On the construction of a rational Fejér rule

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Report TW 438, October 2005

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Keywords : Quadrature, Orthogonal Rational Functions
CR Subject Classification : Primary : G.1.4 (Numerical Analysis; Quadrature and Numerical Differentiation)

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Abstract

We present a method to construct a rational generalization of Fejér's quadrature rule. Compared to similar existing rules, our rule has the advantage that the nodes are the zeros of a Chebyshev orthogonal rational function, which leads to smaller weights and a more stable quadrature rule.

1 Introduction

To compute the integral of a function with respect to the Lebesgue measure on the interval $[-1, 1]$, Fejér's first rule [DR84, p. 84-85] is often an excellent choice. The computational effort is minimal — both nodes and weights are known explicitly — and, using n nodes, it integrates polynomials of degree $n-1$ exactly. Another obvious choice, Gauss-Legendre quadrature, has of course a larger domain of validity — with the same number of nodes, it integrates polynomials of degree $2n-1$ — but at the expense of more computations.

Several generalizations have been made to construct quadrature formulas integrating rational functions with respect to the Lebesgue measure, see. e.g. [Gau99, VAV93, WL00]. In this paper we present a new quadrature rule, a rational variant of Fejér's rule, which requires less computational effort than the formulas from [Gau99] and in some cases of interest is more stable and gives more accurate results than the rule presented in [WL00].

In [VDBGV05] we constructed rational generalizations of the well-known classical Gauss-Chebyshev quadrature formula. These rational quadrature rules integrate functions with arbitrary real poles outside the interval $[-1, 1]$, with respect to the different Chebyshev weight functions $(1-x)^{\alpha}(1+x)^{\beta}$, with α and β belonging to $\{\pm 1/2\}$. They can be constructed in order $O(mn)$ operations, where m is the number of *distinct* poles, for arbitrarily high degree n. The main reason for the efficient computation of these rules is that we have explicit representations for the so-called Chebyshev orthogonal rational functions. These were also introduced in the same article.

Unlike the formulas from [VDBGV05], the quadrature rule constructed in the present paper is not a Gaussian rule, but instead a true rational generalization of Fejér's rule. Fejér's (polynomial) rule is an interpolatory quadrature formula which has nodes at the zeros of the Chebyshev polynomial $T_n(x)$ and which integrates exactly polynomials of degree $n-1$ with respect to the

Lebesgue measure on $[-1, 1]$. The reason for studying an interpolatory rule instead of a Gaussian rule, is that we do not have explicit representations for the Legendre orthogonal rational functions, which makes the computational cost of the Gaussian rule much higher than for the interpolatory rule we present here.

The outline of this paper is as follows. In the next section we present some necessary theoretical preliminaries about orthogonal rational functions and interpolatory quadrature formulas. The main results are presented in section 3, but since the computations are rather technical, all the proofs have been moved to the end of the paper, in section 7. The numerical issues of constructing this quadrature formula are discussed in section 4. In section 5, finally, we give several numerical examples and compare our formulas to some of the abovementioned alternatives.

2 Preliminaries

The complex plane is denoted by $\mathbb{C}$, the Riemann sphere by $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$, the real line by $\mathbb{R}$ and the extended real line by $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$. For the unit circle and its interior we introduce the following notation:

$$\mathbb{T} = \{z : |z| = 1\}, \quad \mathbb{D} = \{z : |z| < 1\}.$$

We will also use $I = [-1, 1]$, $\overline{\mathbb{R}}^I = \overline{\mathbb{R}} \setminus I$ and $\overline{\mathbb{C}}^I = \overline{\mathbb{C}} \setminus I$.

We denote the Joukowski transform $x = \frac{1}{2}(z + z^{-1})$ by $x = J(z)$, mapping the open unit disc $\mathbb{D}$ to the cut Riemann sphere $\overline{\mathbb{C}}^I$ and the unit circle $\mathbb{T}$ to the interval I. The inverse mapping is denoted by $z = J^{-1}(x)$ and is chosen so that $z \in \mathbb{D}$ if $x \in \overline{\mathbb{C}}^I$.

Let there be given a sequence of poles $A = \{\alpha_1, \alpha_2, \ldots\} \in \overline{\mathbb{R}}^I$. The rational function spaces we are dealing with, are defined as follows. For each pole α_k, put

$$Z_k(x) = \frac{x}{1 - x/\alpha_k}, \quad k = 1, 2, \ldots$$

and define the basis functions

$$b_0 \equiv 1, \quad b_k(x) = b_{k-1}(x) Z_k(x), \quad k = 1, 2, \ldots$$

Then a linear vector space of rational functions with poles in $\{\alpha_1, \ldots, \alpha_n\}$ is given by

$$\mathcal{L}_n = \text{span}\{b_0, \ldots, b_n\}.$$

Note that, if all poles are at infinity, then $\mathcal{L}_n = \mathcal{P}_n$, the space of polynomials of degree n. We will also use the notation

$$\pi_n(x) = \prod_{k=1}^{n} \left(1 - \frac{x}{\alpha_k}\right)$$

for the denominator of a function in $\mathcal{L}_n$.

