Title Star Chebyshev series method for computing weighted quadrature formulas

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Abstract

In this paper we study convergence and computation of interpolatory quadrature formulas with respect to a wide variety of weight functions. The main goal is to evaluate accurately a definite integral, whose mass is highly concentrated near some points. The numerical implementation of this approach is based on the calculation of Chebyshev series and some integration formulas which are exact for polynomials. In terms of accuracy, the proposed method can be compared with rational Gauss quadrature formula.

Keywords: Interpolatory quadrature formula, rational quadrature formula, ill-scaled integrand, difficult pole, modified weight function, Chebyshev series

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1. Introduction

A common problem is the evaluation of a definite integral over a bounded interval $[a, b]$. The solution of this problem can be approached in terms of a product integration rule, specially when the integrand has singularities. The

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procedure is to rewrite the integrand as \( F(x)W(x) \), where \( F \) is the integrand and \( W \) is a non-negative weight function.

Suppose that \( w \) is a weight function on \([a, b]\), which is closely related to \( W \) in a sense to be clarified. The integral of \( FW \) can be approximated by a weighted quadrature of the form

\[
\int_a^b F(x)W(x)dx = \sum_{k=1}^n \lambda_{n,k}(W)F(x_{n,k}) + \mathcal{E}_n(F),
\]

where \( \lambda_{n,k}(W) = \int_a^b P_n(x) \left( x - x_{n,k} \right) \frac{P_n'(x_{n,k})}{W(x)}dx \),

and \( P_n(x) = \prod_{k=1}^n (x - x_{n,k}) \) is the \( n \)th (monic) orthogonal polynomial with respect to \( w \).

In the rest of this article, we will maintain the notation used in (2). The aim is to indicate explicitly the weight function to which we refer.

To improve the accuracy of the results, a plausible strategy consists in modifying conveniently the initial factorization, say, \( FW = fGW \), where \( G \geq 0 \), and the main property of \( f \) is to have no singularities.

Roughly speaking, a real-valued function is said to be a difficult function, if it has integrable singularities, or it ranges over very large and very small values (poor scaling). A typical case is one in which the function is meromorphic on a region \( V \supset [a, b] \). In this context, the adjective difficult also applies to the poles of the integrand that are very close to \([a, b]\).

To tackle the integration of a difficult function, the technique of selecting \( G \) as a proper rational function has been used intensively, i.e. \( f = qF/p \) and \( G = p/q \), where \( p \) and \( q \) are polynomials whose roots match the difficult points of \( F \) (cf. [5]–[7],[9]). Monegato [9] considers \( G = \frac{1}{q} \), and calculates \( \lambda_{n,k}(W/q) \) in terms of \( \lambda_{n,k}(W) \). That approach requires the calculation of the integrals \( V_i = \int_a^b x^i W(x)/q(x)dx \), \( i = 0, 1 \). Monegato’s method is based on the partial fraction decomposition of \( 1/q \), and depends on the ability to calculate \( V_i \). The main objective of [9] is to obtain accurate results when the integrand has difficult poles, and this is achieved by applying a non-linear algorithm proposed by Gautschi. A variant of Monegato’s work is given in [5] where it is considered \( \{G_n\} \), defined as \( G_n = p_n/q_n \), \( n \in \mathbb{N} \), where \( \{p_n\} \) and \( \{q_n\} \) are two sequences of polynomials such that \( p_n/q_n = \mathcal{O}(1) \). Moreover, the roots of \( p_n \) coincide with some zeros of the integrand, and the difficult poles of the integrand are neutralized by applying an appropriate change of
variables. The examples in [5] demonstrate that the zeros of the integrand can play a role, but the numerical results are similar to those in [9] when \( p_n \equiv 1 \). A common feature to both papers [5, 9] is that the convergence of the quadrature rules is guaranteed by the following condition (cf. [10]).

\[
\int_{a}^{b} W(x)^2 / w(x) \, dx < \infty.
\]

(3)

The purpose of this paper is to present a flexible approach to evaluate the integral of difficult functions. As a result, they have been derived several methods whose performance is illustrated mainly by means of numerical examples. In a sense, some of these methods are simpler than that of Monegato [9]. Our strategy has been based on constructing interpolatory quadrature formulas with respect to a class of varying weights.

