is in $[-1,1]$.

Of course, the general theory as outlined above in Section 3 remains valid: the zeros of Q_n are real and simple and can be used as nodes in a quadrature formula. But in the case of a finite interval, we would like the nodes to be inside this interval, which is not necessarily true for the zeros of Q_n, as will become clear later on. We have the following theorem.

Theorem 4.1. *Let μ be as defined above and assume none of the poles is in $[-1,1]$. Then the para-orthogonal function $Q_n(z,\tau)$ has at least $n-1$ zeros inside the open interval $(-1,1)$.*

Proof. Fix τ and put $Q_n(z,\tau)=q_n(z,\tau)/\pi_n(z)$. The zeros of $q_n(z,\tau)$ are real and simple, which means we can normalize q_n such that all its coefficients are real. Assume this has been done. Note that a function f is in $(Z_{n-1}/Z_{n*})\mathscr{L}_{n-2}$ iff it can be written as $f(z)=(z-\bar{\alpha}_n)p_{n-2}(z)/\pi_{n-1}(z)$ where $p_{n-2}\in\mathscr{P}_{n-2}$. It follows that $Q_n\perp(z-\bar{\alpha}_n)/\pi_{n-1}(z)$, or

$$\int_{-1}^{1}\frac{q_n(z,\tau)}{|\pi_{n-1}(z)|^2}\,w(z)\,\mathrm{d}z=0.$$

Because of the nonnegativity of $w(z)$ this is only possible if q_n has at least one zero inside $(-1,1)$.

Now suppose there are only $m\leqslant n-1$ zeros $\xi_1,\ldots,\xi_m$ inside the interval. In that case the function $q_n(z,\tau)(z-\xi_1)(z-\xi_2)\cdots(z-\xi_m)$ has constant sign on $(-1,1)$ so that

$$\int_{-1}^{1}\frac{q_n(z,\tau)(z-\xi_1)(z-\xi_2)\cdots(z-\xi_m)}{|\pi_{n-1}(z)|^2}\,w(z)\,\mathrm{d}z\neq 0.$$

This is impossible since $(z-\xi_1)(z-\xi_2)\cdots(z-\xi_m)(z-\bar{\alpha}_n)/\pi_{n-1}(z)$ is an element of $(Z_{n-1}/Z_{n*})\mathscr{L}_{n-2}$. □

Now we would like to settle the question whether there are values of τ for which all the zeros of $Q_n(z,\tau)$ are in the interval. For real α_n this follows immediately from Theorem 5.2. If α_n is not real, we may reason as follows. From the implicit function theorem it follows that the zeros of $Q_n(z,\tau)$ are continuous functions of τ. Because of Lemma 3.2 their graphs do not intersect. Also it is not difficult to show that these functions are monotonous. For a detailed description we refer to [5]. For a certain value τ_c the numerator polynomial of Q_n has degree $n-1$, so one of the zeros tends to infinity. Since $\tau=e^{i\theta}\in\mathbb{T}$ we may as well consider $\arg(\tau)=\theta\in[0,2\pi]$. Now suppose that for every value of θ only $n-1$ zeros are inside the interval. Let us denote them by $\xi_1(\theta),\ldots,\xi_{n-1}(\theta)$, in ascending order. For a certain value θ_1, one of the outer zeros, say $\xi_1(\theta)$, will leave the interval either to approach the zero outside the interval, or to approach infinity. For another value θ_2 a zero $\xi_e(\theta)$ will enter the interval from the other side such that $\xi_e(2\pi)=\xi_{n-1}(0)$. If $\theta_2>\theta_1$ then there are only $n-2$ zeros inside the interval for $\theta\in[\theta_1,\theta_2]$, which is impossible. It follows that $\theta_2\leqslant\theta_1$. For $\theta=\theta_1$ we then have n zeros inside the (closed) interval. To clarify the above discussion, an example is given in Fig. 1. The zeros of $Q_7(z,\tau)$ are shown as functions of $\arg(\tau)$. The poles are at $\{1+i,1-i,-1+i,-1-i,2+i,\ldots\}$ and orthogonality is with respect to the Lebesgue measure. Note that for almost all values of τ there are n zeros inside the interval.