In what follows, the word *measure* will always mean a positive bounded Borel measure μ on I whose support $\mathrm{supp}(\mu) \subset I$ is an infinite set. Given such a measure, the L^2 inner product is defined as

$$\langle f\,, g\rangle = \int_{-1}^{1} f(x)\overline{g(x)}d\mu(x).$$

Orthonormalizing the basis $\{b_0, \ldots, b_n\}$ with respect to this inner product yields the orthonormal rational functions (ORF) $\{\varphi_0, \varphi_1, \ldots, \varphi_n\}$. These functions are unique up to a unimodular constant, which is not relevant for our discussion.

The reproducing kernel $k_n(x, y)$ for the space $\mathcal{L}_n$ is given by

$$k_n(x, y) = \sum_{k=0}^{n} \varphi_k(x)\overline{\varphi_k(y)}.$$

For real y the complex conjugate bar can be omitted, since the orthonormal rational functions have real coefficients with respect to the basis b_k, according to lemma 11.1.1 in [BGVHN99]. This function appears in the expression for the Gaussian quadrature weights, given in the next theorem.

Theorem 2.1. *Let $\{x_{nk}\}_{k=1}^{n}$ be the zeros of the n-th orthogonal rational function φ_n and let $\{\lambda_{nk}\}_{k=1}^{n}$ be defined by*

$$\lambda_{nk} = k_{n-1}(x_{nk}, x_{nk})^{-1}.$$

Then the quadrature formula for

$$I_\mu(f) = \int_{-1}^{1} f(x)d\mu(x)$$

given by

$$I_n(f) = \sum_{k=1}^{n} \lambda_{nk} f(x_{nk})$$

is exact in the space $\mathcal{L}_n \cdot \mathcal{L}_{n-1} = \{gh : g \in \mathcal{L}_n, h \in \mathcal{L}_{n-1}\}$, i.e. $I_n(f) = I_\mu(f)$ for any f in $\mathcal{L}_n \cdot \mathcal{L}_{n-1}$. The space $\mathcal{L}_n \cdot \mathcal{L}_{n-1}$ is called the domain of validity *of this quadrature formula.*

This reduces to the classical Gauss quadrature formula in the case where all poles are at infinity.

In addition to Gaussian quadrature formulas, more general interpolatory quadrature rules are also studied. The most famous example is Fejér's rule, which, using as nodes the n zeros of the Chebyhev polynomial $T_n(x)$, integrates polynomials of degree $n-1$ exactly with respect to the Lebesgue measure on I. Explicit expressions for both nodes and weights are available. The main purpose of this paper is to generalize Fejér's rule to the case of rational functions with arbitrary real poles outside I. The key to most results is a general theorem about interpolatory quadrature formulas which was proved in [VDB04]. Before we proceed to give this theorem, let us introduce some more notation and definitions. Assume we are given a measure $\tilde{\mu}$, different from μ, and we wish to construct a quadrature formula for this measure with nodes $\{x_{nk}\}_{k=1}^n$ such that it has maximal domain of validity. It can be shown [VDB04] that there exist weights $\{A_{nk}\}_{k=1}^n$ such that the formula

$$\sum_{k=1}^{n} A_{nk} f(x_{nk}) \approx \int_{-1}^{1} f(x) d\tilde{\mu}(x)$$

is exact for $f \in \mathcal{L}_{n-1}$. We introduce the function $\mathrm{k}_n(x)$ defined as

$$\mathrm{k}_n(x) = \int k_n(x,t) d\tilde{\mu}(t).$$

Note that this is a function in $\mathcal{L}_n$. The following theorem can be found in [VDB04] and we give it without proof.

Theorem 2.2. *With the definitions of this section we have*

$$A_{nk} = \mathrm{k}_{n-1}(x_{nk})\lambda_{nk}$$

for $k = 1, \ldots, n$.

The relation between modified moments and interpolatory quadrature follows from the observation that

$$\mathrm{k}_n(x) = \sum_{k=0}^{n} \nu_k \varphi_k(x)$$

where

$$\nu_k = \int \varphi_k(x) d\tilde{\mu}(x)$$

are rational modified moments. In the rest of this paper let

$$d\mu(x) = \frac{dx}{\pi\sqrt{1-x^2}}, \quad d\tilde{\mu}(x) = dx$$

and let $\varphi_n(x)$ denote the Chebyshev rational functions orthogonal with respect to μ, as introduced in [VDBGV05]. From this article we get the following theorem.

Theorem 2.3. *The Chebyshev orthogonal rational functions* φ_n *are given by*

$$\varphi_n(x) = \sqrt{\frac{1-\beta_n^2}{2}} \left(\frac{zB_{n-1}(z)}{1-\beta_n z} + \frac{1}{(z-\beta_n)B_{n-1}(z)} \right), \quad n = 1, 2, \ldots$$

where $x = J(z) \in \overline{\mathbb{C}}$ *and* $\alpha_k = J(\beta_k)$*, with* J *the Joukowski transform defined at the beginning of this section. The function* $B_n(z)$ *is a finite Blaschke product,*

$$B_0 \equiv 1, \quad B_n(z) = \frac{z-\beta_1}{1-\beta_1 z} \cdot \frac{z-\beta_2}{1-\beta_2 z} \cdot \cdots \cdot \frac{z-\beta_n}{1-\beta_n z}, \quad n = 1, 2, \ldots$$

It was shown that the Gaussian nodes and weights $\{x_{nk}\}$ and $\{\lambda_{nk}\}$ can be computed very efficiently for arbitrary poles A. The problem of computing the rational Fejér rule thus reduces to the computation of the modified moments ν_k.

