Quadratures associated with pseudo-orthogonal rational functions on the real half line with poles in $[-\infty, 0]$

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Dedicated to Francisco Marcellan Español on the occasion of his 60th birthday

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Abstract

We consider a positive measure on $[0,\infty)$ and a sequence of nested spaces $\mathscr{L}_0 \subset \mathscr{L}_1 \subset \mathscr{L}_2 \cdots$ of rational functions with prescribed poles in $[-\infty, 0]$. Let $\{\varphi_k\}_{k=0}^{\infty}$, with $\varphi_0 \in \mathscr{L}_0$ and $\varphi_k \in \mathscr{L}_k \setminus \mathscr{L}_{k-1}$, $k = 1, 2, \ldots$ be the associated sequence of orthogonal rational functions. The zeros of φ_n can be used as the nodes of a rational Gauss quadrature formula that is exact for all functions in $\mathscr{L}_n \cdot \mathscr{L}_{n-1}$, a space of dimension $2n$. Quasi- and pseudo-orthogonal functions are functions in $\mathscr{L}_n$ that are orthogonal to some subspace of $\mathscr{L}_{n-1}$. Both of them are generated from φ_n and φ_{n-1} and depend on a real parameter τ. Their zeros can be used as the nodes of a rational Gauss-Radau quadrature formula where one node is fixed in advance and the others are chosen to maximize the subspace of $\mathscr{L}_n \cdot \mathscr{L}_{n-1}$ where the quadrature is exact. The parameter τ is used to fix a node at a pre-assigned point. The space where the quadratures are exact has dimension $2n-1$ in both cases but it is in $\mathscr{L}_{n-1} \cdot \mathscr{L}_{n-1}$ in the quasi-orthogonal case and it is in $\mathscr{L}_n \cdot \mathscr{L}_{n-2}$ in the pseudo-orthogonal case.

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1. Introduction

It is well known that the zeros of orthogonal polynomials φ_n with respect to a positive measure μ with support in $[0,\infty)$ are simple and lie in $(0,\infty)$. The zeros x_k, $k = 1, \ldots, n$ of φ_n are nodes of a quadrature formula $Q[f] = \sum_{k=1}^{n} c_k f(x_k)$ with positive weights c_k, the formula being exact on the space $\mathscr{P}_{2n-1}$ of polynomials of degree at most $2n-1$. These are the well-known *Gauss-Christoffel quadrature formulas*. See e.g., (5, Ch. I.6), (6, Ch. I.3), (7, Ch. I.4).

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Furthermore, all the zeros of the *quasi-orthogonal polynomials* $\varphi_n(z,\tau) = \varphi_n(z) - \tau\varphi_{n-1}(z)$, $\tau \in \hat{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$, are real and simple and at least $n-1$ of them lie in $(0,\infty)$. Also these zeros are nodes in a quadrature formula with positive weights, and this formula is exact on $\mathscr{P}_{2n-2}$. See e.g. (5, Ch. II.3), (6, Ch. I.3).

The space $\text{span}\{z^{-p},\ldots,1,\ldots,z^q\}$ with p and q non-negative integers is denoted by $\Lambda_{-p,q}$. The space Λ of all Laurent polynomials is the union of all these $\Lambda_{-p,q}$. Let μ be a positive measure on $[0,\infty)$ such that all the elements of Λ are integrable, and let $\{\varphi_n\}$ denote the *orthogonal Laurent polynomials* with respect to μ obtained by orthogonalization of the basis $\{1,z^{-1},z,z^{-2},z^2,\ldots\}$. Then, again all the zeros of φ_n are simple and lie in $(0,\infty)$. These zeros are the nodes in a quadrature formula with positive weights c_k which is exact on the space $\Lambda_{-2m,2m-1}$ when $n = 2m$ and on the space $\Lambda_{-(2m+1),2m}$ when $n = 2m+1$.

The *quasi-orthogonal Laurent polynomials* are defined as $\varphi_n(z,\tau) = \varphi_n(z) - \tau z^{(-1)^n}\varphi_{n-1}(z)$, $\tau \in \hat{\mathbb{R}}$. These Laurent polynomials in many respects play a role similar to the quasi-orthogonal polynomials in the classical polynomial case. All the zeros of $\varphi_n(z,\tau)$ are real and simple and at least $n-1$ of them lie in $(0,\infty)$. Also these zeros are nodes in a quadrature formula with positive weights which is exact on $\Lambda_{-2m,2m-2}$ when $n = 2m$ and on $\Lambda_{-2m,2m}$ when $n = 2m+1$. For basic properties of orthogonal and quasi-orthogonal Laurent polynomials and their associated quadrature formulas, see e.g., (9; 10; 11).

The Laurent polynomials $\Phi_n(z,\tau) = \varphi_n(z) - \tau\varphi_{n-1}(z)$, $\tau \in \mathbb{R}$ are called *pseudo-orthogonal Laurent polynomials*. All the zeros of $\Phi_n(z,\tau)$ are real and simple and at least $n-1$ of them lie in $(0,\infty)$. These zeros are nodes in a quadrature formula which is exact on $\Lambda_{-(2m-1),2m-1}$ when $n = 2m$ and on $\Lambda_{-(2m+1),2m-1}$ when $n = 2m+1$. However, the weights in the formula are positive for nodes which are positive, but not for the possible node not lying in $(0,\infty)$. For these results see (12).

The theory of *orthogonal rational functions with prescribed poles* can be considered as a generalization of the theory of orthogonal polynomials and orthogonal Laurent polynomials (where the poles are at infinity and at the origin and infinity respectively). Results about quadrature formulas associated with orthogonal and quasi-orthogonal rational functions with poles in the extended real line $\hat{\mathbb{R}}$ can be found in (1) (where an equivalent situation with poles on the unit circle is treated), (2), (4) and references given there. In particular the situation where the support of the orthogonality measure is contained in $[0,\infty)$ and prescribed poles lie in $[-\infty,0]$ was treated in (4).

A study of rational functions generalizing pseudo-orthogonal Laurent polynomials has so far not been undertaken. In this paper, we introduce such functions and develop properties of their zeros and quadrature formulas associated with them.

In Section 2 we describe basic properties of orthogonal rational functions with poles in $[-\infty,0]$, determined by a positive measure μ on $[0,\infty)$. In Section 3 we briefly discuss the quasi-orthogonal rational functions and the quadrature formulas in this situation. In Section 4 we introduce pseudo-orthogonal rational functions and prove basic results on their zeros, while in Section 5 we are concerned with the associated quadrature formulas. The computational aspects of the above quadrature formulas are discussed in Section 6 and they are illustrated with several numerical examples in Section 7. Finally some concluding remarks are given in Section 8.

Possible applications of such quadratures can be found in some special integrals appearing in

theoretical physics or more generally in evaluating any integral transform that can be written as, or transformed into, an integral over the positive real line with an integrand that is the product of a positive (weight) function and a function that is a rational function or that can be well approximated by a rational function with known poles (on $[0,\infty)$). Take for example the Laplace or Hankel transform of $\sin(1/sqrt(p(x)))$ where $p(x)$ is a polynomial with known negative roots which could be as simple as $p(x)=x$ or x^2.

2. Orthogonal rational functions

In (2) and references given there, a general theory of orthogonal rational functions with prescribed poles is developed. In (4) a presentation is given with special regard to the situation where the relevant measures have support in $[0,\infty)$ and the prescribed poles lie in $[-\infty,0]$.

Let $\{\zeta_n\}_{n=1}^{\infty}$ be a sequence of elements in $[-\infty,0]$, possibly repeated. We define $r_0=1$, $r_n(z)=1$ if $\zeta_n=-\infty$, $r_n(z)=(\zeta_n-z)$ if $\zeta_n\neq-\infty$, $n=1,2,\ldots$ and set $D_0=1$, $D_n(z)=r_1(z)r_2(z)\cdots r_n(z)$ for $n=1,2,3,\ldots$. The space $\mathscr{L}_n$ is defined as $\mathscr{L}_n=\{P(z)/D_n(z):P\in\mathscr{P}_n\}$, and we set $\mathscr{L}=\cup_{n=0}^{\infty}\mathscr{L}_n$. We shall also make use of spaces $\mathscr{L}_p\cdot\mathscr{L}_q$ consisting of all products of an element in $\mathscr{L}_p$ and an element in $\mathscr{L}_q$. Similarly we define $\mathscr{L}\cdot\mathscr{L}$. Note that $\mathscr{L}\cdot\mathscr{L}=\mathscr{L}$ if every value ζ_n occurs infinitely many times in the sequence.

Note that the Laurent polynomial situation is obtained when $\zeta_{2m}=-\infty$, $\zeta_{2m+1}=0$ for all m, while the classical polynomial situation is obtained when $\zeta_n=-\infty$ for all n.

Let μ be a positive measure with infinite support in $[0,\infty)$ such that all elements in $\mathscr{L}\cdot\mathscr{L}$ are integrable. Without loss of generality we normalize such that $\int \mathrm{d}\mu(t)=1$. (The integral sign always means integration over $[0,\infty)$ in this paper.) We define the inner product $\langle\cdot,\cdot\rangle$ on $\mathscr{L}$ by $\langle g,h\rangle=\int g(t)\overline{h(t)}\mathrm{d}\mu(t)$, $g,h\in\mathscr{L}$.