From here onwards, we will only consider integrals on the interval \([-1, 1]\).

The paper is organized as follows.

In Section 2 we consider a modification of (1–2) given in terms of a sequence \( \{G_n W\} \), which means that the coefficients are given by \( \lambda_{n,k}(G_m W) \). Then we obtain convergence when the trio \( \{G_n, W, w\} \) satisfies a condition weaker than (3). Section 3 deals with the case \( G = K / q \), where \( K \in L_2(w) \), and focuses on the calculation of \( \lambda_{n,k}(KW/q) \). Here we assume that \( G \) is approximated by \( G_m = p_m / q \), where \( p_m \) is a partial sum of the Chebyshev series expansion of \( K \). The problem reduces to consider \( w(x) = 1/\sqrt{1-x^2} \) and \( W = h_1 w \), where \( h_1 \) is a polynomial. It is clear that \( W \) is a generic weight that includes the four classical Chebyshev weight functions. It is used a technique similar to that by Berriochoa et al [1], to prove an exact formula for \( \lambda_{n,k}(KW/q) \). Unlike the method proposed by Clenshaw and Curtis [4], here we only use the Chebyshev series expansion of a factor \( K \).

The numerical examples of Section 4 allow to appraise the effectiveness of the proposed approach. To facilitate this, we compare our results with those obtained by Gautschi [7], Monegato [9] and Deckers et al [2]. Section 5 is devoted to the calculation of the coefficients of the Chebyshev series expansion, and Section 6 contains some remarks as a conclusion.

Throughout the paper \( \Pi \) denotes the space of all algebraic polynomials, \( \Pi_n = \{ p \in \Pi; \, \deg(p) \leq n \} \), and \( \|f\| = \sup_{x \in [-1,1]} |f(x)| \).
2. Convergence of modified quadrature rules

**Definition 1.** Let $W$ and $w$ be two weight functions on $[-1,1]$, both with infinitely many points of increase. Let $F$ be an integrable function with respect to $W$ and assume that $F = fG$, where $f$ is continuous, and $G$ is a nonnegative function such that $G \in L_1(W)$. Let $\{G_n\}$ be a sequence of positive and continuous functions on $(-1,1)$, such that $G_n \in L_1(W)$, $n \in \mathbb{N}$, and $G_nWdx \to GWdx$, as $n \to \infty$, in the weak * topology of measures. We say that

$$\int_{-1}^{1} F(x)W(x)dx = \sum_{k=1}^{n} \lambda_{n,k}(G_mW)f(x_{n,k}) + E_{n,m}(f) \quad (4)$$

is a modified interpolatory quadrature formula (MIQF) of order $(n,m)$, with respect to the pair $(\{G_n\},w)$, if

$$\lambda_{n,k}(G_mW) = \int_{a}^{b} \frac{P_n(x)}{(x-x_{n,k})P'_n(x_{n,k})} G_m(x)W(x)dx, \quad (5)$$

where $P_n(x) = \prod_{k=1}^{n}(x-x_{n,k})$ is the $n$th (monic) orthogonal polynomial with respect to $w$.

As usual, the term $E_{n,m}(f)$ stands for the quadrature error.

**Proposition 1.** Suppose that (4) is a MIQF with respect to $(\{G_n\},w)$, and let $n$ be fixed. Then

$$\int_{-1}^{1} f(x)G_m(x)W(x)dx = \sum_{k=1}^{n} \lambda_{n,k}(G_mW)f(x_{n,k}) \quad (6)$$

holds for all $f \in \Pi_{n-1}$, and all $m \in \mathbb{N}$.

**Proof.** Just note that $\lambda_{n,k}(G_mW)$ is the $k$th coefficient of the interpolatory rule of polynomial type which corresponds to the weight $G_mW$. \qed

The construction of (4) depends on the integrand $F = fG$, which increases the cost of the numerical procedure. In effect, the quadrature coefficients must be calculated each time one changes $G$. On the other hand, $\{G_n\}$ represents a discretization method.

If $G = p/q$, with $p,q \in \Pi$, then we say that (4) is a rational formula.
To study the convergence of a MIQF, we assume that $m = m(n)$ is an increasing sequence of integers. For simplicity, we will write $G_n$ and $E$, instead of $G_{m(n)}$ and $E_{n,m(n)}$, respectively.