The following section describes two different approaches to compute the ν_k. Which approach is preferable, depends on the location of the poles, as illustrated in sections 4 and 5.

3 Computing the modified moments

As we mentioned in the introduction, this section only contains the results. All proofs can be found in section 7. Both methods are based on decomposing φ_k into functions which can be integrated 'exactly'.

3.1 Chebyshev polynomials

This method is based on an explicit representation of the numerator of φ_k in terms of Chebyshev polynomials, as given in the following theorem.

Theorem 3.1. *The Chebyshev rational function $\varphi_k(x)$ can be written as*

$$\varphi_k(x) = \sqrt{2} \cdot \frac{\sqrt{1-\beta_k^2}}{\prod_{i=1}^{k}(1+\beta_i^2)} \cdot \frac{\sum_{i=0}^{\prime k} \left[c_i^{(k)} + c_{-i}^{(k)}\right] T_i(x)}{\pi_k(x)}$$

where $\sum_i' a_i = a_0/2 + a_1 + a_2 + \ldots$ and the coefficients $c_i^{(k)}$ can be computed recursively from

$$c_i^{(k+1)} = c_{i-1}^{(k)} - (\beta_k + \beta_{k+1})c_i^{(k)} + \beta_k\beta_{k+1}c_{i+1}^{(k)} \tag{3.1}$$

with the initial conditions $c_0^{(1)} = -\beta_1$ and $c_1^{(1)} = 1$, and the convention that $c_i^{(k)} = 0$ for $i \le -k$ or $i > k$ (from which it also follows that $c_k^{(k)} = 1$ for all k). The function $T_i(x)$ is a Chebyshev polynomial of degree i.

Furthermore, if all poles are equal to $\alpha = J(\beta)$, then explicit expressions for the coefficients $c_i^{(k)}$ are given by

$$c_i^{(k)} = (-\beta)^{k-i}\binom{2k-1}{k-i}. \tag{3.2}$$

Using this theorem, the computation of the modified moments ν_k comes down to computing the 'moments' $\int_{-1}^{1} T_i(x)/\pi_k(x)dx$. This can be done recursively, as described in [WL00] for the case where all poles are different from each other. If there are repeated poles, some (technical) modifications are needed, but we do not go into details.

3.2 Interval Blaschke products

Now we decompose $\varphi_k(x)$ as follows,

$$\varphi_k(x) = \sum_{i=0}^{k} a_i^{(k)} f_i(x) \tag{3.3}$$

where $f_0 \equiv 1$ and

$$f_i(x) = \left(\frac{1-\alpha_i x}{x-\alpha_i}\right)^j, \quad i = 1, 2, \ldots, \quad j = 1, 2, \ldots, \#\alpha_i$$

and $\#\alpha_i$ denotes the multiplicity of the pole α_i. Note that these functions are in fact real Blaschke products on the interval $[-1, 1]$, i.e. $|f_i(x)| < 1$ for $x \in (-1, 1)$ and $|f_i(x)| = 1$ for $x = \pm 1$. Equation (3.3) can be written in matrix form for $k = 0, \ldots, n-1$ as $\mathbf{\Phi} = \mathbf{AF}$, where $\mathbf{\Phi} = [\varphi_0 \cdots \varphi_{n-1}]^T$, the lower triangular matrix $\mathbf{A}$ contains the coefficients $a_i^{(k)}$ and $\mathbf{F} = [f_0 \cdots f_{n-1}]^T$.

The following theorem is needed for the computation of the matrix $\mathbf{A}$.

Theorem 3.2. *Put by definition $\mathbf{B} = [b_i^{(k)}] = \mathbf{A}^{-1}$. The entries $b_i^{(k)}$ are given by*

$$b_i^{(k)} = \langle f_k \,, \varphi_i \rangle_\mu \,. \tag{3.4}$$

It is clear that $b_0^{(0)} = 1$. Explicit expressions for the other coefficients are available in the following two cases.

1. *If all poles are equal to $\alpha \neq \infty$, we have*

$$\begin{aligned} b_i^{(k)} &= \sqrt{\frac{1-\beta^2}{2}} \frac{1}{2^{k-1}} \sum_{j=0}^{\lfloor (k-i)/2 \rfloor} \binom{k}{j} (-\beta)^{k-2j-i}, \quad i \geq 1, \\ b_0^{(k)} &= \frac{1}{2^{k-1}} \sum_{j=0}^{\lfloor k/2 \rfloor} \binom{k}{j} (-\beta)^{k-2j} - \frac{1}{2^k} \binom{k}{k/2} (1 - k \bmod 2), \end{aligned} \tag{3.5}$$

   where $\lfloor x \rfloor$ denotes the largest integer less than or equal to x. Note that the last term in the second formula only appears when k is even.

2. *If all poles are different from each other, we have*

$$\begin{aligned} b_i^{(k)} &= \sqrt{\frac{1-\beta_i^2}{2}} \frac{1-\beta_k^2}{1-\beta_i\beta_k} B_{i-1}(\beta_k), \quad i \geq 1, \\ b_0^{(k)} &= -\beta_k. \end{aligned}$$

In all formulas $\alpha_i = J(\beta_i)$ and $\alpha = J(\beta)$.