We construct the *orthonormal sequence* $\{\varphi_n\}_{n=0}^{\infty}$ in $\mathscr{L}$ such that $\varphi_0\in\mathscr{L}_0$, $\varphi_n\in\mathscr{L}_n\setminus\mathscr{L}_{n-1}$ for $n=1,2,3,\ldots$, for example by the Gram-Schmidt orthonormalization of the basis $\{(z-a)^n/D_n(z)\}_{n=0}^{\infty}$, $a>0$. Note that in this construction the $\varphi_n(x)$ can be normalized such that the $\varphi_n(x)$ are real for real x. We may write for $n=1,2,3,\ldots$

$$\varphi_n(z)=\frac{P_n(z)}{D_n(z)},\quad \text{where } P_n=p_{nn}z^n+\cdots+p_{0n}\in\mathscr{P}_n\setminus\mathscr{P}_{n-1}. \tag{2.1}$$

All the zeros of the polynomial P_n are simple and lie in $(0,\infty)$. (See (4, Section 8).) We may then normalize φ_n, $n=1,2,\ldots$ as we did in (4, Eq. (3.1))

$$\begin{aligned}&\operatorname{sign}P_n(\zeta_{n-1})=\operatorname{sign}P_{n-1}(\zeta_{n-1})\ \text{ if }\ \zeta_{n-1}\neq-\infty,\\&\operatorname{sign}p_{nn}=\operatorname{sign}p_{n-1,n-1}\ \text{ if }\ \zeta_{n-1}=-\infty,\\&p_{11}>0.\end{aligned}$$

Note that P_k has all its zeros in $(0,\infty)$. Thus the sign of its function values to the left of the leftmost zero will be the same as or opposite to the sign of its leading coefficient, depending on k being even or odd. In the case of $-\infty<\zeta_{n-1}<0$, the above sign normalization means that we must have $p_{nn}/p_{n-1,n-1}<0$. Moreover, because the product of the zeros of P_k is given by $(-1)^k p_{0,k}/p_{k,k}$, this must be positive. In other words, if we use this fact for $k=n$ and $k=n-1$, we

get $\operatorname{sign}(p_{nn}/p_{n-1,n-1}) = -\operatorname{sign}(p_{0,n}/p_{0,n-1})$. Thus the previous normalization can be rewritten as $(n = 1,2,\ldots)$

$$\begin{aligned} &p_{nn}/p_{n-1,n-1} < 0 \text{ i.e. } p_{0n}/p_{0,n-1} > 0 \text{ if } \zeta_{n-1} \neq -\infty, \\ &p_{nn}/p_{n-1,n-1} > 0 \text{ i.e. } p_{0n}/p_{0,n-1} < 0 \text{ if } \zeta_{n-1} = -\infty, \\ &p_{11} > 0. \end{aligned} \tag{2.2}$$

The *functions σ_n of the second kind* are defined by

$$\sigma_n(z) = \int \frac{\varphi_n(t) - \varphi_n(z)}{t - z} \mathrm{d}\mu(t), \quad n = 0,1,2,\ldots. \tag{2.3}$$

Note that σ_n is of the form $\sigma_n(z) = S_n(z)/D_n(z)$, where $S_n \in \mathscr{P}_{n-1}$, and thus σ_n belongs to $\mathscr{L}_n$.

The functions φ_n and σ_n satisfy a *three-term recurrence relation*. From this follows a *confluent Christoffel-Darboux type formula*, from which it can be deduced that between two consecutive zeros of φ_n, there is exactly one zero of φ_{n-1}. See (4, Section 5). Furthermore the recurrence relation leads to the *determinant formula*

$$\sigma_n(z)\varphi_{n-1}(z) - \sigma_{n-1}(z)\varphi_n(z) = (-1)^n \frac{W_1 W_2 \cdots W_n}{r_{n-1}(z) r_n(z)}, \tag{2.4}$$

where all the constants W_k are negative. (See (4, Sections 10, 12).)

The following result, which we shall need in Section 3, seems not to have been stated in the literature.

Proposition 2.1. *Between two consecutive zeros of φ_n, there is exactly one zero of σ_n.*

PROOF. Let ξ and η be two consecutive zeros of φ_n, $\xi < \eta$. Since the zeros of φ_{n-1} separate the zeros of φ_n as stated above, the values $\varphi_{n-1}(\xi)$ and $\varphi_{n-1}(\eta)$ have opposite sign. For $z \in (0,\infty)$ the right-hand side of (2.4) does not change sign. It follows that $\sigma_n(\xi)\varphi_{n-1}(\xi)$ and $\sigma_n(\eta)\varphi_{n-1}(\eta)$ are nonzero and have the same sign. Consequently $\sigma_n(\xi)$ and $\sigma_n(\eta)$ must have opposite sign. Then by the intermediate value theorem for continuous functions there is a $\zeta \in (\xi,\eta)$ such that $\sigma_n(\zeta) = 0$. The result now follows since $\sigma_n(z)$ has at most $n-1$ different zeros. ∎

For the sake of completeness, with regard to the main theme in this paper, we state an *analog of the classical Gauss-Christoffel quadrature formula*. For a proof see (1), (2, Chap. 11.6), (4, Section 6).

Theorem 2.2. *Let $x_{1,n}, x_{2,n}, \ldots, x_{n,n}$ be the n distinct zeros of φ_n. Then there exist positive weights $c_{1,n}, c_{2,n}, \ldots, c_{n,n}$ such that*

$$\int f(t)\mathrm{d}\mu(t) = \sum_{k=1}^{n} c_{k,n} f(x_{k,n})$$

for all $f \in \mathscr{L}_n \cdot \mathscr{L}_{n-1}$.

3. Quasi-orthogonal rational functions

The functions which in most respects generalize quasi-orthogonal polynomials are the *quasi-orthogonal rational functions* $\varphi_n(z,\tau)$ defined as follows:

$$\varphi_n(z,\tau) = \varphi_n(z) - \tau\frac{r_{n-1}(z)}{r_n(z)}\varphi_{n-1}(z), \quad \tau \in \hat{\mathbb{R}},\ \ n \geq 1 \tag{3.5}$$

with $\varphi_n(z,\infty)$ meaning $\frac{r_{n-1}(z)}{r_n(z)}\varphi_{n-1}(z)$. We may write $\varphi_n(z,\tau) = P_n(z,\tau)/D_n(z)$, where $P_n(z,\tau)$ is a polynomial in z of degree n.

Although it is quite obvious, it seems that their orthogonality property has not been stated explicitly in the literature. We give it here for completeness.

Theorem 3.1. *The quasi-orthogonal rational function $\varphi_n(z,\tau)$ is orthogonal to*

$$\mathscr{L}_{n-1}(\zeta_n) = \frac{r_n(z)}{r_{n-1}(z)}\mathscr{L}_{n-2} = \left\{\frac{Y_{n-1}(z)}{D_{n-1}(z)} : Y_{n-1}(z) \in \mathscr{P}_{n-1},\ \ Y_{n-1}(\zeta_n) = 0\right\}.$$

By $Y_{n-1}(\infty)$ we mean its coefficient of z^{n-1}.

PROOF. If $f \in \mathscr{L}_{n-1}(\zeta_n)$ then $f = \frac{r_n p_{n-2}}{D_{n-1}}$ with $p_{n-2} \in \mathscr{P}_{n-2}$. So, using the orthogonality of φ_n and φ_{n-1},

$$\langle f(z), \varphi_n(z,\tau)\rangle = -\tau\left\langle \frac{r_n p_{n-2}}{D_{n-1}}, \frac{r_{n-1}}{r_n}\varphi_{n-1}\right\rangle = -\tau\left\langle \frac{p_{n-2}}{D_{n-2}}, \varphi_{n-1}\right\rangle = 0$$

which proves the theorem. ∎

The *functions of the second kind* $\sigma_n(z,\tau)$ are defined as

$$\sigma_n(z,\tau) = \sigma_n(z) - \tau\frac{r_{n-1}(z)}{r_n(z)}\sigma_{n-1}(z). \tag{3.6}$$

In general these functions cannot be written as

$$\int \frac{\varphi_n(t,\tau) - \varphi_n(z,\tau)}{t-z}\mathrm{d}\mu(t).$$

It is proved in (2, Lemma 11.5.2) without restrictions on μ and the ζ_m that $P_n(z,\tau)$ has n simple zeros, all lying in $(-\infty,\infty)$. We shall give more precise information on the location of the zeros when μ has support in $[0,\infty)$ and all ζ_n are contained in $[-\infty,0]$.

Proposition 3.2. *The quasi-orthogonal rational function $\varphi_n(z,\tau)$ has at least $n-1$ simple zeros in $(0,\infty)$.*

PROOF. Let $x_{k,n}(\tau)$, $k = 1,2,\ldots,q$ be the distinct positive zeros of odd order of $\varphi_n(z,\tau)$. Then we may write

$$\varphi_n(z,\tau) = \frac{k_n\Big(z - x_{1,n}(\tau)\Big)\cdots\Big(z - x_{q,n}(\tau)\Big)}{D_n(z)} Q_{n-q}(z,\tau)$$

where $Q_{n-q}(z,\tau)$ is a polynomial in z of degree at most $n-q$ and k_n is a real constant. This polynomial $Q_{n-q}(z,\tau)$ does not change sign on $(0,\infty)$ since all its zeros in $(0,\infty)$ are of even order and non-real zeros appear in conjugate pairs.

Set $R(z,\tau) = \frac{r_n(z)}{r_{n-1}(z)} S(z,\tau)$ with

$$S(z,\tau) = \frac{\Big(z - x_{1,n}(\tau)\Big)\cdots\Big(z - x_{q,n}(\tau)\Big)}{D_q(z)}.$$

Note that $S(z,\tau) \in \mathscr{L}_q$ and that also $R(z,\tau)\varphi_n(z,\tau)$ does not change sign on $(0,\infty)$. Consequently $\int R(t)\varphi_n(t,\tau)\mathrm{d}\mu(t) \neq 0$ since μ has infinite support.