5. Real poles

Everything which was said before holds for arbitrary complex poles and is therefore also valid for real poles. In the case of real poles, however, the para-orthogonal functions $Q_n(z,\tau)$ are (up to a factor depending only on τ) equal to $\phi_n(z)$ (this is also true if only the pole α_n is real). This follows immediately from the remark after Lemma 3.1. Now one defines quasi-orthogonal functions, similar to the para-orthogonal functions, as follows:

$$\tilde{Q}_n(z,\tau)=\phi_n(z)+\tau\,\frac{Z_n(z)}{Z_{n-1}(z)}\,\phi_{n-1}(z),\qquad \tau\in\mathbb{R},\ n\geqslant 1.$$

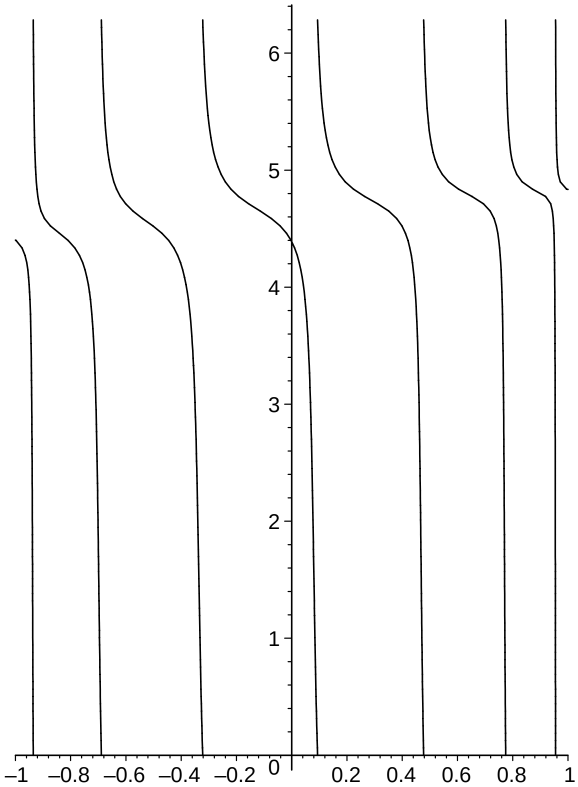

Fig. 1. Zeros of $Q_7(z,\tau)$ as a function of $\arg(\tau)$.

We set by definition

$$\tilde{Q}_n(z,\infty) = \frac{Z_n(z)}{Z_{n-1}(z)}\,\phi_{n-1}(z).$$

It is easily checked that also in this case we have $\tilde{Q}_n \perp (Z_{n-1}/Z_{n*})\mathscr{L}_{n-2}$ (note that $Z_{n*} = Z_n$). If we put $\tau = 0$ we obtain the orthogonal rational function ϕ_n.

These quasi-orthogonal rational functions have basically the same properties as the para-orthogonal functions defined above. We have the following lemma (with the usual definition of regularity), as proved in [1].

Lemma 5.1. *Let $\phi_n(z)$ be an orthonormal rational function with real poles $\{\alpha_1, \alpha_2, \dots, \alpha_n\} \subset \mathbb{R}\backslash\{0\}$ and $\tilde{Q}_n(z,\tau) = \phi_n(z) + \tau(Z_n(z)/Z_{n-1}(z))\phi_{n-1}(z)$, $\tau \in \hat{\mathbb{R}}$ the associated quasi-orthogonal function. If $\tilde{Q}_n(z,\tau)$ is regular, then $\tilde{Q}_n(z,\tau)$ has n simple zeros on $\hat{\mathbb{R}}$.*

Again the zeros of $\tilde{Q}_n$ are used as nodes in a quadrature formula. In [1] it is shown that Theorem 3.3 holds with $\tilde{Q}_n$ in place of Q_n and ξ_k the zeros of $\tilde{Q}_n$.

Now let us restrict our attention to the case of a finite interval as in Section 4. Under the same conditions on the measure μ and using the orthogonality of ϕ_n, the following theorem is easily proved. We already know that the zeros of ϕ_n are real. Note that for all poles at infinity we recover a well-known property of zeros of orthogonal polynomials.