For the general case where there are both repeated and different poles, the explicit formulas are too complicated to be of use. We come back to this in section 4.

To be able to compute the modified moments ν_k, we also need the integrals $\int_{-1}^{1} f_k(x)dx$. The next theorem shows how they can be computed.

Theorem 3.3. *For $|\alpha| > 1$, define the integrals*

$$I_m^{(\alpha)} = \int_{-1}^{1} \left(\frac{1-\alpha x}{x-\alpha} \right)^m dx.$$

They satisfy the (backward) recurrence relation

$$I_{m-1}^{(\alpha)} = \left(1 - \frac{1}{\alpha^2}\right) \frac{1-(-1)^m}{m} - \frac{2}{\alpha} I_m^{(\alpha)} - \frac{1}{\alpha^2} I_{m+1}^{(\alpha)},$$

and the series expansions

$$I_m^{(\alpha)} = \frac{2}{m+1} + \frac{4m}{\alpha^2}\sum_{j=0}^{\infty}\frac{1}{(2j+m+3)(2j+m+1)}\frac{1}{\alpha^{2j}}, \quad m \text{ even},$$

$$I_m^{(\alpha)} = -\frac{4m}{\alpha}\sum_{j=0}^{\infty}\frac{1}{(2j+m+2)(2j+m)}\frac{1}{\alpha^{2j}}, \quad m \text{ odd}.$$

As explained in section 4, we use the backward recurrence relation for stability reasons. The series expansions are of course needed to start this recurrence. If all poles are different from each other, we only need integrals of type $I_1^{(\alpha)}$, which can be computed explicitly,

$$I_1^{(\alpha)} = (\alpha^2 - 1)\log\frac{\alpha+1}{\alpha-1} - 2\alpha.$$

The previous two theorems contain all the information we need to solve the lower triangular system

$$\int_{-1}^{1}\mathbf{F}dx = \mathbf{A}^{-1}\int_{-1}^{1}\mathbf{\Phi}dx,$$

thus providing the modified moments ν_k.

4 Numerical issues

While the previous section only presented the theoretical formulas to compute the modified moments, in this section we discuss some numerical considerations to determine which method is more suitable, depending on the location of the poles. Some examples are given as illustration. All computations from this and the following section were done in Matlab 7 on a Pentium III (Coppermine) with a CPU speed of 733 MHz.

4.1 Chebyshev polynomials

The applicability of this method depends on the size of the coefficients $d_i^{(k)} = c_i^{(k)} + c_{-i}^{(k)}$ and the integrals $I_i^{(k)} = \int_{-1}^{1} T_i(x)/\pi_k(x)dx$. We first consider two limit cases.

In the case where all poles are at infinity (corresponding to the classical Fejér rule), we obviously have $\varphi_k(x) = \sqrt{2}\,T_k(x)$. The coefficients $d_i^{(k)}$ satisfy $d_i^{(k)} = 0$ for $i < k$ and $d_k^{(k)} = 1$, and the values of $I_i^{(k)}$ remain bounded. From a numerical point of view, computing the modified moments ν_k in this case is a perfectly well-conditioned problem. It is safe to say that this will also be true for poles far from the interval $[-1, 1]$ (e.g. poles tending to infinity), since in that case the rational function φ_k is still very much 'polynomial-like'.

The other limit case corresponds to all poles equal to $\alpha = 1$. This is of course not allowed in practice, but it is interesting to study the growth of the coefficients $d_i^{(k)}$. It follows from equation (3.1) that in this case

$$d_i^{(k+1)} = d_{i-1}^{(k)} - 2d_i^{(k)} + d_{i+1}^{(k)}.$$

Table 1: Size of coefficients and relative error when $n = 15$.

α_k	$\max_i \lvert d_i^{(n)} \rvert$	$\max_i \lvert I_i^{(n)} \rvert$	rel. err. ν_n
$2k$	$1.68e+00$	$7.96e-17$	$1.95e-09$
$(-1)^k 2k$	$1.00e+00$	$5.15e-17$	$2.89e-12$
1.001	$7.47e+07$	$7.14e+40$	$2.87e+34$
$1+2^{-k}$	$6.44e+06$	$2.81e+31$	$7.74e+18$
$(-1)^k(1+2^{-k})$	$3.58e+02$	$5.22e+12$	$2.51e-02$

Together with the fact that $d_k^{(k)} = 1$, it can easily be proved by induction that we have the following explicit formula,

$$d_i^{(k)} = (-1)^{k-i} \binom{2k}{k-i},$$

which means that for large k and small i this coefficient becomes very large. The same will be true if all poles are equal to α very close to 1 or -1, as follows from equation (3.2). In general, since the coefficients are continuous functions of the poles, if all poles are close to the interval (and at the same side), these coefficients can become very large. In that case also the integrals $I_i^{(k)}$ can be very large, but the modified moments ν_k are typically of order $O(1)$. It is well-known that summing very large numbers to obtain a small number is an ill-conditioned problem.