Now assume that $q < n-1$. Then $\langle R(z,\tau), \varphi_n(z)\rangle = 0$ since $R(z,\tau) \in \mathscr{L}_{n-1}$. Furthermore

$$\left\langle R(z,\tau), \frac{r_{n-1}(z)}{r_n(z)}\varphi_{n-1}(z)\right\rangle = \left\langle \frac{r_n(z)}{r_{n-1}(z)} S(z,\tau), \frac{r_{n-1}(z)}{r_n(z)}\varphi_{n-1}(z)\right\rangle = \langle S(z,\tau), \varphi_{n-1}(z)\rangle = 0,$$

since $S(z,\tau) \in \mathscr{L}_q \subset \mathscr{L}_{n-2}$. Thus $\int R(t,\tau)\varphi_n(t,\tau)\mathrm{d}\mu(t) = 0$. This is a contradiction and hence $q \geq n-1$. From this the result follows. ∎

For the sake of completeness, we state as a theorem a special case of a quadrature formula which is valid without restrictions on the location of the support of μ and of ζ_n. For a proof of the general result, see e.g., (1, Section 5), (2, Chapter 11.6). As before we assume $\operatorname{supp}\mu \subset [0,\infty)$ and $\zeta_k \in [-\infty, 0]$ for all k. Note that $\varphi_n(z,\infty)$ will have only $n-1$ zeros, but if $\tau \neq \infty$ then $\varphi_n(z,\tau)$ always has n zeros, one of which could be at ∞.

Theorem 3.3. *Suppose $\tau \neq \infty$. Let $x_{1,n}(\tau),\ldots,x_{n,n}(\tau)$ be the zeros of $\varphi_n(z,\tau)$, and assume that the one possible zero outside $(0,\infty)$ does not coincide with any ζ_k. Then there exist positive constants $\kappa_{1,n}(\tau),\ldots,\kappa_{n,n}(\tau)$ such that*

$$\int f(t)\mathrm{d}\mu(t) = \sum_{k=1}^{n} \kappa_{k,n}(\tau) f(x_{k,n}(\tau)) \tag{3.7}$$

for all $f \in \mathscr{L}_{n-1}\cdot\mathscr{L}_{n-1}$.

Remark 3.1. If $\tau \neq \infty$, we may write $P_n(z,\tau) = p_{0,n}(\tau) + \cdots + p_{n,n}(\tau)z^n$. Assume $\zeta_{n-1} \neq -\infty$. Then

$$p_{0,n}(\tau) = p_{0,n} - \tau\zeta_{n-1}p_{0,n-1} \text{ and } p_{n,n}(\tau) = p_{n,n} + \tau p_{n-1,n-1}$$

(cf. Section 2). We have

$$x_{1,n}(\tau)\cdots x_{n,n}(\tau) = (-1)^n\frac{p_{0,n}(\tau)}{p_{n,n}(\tau)} = (-1)^n\frac{p_{0,n} - \tau\zeta_{n-1}p_{0,n-1}}{p_{n,n} + \tau p_{n-1,n-1}}.$$

The product changes sign when $\tau = \frac{p_{0,n}}{\zeta_{n-1}p_{0,n-1}}$ and when $\tau = -\frac{p_{n,n}}{p_{n-1,n-1}}$. For $\tau = 0$ the product is positive since all the zeros are positive. Because $\frac{p_{0,n}}{\zeta_{n-1}p_{0,n-1}} < 0$ and $-\frac{p_{n,n}}{p_{n-1,n-1}} > 0$ we conclude that all the zeros of $P_n(z,\tau)$ are positive when $\tau \in \left(\frac{p_{0,n}}{\zeta_{n-1}p_{0,n-1}}, -\frac{p_{n,n}}{p_{n-1,n-1}}\right)$. Similarly we find that all the zeros are positive when $\tau \in \left(\frac{p_{0,n}}{p_{0,n-1}}, \infty\right)$ if $\zeta_{n-1} = -\infty$. More generally, it is not difficult to see that it is always possible to choose a τ such that $P_n(z,\tau)$ vanishes at an arbitrary chosen point $x_* \in \hat{\mathbb{R}}$. Indeed, since $P_n(z,\tau) = P_n(z) - \tau r_{n-1}(z)P_{n-1}(z)$, it is clear that it suffices to choose $\tau(x_*) = P_n(x_*)/[r_{n-1}(x_*)P_{n-1}(x_*)]$ to get $P_n(x_*, \tau(x_*)) = 0$. This also holds with proper adaptations if x_* is a zero of P_{n-1}, or equal to ζ_{n-1}, or infinity. The endpoints of the intervals for τ given above correspond to the case where x_* is at one of the boundaries of the interval $[0,\infty]$, i.e., on the verge of leaving the interval with positive nodes.

The situation is sketched in Figure 1. It is seen that for finite ζ_{n-1} the zeros of $\varphi_n(z,\tau)$ are

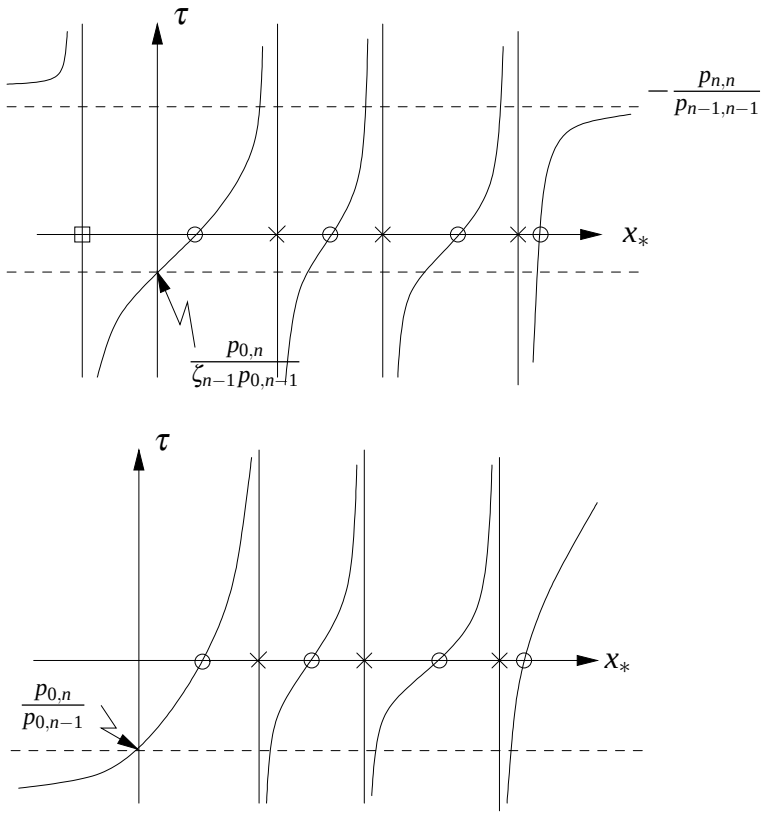

Figure 1: Plot of $\tau(x_*) = \frac{P_n(x_*)}{r_{n-1}(x_*)P_{n-1}(x_*)}$. The situation with $n = 4$ and ζ_3 finite (top) or $-\infty$ (bottom). The circles indicate the zeros of P_4 and the crosses the zeros of P_3. The square is ζ_3.

monotonically shifting to the right as τ increases from $\frac{p_{0,n}}{\zeta_{n-1}p_{0,n-1}}$ to $-\frac{p_{n,n}}{p_{n-1,n-1}}$. At the topmost endpoint for τ, the rightmost zero of $\varphi_n(z,\tau)$ is leaving the interval $[0,+\infty]$ at $+\infty$ (to re-enter at $-\infty$) while at the the bottommost endpoint of the interval for τ, the leftmost zero of $\varphi_n(z,\tau)$ leaves

the interval $[0,+\infty]$ at 0 (and becomes negative). All the other zeros of $\varphi_n(z,\tau)$ are caught in the intervals fixed by the zeros of φ_{n-1}.

For $\zeta_{n-1}=-\infty$, the situation is sketched at the bottom of the figure. For all values of τ larger than $\frac{p_{0,n}}{p_{0,n-1}}$ all the zeros of $\varphi_n(z,\tau)$ are positive and are monotonically increasing in between two consecutive zeros of φ_{n-1} as τ increases. If τ becomes less than $\frac{p_{0,n}}{p_{0,n-1}}$ then the leftmost zero is leaving the interval $[0,\infty]$ at 0.

In view of our previous observations, it will be proved that the general form of the plots of $\tau(x_*)$ is indeed as sketched in Figure 1 if we prove the monotonicity of this function.

Proposition 3.4. *For increasing x, the function* $\tau(x)=\frac{P_n(x)}{r_{n-1}(x)P_{n-1}(x)}$ *jumps from* $+\infty$ *to* $-\infty$ *in each of its poles while it is monotonically increasing from* $-\infty$ *to* $+\infty$ *in between.*

PROOF. We first note that

$$\tau(x)=\frac{P_n(x)}{r_{n-1}(x)P_{n-1}(x)}=\frac{\varphi_n(x)r_n(x)}{\varphi_{n-1}(x)r_{n-1}(x)}.$$

Taking the derivative gives

$$\frac{\mathrm{d}\tau(x)}{\mathrm{d}x}=\frac{r_{n-1}(x)\varphi_{n-1}(x)[r_n(x)\varphi_n(x)]'-[r_{n-1}(x)\varphi_{n-1}(x)]'r_n(x)\varphi_n(x)}{\left(r_{n-1}(x)\varphi_{n-1}(x)\right)^2}$$

Next we recall the confluent form of the Christoffel-Darboux formula given in (4, Theorem 5.1)

$$r_{n-1}(x)\varphi_{n-1}(x)[r_n(x)\varphi_n(x)]'-[r_{n-1}(x)\varphi_{n-1}(x)]'r_n(x)\varphi_n(x)=U_n\sum_{k=0}^{n-1}\varphi_k(x)^2,$$

where according to (4, Eq. (4.2))

$$U_n=\begin{cases}\dfrac{P_n(\zeta_{n-1})}{P_{n-1}(\zeta_{n-1})} & \text{if } \zeta_{n-1}\neq-\infty\\[2ex] \dfrac{p_{n,n}}{p_{n-1,n-1}} & \text{if } \zeta_{n-1}=-\infty\end{cases}$$

and thus, because of our normalization $U_n>0$ for $n=1,2,3,\ldots$.
If we plug this into the expression for the derivative of τ we see that $\tau'(x)>0$ as was to be proved.