Theorem 5.2. *Let ϕ_n be an orthogonal rational function on the interval $[-1,1]$ with poles outside this interval. Then the zeros of ϕ_n are simple and contained in the open interval $(-1,1)$.*

Since we assumed that all the poles are outside the interval of integration it follows from the previous theorem that $\tilde{Q}_n(z,0)$ is regular and that there are n simple zeros inside the interval. Using a similar argument as in Theorem 4.1 we have the following result.

Theorem 5.3. *Let μ be as defined above and assume none of the poles is in $[-1,1]$. Then the quasi-orthogonal function $\tilde{Q}_n(z,\tau)$ has at least $n-1$ zeros inside the open interval $(-1,1)$.*

If $\tau=\infty$ one of the zeros of $\tilde{Q}_n$ is the pole α_{n-1} which is outside the interval.

6. Zeros of orthogonal rational functions

It is a well-known property of orthogonal polynomials that their zeros are the eigenvalues of a tridiagonal matrix, the Jacobi matrix, containing the recursion coefficients. In this section, we derive a similar property for orthogonal rational functions, but here the zeros are eigenvalues of a quadratic eigenvalue problem.

Taking the numerator of the recurrence relation (2.1) and rearranging yields

$$
\begin{aligned}
&-\alpha_{n-1}C_n p_{n-2}(z)+B_n p_{n-1}(z)+\frac{1}{\alpha_n}p_n(z)\\
&\quad=\left[-\left(\frac{\alpha_{n-1}}{\bar{\alpha}_{n-2}}+1\right)C_n p_{n-2}(z)+\left(\frac{B_n}{\alpha_{n-1}}-A_n\right)p_{n-1}(z)\right]z+\frac{C_n}{\bar{\alpha}_{n-2}}p_{n-2}(z)z^2.
\end{aligned}
$$

This equation can be written down for every n and after collecting the coefficients in $n\times n$-matrices we obtain the following expression:

$$
\begin{bmatrix}
B_1 & \frac{1}{\alpha_1} & & & \\
-\alpha_1 C_2 & B_2 & \frac{1}{\alpha_2} & & \\
 & \ddots & \ddots & \ddots & \\
 & & -\alpha_{n-2}C_{n-1} & B_{n-1} & \frac{1}{\alpha_{n-1}}\\
 & & & -\alpha_{n-1}C_n & B_n
\end{bmatrix}
\begin{bmatrix}
p_0(z)\\ p_1(z)\\ \vdots \\ p_{n-2}(z)\\ p_{n-1}(z)
\end{bmatrix}
$$

$$= \begin{bmatrix} \frac{B_1}{\alpha_0} - A_1 & & & & \\ -(\frac{\alpha_1}{\bar{\alpha}_0}+1)C_2 & \frac{B_2}{\alpha_1} - A_2 & & & \\ \ddots & \ddots & & & \\ & -(\frac{\alpha_{n-2}}{\bar{\alpha}_{n-3}}+1)C_{n-1} & \frac{B_{n-1}}{\alpha_{n-2}} - A_{n-1} & \\ & & -(\frac{\alpha_{n-1}}{\bar{\alpha}_{n-2}}+1)C_n & \frac{B_n}{\alpha_{n-1}} - A_n \end{bmatrix} \begin{bmatrix} p_0(z) \\ p_1(z) \\ \vdots \\ p_{n-2}(z) \\ p_{n-1}(z) \end{bmatrix} z$$

$$+ \begin{bmatrix} 0 & & & & \\ \frac{C_2}{\bar{\alpha}_0} & & & & \\ & \ddots & & & \\ & & \frac{C_{n-1}}{\bar{\alpha}_{n-3}} & & \\ & & & \frac{C_n}{\bar{\alpha}_{n-2}} & 0 \end{bmatrix} \begin{bmatrix} p_0(z) \\ p_1(z) \\ \vdots \\ p_{n-2}(z) \\ p_{n-1}(z) \end{bmatrix} z^2 - \frac{1}{\alpha_n} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ p_n(z) \end{bmatrix}.$$