The previous considerations are illustrated in table 1, which shows the maximum absolute values of $d_i^{(n)}$, $I_i^{(n)}$ and the relative error on ν_n for different locations of the poles when $n = 15$. Note that the accuracy seems to be higher for poles which are more or less symmetric with respect to the origin. This is due to the computation of the integrals $I_i^{(k)}$ using the algorithm from [WL00]. As mentioned by the authors, their algorithm seems to be unstable for poles which are all at the same side of the interval. However, some digits are also lost in the case of $\alpha_k = (-1)^k 2k$. It is not immediately clear what causes this loss. Obviously, when there are many poles close to the interval (at one or both sides), all digits are lost because the integrals $I_i^{(k)}$ become too large.

4.2 Interval Blaschke products

If there are both repeated and different poles, it is very difficult to derive explicit formulas for the inner products (3.4). However, the functions f_k and φ_i all belong to $\mathcal{L}_{n-1}$, so we can compute the inner products *exactly* using the n-point Gauss-Chebyshev quadrature formula which we already computed (see section 2).

In the case where all poles are equal, we can simplify the computations as follows. If, for fixed k, we only consider the sum in (3.5) and denote it by

$$\tilde{b}_i = \sqrt{\frac{2}{1-\beta^2}} 2^{k-1} b_{k-2i}^{(k)}$$

Table 2: Condition number for the matrix $\mathbf{B}$ when $n = 15$.

α_k	cond $\mathbf{B}$
$2k$	$4.32e + 24$
$(-1)^k 2k$	$4.11e + 19$
1.001	$1.10e + 06$
$1 + 2^{-k}$	$4.19e + 05$
$(-1)^k(1 + 2^{-k})$	$1.06e + 03$

then it is easily checked that we have the recurrence formula

$$\tilde{b}_i = \beta^2 \tilde{b}_{i-1} + \binom{k}{i}$$

and $\tilde{b}_0 = 1$. For the other coefficients it holds that $b^{(k)}_{k-2i-1} = -\beta b^{(k)}_{k-2i}$.

Similarly, if all poles are different, there is no need to recompute the Blaschke product for each i. Obviously,

$$B_{i-1}(\beta_k) = B_{i-2}(\beta_k)\frac{\beta_k - \beta_{i-1}}{1 - \beta_k \beta_{i-1}}.$$

Taking into account the above considerations seriously reduces the computational cost of this approach. In fact, this makes the difference between a complexity of order $O(n^2)$ and $O(n^3)$.

As for the integrals $I^{(\alpha)}_m$, we use the backward recurrence relation because it is stable. The homogeneous solution of this recurrence consists of the two modes $(-1/\alpha)^k$ and $k(-1/\alpha)^k$ which both remain bounded for $k \to \infty$ because $|\alpha| > 1$. For the forward recurrence the homogeneous solution consists of $(-\alpha)^k$ and $k(-\alpha)^k$ which both become unbounded. However, for poles very close to the interval, or for small values of m, it is preferable to use the forward recurrence since it does not need the series expansions (which converge very slowly if $|\alpha| \approx 1$).

Finally, the applicability of this method depends on the condition number of the matrix $\mathbf{B}$, which corresponds roughly to the number of digits lost in solving the lower triangular system. In table 2 we show the 2-norm condition number for different locations of the poles when $n = 15$. Contrary to the method based on Chebyshev polynomials, this approach fails completely when the poles are far from the interval, and seems to work rather well for poles *extremely* close to the interval. This is confirmed by figure 1, which shows the error growth (the relative error divided by the machine precision) for the modified moments ν_k and the same locations of the poles as in table 2. For poles tending to infinity, all digits are lost very quickly. However, when the poles converge to the interval exponentially, only a few digits are lost. Also, the integrals $I^{(\alpha)}_m$ remain bounded as is obvious from their definition. This kind of behaviour is exactly what we want and shows that this method is perfectly complementary to the method based on Chebyshev polynomials.

Figure 1: Error growth of ν_k for different locations of the poles.

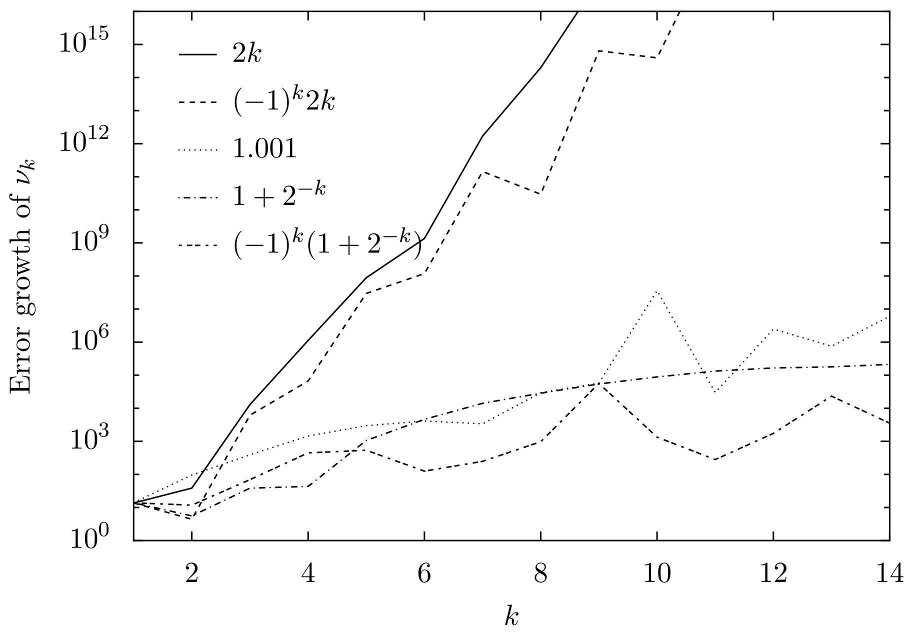

Table 3: Relative error for I_1 with $\omega = 1.1$.

