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Recurrence Relations for Orthogonal Rational Functions

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Abstract It is well known that members of families of polynomials, that are orthogonal with respect to an inner product determined by a nonnegative measure on the real axis, satisfy a three-term recursion relation. Analogous recursion formulas are available for orthogonal Laurent polynomials with a pole at the origin. This paper investigates recursion relations for orthogonal rational functions with arbitrary prescribed real or complex conjugate poles. The number of terms in the recursion relation is shown to be related to the structure of the orthogonal rational functions.

Keywords orthogonal rational function · recursion formulas

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1 Introduction

Let μ be a nondecreasing function on the finite or infinite real interval $[a, b]$ with infinitely many points of increase, and introduce the inner product

$$< f, g >= \int_a^b f(x)g(x)d\mu \tag{1}$$

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and associated norm $\|f\| =< f, f >^{1/2}$. Assume that all moments

$$\mu_j = \int_a^b x^j d\mu, \qquad j = 0, 1, 2, \dots ,$$

exist. Then it is well known that there is an infinite sequence of orthogonal polynomials associated with this inner product and that they satisfy a three-term recursion formula; see, e.g., Brezinski [3] or Szegő [17].

We are interested in investigating the structure of recursion relations of orthogonal rational functions with prescribed poles. We tacitly assume that the measure is such that all necessary moments exist and first consider monic orthogonal Laurent polynomials with a pole at the origin,

$$\phi_j(x) = \begin{cases} x^j + \displaystyle\sum_{k=-j+1}^{j-1} c_{j,k} x^k, & j = 0, 1, 2, \dots , \\ x^j + \displaystyle\sum_{k=j+1}^{-j} c_{j,k} x^k, & j = -1, -2, -3, \dots . \end{cases} \tag{2}$$

Thus, $\phi_0(x) = 1$, and, for $j \geq 1$, $\phi_j(x)$ is the product of x^{-j+1} and a polynomial in x. Similarly, for $j \leq -1$, $\phi_j(x)$ can be expressed as x^j times a polynomial in x. The first $2k + 1$ monic orthogonal Laurent polynomials

$$\phi_0, \phi_1, \phi_{-1}, \phi_2, \phi_{-2}, \dots , \phi_k, \phi_{-k} \tag{3}$$

form an orthogonal basis for the space $\text{span}\{1, x, x^{-1}, x^2, x^{-2}, \dots , x^k, x^{-k}\}$. Njåstad and Thron [15] showed that the Laurent polynomials (2) ordered according to (3) satisfy short recursion relations. This result, as well as other properties of these Laurent polynomials, are discussed by Jones and Njåstad [13].

Recursion relations for monic orthogonal Laurent polynomials of the form

$$\phi_j(x) = \begin{cases} x^j + \displaystyle\sum_{k=-\lfloor (j-1)/n \rfloor}^{j-1} c_{j,k} x^k, & j = 1, 2, 3, \dots , \\ x^j + \displaystyle\sum_{k=j+1}^{-nj} c_{j,k} x^k, & j = -1, -2, -3, \dots , \end{cases} \tag{4}$$

with n a fixed positive integer and $\phi_0(x) = 1$ are studied in [11,12] by matrix methods. Here $\lfloor \alpha \rfloor$ denotes the largest integer smaller than or equal to $\alpha \geq 0$. The $k(n + 1)$ monic orthogonal Laurent polynomials

$$\phi_0, \phi_1, \dots , \phi_n, \phi_{-1}, \phi_{n+1}, \dots , \phi_{2n}, \phi_{-2}, \phi_{2n+1}, \dots , \phi_{kn}$$

form a basis for the space

$$\text{span}\{1, x, x^2, \dots , x^n, x^{-1}, x^{n+1}, \dots , x^{2n}, x^{-2}, x^{2n+1}, \dots , x^{kn}\}. \tag{5}$$

Thus, for $n = 1$ the Laurent polynomials (4) simplify to (2). Recently, Díaz-Mendoza et al. [7] presented recursion relations for more general sequences of orthogonal Laurent polynomials with a pole at the origin. An increase of the numerator degree may be followed by an increase in the denominator or numerator degrees; an increase of the denominator degree must be followed by an increase in the numerator degree.

It is the purpose of the present paper to investigate recurrence relations for orthonormal rational functions with a few prescribed real or complex conjugate poles. We show that these functions, under some restrictions on the ordering of the poles, satisfy short recursion relations, analogous to the three-term recursion relation for orthogonal polynomials. The number of terms in the recursion relations for orthonormal rational functions with prescribed poles depends both on the number of distinct poles and on the order in which the poles enter in the sequence of orthonormal rational functions.