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Since this τ gives us the freedom of fixing a zero, i.e., a node of the quadrature formula, we can use this to construct rational Gauss-Radau formulas, which are formulas that prescribe one node and choose the other nodes in an optimal way so as to obtain a maximal domain of validity of the quadrature formula, which in this case is $\mathscr{L}_{n-1}\cdot\mathscr{L}_{n-1}$, a space of dimension $2n-1$.

4. Pseudo-orthogonal rational functions

We continue to consider a measure μ with infinite support in $[0,\infty)$ and rational functions with prescribed poles $\zeta_k \in [-\infty, 0]$.

The *pseudo-orthogonal rational functions* $\Phi_n(z,\tau)$ are defined as

$$\Phi_n(z,\tau) = \varphi_n(z) - \tau\varphi_{n-1}(z), \quad \tau \in \hat{\mathbb{R}}, \quad n \geq 1 \tag{4.8}$$

with $\Phi_n(z,\infty)$ meaning $\varphi_{n-1}(z)$. We may write $\Phi_n(z,\tau) = \Pi_n(z,\tau)/D_n(z)$ where Π_n is a polynomial of degree at most n.

The orthogonality property of pseudo-orthogonal rational functions is much simpler than for quasi-orthogonal rational functions since $\Phi_n(z,\tau)$ will be obviously orthogonal to $\mathscr{L}_{n-2}$ (which has the same dimension as $\mathscr{L}_{n-1}(\zeta_n)$ for the quasi-orthogonal functions).

We also consider *functions of the second kind* $\Sigma_n(z,\tau)$ defined as

$$\Sigma_n(z,\tau) = \sigma_n(z) - \tau\sigma_{n-1}(z). \tag{4.9}$$

These functions may also be written as

$$\Sigma_n(z,\tau) = \int \frac{\Phi_n(t,\tau) - \Phi_n(z,\tau)}{t-z} \mathrm{d}\mu(t). \tag{4.10}$$

(Cf. the functions of the second kind associated with the quasi-orthogonal functions where a similar representation does not hold in general.)

Proposition 4.1. *$\Phi_n(z,\tau)$ has at least $n-1$ simple zeros lying in $(0,\infty)$.*

PROOF. Let $\xi_{1,n}(\tau),\ldots,\xi_{q,n}(\tau)$ be the positive zeros of odd order of $\Phi_n(z,\tau)$. Then we may write

$$\Phi_n(z,\tau) = \frac{\gamma_n\,(z-\xi_{1,n}(\tau))\cdots\big(z-\xi_{q,n}(\tau)\big)}{D_n(z)} Q_{n-q}(z,\tau)$$

where $Q_{n-q}(z,\tau)$ is a polynomial in z of degree at most $n-q$ and γ_n a real constant. This polynomial $Q_n(z,\tau)$ does not change sign on $(0,\infty)$, since all the zeros in $(0,\infty)$ are of even order and non-real zeros appear in conjugate pairs. Set

$$R(z,\tau) = \frac{(z-\xi_{1,n}(\tau))\cdots(z-\xi_{q,n}(\tau))}{D_q(z)}.$$

It follows that $R(z,\tau)\Phi_n(z,\tau)$ does not change sign for $z \in (0,\infty)$.
Consequently $\int R(t,\tau)\Phi_n(t,\tau)\mathrm{d}\mu(t) \neq 0$ since μ has infinite support.

Now assume that $q < n-1$. Then $\langle R(z,\tau), \varphi_n(z)\rangle = 0$ and $\langle R(z,\tau), \varphi_{n-1}(z)\rangle = 0$ since $R(z,\tau) \in \mathscr{L}_q \subset \mathscr{L}_{n-2}$. This is a contradiction, and hence $q \geq n-1$. From this the result follows. ∎

Remark 4.1. When $\Pi_n(z,\tau) = P_n(z) - \tau r_n(z)P_{n-1}(z)$ is of degree less than n, then $\Phi_n(z,\tau)$ has only $n-1$ zeros. Otherwise $\Phi_n(z,\tau)$ has n real simple zeros, one of which may lie in $(-\infty, 0]$.

We may write $\Pi_n(z,\tau) = \pi_{0,n}(\tau) + \cdots + \pi_{n,n}(\tau)z^n$. Assume $\zeta_n \neq -\infty$. Then

$$\pi_{0,n}(\tau) = p_{0,n} - \tau\zeta_n p_{0,n-1} \text{ and } \pi_{n,n}(\tau) = p_{n,n} + \tau p_{n-1,n-1}.$$

We have

$$\xi_{1,n}(\tau)\cdots\xi_{n,n}(\tau) = (-1)^n \frac{\pi_{0,n}(\tau)}{\pi_{n,n}(\tau)} = (-1)^n \frac{p_{0,n} - \zeta_n\tau p_{0,n-1}}{p_{n,n} + \tau p_{n-1,n-1}}.$$

For $\tau = 0$ the product is positive since all the zeros are positive. The product changes sign when $\tau = \frac{p_{0,n}}{\zeta_n p_{0,n-1}}$ and when $\tau = -\frac{p_{n,n}}{p_{n-1,n-1}}$. Because $\frac{p_{0,n}}{\zeta_n p_{0,n-1}} < 0$ and $-\frac{p_{n,n}}{p_{n-1,n-1}} > 0$ we conclude that all the zeros are positive when $\tau \in \left(\frac{p_{0,n}}{\zeta_n p_{0,n-1}}, -\frac{p_{n,n}}{p_{n-1,n-1}}\right)$. Similarly we find that all the zeros are positive when $\tau \in \left(\frac{p_{0,n}}{p_{0,n-1}}, \infty\right)$ if $\zeta_n = -\infty$.

Moreover, just as in the quasi-orthogonal case, it is always possible to choose $\tau \in \hat{\mathbb{R}}$ such that $\Pi_n(z,\tau)$ has a zero (in a generalized sense explained in the previous section in Remark 3.1) at some preassigned point $x_* \in \hat{\mathbb{R}}$. The boundaries of the intervals given above are obtained for $x_* = 0$ or $x_* = \infty$. Note again that by an appropriate choice of τ we can construct a rational Gauss-Radau formula with a prefixed node anywhere on $\hat{\mathbb{R}}$ while the other nodes are chosen in an optimal way so as to get a maximal domain of validity. This domain of validity is now $\mathscr{L}_n \cdot \mathscr{L}_{n-2}$, (see Theorem 5.1 below) again a space of dimension $2n-1$, but in general different from the space $\mathscr{L}_{n-1} \cdot \mathscr{L}_{n-1}$ which was the space where the quadrature formula was exact in the quasi-orthogonal case. Also the interpretation of Figure 1 is applicable, the only difference is that r_{n-1} has to be replaced by r_n and hence ζ_{n-1} by ζ_n.

The proof of Proposition 3.4 cannot just be repeated because the Christoffel-Darboux relation is not directly applicable. However, it should be clear that the function $\tau(x) = \frac{P_n(x)}{r_{n-1}(x)P_{n-1}(x)}$ in the quasi-orthogonal case has to be replaced by $\tau(x) = \frac{P_n(x)}{r_n(x)P_{n-1}(x)} = \frac{\varphi_n(x)}{\varphi_{n-1}(x)}$ in the pseudo-orthogonal case. Thus, we have in both cases almost the same rational function. Only the pole ζ_{n-1} has been replaced by ζ_n. This results in plots like in Figure 1 which may or may not be flipped upside-down. For completeness we give an outline of a proof of this property.

Proposition 4.2. *There are two situations: (A) when the points ζ_n and ζ_{n-1} are both finite or both $-\infty$ and (B) when one of then is $-\infty$ and the other is finite. When x incleases from $-\infty$ to $+\infty$, then in each of its poles, the function $\tau(x) = \frac{P_n(x)}{r_n(x)P_{n-1}(x)}$ jumps from $-\infty$ to $+\infty$ in case (A) and from $+\infty$ to $-\infty$ in case (B) and it varies monotonically in between successive poles.*

PROOF. Let us denote the above function $\tau(x)$ for the pseudo-orthogonal case by $\tau_P(x)$ while we denote $\tau_Q(x) = \frac{P_n(x)}{r_{n-1}(x)P_{n-1}(x)}$ for the quasi-orthogonal case. We distinguish several cases:

- $\zeta_{n-1} = \zeta_n = -\infty$. Here $\tau_P(x) = \tau_Q(x) = \frac{P_n(x)}{P_{n-1}(x)}$, and the monotonicity is the same.

- ζ_{n-1} and ζ_n are both finite. Then the difference is that the finite pole ζ_{n-1} is replaced by another finite pole ζ_n. This gives a graph for τ_Q that is similar to the top graph of Figure 1, except that the leftmost vertical asymptote is not at ζ_{n-1} but at ζ_n.
- $\zeta_{n-1} = -\infty$ and ζ_n finite. Then $\tau_P(x) = \frac{P_n(x)}{r_n(x)P_{n-1}(x)}$ while $\tau_Q(x) = \frac{P_n(x)}{P_{n-1}(x)}$. The graph of $\tau_Q(x)$ is the bottom situation of Figure 1. Since $\tau_P(x) = \tau_Q(x)/(\zeta_n - x)$, τ_P has the same zeros and the same poles (vertical asymptotes) as τ_Q, with an extra pole in ζ_n. Since $\zeta_n - x$ is negative to the right of ζ_n and positive to the left, it will flip the graph upside down on the positive real axis and go to $+\infty$ ($-\infty$) when approaching the zeros of P_{n-1} from the right (left) while for $x \to \pm\infty$ it has a limit $-\frac{p_{nn}}{p_{n-1,n-1}} < 0$. On the negative real axis, it will grow to $+\infty$ when approaching the extra pole ζ_n from the right and to $-\infty$ when approaching it from the left. Consider the poles $\pi_1, \ldots, \pi_n$ of τ_P ordered cyclically and define $I_k = (\pi_k, \pi_{k+1})$, $k = 1, \ldots, n-1$ and $I_n = (\pi_n, \pi_1) = \{x > \pi_n\} \cup \{x < \pi_1\}$. Then in each interval I_k the function τ_P is continuous and ranges from $+\infty$ to $-\infty$. Thus for every real τ^* there will be be at least one value of x in each interval I_k solving $\tau_P(x) = \tau^*$. Because all these x-values are zeros of an algebraic polynomial of degree at most n, there can be at most n of them, which means that τ_P is one-to-one and thus monotonic in each interval I_k. Hence the graph of $\tau_P(x)$ looks like the top graph in Figure 1, but flipped upside down, i.e., with the τ-axis pointing downwards.
- $\zeta_n = -\infty$ and ζ_{n-1} finite. The situation is like in the previous one. Now $\tau_P(x) = r_{n-1}(x)\tau_Q(x)$ with τ_Q like the top graph of Figure 1. The factor r_{n-1} removes the pole at ζ_{n-1} and since $r_{n-1}(x)$ is negative to the right of it and positive to the left, it will again flip the figure upside down. By our sign normalization $\tau_P(\zeta_{n-1}) = \frac{P_n(\zeta_{n-1})}{P_{n-1}(\zeta_{n-1})} > 0$. Clearly $\tau_P(x)$ will become infinite at infinity. Since there is no sign change to the left of ζ_{n-1}, the limit at $-\infty$ will be $+\infty$. This implies $\frac{p_{nn}}{p_{n-1,n-1}} < 0$, so that the limit at $x = +\infty$ will be $-\infty$. Monotonicity follows as above (now one pole being at ∞) and we end up with a situation like in the bottom graph of Figure 1, but flipped upside down.