n	ORF	WL
2	$4.15e-01$	$1.42e-02$
4	$1.76e-03$	$8.87e-04$
8	$1.36e-08$	$4.51e-08$
12	$9.41e-14$	$2.36e-13$
16	$< \epsilon_{\text{mach}}$	$4.44e-16$

5 Examples

In this section we apply our quadrature formula based on orthogonal rational functions (ORF) to some test integrals and compare the accuracy and stability with the results obtained using the formulas from [WL00]. In all examples, the 'exact' result was obtained from a multiprecision computation in Maple.

For the first example we follow [WL00] and [Gau99] and compute

$$I_1 = \int_{-1}^{1} \frac{\pi x/\omega}{\sin(\pi x/\omega)} dx, \quad \omega > 1.$$

The integrand has poles at the integer multiples of ω, so we choose the sequence of poles $A = \{\omega, -\omega, 2\omega, -2\omega, \ldots\}$. Table 3 shows the relative error in the quadrature rule using our approach (ORF) based on Chebyshev polynomials and the method from Weideman and Laurie (WL) for the case $\omega = 1.1$. It seems that with increasing n, our quadrature formula is a little more accurate, but

Table 4: Relative error for I_1 with $\omega = 1.001$.

n	ORF	WL
2	$2.96e+00$	$1.79e-01$
4	$8.85e-03$	$3.89e-03$
8	$4.78e-08$	$2.07e-07$
12	$1.33e-13$	$1.56e-12$
16	$5.17e-14$	$1.75e-14$

Table 5: Relative error for I_2 with $\alpha = -2.5$.

n	ORF	WL
2	$2.52e-03$	$4.06e-04$
4	$2.26e-06$	$1.86e-06$
8	$6.20e-12$	$2.58e-11$
12	$5.55e-16$	$2.86e-12$
16	$2.22e-16$	$3.11e-11$

the difference is very small. For $n = 16$ Matlab returned a relative error of 0 for our method, which means less than machine precision, which is approximately $2.22e-16$. In all cases the weights were positive and less than 1.

In table 4 we repeat this experiment but now with $\omega = 1.001$. The results are comparable to the previous case, but it seems that we cannot get more than approximately 14 correct digits due to roundoff errors. Again all weights were positive and less than 1.

The next example is

$$I_2 = \int_{-1}^{1} \frac{1}{\sqrt{(x+3)(x+2)}} dx.$$

As noted by Van Assche in [VAV93], the integrand is in fact a Stieltjes function and can be well approximated by a rational function with poles on the branch cut $[-3, -2]$. First we take all poles equal to $\alpha = -2.5$. Table 5 gives the results. In our approach, we used the method based on Blaschke products, but the other method (Chebyshev polynomials) gave similar results. It is worth mentioning that for $n = 16$, even though the condition number of the matrix $\mathbf{B}$ was of order $O(10^5)$, the quadrature sum is accurate up to machine precision. It is not uncommon in numerical integration to obtain an accurate approximation to the integral even with quadrature weights which are not very accurate. Also note that in this case the WL formula seems to stagnate at more or less 12 correct digits. We also noticed several negative weights in this formula, while the weights in our formula were all positive. Next we take all poles different from each other as in the second example of [VAV93]. They are the zeros of successive Chebyshev polynomials $T_{3^m}(x)$, transformed to $[-3, -2]$ and ordered in such a way that they are dense on this interval. For more information we refer

Table 6: Relative error for I_2 with α_k distributed over $[-3, -2]$.

n	ORF	WL
2	$4.72e-03$	$2.51e-04$
4	$7.47e-08$	$6.88e-08$
8	$4.67e-14$	$1.20e-10$
12	$3.33e-16$	$2.99e-03$
16	$1.11e-16$	$3.42e+01$

Table 7: Relative error for I_3 with $\omega = 1.1$.

n	ORF	WL	OF
5	$4.56e-02$	$5.52e-01$	$1.86e-01$
10	$1.18e-04$	$4.34e+00$	$3.84e-02$
20	$3.14e-13$	$5.88e+14$	$7.38e-04$
30	$7.33e-15$	$2.04e+28$	$4.66e-06$

to the article. The results are shown in table 6. This time we used the method based on Chebyshev polynomials for the ORF rule. Note that with increasing n, all digits are lost in the WL rule, while this does not occur in our method. This is very remarkable since both methods use the integrals $I_i^{(k)}$. The loss of accuracy must therefore occur not in the computation of these integrals, but when combining these integrals to obtain the quadrature weights. We mention that some of the weights in the WL rule were negative and of order $O(10^2)$. All weights in the ORF rule were positive and less than 1.