Since the poles are fixed, the rational functions are Padé-type approximants. An elegant treatment of Padé-type approximants is provided by Brezinski [3]; see also [4,1].

Our interest in rational functions with prescribed poles stems from the fact that they are better suited to approximating certain functions in regions of the complex plane than polynomials and Padé approximants with “free” poles. This has been discussed and illustrated, e.g., by Ambroladze and Wallin [1] and Druskin and Knizhnerman [8]. More recent results on the approximation by rational functions with fixed poles can be found in [2,9,14]. Numerical examples concerned with the approximation of matrix functions by rational functions with fixed poles are described in [8,9,11,12,14].

This paper is organized as follows. Section 2 describes short recursion formulas for orthogonal rational functions with prescribed poles. These recursion relations are believed to be new. We remark that there are other kinds of known short recursion relations for orthogonal rational functions, in which the “coefficients” depend on the independent variable x. These recursion formulas are commented on at the end of Section 2. Section 3 describes a Stieltjes-type procedure based on the recursion formulas of Section 2. This procedure provides a recursive approach to generating a sequence of orthonormal rational functions with fixed poles. A numerical example is presented in Section 4 and concluding remarks can be found in Section 5.

2 Recurrence relations for orthonormal rational functions

Let $\mathcal{P}$ denote the space of all polynomials with real coefficients and introduce the linear space of rational functions with real or complex conjugate poles $\alpha_1, \alpha_2, \alpha_3, \ldots$,

$$\mathcal{Q} = \operatorname{span}\left\{ \frac{1}{(x-\alpha_k)^s} \;:\; s \in \mathbb{N}, \quad \alpha_k \notin [a,b] \;\text{ and }\; |\alpha_k| < \infty \right\},$$

where as usual $\mathbb{N}$ denotes the set of positive integers. Let $\bar{\alpha}_j$ denote the complex conjugate of the pole α_j and assume that α_j has a nonvanishing imaginary part. Then, in order to avoid complex arithmetic, we replace each pair of rational functions

$$\frac{1}{(x-\alpha_j)^s} \quad \text{and} \quad \frac{1}{(x-\bar{\alpha}_j)^s}$$

in $\mathcal{Q}$ by

$$\frac{1}{(x^2+p_jx+q_j)^s} \quad \text{and} \quad \frac{x}{(x^2+p_jx+q_j)^s},$$

where

$$x^2+p_jx+q_j = (x-\alpha_j)(x-\bar{\alpha}_j) \tag{6}$$

with p_j and q_j real. This change of basis makes it possible to use real arithmetic only when approximating real-valued functions.

Introduce the linear space

$$\mathcal{P}+\mathcal{Q} = \text{span}\{1,\ x^s,\ \frac{1}{(x-\alpha_k)^s},\ \frac{1}{(x^2+p_jx+q_j)^s},\ \frac{x}{(x^2+p_jx+q_j)^s}\ :$$

$$s\in\mathbb{N},\ \alpha_k\in\mathbb{R}\backslash[a,b],\ \alpha_j\in\mathbb{C}\backslash\mathbb{R},\ |\alpha_k|,|\alpha_j|<\infty\},$$

where the p_j and q_j are defined by (6) with the imaginary part of α_j nonvanishing. Let $\Psi = \{\psi_0,\psi_1,\psi_2,\dots\}$ denote an elementary basis for this space, i.e., $\psi_0(x)=1$ and each $\psi_\ell(x)$ for $\ell=1,2,\dots$ is one of the functions

$$x^s,\ \frac{1}{(x-\alpha_k)^s},\ \frac{1}{(x^2+p_jx+q_j)^s},\ \frac{x}{(x^2+p_jx+q_j)^s}$$

for some positive integers k, j, and s. Application of the Gram-Schmidt process with respect to the inner product (1) and associated norm to the basis Ψ yields a basis of orthonormal rational functions with the prescribed finite poles $\alpha_1,\alpha_2,\alpha_3,\dots$,

$$\Phi = \{\phi_0,\phi_1,\phi_2,\dots\}.$$

The recursion relations for the ϕ_j depend on the ordering of the basis functions ψ_j of Ψ. We write $\psi_j \prec \psi_k$ if the basis function ψ_j comes before ψ_k. The ordering of the basis Ψ is said to be *natural* if it satisfies the following three conditions:

1. $x^s \prec x^{s+1}$ for all integers $s\geq 0$.
2. $\frac{1}{(x-\alpha_k)^s} \prec \frac{1}{(x-\alpha_k)^{s+1}}$ for all positive integers s and every pole α_k.
3. $\frac{1}{(x^2+p_jx+q_j)^s} \prec \frac{x}{(x^2+p_jx+q_j)^s} \prec \frac{1}{(x^2+p_jx+q_j)^{s+1}}$ for all positive integers s and every pair $\{p_j,q_j\}$.