We now have an equation of the form $-\mathscr{C}_n p(z) = \mathscr{B}_n p(z)z + \mathscr{A}_n p(z)z^2 - 1/\alpha_n q(z)$ with $\mathscr{A}_n, \mathscr{B}_n, \mathscr{C}_n \in \mathbb{C}^{n\times n}$ and $p(z), q(z) \in \mathbb{C}^n[z]$. Let λ be a zero of p_n then this reduces to the following quadratic eigenvalue problem:

$$(\mathscr{A}_n\lambda^2 + \mathscr{B}_n\lambda + \mathscr{C}_n)p(\lambda) = 0. \tag{6.1}$$

Thus, we have proved that the zeros of ϕ_n satisfy a quadratic eigenvalue problem. In general, a quadratic eigenvalue problem of size n has $2n$ eigenvalues. It can be shown, however [5], that due to the specific structure of the matrices $\mathscr{A}_n$, $\mathscr{B}_n$ and $\mathscr{C}_n$ there are only n finite eigenvalues, so Eq. (6.1) does not introduce spurious solutions.

Now consider the quadratic matrix equation

$$\mathscr{A}_n X^2 + \mathscr{B}_n X + \mathscr{C}_n = 0. \tag{6.2}$$

If S is a solution of (6.2) then

$$\mathscr{A}_n\lambda^2 + \mathscr{B}_n\lambda + \mathscr{C}_n = -(\mathscr{B}_n + \mathscr{A}_n S + \mathscr{A}_n\lambda)(S - \lambda I_n).$$

This means that every eigenvalue–eigenvector pair of S is also an eigenvalue–eigenvector pair for the quadratic eigenvalue problem. Since there are only n eigenvalues in our case, the existence of a solution S implies that its eigenvalues are the zeros of $\phi_n(z)$. The eigenvectors v_i corresponding to the zeros λ_i of $\phi_n(z)$ are

$$v_1 = \begin{bmatrix} p_0(\lambda_1) \\ p_1(\lambda_1) \\ p_2(\lambda_1) \\ \vdots \\ p_{n-2}(\lambda_1) \\ p_{n-1}(\lambda_1) \end{bmatrix}, v_2 = \begin{bmatrix} p_0(\lambda_2) \\ p_1(\lambda_2) \\ p_2(\lambda_2) \\ \vdots \\ p_{n-2}(\lambda_2) \\ p_{n-1}(\lambda_2) \end{bmatrix}, \ldots, v_n = \begin{bmatrix} p_0(\lambda_n) \\ p_1(\lambda_n) \\ p_2(\lambda_n) \\ \vdots \\ p_{n-2}(\lambda_n) \\ p_{n-1}(\lambda_n) \end{bmatrix}.$$

Since the polynomials $p_k(z)$ all have degree exactly k, these vectors are linearly independent. It follows that $S = V\Lambda V^{-1}$ with $V = [v_1 \ \cdots \ v_n]$ and $\Lambda = \mathrm{diag}(\lambda_i)$ forms a solution to (6.2). We have thus proved the following theorem.

Theorem 6.1. *With* $\mathscr{A}_n$, $\mathscr{B}_n$ and $\mathscr{C}_n$ *as defined above, the zeros of the orthonormal rational function* $\phi_n(z)$ *are the solutions of the quadratic eigenvalue problem*

$$(\mathscr{A}_n\lambda^2 + \mathscr{B}_n\lambda + \mathscr{C}_n)p(\lambda) = 0$$

and the eigenvalues of any matrix X *solving*

$$\mathscr{A}_nX^2 + \mathscr{B}_nX + \mathscr{C}_n = 0.$$

Numerical experiments have indicated that this quadratic eigenvalue problem is very ill-conditioned. Further research needs to be done to investigate this. In another contribution of these proceedings [2] it is shown that the zeros of ϕ_n also satisfy a generalized eigenvalue problem, which seems to be less ill-conditioned. For a more detailed description of solving quadratic eigenvalue problems and quadratic matrix equations, we refer to [3,4].

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