This concludes the proof. ∎

Proposition 4.3. *The functions of the second kind $\Sigma_n(z,\tau)$ may be written in the form*

$$\Sigma_n(z,\tau) = \frac{[p_{n,n} + \tau p_{n-1,n-1}]z^{n-1} + O(z^{n-2})}{D_n(z)} \tag{4.11}$$

when $\zeta_n \neq -\infty$ and

$$\Sigma_n(z,\tau) = \frac{p_{n,n}z^{n-1} + O(z^{n-2})}{D_n(z)} \tag{4.12}$$

when $\zeta_n = -\infty$.

PROOF. Since $\varphi_n(z) = P_n(z)/D_n(z)$ we may write

$$\sigma_n(z) = \int \frac{\varphi_n(t) - \varphi_n(z)}{t - z} \mathrm{d}\mu(t) = \frac{1}{D_n(z)} \int \frac{P_n(z)D_n(t) - D_n(z)P_n(t)}{D_n(t)(t-z)} \mathrm{d}\mu(t).$$

Set $\gamma=(-1)^n$ if $\deg D_n(z)=n$, $\gamma=0$ if $\deg D_n(z)<n$. Expanding in powers of z we get

$$P_n(z)D_n(t)-D_n(z)P_n(t)=p_{n,n}z^nD_n(t)-\gamma z^nP_n(t)+O(z^{n-1})$$

and by division by $t-z$ this leads to

$$\frac{P_n(z)D_n(t)-D_n(z)P_n(t)}{t-z}=[p_{n,n}D_n(t)-\gamma P_n(t)]\,z^{n-1}+O(z^{n-2}).$$

Thus

$$\begin{aligned}\sigma_n(z) &= \frac{z^{n-1}}{D_n(z)}\int\frac{p_{n,n}D_n(t)-\gamma P_n(t)}{D_n(t)}\mathrm{d}\mu(t)+\frac{1}{D_n(z)}\int\frac{O(z^{n-2},t)}{D_n(t)}\mathrm{d}\mu(t)\\ &= \frac{z^{n-1}}{D_n(z)}\left[\int p_{n,n}\mathrm{d}\mu(t)-\gamma\int\varphi_n(t)\mathrm{d}\mu(t)\right]+\frac{1}{D_n(z)}\int\frac{O(z^{n-2},t)}{D_n(t)}\mathrm{d}\mu(t).\end{aligned}$$

The first integral in the last line equals $p_{n,n}$ by the normalization of μ, and the second integral vanishes because of the orthogonality property if $n\geq 1$. Thus

$$\sigma_n(z)=\frac{p_{n,n}z^{n-1}}{D_n(z)}+\frac{O(z^{n-2})}{D_n(z)}. \tag{4.13}$$

Similarly

$$\sigma_{n-1}(z)=\frac{p_{n-1,n-1}z^{n-2}}{D_{n-1}(z)}+\frac{O(z^{n-3})}{D_{n-1}(z)}.$$

Consequently

$$\Sigma_n(z,\tau)=\left[\frac{p_{n,n}z^{n-1}}{D_n(z)}+\frac{O(z^{n-2})}{D_n(z)}\right]-\tau\left[\frac{p_{n-1,n-1}r_n(z)z^{n-2}}{D_n(z)}+\frac{O(z^{n-2})}{D_n(z)}\right].$$

Hence

$$\Sigma_n(z,\tau)=\frac{[p_{n,n}+\tau p_{n-1,n-1}]\,z^{n-1}}{D_n(z)}+\frac{O(z^{n-2})}{D_n(z)}$$

when $\zeta_n\neq-\infty$ and

$$\Sigma_n(z,\tau)=\frac{p_{n,n}z^{n-1}}{D_n(z)}+\frac{O(z^{n-2})}{D_n(z)}$$

when $\zeta_n=-\infty$. ∎

Proposition 4.4. *Between two consecutive positive zeros of $\Phi_n(z,\tau)$ there is exactly one zero of $\Sigma_n(z,\tau)$.*

PROOF. Let τ be given, and assume that there is a common zero z_0 of $\Phi_n(z,\tau)$ and $\Sigma_n(z,\tau)$. Then $\sigma_n(z_0)\varphi_{n-1}(z_0)-\sigma_{n-1}(z_0)\varphi_n(z_0)=0$, which contradicts the determinant formula (2.4). Hence $\Phi_n(z,\tau)$ and $\Sigma_n(z,\tau)$ have no common zero.

For $\tau=0$, the zeros of $\Phi_n(z,\tau)$ and $\Sigma_n(z,\tau)$ separate each other in the sense of the statement we wish to prove, according to Proposition 2.1. Since $\Phi_n(z,\tau)$ and $\Sigma_n(z,\tau)$ have no common zero, it follows by the continuity of the zeros with respect to τ that the zeros of $\Phi_n(z,\tau)$ and $\Sigma_n(z,\tau)$ separate each other as stated for arbitrary τ. ∎

5. Quadratures associated with pseudo-orthogonal rational functions

As before we consider a measure μ with infinite support in $[0,\infty)$ and rational functions with prescribed poles ζ_m in $[-\infty,0]$.

Theorem 5.1. *Let $\xi_{1,n}(\tau),\ldots,\xi_{n,n}(\tau)$ denote the zeros of $\Phi_n(z,\tau)$ and assume that the one possible zero outside $(0,\infty)$ does not coincide with any ζ_m. Then there exist constants $\lambda_{1,n}(\tau),\ldots,\lambda_{n,n}(\tau)$ such that*

$$\int F(t)\mathrm{d}\mu(t) = \sum_{k=1}^{n} \lambda_{k,n}(\tau) F\left(\xi_{k,n}(\tau)\right) \tag{5.14}$$

for all $F \in \mathscr{L}_n \cdot \mathscr{L}_{n-2}$.

PROOF. For each k there is a unique element $L_{k,n}(z,\tau)$ in $\mathscr{L}_{n-1}$ satisfying $L_{k,n}\left(\xi_{j,n}(\tau),\tau\right) = \delta_{kj}$ for $j = 1,\ldots,n$. Set $\lambda_{k,n}(\tau) = \int L_{k,n}(t,\tau)\mathrm{d}\mu(t)$.

Let $F \in \mathscr{L}_n \cdot \mathscr{L}_{n-2}$ and set $F_n(z) = \sum_{k=1}^{n} F\left(\xi_{k,n}(\tau)\right) L_{k,n}(z,\tau)$, $f_n(z) = F(z) - F_n(z)$. Then $F_n \in \mathscr{L}_{n-1}$ and $f_n \in \mathscr{L}_n \cdot \mathscr{L}_{n-2}$. Furthermore $f_n\left(\xi_{j,n}(\tau)\right) = 0$ for $j = 1,\ldots,n$. Consequently we may write $f_n(z) = \Phi_n(z,\tau)\cdot Q_{n-2}(z,\tau)$, where $Q_{n-2}(z,\tau) \in \mathscr{L}_{n-2}$. Hence $\int f_n(t)\mathrm{d}\mu(t) = \langle \Phi_n(z,\tau), Q_{n-2}(z,\tau)\rangle = 0$. Consequently

$$\int F(t)\mathrm{d}\mu(t) = \sum_{k=1}^{n} F\left(\xi_{k,n}(\tau)\right) \int L_{k,n}(t,\tau)\mathrm{d}\mu(t) = \sum_{k=1}^{n} \lambda_{k,n}(\tau) F\left(\xi_{k,n}(\tau)\right).$$

■

Remark 5.1. An argument for the positivity of the weights $\lambda_{k,n}(\tau)$ similar to that for the positivity of the weights $\kappa_{k,n}(\tau)$ given in (2, Chap. 11.6) is not possible. The reason is that the function $\left[L_{k,n}(z,\tau)\right]^2$ does in general not belong to $\mathscr{L}_n \cdot \mathscr{L}_{n-2}$, and hence the quadrature formula (5.14) can not be applied to this function. We shall however give another type of argument for the positivity of the weights corresponding to those nodes which lie in $(0,\infty)$.

Proposition 5.2. *The weights $\lambda_{k,n}(\tau)$ may be written as*

$$\lambda_{k,n}(\tau) = \frac{\Sigma_n\left(\xi_{k,n}(\tau),\tau\right)}{\Phi_n'\left(\xi_{k,n}(\tau),\tau\right)} \tag{5.15}$$

for $k = 1,2,\ldots,n$. Here $\Phi_n'\left(\xi_{k,n}(\tau),\tau\right) = \frac{\mathrm{d}}{\mathrm{d}z}\left[\Phi_n(z,\tau)\right]_{z=\xi_{k,n}(\tau)}$.