The following result brings us closer to the theory in [10].

**Proposition 2.** Let $E_n$ be the error functional of a MIQF with respect to $(\{G_n\}, w)$, with $G_n = G$, for all $n$. If condition (3) holds true, then

1. $\lim_n E_n(f) = 0$, and
2. $\lim_n \sum_{k=1}^{n} |\lambda_{n,k}(GW)| f(x_{n,k}) = \int_{-1}^{1} f(x)G(x)W(x)dx$,

for all bounded Riemann integrable functions $f$.

**Proof.** Let $M > 0$ such that $G(x) \leq M$ for all $x \in [-1, 1]$. According to [10, Theorem 1], we only have to check that

$$\int_{-1}^{1} (W(x)G(x))^2 dx/w(x) \leq M^2 \int_{-1}^{1} W(x)^2 dx/w(x) < \infty.$$ 

The following result is proved using the technique of [10] (See also [5]).

**Proposition 3.** If (4) represents a MIQF with respect to $(\{G_n\}, w)$, and $G_n \in L_2(W^2/w)$, $n \in \mathbb{N}$, then $\sum_{j=1}^{n} |\lambda_{n,j}(G_nW)| = O(\rho_n)$, where

$$\rho_n = \left( \int_{-1}^{1} \frac{G_n(x)^2W(x)^2}{w(x)} dx \right)^{1/2}.$$ 

Moreover, if $\sup_n \rho_n < \infty$, then $\lim_n E_n(f) = 0$ for all $f$ continuous.

**Proof.** Consider the orthonormal basis of polynomials with respect to $w$, and let $S_{n,m}$ be the $m$th partial sum of the corresponding Fourier series of $WG_n/w \in L_2(w)$. Taking into account that $\deg(P_n(x)/(x-x_{n,j})) = n-1$, we can write

$$\lambda_{n,j}(G_nW) = \int_{-1}^{1} \frac{P_n(x)S_{n,n-1}(x)}{P_n'(x_{n,j})(x-x_{n,j})} w(x)dx.$$ 

Now we use the orthogonality of $P_n$ with respect to the following polynomial

$$\frac{S_{n,n-1}(x) - S_{n,n-1}(x_{n,j})}{x-x_{n,j}},$$

with degree $n-2$, to obtain that

$$\lambda_{n,j}(G_nW) = S_{n,n-1}(x_{n,j})c_{n,j},$$ 

(8)
where $c_{n,j}$ are the coefficients of the Gauss rule associated with $w$. By writing $c_{n,j} = c_{1/2}c_{n,j}$ and adding the first $n$ coefficients in (8) we can use the Cauchy-Schwartz inequality to obtain the following estimate

$$\sum_{j=1}^{n} |\lambda_{n,j}(G_n W)| \leq \left( \sum_{j=1}^{n} c_{n,j} S_{n,n-1}^2(x_{n,j}) \right)^{1/2} \left( \sum_{j=1}^{n} c_{n,j} \right)^{1/2}. \quad (9)$$

Because $\deg(S_{n,n-1}^2) = 2n - 2$, we can apply to $S_{n,n-1}^2$ the exactness condition for the Gauss quadrature formula associated with $w$. The Bessel inequality allows us to obtain

$$\sum_{j=1}^{n} |\lambda_{n,j}(G_n W)| \leq \rho_n \left( \int_{-1}^{1} w(x) dx \right)^{1/2}, \quad (10)$$

which proves the first part of the proposition.

Now let $L_n(f) = \int_{-1}^{1} f(x)G_n(x)W(x)dx - \sum_{k=1}^{n} \lambda_{n,k}(G_n W)f(x_{n,k})$, where $f$ is continuous on $[-1,1]$. It follows that

$$\left| \int_{-1}^{1} f(x)G_n(x)W(x)dx \right| \leq \rho_n \|f\| \left( \int_{-1}^{1} w(x) dx \right)^{1/2}.$$

Now suppose that $\sup_n \rho_n < \infty$. From (10), it follows the asymptotical stability of the quadrature formula. Moreover, $\{L_n\}$ is uniformly bounded. From the exactness condition (Proposition 1) one obtains that $\lim_n L_n(f) = 0$ for all $f$ continuous on $[-1,1]$.