For the final example we look at the integral

$$I_3 = \int_{-1}^{1} \sin \frac{1}{\omega - x} dx, \quad \omega > 1$$

whose integrand has an essential singularity in ω. We take all poles equal to $\alpha = \omega$ and use the method based on Blaschke products. In table 7 we compare our results with the WL rule and the ordinary (polynomial-based) Fejér rule (OF). This time the WL rule fails completely, not only because of loss of accuracy in the construction of the rule, but also because the weights are very large and of mixed sign. For $n = 20$ the largest weight was of order $O(10^{20})$. Note that our method performs very well (even though for $n = 30$ the condition number of the matrix $\mathbf{B}$ was equal to $1.59e + 11$). All the computed weights were positive and less than 1.

6 Conclusion

For the cases where the WL quadrature rule from [WL00] works well, there is not really a need to use our formulas. ALthough the results are a little better, this is at the expense of considerably more computations. However, for poles close to the interval, or at the same side of the interval, the WL rule fails, either because of rounding errors or because the weights become very large and of mixed sign. In this case the examples indicate that our rule performs much better, especially when the computations are done using the interval Blaschke products. The weights remain small and the presence of poles attract the nodes to the endpoints (we refer to [VDBGV05] for a detailed explanation).

7 Proofs

In all proofs in this section, we use $x = J(z)$ and $\alpha_k = J(\beta_k)$ where J is the Joukowski transform.

Proof of theorem 3.1. From theorem 2.3 and the fact that

$$\pi_n(x) = \frac{\prod_{k=1}^{n}(1-\beta_k z)(z-\beta_k)}{z^n \prod_{k=1}^{n}(1+\beta_k^2)}$$

we get that

$$\varphi_n(x) = \sqrt{\frac{1-\beta_n^2}{2}}\frac{z^{-(n-1)}(z-\beta_n)\prod_{k=1}^{n-1}(z-\beta_k)^2 + z^{-n}(1-\beta_n z)\prod_{k=1}^{n-1}(1-\beta_k z)^2}{\pi_n(x)\prod_{k=1}^{n}(1+\beta_k^2)}.$$

If we put

$$z^{-(n-1)}(z-\beta_n)\prod_{k=1}^{n-1}(z-\beta_k)^2 = \sum_{k=-(n-1)}^{n} c_k^{(n)} z^k$$

then the numerator equals

$$z^{-(n-1)}(z-\beta_n)\prod_{k=1}^{n-1}(z-\beta_k)^2 + z^{-n}(1-\beta_n z)\prod_{k=1}^{n-1}(1-\beta_k z)^2 =$$
$$\sum_{k=-(n-1)}^{n} c_k^{(n)}(z^k + z^{-k}) = 2\sum_{k=1}^{n-1}(c_k^{(n)} + c_{-k}^{(n)})T_k(x) + 2(T_n(x) + c_0^{(n)}).$$

To find the coefficients $c_k^{(n)}$ write

$$\begin{aligned} z^{-n}(z-\beta_{n+1})\prod_{k=1}^{n}(z-\beta_k)^2 &= z^{-1}(z-\beta_{n+1})(z-\beta_n)z^{-(n-1)}(z-\beta_n)\prod_{k=1}^{n-1}(z-\beta_k)^2 \\ &= z^{-1}(z-\beta_{n+1})(z-\beta_n)\sum_{k=-(n-1)}^{n} c_k^{(n)} z^k \\ &= \sum_{k=-n}^{n+1}[c_{k-1}^{(n)} - (\beta_n+\beta_{n+1})c_k^{(n)} + \beta_n\beta_{n+1}c_{k+1}^{(n)}]z^k \end{aligned}$$

if we take the convention that $c_k^{(n)} = 0$ for $k \leq -n$ or $k > n$. This yields the recurrence relation (3.1).

If all poles are equal, formula (3.2) follows (by induction) from this recurrence relation using the well-known recurrence for binomial numbers. □

Proof of theorem 3.2. Formula (3.4) follows from the orthogonality of the φ_k. We only prove the explicit expressions corresponding to all poles equal. If all poles are different, the reasoning is analogous and the computations are easier.

If all poles are equal to α, the functions f_k have the form

$$f_k(x) = \left(\frac{1-\alpha x}{x-\alpha}\right)^k, \quad k = 1, 2, \ldots$$

From the definition of the Joukowski transform it follows that

$$f_k(x) = \frac{1}{2^k}\left(\frac{1-\beta z}{z-\beta} + \frac{z-\beta}{1-\beta z}\right)^k$$

so the inner product becomes

$$\langle f_k\,, \varphi_i\rangle_\mu = 2\Re\left\{\frac{1}{2\pi\mathbf{i}}\sqrt{\frac{1-\beta^2}{2}}\frac{1}{2^k}\oint_{\mathbb{T}}\left(\frac{1-\beta z}{z-\beta} + \frac{z-\beta}{1-\beta z}\right)^k \frac{(z-\beta)^{i-1}}{(1-\beta z)^i}dz\right\}$$

where $\Re$ denotes the real part and $\mathbb{T}$ is the complex unit circle. Using the residue theorem then gives

$$\langle f_k\,, \varphi_i\rangle_\mu = \sqrt{\frac{1-\beta^2}{2}}\frac{1}{2^{k-1}}\operatorname{Res}\left\{\left(\frac{1-\beta z}{z-\beta} + \frac{z-\beta}{1-\beta z}\right)^k \frac{(z-\beta)^{i-1}}{(1-\beta z)^i}, \beta\right\}$$