We now show that orthonormal rational functions with prescribed poles corresponding to any natural ordering satisfy four types of recurrence relations.

Theorem 1 *Let the basis $\Psi = \{\psi_0, \psi_1, \psi_2, \dots\}$ satisfy the requirements of natural ordering. Assume that every sequence of m_1 consecutive basis functions $\psi_k, \psi_{k+1}, \dots, \psi_{k+m_1-1}$ contains at least one power x^ℓ, and that between every pair of basis functions*

$$\left\{ \frac{1}{(x^2+p_jx+q_j)^s}, \frac{x}{(x^2+p_jx+q_j)^s} \right\}, \qquad s = 1, 2, 3, \dots ,$$

there are at most m_2 basis functions. Then the orthonormal rational functions $\phi_0, \phi_1, \phi_2, \dots$ with prescribed poles satisfy a $(2m+1)$-term recurrence relation of the form

$$x\phi_k(x) = \sum_{i=-m}^{m} c_{k,k+i}\phi_{k+i}(x), \qquad k = 0, 1, 2, \dots , \tag{7}$$

with $m = \max\{m_1, m_2 + 1\}$. By convention, coefficients $c_{k,k+i}$ and functions ϕ_{k+i} with negative index $k+i$ are defined to be zero.

Proof It follows from the ordering that

$$x\phi_k(x) \in \operatorname{span}\{\phi_0, \phi_1, \dots, \phi_{k+m-1}, \phi_{k+m}\}, \qquad k = 0, 1, 2, \dots , \tag{8}$$

i.e.,

$$x\phi_k(x) = \sum_{i=0}^{k+m} c_{k,i}\phi_i(x), \qquad c_{k,i} =< x\phi_k, \phi_i > .$$

Replacing k by i in (8) and using the fact that $c_{k,i} =< \phi_k, x\phi_i >$ yields $c_{k,i} = 0$ for $i < k - m$.

Remark 1 If $\mathcal{Q}$ is not empty, i.e., if there are finite poles, then we can order the basis Ψ to get the smallest possible value of m, which is 2, corresponding to $m_1 = 2$ and $m_2 = 1$. In this case, we obtain (at most) a five-term recurrence relation.

Remark 2 If $\mathcal{Q}$ is empty, then $m = 1$ and we obtain the standard three-term recurrence relation for orthonormal polynomials.

Theorem 2 *Let the basis $\Psi = \{\psi_0, \psi_1, \psi_2, \dots\}$ satisfy the requirements of natural ordering and let α_ℓ be a real pole of this basis. Assume that every sequence of m_1 consecutive basis functions $\psi_k, \psi_{k+1}, \dots, \psi_{k+m_1-1}$ contains at least one power $(x-\alpha_\ell)^{-t}$, $t \geq 1$, and that between every pair of basis functions*

$$\left\{ \frac{1}{(x^2+p_jx+q_j)^s}, \frac{x}{(x^2+p_jx+q_j)^s} \right\}, \qquad s = 1, 2, 3, \dots ,$$

there are at most m_2 functions. Then the basis of orthonormal rational functions $\phi_0, \phi_1, \phi_2, \dots$ with prescribed poles satisfy a $(2m+1)$-term recurrence relation of the form

$$\frac{1}{x-\alpha_\ell}\,\phi_k(x) = \sum_{i=-m}^{m} c_{k,k+i}^{(\ell)}\phi_{k+i}(x), \qquad k = 0, 1, 2, \dots , \tag{9}$$

with $m = \max\{m_1, m_2 + 1\}$*. Coefficients* $c_{k,k+i}^{(\ell)}$ *and functions* ϕ_{k+i} *with negative index* $k+i$ *are defined to be zero.*

Proof The result can be shown similarly as Theorem 1. For instance, we expand expressions of the form $(x-\alpha_\ell)^{-1}(x^2+p_jx+q_j)^{-s}$ in terms of the functions $(x-\alpha_\ell)^{-1}$, $(x^2+p_jx+q_j)^{-s}$, $x(x^2+p_jx+q_j)^{-s}$, $(x^2+p_jx+q_j)^{-s+1}$, $x(x^2+p_jx+q_j)^{-s+1}, \ldots$ for suitable values of s.