Using that $|E_n(f)| \leq \left| \int_{-1}^{1} f(G - G_n)Wdx \right| + |L_n(f)|$, the second part of the proposition is also proved. \hfill \square

If $\{G_n\}$ satisfies $G_n \leq C_0$, $n \in \mathbb{N}$, then the asymptotical stability of the corresponding MIQF can be obtained by assuming condition (3) (cf. [5]).

Let $W(x) = 1/(1 - x^2)^{\delta}$ and $h(x) = (1 - x^2)^{\eta}$ with $3/4 \leq \delta < 1$ and $\delta - 3/4 < \eta$. Let $w(x) = 1/\sqrt{1 - x^2}$. It implies that $h \in \mathcal{L}_2(W^2/w)$ and (3) is not fulfilled. If $G_n \leq h$, $n \in \mathbb{N}$, then $\sup_n \rho_n < \infty$, where $\rho_n$ is given by (7). We conclude that the assumptions of Proposition 3 are weaker than those of [10, Theorem 1] and [5, Lemma 1].

As expected, the rate of convergence of the quadrature error depends heavily on the approximation properties of both functions $f$ and $G$. 6
Proposition 4. Let $\mathcal{E}_n$ be the $n$th error functional of a MIQF with respect to $(\{G_n\}, w)$. Let us suppose that $\limsup_n \rho_n^{1/n} \leq 1$, where $\rho_n$ is given by (7). If we also have that $\limsup_n \|G - G_n\|^{1/n} < 1$, and $f$ is analytic on $[-1, 1]$, then $\limsup_n |\mathcal{E}_n(f)|^{1/n} < 1$.

Proof. For every $n$, let $p_{n-1}^* \in \Pi_{n-1}$ be the polynomial of best approximation to $f$ on $[-1, 1]$, in the uniform norm. We obtain that

$$|\mathcal{E}_n(f)| \leq \|f\| \|G - G_n\| M_1 + \|f - p_{n-1}^*\| \rho_n (1 + M_2),$$

where $M_1 = \int_{-1}^1 W(x)dx$ and $M_2 = \left( \int_{-1}^1 w(x)dx \right)^{1/2}$.

Now, we only have to apply the theorem of Bernstein-Walsh which asserts that $\limsup_n \|f - p_{n-1}^*\|^{1/n} < 1$. \hfill \Box

3. Calculation of quadrature coefficients

For every $p \in \Pi$ we define $\tilde{p}(z) = z^n p((z + 1/z)/2)$, where $n = \deg(p)$. If $p(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_0$, with $a_n \neq 0$, then $\deg(\tilde{p}) = 2n$ and $\tilde{p}(0) = a_n/2^n \neq 0$. Besides, $\tilde{p}(\zeta) = 0$ if and only if $\tilde{p}(1/\zeta) = 0$, $\zeta \neq 0$.

If $p_1 \in \Pi_{n_1}$ and $p_2 \in \Pi_{n_2}$, then $\tilde{p}_1 \tilde{p}_2 = \tilde{p}_1 \tilde{p}_2$.

In the sequel, we give a more specific meaning to the previous notation.

Set $w(x) = 1/\sqrt{1 - x^2}$ and $W_1 = w/\pi$. Now we restrict our attention to those weight functions which have the form $W = h_1 W_1$, where $h_1$ is an algebraic polynomial non-negative on $[-1, 1]$. Notice that condition (3) holds true, in effect, $\int_{-1}^1 W^2 dx/w = \int_{-1}^1 h_1^2 w dx/\pi^2 < \infty$.

Let $K$ be a positive and continuous function on $[-1, 1]$, whose Chebyshev coefficients are defined as usual, i.e.

$$A_0 = \int_{-1}^1 K(x) T_0(x) W_1(x) dx, \quad A_j = 2 \int_{-1}^1 K(x) T_j(x) W_1(x) dx, \quad j = 1, 2, ...$$

where $T_j$ is the $j$th Chebyshev orthogonal polynomial of the first kind.

Set $G = K/q$ where $q$ is a polynomial positive on $[-1, 1]$. The following results are given for MIQFs with respect to $(\{G_n\}, w)$, where $G_n = \sum_{j=0}^n A_j T_j/q$, $n \in \mathbb{N}$.