PROOF. The function $t \to \frac{\Phi_n(t,\tau)-\Phi_n(z,\tau)}{t-z}$ belongs to $\mathscr{L}_n$, hence to $\mathscr{L}_n\cdot\mathscr{L}_{n-2}$. Using the form (4.10) of the function $\Sigma_n(z,\tau)$ we find by applying Theorem 5.1 that

$$\Sigma_n(z,\tau) = \int \frac{\Phi_n(t,\tau)-\Phi_n(z,\tau)}{t-z}\mathrm{d}\mu(t) = \sum_{k=1}^{n} \lambda_{k,n}(\tau)\frac{-\Phi_n(z,\tau)}{\xi_{k,n}(\tau)-z}$$

(taking into account that $\Phi_n\left(\xi_{k,n}(\tau),\tau\right)=0$). Thus

$$\frac{\Sigma_n(z,\tau)}{\Phi_n(z,\tau)}=\sum_{j=1}^{n}\frac{\lambda_{j,n}(\tau)}{z-\xi_{j,n}(\tau)}$$

and hence

$$\frac{\left(z-\xi_{k,n}(\tau)\right)\Sigma_n(z,\tau)}{\Phi_n(z,\tau)-\Phi_n\left(\xi_{k,n}(\tau),\tau\right)}=\sum_{j=1}^{n}\lambda_{j,n}(\tau)\frac{z-\xi_{k,n}(\tau)}{z-\xi_{j,n}(\tau)}.$$

Letting z tend to $\xi_{k,n}(\tau)$ in this equation we obtain

$$\lambda_{k,n}(\tau)=\frac{\Sigma_n(\xi_{k,n}(\tau),\tau)}{\frac{\mathrm{d}}{\mathrm{d}z}[\Phi_n(z,\tau)]_{z=\xi_{k,n}(\tau)}}.$$

■

Theorem 5.3. *The weights $\lambda_{k,n}(\tau)$ corresponding to positive nodes $\xi_{k,n}(\tau)$ are positive.*

PROOF. Let the zeros of $\Phi_n(z,\tau)$ be ordered such that $\xi_{1,n}(\tau)<\xi_{2,n}(\tau)<\cdots<\xi_{n,n}(\tau)$. Then at most $\xi_{1,n}(\tau)$ can be negative. The function $\Sigma_n(z,\tau)$ has $n-1$ zeros. According to Proposition 4.4 there is exactly one such zero in the interval $(\xi_{j,n}(\tau),\xi_{j+1,n}(\tau))$ which is contained in $(0,\infty)$.

We may write

$$\Phi_n(z,\tau)=\frac{[p_{n,n}+\tau p_{n-1,n-1}]\,M_n(z)}{D_n(z)},\ \ M_n(z)=\prod_{k=1}^{n}\Big(z-\xi_{k,n}(\tau)\Big),$$

(cf. Remark 4.1) and

$$\Sigma_n(z,\tau)=\frac{[p_{n,n}+\tau p_{n-1,n-1}]\,N_{n-1}(z)}{D_n(z)},\ \ N_{n-1}(z)=\prod_{k=1}^{n}\Big(z-\eta_{k,n-1}(\tau)\Big),$$

where $\eta_{k,n-1}(\tau)$ are the zeros of $\Sigma_n(z,\tau)$ (cf. Proposition 4.3). Set $s=\operatorname{sign}D_n(x)\cdot\operatorname{sign}\,[p_{n,n}+\tau p_{n-1,n-1}]$ for $x>\xi_{n,n}(\tau)$. We observe that $\operatorname{sign}\Phi_n(x,\tau)=s$ for $x>\xi_{n,n}(\tau)$. Similarly we find that $\operatorname{sign}\Sigma_n(x,\tau)=s$ for $x\geq\xi_{n,n}(\tau)$ since the largest zero of $\Sigma_n(z,\tau)$ lies in $(\xi_{n-1,n}(\tau),\xi_{n,n}(\tau))$.

Because $s\cdot\Phi_n(z,\tau)$ is increasing for $x\geq\xi_{n,n}$ and zeros are simple, it follows that $\operatorname{sign}\Phi_n'\left(\xi_{n,n}(\tau),\tau\right)=s$. Taking into account Proposition 5.2, we conclude that $\lambda_{n,n}(\tau)$ is positive.

From the separation property of Proposition 4.4 we find that $\operatorname{sign}\Phi_n'\left(\xi_{n-1,n}(\tau),\tau\right)=-s$ and $\operatorname{sign}\Sigma_n\left(\xi_{n-1,n}(\tau),\tau\right)=-s$. Thus again it follows from Proposition 5.2 that $\lambda_{n-1,n}(\tau)$ is positive.

Repeatedly using this argument, we conclude that $\lambda_{k,n}(\tau)$ is positive as long as $\xi_{k,n}(\tau)$ is positive.

■

6. Computational aspects

Given a positive measure μ on $[0,\infty)$ with $\int \mathrm{d}\mu(t) = 1$, and a sequence of numbers $\{\zeta_k\}$ in $[-\infty, 0]$, it is known that the sequence of orthogonal rational functions $\{\varphi_k\}$ with $\varphi_n \in \mathscr{L}_n \setminus \mathscr{L}_{n-1}$ satisfy a recurrence relation which we formulate in the next theorem that was proved in (4, Theorems 3.1 and 4.1).

Theorem 6.1. *The orthogonal rational functions φ_n satisfy the following recursion*

$$\varphi_n(z) = \frac{U_n z^{\gamma_{n-1}} + V_n r_{n-1}(z)}{r_n(z)} \varphi_{n-1}(z) + \frac{W_n r_{n-2}(z)}{r_n(z)} \varphi_{n-2}(z), \quad n = 1, 2, \ldots \tag{6.16}$$

with initial conditions $\varphi_{-1} = 0$ and $\varphi_0 = 1$ and where $r_{-1} = 1$ and the $r_n(z)$, $n \geq 0$ are as before, the U_n, V_n, W_n are constants while γ_n is defined as

$$\gamma_n = 0 \ \text{ if } \zeta_n \neq -\infty \text{ and } 1 \text{ otherwise, } n \geq 0, \ (\zeta_0 = -\infty).$$

With a proper sign normalization as in (4), it can be arranged that $U_n > 0$ and $W_n = -U_n/U_{n-1} < 0$.

In the same paper it is also explained how to compute the nodes and the weights of the rational Gauss quadrature formula associated with these functions which was formulated in Theorem 2.2. For a proof see (4, Section 7).

Theorem 6.2. *Define $c_k = -V_k/U_k$ and $d_k = 1/U_k$, where U_j, V_j are as in the previous theorem. Furthermore set*

$$J_n = \operatorname{tridiag} \begin{pmatrix} d_1, d_2, \ldots, d_{n-1} \\ c_1, c_2, c_3, \ldots, c_{n-1}, c_n \\ d_1, d_2, \ldots, d_{n-1} \end{pmatrix}, \qquad \begin{aligned} I_n^{\gamma} &= \operatorname{diag}(\gamma_0, \gamma_1, \ldots, \gamma_{n-1}), \\ Z_n &= \operatorname{diag}(\rho_0, \rho_1, \ldots, \rho_{n-1}), \end{aligned}$$

where γ_k as in the previous theorem and

$$\rho_k = \zeta_k \ \text{ if } \zeta_k \neq -\infty \text{ and } 1 \text{ otherwise.}$$

Finally define $I_n^{1-\gamma} = I_n - I_n^{\gamma}$ with I_n the unit matrix of size n, and $A_n = J_n Z_n - I_n^{1-\gamma}$ and $B_n = J_n I_n^{1-\gamma} + I_n^{\gamma}$. Then the n eigenvalues $\{x_{k,n}\}_{k=1}^n$ for the pencil (A_n, B_n) are the nodes of the n-point rational Gaussian quadrature formula and if $E_k = [e_{1,k}, \ldots, e_{n,k}]^T$ is the (right) eigenvector corresponding to $x_{k,n}$, normalized by $E_k^T E_k = 1$, then the corresponding weight in the quadrature formula is given by $c_{k,n} = e_{1,k}^2$.

Remark 6.1. Note that I_n^{γ} has a 1 for each infinite ζ_k while $I_n^{1-\gamma}$ does the opposite. Hence, if all $\zeta_k = -\infty$, then $B_n = I_n$ which gives the classical eigenvalue problem of the polynomial case. The case of all finite poles, i.e., $I_n^{\gamma} = 0$ whence $(A_n, B_n) = (J_n Z_n - I_n, J_n)$ was discussed in (3). It is a rational generalization of the classical numerical method to compute polynomial Gauss-Christoffel quadrature formulas via an eigenvalue decomposition if the Jacobi matrix is known. A recent survey for the polynomial case can be found in e.g., (7). See also (8) for related software.

Quasi-orthogonal rational functions

For the nodes and weights of the quadrature formulas associated with the quasi-orthogonal and pseudo-orthogonal rational functions, one has to modify trailing coefficients in the recurrence as we shall explain now.

Since the quasi-orthogonal rational functions are given by $\varphi_n(x,\tau) = \varphi_n(z) - \tau\frac{r_{n-1}(z)}{r_n(z)}\varphi_{n-1}(z)$, it follows from the recurrence relation (6.16) that for $n \geq 1$ we can generate $\varphi_1, \ldots, \varphi_{n-1}$ as before and in the final step set

$$\varphi_n(z,\tau) = \frac{U_n z^{\gamma_{n-1}} + V_n' r_{n-1}(z)}{r_n(z)}\varphi_{n-1}(z) + \frac{W_n r_{n-2}(z)}{r_n(z)}\varphi_{n-2}(z),$$

where $V_n' = V_n - \tau$ if τ is finite. Thus the computational procedure can be used as before, only V_n has to be modified.