Remark 3 The basis Ψ determined by the ordering (5) corresponds to $m_1 = n+1$ and $m_2 = 0$ for $k \geq 1$ in Theorem 2. Therefore, the sum (9) has $2n+3$ terms for large k.

Theorem 3 *Let the basis* $\Psi = \{\psi_0, \psi_1, \psi_2, \ldots\}$ *satisfy the requirements of natural ordering, and assume that every sequence of* m *consecutive basis functions* $\psi_k, \psi_{k+1}, \ldots, \psi_{k+m-1}$ *contains at least one function* $(x^2+p_jx+q_j)^{-s}$ *for some integer* $s \geq 1$*. Then the orthonormal rational functions* $\phi_0, \phi_1, \phi_2, \ldots$ *with prescribed poles satisfy a* $(4m-3)$*-term recurrence relation of the form*

$$\frac{1}{x^2+p_jx+q_j}\,\phi_k(x) = \sum_{i=-2m+2}^{2m-2} c_{k,k+i}^{(j)}\phi_{k+i}(x), \qquad k = 0, 1, 2, \ldots \ . \tag{10}$$

Coefficients $c_{k,k+i}^{(j)}$ *and functions* ϕ_{k+i} *with negative index* $k+i$ *are defined to be zero.*

Proof The result follows similarly as Theorem 2. Here we only note that every sequence of $2m-1$ consecutive basis functions ψ_j contains functions $(x^2+p_jx+q_j)^{-s}$ and $x(x^2+p_jx+q_j)^{-s-1}$ for some positive integer s.

Theorem 4 *Let the conditions of Theorem 3 hold. Then the orthonormal rational functions* $\phi_0, \phi_1, \phi_2, \ldots$ *with prescribed poles satisfy a* $(4m-1)$*-term recurrence relation of the form*

$$\frac{x}{x^2+p_jx+q_j}\,\phi_k(x) = \sum_{i=-2m+1}^{2m-1} \hat{c}_{k,k+i}^{(j)}\phi_{k+i}(x), \qquad k = 0, 1, 2, \ldots \ .$$

Coefficients $\hat{c}_{k,k+i}^{(j)}$ *and functions* ϕ_{k+i} *with negative index* $k+i$ *are defined to be zero.*

Proof The result can be shown in the same manner as Theorem 3.

We remark that there are other approaches to derive short recursion relations for orthogonal rational functions with prescribed poles. When the measure that defines the inner product lives on the unit circle, recursion formulas can be expressed with the aid of CMV-like matrices; see Bultheel and Cantero [5]. These matrices are five-diagonal, but differ from the matrices mentioned in Remark 1. Three-term recursion relations for orthogonal rational functions are described by Bultheel et al. [6]. Here the "coefficients" involve linear fractional transformations. The recursion formulas of the present paper differ from standard three-term recursion formulas for orthogonal polynomials only in that more terms with constant coefficients are required; cf. Remark 1. Which one of these recursion formulas is most convenient to use depends on the application at hand.

3 A Stieltjes-type procedure

This section describes a procedure of Stieltjes-type for the generation of an orthonormal basis for the space $\mathcal{P}+\mathcal{Q}$. The "standard" Stieltjes procedure is a recursive scheme for determining orthonormal polynomials of increasing degree by evaluating recursion coefficients of the three-term recursion formula and appropriate inner products in suitable order; see, e.g., Gautschi [10] for details. The algorithm below is an analog of the standard Stieltjes procedure for the computation of bases $\{\phi_0, \phi_1, \ldots, \phi_n\}$ or $\{\phi_0, \phi_1, \ldots, \phi_{n+1}\}$ of orthonormal rational functions with prescribed poles for the spaces $\text{span}\{\psi_0, \psi_1, \ldots, \psi_n\}$ or $\text{span}\{\psi_0, \psi_1, \ldots, \psi_{n+1}\}$; the latter basis is determined when $\psi_n(x) = (x^2 + p_j x + q_j)^{-s}$ for some $s \in \mathbb{N}$. The recursions of the algorithm are obtained from the relations derived in the previous section.