Lemma 1 is a consequence of [8, Theorem 5.2].

Lemma 1. If $K \in \mathcal{L}_2(w)$, then $G_n Wdx \rightarrow GWdx$, as $n \rightarrow \infty$, in the weak * topology of measures.
Theorem 1. Let \( q \in \Pi_m \setminus \Pi_{m-1} \) be such that \( q(x) > 0 \) for all \( x \in [-1, 1] \). Set \( h_1/q = p_1 + p_2/q \), where \( p_i \in \Pi_n \), \( i = 1, 2 \) and \( n_2 < m \). Let \( P = \sum_{i=0}^n b_i T_i \), where \( b_i \in \mathbb{R} \), \( i = 0, \ldots, n \). If \( K \in \mathcal{L}_2(w) \), then

\[
2 \int_{-1}^1 P(x)K(x)h_1(x)W_1(x)/q(x)dx =
\]

\[
\Re \left( \sum_{j=0}^{n_1+n} A_j \text{Res} \left( \frac{\tilde{p}_1(z)V_n(z)}{z^{n_1+1-j}}, 0 \right) + \sum_{j=0}^\infty A_j \sum_{i=0}^s \text{Res} \left( \frac{V_n(z)R(z)}{z^{n_2+1-m-j}}, z_i \right) \right)
\]

where \( z_1, \ldots, z_s \) are the \( s \) distinct zeros of \( \tilde{q} \) in the unit disk, \( s \leq m \), \( z_0 = 0 \), \( R(z) = \tilde{p}_2(z)/\tilde{q}(z) \), \( V_n(z) = \sum_{i=0}^n b_i (z^i + z^{-i}) \), and \( \text{Res}(F, z) \) is the residue of \( F \) at \( z \).

Proof. If \( q \in \Pi_m \) possesses \( s \) distinct zeros in \( \mathbb{R}\setminus[-1, 1] \), then, using the properties of the transform \( q \to \tilde{q} \), one obtains that \( \tilde{p}_2(z)/\tilde{q}(z) \) has \( s \) distinct poles \( z_i \neq 0 \) in the unit disk.

Let \( H(\theta) = \frac{h_1(\cos(\theta))}{q(\cos(\theta))} \). The following equalities hold true.

\[
\int_{-1}^1 \left( \frac{PKh_1W_1}{q} \right)(x)dx = \frac{1}{2\pi} \int_{-\pi}^{\pi} P(\cos(\theta))H(\theta) \sum_{j=0}^\infty A_j \cos(j\theta) d\theta =
\]

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{s=0}^n b_s \cos(s\theta)H(\theta) \sum_{j=0}^\infty A_j e^{ij\theta} d\theta +
\]

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{s=0}^n b_s \cos(s\theta)H(\theta) \sum_{j=0}^\infty A_j e^{ij\theta} d\theta =
\]

\[
\frac{1}{2} \Re \left( \frac{1}{2\pi i} \int_{|z|=1} V_n(z) \left( \frac{\tilde{p}_1(z)}{z^{n_1}} + \frac{z^m \tilde{p}_2(z)}{z^{n_2} \tilde{q}(z)} \right) \sum_{j=0}^\infty A_j z^{j-1} dz \right)
\]

From Lemma 1 we obtain that

\[
\int_{-1}^1 \left( \frac{PKh_1W_1}{q} \right)(x)dx = \frac{1}{2} \Re \left( \sum_{j=0}^\infty A_j \left( \frac{1}{2\pi i} \int_{|z|=1} V_n(z) \tilde{p}_1(z) z^{j-1} dz + \right) \right).
\]

The proof finishes after applying the residue theorem. \( \square \)
Notice that $V_n(z) = \sigma(z)/z^n$, where $\sigma \in \Pi_{2n}$.

Next we prove three corollaries of Theorem 1.

**Corollary 1.** Let $P = \sum_{i=0}^{n} b_i T_i$, where $b_i \in \mathbb{R}$, $i = 0, \ldots, n$. If $K \in \mathcal{L}_2(w)$ then the following formula takes place.

$$
\int_{-1}^{1} P(x)(Kh_1 W_1)(x)dx = \frac{1}{2} \Re \left( \sum_{j=0}^{d+n} A_j \Res \left( \frac{V_n(z) \tilde{h}_1(z)}{z^{-j+d+1}}, 0 \right) \right),
$$

(12)

where $d = \deg(h_1)$ and $V_n(z) = \sum_{i=0}^{n} b_i (z^i + z^{-i})$.