If τ is infinite, then $\varphi_n(x,\tau) = \frac{r_{n-1}(z)}{r_n(z)}\varphi_{n-1}(z)$. Here the zeros of $\varphi_n(x,\tau)$ are the zeros of φ_{n-1} and ζ_{n-1} (which could be infinite). Thus the computational procedure can stop with a problem of size $n-1$ instead of size n.

Pseudo-orthogonal rational functions

In the case of pseudo-orthogonal rational functions, the modification of the parameters in the recurrence is more complicated. We start again from the definition and see that

$$\Phi_n(z,\tau) = \frac{U_n z^{\gamma_{n-1}} + V_n r_{n-1}(z) - \tau r_n(z)}{r_n(z)}\varphi_{n-1}(z) + \frac{W_n r_{n-2}(z)}{r_n(z)}\varphi_{n-2}(z).$$

But now there are different possibilities depending on ζ_{n-1}, ζ_n and τ being finite or not.

If $\tau = \infty$, then $\Phi_n(z,\tau) = \varphi_{n-1}(z)$ and we can use the recursion for the orthogonal rational functions and stop at $n-1$ instead of n. So, let us assume that $\tau \neq \infty$. Then, if $\zeta_{n-1} = -\infty$, hence $\gamma_{n-1} = 1$ and $r_{n-1} = 1$ so that we may set $U_n z + V_n - \tau r_n(z) = U_n' z + V_n'$ with $U_n' = U_n$ and $V_n' = V_n - \tau$ if $\zeta_n = -\infty$ (i.e., $r_n = 1$) and $U_n' = U_n + \tau$ and $V_n' = V_n - \tau\zeta_n$ if ζ_n is finite.

If on the other hand ζ_{n-1} is finite and hence $\gamma_{n-1} = 0$, then $U_n + V_n(\zeta_{n-1} - z) - \tau r_n(z) = U_n' + V_n'(\zeta_{n-1} - z)$ with $U_n' = U_n - \tau$ and $V_n' = V_n$ if $\zeta_n = \infty$ (i.e., $r_n = 1$) and $U_n' = U_n + \tau(\zeta_{n-1} - \zeta_n)$ and $V_n' = V_n - \tau$ if ζ_n is finite. We can summarize this in the following table:

	$\zeta_{n-1} = -\infty$	$\zeta_{n-1} \neq -\infty$
$\zeta_n = -\infty$	$U_n' = U_n$ $V_n' = V_n - \tau$	$U_n' = U_n - \tau$ $V_n' = V_n$
$\zeta_n \neq -\infty$	$U_n' = U_n + \tau$ $V_n' = V_n - \tau\zeta_n$	$U_n' = U_n + \tau(\zeta_{n-1} - \zeta_n)$ $V_n' = V_n - \tau$

There is however an extra caveat. We have modified the U_n and V_n but the $W_n = -U_n/U_{n-1}$ is still unaltered, using the old value of U_n. The result is that c_n in the matrix J_n is replaced by $c_n' = -V_n'/U_n'$, and the element $d_{n-1} = 1/U_{n-1}$ in the upper diagonal is left unaltered. However on the lower diagonal $d_{n-1} = 1/U_{n-1}$ was the result of $-W_n/U_n$ where $W_n = -U_n/U_{n-1}$, whereas

now this element is $d'_{n-1} = \frac{U_n}{U_{n-1}U'_n} = d_{n-1}\frac{U_n}{U'_n}$ and the matrix J is not symmetric anymore unless $\zeta_{n-1} = \zeta_n = -\infty$. This however is not an extra complication since the pencil that matters (A_n, B_n) wasn't symmetric anyway.

These modifications of the matrix pencil will guarantee that the correct nodes are obtained. Computing the corresponding weights can however not be done as in the quasi-orthogonal case. This can be seen as follows. Let $x_k = x_{k,n}(\tau)$ be the nodes of the quadrature formula and $w_k = \lambda_{k,n}(\tau)$ the corresponding weights. Define the $n \times n$ matrix F with entries $F_{k,j} = \varphi_{j-1}(x_k)$ for $k, j = 1, \ldots, n$, and let W be the diagonal matrix of the weights $W = \mathrm{diag}\,(w_1, \ldots, w_n)$. Clearly the (i, j) entry of the product $F^T W F$ is given by

$$\sum_{k=1}^{n} w_k \varphi_i(x_k)\varphi_j(x_k) \approx \int_0^\infty \varphi_i(x)\varphi_j(x)d\mu(x) = \delta_{ij}, \;\; 0 \le i, j \le n-1$$

where equality will hold, so that $F^T W F = I$, the identity matrix, as long as the quadrature formula is exact in $\mathscr{L}_{n-1} \cdot \mathscr{L}_{n-1}$. This is true in the quasi-orthogonal case. Inverting the relation $F^T W F = I$ gives $F F^T = W^{-1}$, which leads to the well known formula $w_k^{-1} = \sum_{i=0}^{n-1} \varphi_i^2(x_k)$.

In the pseudo-orthogonal case, the quadrature formula is only exact in $\mathscr{L}_n \cdot \mathscr{L}_{n-2}$. Consequently we have $F^T W F = G$ where G is the identity matrix, except for its (n, n) element, which is an unknown element $\omega_n = \sum_{j=1}^{n} w_j \varphi_{n-1}^2(x_j)$. Hence the weights are given by $W^{-1} = F G^{-1} F^T$. I.e., $w_k^{-1} = \sum_{i=0}^{n-2} \varphi_i^2(x_k) + \omega_n^{-1}\varphi_{n-1}^2(x_k)$. Note that the the columns of the matrix F^T are the eigenvectors of the pencil (A_n, B_n), which we have already computed. A possibility to use the availability of these eigenvectors is to solve for the positive root ω_n of the equation $\sum_{k=1}^{n} w_k(\omega_n) = 1$. This is in general a very smooth curve that is almost linear in the interesting region. Hence just a couple of iterations is sufficient. Once ω_n is known, also the w_k can be evaluated.

7. Numerical examples

Example 7.1. Let us take a classical example of the Laguerre polynomials $\varphi_n = L_n$. These are orthogonal with respect to the weight $w(x) = \exp(-x)$ on $[0, \infty)$. These are orthogonal rational functions with all their poles at infinity, and hence all γ_k and $r_k(x)$ are 1. The latter fact implies that here the pseudo- and the quasi-orthogonal rational functions coincide, as they will always do in the polynomial case. They satisfy the recurrence relation

$$L_{-1} = 0, \;\; L_0 = 1, \;\; L_n(x) = (U_n x + V_n)L_{n-1}(x) + W_n L_{n-2}(x), \;\; n = 1, 2, \ldots$$

and if we use the sign normalization that we adopted in this paper, then

$$U_n = \frac{1}{n}, \;\; V_n = \frac{1-2n}{n}, \;\; W_n = \frac{1-n}{n}.$$

The Figure 1 now is like in Figure 2, where we took $n = 6$. As can be seen on this graph, any value of τ above $p_{0,6}/p_{0,5}$ will give positive nodes for the [pseudo/quasi]-orthogonal polynomials. This is true for any n because the constant terms are always $p_{0,k} = (-1)^k$.

The nodes and the weights of a quadrature formula are obtained by solving an ordinary eigenvalue problem for the tridiagonal matrix J_n as given in Theorem 6.2 with $d_k = 1/U_k = k$ and

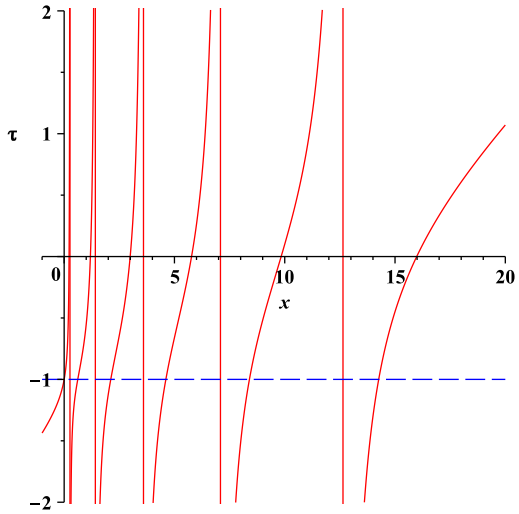

Figure 2: Plot of $\tau(x_*) = \frac{P_n(x_*)}{P_{n-1}(x_*)}$. The situation is for $n = 6$. The horizontal dashed line is at $p_{0,6}/p_{0,5} = -1$.

$c_k = -V_k/U_k = 2k-1$, except for the last one c_n which is $-V_n'/U_n = (V_n - \tau)/U_n = n(2+\tau) - 1$. It is well known that the formula will be exact in the space of polynomials of degree at most $2n-2$, unless $\tau = 0$ or $\tau = \infty$, in which case it becomes a Gauss-Laguerre formula which will be exact for all polynomials of degree up to $2n-1$ if $\tau = 0$ or of degree up to $2n-3$ if $\tau = \infty$. You can imagine the nodes of the quadrature formula by drawing a horizontal line for some value of τ in Figure 2. The corresponding nodes are then the abscissas of the intersections with the curvy parts of the graph. As can be seen, the nodes all move slightly to the right with increasing values of τ, while the rightmost one escapes to ∞, the leftmost one is caught in a narrow interval $[0, x_{0,n-1}]$ where $x_{0,n-1}$ is the leftmost zero of L_{n-1}, determining the first vertical asymptote, which in this case is at $x_{0,5} \approx 0.264$. Note that only one of the nodes can go to ∞, since all the others are captured in between the zeros of L_{n-1} which define the location of the vertical asymptotes. So none of them can go beyond the rightmost asymptote, which is in this case $x_{5,5} \approx 12.64$.

For the generalized Laguerre polynomials $L_n^{(\alpha)}$, the situation is quite similar. With increasing α, the dashed line on Figure 1 shifts down and the vertical asymptotes all move to the right widening the distance between them.