We assume that the functions $\psi_0, \psi_1, \psi_2, \ldots$ satisfy the requirements of natural ordering and that there are no functions between the pair of functions $\{(x^2+p_jx+q_j)^{-s}, x(x^2+p_jx+q_j)^{-s}\}$. The algorithm below determines integers m and p for every new basis function to be included. Their values will be discussed in Theorem 5 below. We say that a function ϕ_m "contains" x^{s-1} if ϕ_m can be written as a linear combination with nonvanishing coefficients of linearly independent functions, one of which is x^{s-1}.

Algorithm 3.1: Stieltjes-type procedure
$\phi_0 := \psi_0/||\psi_0||$; $k := 1$;
while $k \leq n$ **do**
  if $\psi_k(x) = x^s$ for some $s \in \mathbb{N}$ **then**
    if $s = 1$ **then**
      $p := -1$; $m := 0$;
    else
      let $m \leq k-1$ be (the largest) integer such that ϕ_m "contains" x^{s-1};
      let p be (the largest) integer such that
        $\forall j \leq p,\ \ x\phi_j(x) \in \text{span}\{\phi_0, \ldots, \phi_{m-1}\}$;
    end
    $v(x) := x\phi_m(x)$;
    for $i = p+1, \ldots, k-1$ **do**
      $c_{k-1,i} :=< v, \phi_i >$; $v := v - c_{k-1,i}\phi_i$;
    end
    $\phi_k := v/||v||$; $k := k+1$;
  end
  if $\psi_k(x) = (x - \alpha_\ell)^{-s}$ for some $s \in \mathbb{N}$ **then**
    if $s = 1$ **then**

$p := -1$; $m := 0$;
else
let $m \le k-1$ be (the largest) integer such that ϕ_m "contains" $(x-\alpha_\ell)^{-(s-1)}$;
let p be (the largest) integer such that $\forall j \le p$, $(x-\alpha_\ell)^{-1}\phi_j(x) \in \text{span}\{\phi_0, \ldots, \phi_{m-1}\}$;
end
$v(x) := (x-\alpha_\ell)^{-1}\phi_m(x)$;
for $i = p+1, \ldots, k-1$ **do**
$c_{k-1,i} :=< v, \phi_i >$; $v := v - c_{k-1,i}\phi_i$;
end
$\phi_k := v/||v||$; $k := k+1$;
end
if $\psi_k(x) = (x^2 + p_r x + q_r)^{-s}$ for some $s \in \mathbb{N}$ **then**
if $s = 1$ **then**
$p := -1$; $m := 0$;
else
let $m \le k-1$ be (the largest) integer such that ϕ_m "contains" $(x^2 + p_r x + q_r)^{-(s-1)}$;
let p be (the largest) integer such that $\forall j \le p$, $(x^2 + p_r x + q_r)^{-1}\phi_j(x) \in \text{span}\{\phi_0, \ldots, \phi_{m-1}\}$;
end
$v_1(x) := (x^2 + p_r x + q_r)^{-1}\phi_m(x)$; $v_2(x) := x(x^2 + p_r x + q_r)^{-1}\phi_m(x)$;
for $i = p+1, \ldots, k-1$ **do**
$c_{k-1,i} :=< v_1, \phi_i >$; $v_1 := v_1 - c_{k-1,i}\phi_i$;
$d_{k-1,i} :=< v_2, \phi_i >$; $v_2 := v_2 - d_{k-1,i}\phi_i$;
end
$\phi_k := v_1/||v_1||$; $\beta :=< v_2, \phi_k >$;
$v_2 := v_2 - \beta\phi_k$; $\phi_{k+1} := v_2/||v_2||$;
$k := k+2$;
end
end

The last part of the algorithm is executed when pairs of new functions $\{(x^2+p_jx+q_j)^{-s}, x(x^2+p_jx+q_j)^{-s}\}$ are introduced. Then two new functions v_1 and v_2 are defined and the latter is ortogonalized against the former.

To make the algorithm attractive for computation, we have to find an efficient way to determine the integers m and p in each step. One way to achieve this is described in the following theorem. The theorem imposes new constraints on the ordering of the functions ψ_j. A benefit of these constraints is that the largest possible value of m (which is $k-1$) is attained (with the exception of $m = k-2$ in only one case). The large value of m ensures short recurrence relations.