(since β is real, the residue at β is real as well, so the real part can be omitted from the formula). Using the binomial theorem, the integrand can be written as

$$\left(\frac{1-\beta z}{z-\beta} + \frac{z-\beta}{1-\beta z}\right)^k \frac{(z-\beta)^{i-1}}{(1-\beta z)^i} = \sum_{j=0}^{k}\binom{k}{j}\left(\frac{1-\beta z}{z-\beta}\right)^{k-2j-i}\frac{1}{z-\beta}$$

and the numerator in the summand equals

$$(1-\beta z)^{k-2j-i} = \sum_{m=0}^{k-2j-i}\binom{k-2j-i}{m}(1-\beta^2)^{k-2j-i-m}(-\beta)^m(z-\beta)^m.$$

Since the residue is a linear function of its argument, we finally get

$$b_i^{(k)} = \langle f_k\,, \varphi_i\rangle_\mu = \sqrt{\frac{1-\beta^2}{2}}\frac{1}{2^{k-1}}\sum_{j=0}^{\lfloor (k-i)/2\rfloor}\binom{k}{j}(-\beta)^{k-2j-i}.$$

The coefficient corresponding to $\varphi_0 \equiv 1$ can be found by similar reasoning, starting from

$$b_0^{(k)} = \langle f_k\,, 1\rangle_\mu = \frac{1}{2^k}\operatorname{Res}\left\{\left(\frac{1-\beta z}{z-\beta}+\frac{z-\beta}{1-\beta z}\right)^k\frac{1}{z},\beta\right\}+ \frac{1}{2^k}\operatorname{Res}\left\{\left(\frac{1-\beta z}{z-\beta}+\frac{z-\beta}{1-\beta z}\right)^k\frac{1}{z},0\right\}.$$

Some computations yield that the first residue equals

$$\operatorname{Res}\left\{\left(\frac{1-\beta z}{z-\beta}+\frac{z-\beta}{1-\beta z}\right)^k\frac{1}{z},\beta\right\} = (-1)^k\sum_{j=0}^{\lfloor k/2\rfloor}\binom{k}{j}\left(\beta^{k-2j}-\frac{1}{\beta^{k-2j}}\right)$$

while the second residue obviousely equals

$$\operatorname{Res}\left\{\left(\frac{1-\beta z}{z-\beta}+\frac{z-\beta}{1-\beta z}\right)^k\frac{1}{z},0\right\} = (-1)^k\left(\beta+\frac{1}{\beta}\right)^k.$$

Adding both terms and doing some algebra finishes the proof. □

Proof of theorem 3.3. To find the recurrence relation, note that we have

$$\frac{d}{dx}\left(\frac{1-\alpha x}{x-\alpha}\right)^m = \frac{m}{\alpha^2-1}\left[\left(\frac{1-\alpha x}{x-\alpha}\right)^{m+1}+ 2\alpha\left(\frac{1-\alpha x}{x-\alpha}\right)^m+\alpha^2\left(\frac{1-\alpha x}{x-\alpha}\right)^{m-1}\right].$$

Integrating both sides from -1 to 1 gives

$$1-(-1)^m = \frac{m}{\alpha^2-1}\left(I_{m+1}^{(\alpha)}+2\alpha I_m^{(\alpha)}+\alpha^2 I_{m-1}^{(\alpha)}\right).$$

Rearranging terms then yields the recurrence relation.

The series expansions are much more difficult to derive. If we define the generating function $I^{(\alpha)}(z)$ as the (formal) series

$$I^{(\alpha)}(z) = \sum_{m=0}^{\infty} I_m^{(\alpha)} z^m,$$

then using the recurrence relation and following the procedure outlined in [GKP94, Chap. 7], we find the explicit expression

$$I^{(\alpha)}(z) = \frac{(\alpha^2-1)z}{(1+\alpha z)^2}\log\frac{(1+z)(\alpha+1)}{(1-z)(\alpha-1)}+\frac{2}{1+\alpha z}.$$

A Taylor series expansion for this function now gives expressions for the integrals $I_m^{(\alpha)}$. We omit the computations, which are cumbersome but straightforward, and only give the result,

$$I_m^{(\alpha)} = (-\alpha)^{m-1}\left((\alpha^2-1)m\log\frac{\alpha+1}{\alpha-1}-2\alpha\right)+2(\alpha^2-1)c_m^{(\alpha)}, \quad m=0,1,\ldots \tag{7.1}$$

where the constants $c_m^{(\alpha)}$ are given by

$$c_m^{(\alpha)} = \sum_{i=0}^{\lfloor m/2 \rfloor - 1} \frac{m-2i-1}{2i+1} (-\alpha)^{m-2-2i}$$

and an empty sum is equal to zero. These expressions, however, are not very useful (especially for large m and α), because of heavy cancellation when summing both terms in (7.1). In fact, if we compute a Laurent series expansion for $I_m^{(\alpha)}$ as a function of α, all terms with positive powers of α cancel against each other (there is only a finite number of such terms) and we are left with only powers of $1/\alpha$. This Laurent series expansion corresponds to the last formulas in theorem 3.3. Again we omit the computations. □

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