Example 7.2. As a second example, we take the weight $w(x) = x^{10}\exp(-x)$ on $[0,\infty)$ but now we choose the poles $\zeta_k = -k$, $k = 1, 2, \ldots$. Because all the poles are finite we have $\gamma_k = 0$ and $r_k(x) = -(x+k)$ for $k = 1, 2, \ldots$. In Figure 3 we have again plotted $\tau(x_*) = \frac{P_n(x_*)}{r_n(x_*)P_{n-1}(x_*)}$ (that is for the pseudo-orthogonal rational functions, otherwise, for the quasi-orthogonal case, r_n should be replaced by r_{n-1}). The lower dashed line is at $p_{0,6}/(\zeta_6 p_{0,5}) \approx -2.411$ and the upper dashed line is at $-p_{6,6}/p_{5,5} \approx 2.618$. For any value in between these two, the zeros, i.e., the nodes of the corresponding quadrature formula will be positive. As τ approaches the upper limit, one node escapes via $+\infty$ and re-enters the scene at $-\infty$. On the other hand, when τ decreases below its

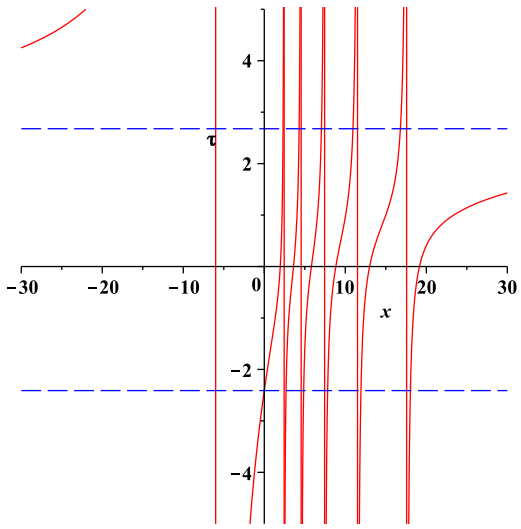

Figure 3: Plot of $\tau(x_*) = \frac{P_n(x_*)}{r_n(x_*)P_{n-1}(x_*)}$. The situation is for $n = 6$. The lower horizontal dashed line is at $p_{0,6}/(\zeta_6 p_{0,5}) \approx -2.411$. The upper horizontal dashed line is at $-p_{6,6}/p_{5,5} \approx 2.618$. For values of τ in between these two, the zeros of the pseudo-orthogonal rational functions will all be positive. Outside of these, one node of the quadrature formula will be negative.

lower boundary, there will be one negative node, but it is confined to the interval $[\zeta_n, 0]$ which is in this example $[-6, 0]$. The recurrence coefficients are

k	1	2	3	4	5	6
U_k	3.399036238	24.37108298	22.73199847	24.34601961	27.56340367	31.64057192
V_k	−34.32314924	2.712439604	2.912097258	2.988112327	3.058306563	3.116475765

For $\tau = 0$ we get the rational Gauss-Laguerre quadrature formula. For example for $n = 6$, rounded values for nodes x_k and weights w_k are given in the next table.

k	1	2	3	4	5	6
x_k	$1.9155e+1$	$1.3001e+1$	$8.8324e+0$	$5.8171e+0$	$3.6035e+0$	$1.9696e+0$
w_k	$6.8670e-2$	$4.2423e-1$	$4.0824e-1$	$9.3581e-2$	$5.2373e-3$	$4.7749e-5$

Any element from $\mathscr{L}_n \cdot \mathscr{L}_{n-1}$ which is of the form $P_{2n-1}/(D_n D_{n-1})$ with P_{2n-1} a random polynomial of degree at most $2n-1$ integrates up to machine precision[2] by this quadrature formula, where in this case $n = 6$.

For positive τ, the nodes shift to the right. For negative τ they shift to the left. For example,

[2] All computations were done using the numerics from Maple 14, which guarantees about 10 decimal digits. The relative error of the computed integral is approximately 10^{-10}.

when $\tau = 0.5$, the nodes and weights become for the pseudo-orthogonal case

k	1	2	3	4	5	6
x_k	$2.0376e+1$	$1.3869e+1$	$9.4440e+0$	$6.2287e+0$	$3.8587e+0$	$2.1055e+0$
w_k	$4.0857e-2$	$3.6087e-1$	$4.5826e-1$	$1.3121e-1$	$8.7065e-3$	$8.9134e-5$

This quadrature formula is exact (up to machine precision) for any randomly generated element in $\mathscr{L}_n \cdot \mathscr{L}_{n-2}$. If we want to force a node at the origin, we should take $\tau = p_{0,6}/(\zeta_6 p_{0,5}) \approx -2.885$. The computed nodes and weights are

k	1	2	3	4	5	6
x_k	$1.8039e+1$	$1.1935e+1$	$7.8215e+0$	$4.8633e+0$	$2.6873e+0$	$-1.4413e-9$
w_k	$1.1432e-1$	$5.1805e-1$	$3.2727e-1$	$3.9669e-2$	$6.9465e-4$	$1.9053e-9$

The smallest node is numerically zero, but it also gets an almost zero weight.

For τ going to $\pm\infty$, the nodes approach the zeros of φ_{n-1} and ζ_n. The first $n-1$ nodes have positive weights. In this example, the negative node has a very small quadrature weight. It can not be neglected though because the function values for the negative node can be very large because it can be very close to a pole of the function.

Example 7.3. One final example. For the weight we choose $w(x) = x^{10}\exp(-x^2)$. We select for the poles ζ_k, $k \geq 1$ from the sequence $-\infty, -1, -\infty, -3, -\infty, -5, -\infty, -7, -\infty, \ldots$. For $n = 6$ and considering the pseudo-orthogonal case, the plot of $\tau(x)$ is given in the left graph of Figure 4. If we choose the poles in the sequence $-1, -\infty, -3, -\infty, -5, -\infty, -7, -\infty, \ldots$, then we get the right graph. Note that, because now $-\infty$ is involved, the sign has changed and we get an upside-down image of the previous examples. The discussion is however essentially the same, and for a random element from $\mathscr{L}_n \cdot \mathscr{L}_{n-2}$, the quadrature formula computes the integrals up to machine precision.

8. Conclusion

For integrals over the positive real axis and spaces of rational functions with poles in $[-\infty, 0]$, one may construct orthogonal rational functions $\{\varphi_k\}_{k\geq 0}$. The zeros of φ_n can be used as the nodes of a quadrature formula exact in the space $\mathscr{L}_n \cdot \mathscr{L}_{n-1}$. All these nodes are in $(0, \infty)$ and get positive weights. The quasi-orthogonal rational functions $\varphi_n(x, \tau)$ have zeros that can be used as the nodes of quadrature formulas to integrate exactly any function in $\mathscr{L}_{n-1} \cdot \mathscr{L}_{n-1}$. All these nodes are positive with positive weights for τ in a finite or half-infinite interval. Outside that interval, one of the nodes will be negative. However, if the negative node does not coincide with one of the prescribed poles of the orthogonal rational functions, then all the weights are positive. The situation for pseudo-orthogonal rational functions $\Phi_n(x, \tau)$ is very similar. They have zeros that can be used as the nodes of quadrature formulas to integrate exactly any function in $\mathscr{L}_n \cdot \mathscr{L}_{n-2}$. All these nodes are positive with positive weights for τ in a finite or half-infinite interval. Outside that interval, one of the nodes will be negative. Assuming that it does not coincide with one of the poles of the orthogonal rational functions, then the weights associated with positive nodes will be positive.

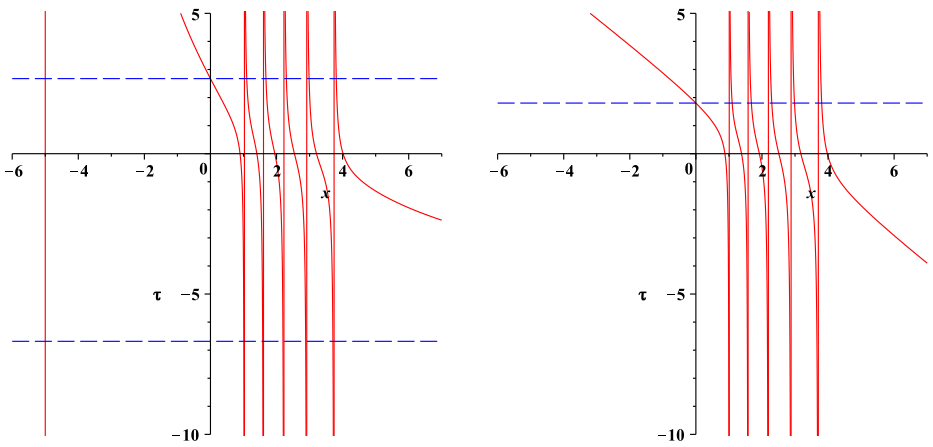

Figure 4: Plot of $\tau(x_*) = \frac{\varphi_n(x_*)}{\varphi_{n-1}(x_*)}$. The situation is for $n = 6$. On the left the poles are $-\infty, -1, -\infty, -3, -\infty$. The nodes (and weights) of the quadrature formula are guaranteed to be positive for $\tau \in (-6.684..., 2.675...)$. On the right the poles are $-1, -\infty, -3, -\infty, -5$ and the nodes (and weights) of the quadrature formula are guaranteed to be positive for $\tau < 1.8036...$.

In both cases, the parameter τ can be used to place a node at some preassigned place and hence produce a Radau-type formula.

The numerical procedure to compute the nodes and the weights can be performed in a way that is comparable but somewhat more complicated than in the polynomial case. One has to solve a generalized eigenvalue problem for a pencil with tridiagonal matrices. If all the poles are at infinity, this generalized problem reduces to the classical ordinary eigenvalue problem for the Jacobi-matrix. For the computation of the weights in the pseudo-orthogonal case, the fact that the quadrature formula is not exact in $\mathscr{L}_{n-1} \cdot \mathscr{L}_{n-1}$ causes extra problems. Therefore because of the similarity of approximation power of the quadratures for the pseudo- and the quasi-orthogonal case, it is numerically advantageous to use the quasi-orthogonal rational functions instead of the pseudo-orthogonal ones.

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