Theorem 5 *Let the functions $\psi_0, \psi_1, \ldots,$ be naturally ordered, and assume in addition that 1) there is a positive power of x between any two rational functions with different poles and 2) if $\psi_i(x) = (x^2+p_jx+q_j)^{-s}$ then $\psi_{i-1}(x) =$*

x^d, $\psi_{i+1}(x) = x(x^2 + p_j x + q_j)^{-s}$ and $\psi_{i+2}(x) = x^{d+1}$. The positive integers m and p in Algorithm 3.1 can be determined in the following way:

- *$m = k - 1$ unless $\psi_{k-1}(x) = x(x^2 + p_j x + q_j)^{-g}$, in which case $m = k - 2$,*
- *$p = r - 1$ where ψ_r denotes a basis function having the same pole(s) as ψ_k but of less order for one (of less order for two if $r = k - 1$).*

Proof The assertion about p follows directly from Theorems 1, 2, 3, and 4. It remains to show the assertion about m. First assume that $\psi_k(x) = x^s$, $s \in \mathbb{N}$. We consider three possibilities:

- If $\psi_{k-1}(x) = x^{s-1}$, then the assertion is obvious.
- If $\psi_{k-1}(x) = (x - \alpha_\ell)^{-d}$ for some $d \in \mathbb{N}$, then

$$(x - \alpha_\ell)\phi_{k-1}(x) = A_k x^s + A_{k-2}\phi_{k-2} + \sum_{j=0}^{k-3} A_j \phi_j(x)$$

  for some coefficients A_ℓ. Since $x - \alpha_\ell$ does not change sign in the interval $[a, b]$, we have that $< (x - \alpha_\ell)\phi_{k-1}, \phi_{k-1} > \neq 0$. Therefore, $A_k \neq 0$.
- If $\psi_{k-1}(x) = x(x^2 + p_j x + q_j)^{-g}$ then $\psi_{k-2}(x) = (x^2 + p_j x + q_j)^{-g}$ and $\psi_{k-3}(x) = x^{s-1}$. The function ϕ_{k-2} is given by the sum

$$\phi_{k-2}(x) = \frac{1}{x^2 + p_j x + q_j}\phi_{k-3}(x) - B_{k-3}\phi_{k-3}(x) - \sum_{j=0}^{k-4} B_j \phi_j(x),$$

  in which only the second term, $B_{k-3}\phi_{k-3}(x)$, may contain x^{s-1}. The assertion now follows from the fact that

$$B_{k-3} =< \frac{1}{x^2 + p_j x + q_j}\phi_{k-3}, \phi_{k-3} > \neq 0.$$

We turn to the situation when $\psi_k(x) = (x - \alpha_\ell)^{-s}$ for some $s \in \mathbb{N}$ and have to distinguish two cases:

- If $\psi_{k-1}(x) = (x - \alpha_\ell)^{-s+1}$, then the assertion is obvious.
- If $\psi_{k-1}(x) = x^d$, then we have that

$$\frac{1}{x - \alpha_\ell}\phi_{k-1}(x) = \tilde{A}_k \frac{1}{(x - \alpha_\ell)^s} + \tilde{A}_{k-2}\phi_{k-2}(x) + \sum_{j=0}^{k-3} \tilde{A}_j \phi_j(x),$$

  and it follows from $< (x - \alpha_\ell)^{-1}\phi_{k-1}, \phi_{k-1} > \neq 0$ that $\tilde{A}_k \neq 0$.

To complete the proof it suffices to show that if $\psi_k(x) = (x^2 + p_j x + q_j)^{-s}$, then $(x^2 + p_j x + q_j)^{-1}\phi_{k-1}(x)$ cannot belong to span$\{\phi_0, \phi_1 \ldots, \phi_{k-1}\}$. Because $\psi_{k-1}(x) = x^d$, we have that

$$\frac{1}{x^2 + p_j x + q_j}\phi_{k-1}(x) = \bar{A}_k \frac{x}{(x^2 + p_j x + q_j)^s} + \bar{A}_{k-1}\frac{1}{(x^2 + p_j x + q_j)^s} + \bar{A}_{k-2}\phi_{k-2}(x) + \sum_{j=0}^{k-3} \bar{A}_j \phi_j(x).$$

Since $< (x^2+p_jx+q_j)^{-1}\phi_{k-1}, \phi_{k-1} > \neq 0$, we conclude that both coefficients $\bar{A}_k$ and $\bar{A}_{k-1}$ cannot vanish.

Let the functions $\psi_0, \psi_1, \psi_2, \dots, \psi_n$ be ordered in the following way:

$$1, x, \frac{1}{x-\alpha_1}, x^2, \frac{1}{(x-\alpha_1)^2}, x^3, \dots, \frac{1}{(x-\alpha_1)^{k_1}}, x^{k_1+1}, \frac{1}{x-\alpha_2}, x^{k_1+2}, \dots,$$
$$\frac{1}{(x-\alpha_2)^{k_2}}, x^{k_1+k_2+1}, \dots, \frac{1}{(x-\alpha_\ell)^{k_\ell}}, x^{k_1+\dots+k_\ell+1}, \frac{1}{x^2+p_1x+q_1},$$
$$\frac{x}{x^2+p_1x+q_1}, x^{K+1}, \dots, \frac{1}{(x^2+p_1x+q_1)^{s_1}}, \frac{x}{(x^2+p_1x+q_1)^{s_1}},$$
$$x^{K+s_1}, \frac{1}{x^2+p_2x+q_2}, \frac{x}{x^2+p_2x+q_2}, x^{K+s_1+1}, \dots,$$

where $K = k_1+k_2+\dots+k_\ell+1$. Then, if $p \geq 0$, we have $p+1 = r = k-2$ (while we deal with only real poles) or $p+1 = r = k-3$ (after we involved the first pair of complex conjugate poles). In other words, all orthonormal rational functions ϕ_j are generated by three-term or four-term recurrence relations, except for $w-1$ of them, where w is the number of distinct poles. If $\psi_j(x) = (x-\alpha_k)^{-1}$, $k \geq 2$, or $\psi_j(x) = (x^2+p_tx+q_t)^{-1}$ or $\psi_j(x) = x(x^2+p_tx+q_t)^{-1}$, then ϕ_j is generated by a recurrence relation containing all the functions $\phi_0, \phi_1, \dots, \phi_{j-1}$.

4 An application to least-squares approximation

We consider the computation of the best least-squares rational approximation with fixed poles on an interval $[a, b]$ of a real-valued function f with poles outside but very close to this interval. It is the purpose of this example to illustrate that it can be beneficial to use orthogonal rational functions to approximate f instead of polynomials. It is well known that the Stieltjes procedure for generating orthogonal polynomials by using their three-term recursion relation may suffer from loss of orthogonality due to propagated round-off errors; see, e.g., [16] for an example.

Let $d\mu = dx$ in (1). We would like to solve the problem

$$\min_{g \in S} ||f-g||, \quad S = \text{span}\{\psi_0, \psi_1, \dots, \psi_n\}.$$

The solution $\hat{g}$ can be determined by first applying Algorithm 3.1 to compute an orthonormal basis $\phi_0, \phi_1, \dots, \phi_n$ of S. Then

$$\hat{g}(x) = \sum_{j=0}^{n} < f, \phi_j > \phi_j(x).$$

Specifically, let the function f be given by

$$f(x) = \frac{e^{-3x}}{(x^2-x+13/50)\ln^2(x-0.2)}.$$

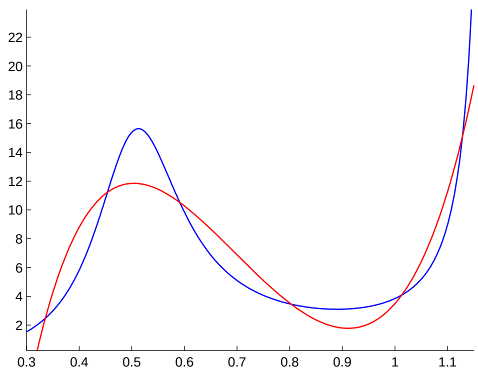

Fig. 1 The function f (blue line) and its the best least-squares approximation from the space S_1

Thus, f has poles at 1.2 and $0.5 \pm i\,0.1$. We would like to approximate f in the interval $[0.3, 1.15]$. Note that the poles of f are very close to this interval. Letting

$$S = S_1 = \mathrm{span}\{1, x, \ldots, x^5\} \tag{11}$$

yields a very poor approximation of f, especially around 0.5 and 1.15, as can be seen in Figure 1. We will comment on the computational details below.

If we use rational approximants with a pole at 1.2, i.e., if we take

$$S = S_2 = \mathrm{span}\left\{1, x, \frac{1}{x-1.2}, x^2, \frac{1}{(x-1.2)^2}, x^3\right\}, \tag{12}$$

then we obtain a smaller approximation error. The rational approximant yields a better approximation of f than the polynomial approximant at the right end point of the interval $[0.3, 1, 15]$, but the error is still large around 0.5; see Figure 2.

When we include all the poles by letting

$$S = S_3 = \mathrm{span}\left\{1, \frac{1}{x-1.2}, x, \frac{1}{x^2-x+13/50}, \frac{x}{x^2-x+13/50}, x^2\right\}, \tag{13}$$

we obtain a very accurate approximation of f as is displayed in Figure 3.

Algorithm 3.1 is applied to the elementary bases of S_1, S_2, and S_3, with the basis functions ordered as displayed in (11), (12), and (13), respectively. When $S = S_1$ and $S = S_2$ all the functions $\phi_j(x)$, $j = 0, 1, \ldots, 5$, are generated by three-term recurrences. In the case when $S = S_3$, the function $\phi_5(x)$ is generated by a four-term recurrence relation, whereas the recurrences for $\phi_3(x)$ and $\phi_4(x)$ are full.

The algorithm is an extension of the Stieltjes procedure and, similar to the latter, it may suffer from loss of orthogonality in finite precision arithmetic. In

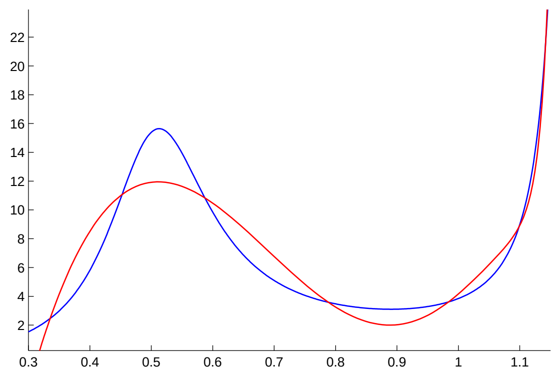

Fig. 2 The function f (blue line) and its the best least-squares approximation from the space S_2

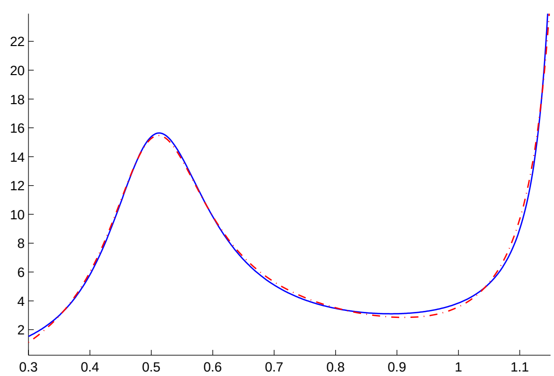

Fig. 3 The function f (blue line) and its the best least-squares approximation from the space S_3

order to illustrate the potential of Algorithm 3.1, we implemented it in MATLAB using symbolic computation to store rational functions and to evaluate the required inner products $< \phi_i, \phi_j >$. The computed values were rounded to double precision arithmetic ($\varepsilon_{\text{machine}} = 2.22 \cdot 10^{-16}$), and we evaluated the Fourier coefficients $< f, \phi_j >$ with the MATLAB function `quadl` with tolerance $1 \cdot 10^{-15}$. The computations were quite rapid and this illustrates that it is feasible to use symbolic arithmetic and to evaluate the inner products $< f, \phi_j >$ accurately for some problems.

However, this approach is not feasible for all problems for which the application of Algorithm 3.1 may be of interest. In general, the Fourier coefficients should be computed recursively according to

$$\begin{array}{lll} c_0 := < f, \phi_0 >, & f_0 := f - c_0\phi_0, & \\ c_j := < f_{j-1}, \phi_j >, & f_j := f_j - c_j\phi_j, & j = 1, 2, \ldots \, . \end{array}$$

The sensitivity of Algorithm 3.1 to round-off errors introduced during the computations is likely to depend on both the inner product and on the set of functions $\{\psi_0, \psi_1, \ldots, \psi_n\}$ to be orthogonalized. A study of the numerical properties of Algorithm 3.1 will be presented elsewhere.

5 Conclusion and extensions

We have shown that orthonormal rational functions with prescribed poles satisfy short recursion relations (7), (9), and (10) under fairly general conditions. These recursion formulas form the foundation of a Stieltjes-type procedure for the recursive generation of orthonormal rational functions with specified poles. An application to least-squares approximation is discussed in the present paper. Many other applications can be envisioned, including the approximation of matrix functions and rational Gauss quadrature. These applications will be considered in forthcoming work.

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