In particular,

$$
\int_{-1}^{1} P(x)(KW_1)(x)dx = \frac{1}{2} \left( A_0 b_0 + \sum_{j=0}^{n} A_j b_j \right).
$$

(13)

**Proof.** To prove (12), we only have to put $H(\theta) = h_1(\cos(\theta))$ in Theorem 1. Equation (13) follows easily by direct calculation of the residues. \qed

**Corollary 2.** Let $P = \sum_{i=0}^{n} b_i T_i$, where $b_i \in \mathbb{R}$, $i = 0, \ldots, n$. Let $q \in \Pi_m \setminus \Pi_{m-1}$ be such that $q(x) > 0$ for all $x \in [-1, 1]$. If $z_1, \ldots, z_s$ are the $s$ distinct zeros of $\tilde{q}$ in the unit disk, then

$$
\int_{-1}^{1} P(x)h_1(x)W_1(x)/q(x)dx = \frac{1}{2} \Re \left( \Res \left( \frac{\tilde{p}_1(z)V_n(z)}{z^{n_1+1}}, 0 \right) + \sum_{i=0}^{s} \Res \left( \frac{V_n(z) \tilde{p}_2(z)}{q(z)z^{n_2+1-m}, z_i} \right) \right),
$$

(14)

where $n_i = \deg(p_i)$, $i = 1, 2$, $z_0 = 0$ and $V_n(z) = \sum_{i=0}^{n} b_i (z^i + z^{-i})$.

**Proof.** The proof is reduced to put $K \equiv 1$ in Theorem 1. \qed

**Corollary 3.** Let $q \in \Pi_m \setminus \Pi_{m-1}$, $m \geq 1$, and $q(x) > 0$ for all $x \in [-1, 1]$. Suppose that $P = \sum_{i=0}^{n} b_i T_i$, where $b_i \in \mathbb{R}$, $i = 0, \ldots, n$. If $K \in \mathcal{L}_2(w)$, then

$$
\int_{-1}^{1} P(x)dx/q(x) = R \left( \sum_{j=0}^{\infty} A_j \sum_{k=0}^{s} \Res \left( \frac{V_n(z)}{q(z)z^{1-m-j}}, z_k \right) \right),
$$

(15)

where $A_{2j} = -2/(4j^2 - 1)$, $A_{2j-1} = 0$, $j = 1, 2, \ldots$, and $A_0 = 1$. Moreover, $z_1, \ldots, z_s$ are the $s$ distinct zeros of $\tilde{q}$ in the unit disk, $z_0 = 0$, $V_n(z) = \sum_{i=0}^{n} b_i (z^i + z^{-i})$ and $\Res(F, z)$ is the residue of $F$ at $z$. 

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Proof. (15) follows from Theorem 1 when \( p_1 \equiv 0, p_2 \equiv h_1 \equiv 1, K(x) = \pi \sqrt{1 - x^2} \), and every \( A_j \) is replaced by their exact expression (cf. [8]). \( \square \)

If \( \deg(h_1) \) is too large, then we recommend the use of equation (12) of Corollary 1, to facilitate the calculation of coefficients \( A_j \).

The presence of \( q \) and \( K \) at the same time might appear to be over-abundant. Actually, we can assign all the benign poles to \( K \), while those that have proven to be difficult must be zeros of \( q \). Corollary 3 includes the presence of both \( K \) and \( q \), and also provides a closed formula for the coefficients \( A_j \). This corollary allows us to tackle the problem of computing \( \int_{-1}^{1} F(x)W(x)dx \) when \( W \equiv 1 \) and \( F = f/q \). This \( F \) is meromorphic and the zeros of \( q \) should be difficult poles. In principle, an adverse fact is that \( K(x) = \sqrt{1 - x^2} \) has singularities at \( \pm 1 \), which makes its Chebyshev series slowly converging. However, the numerical results are acceptably accurate, as demonstrated by some examples. If we are using (12), (13) or (14), then no matter what is the speed of convergence of the Chebyshev series, because these formulas are given in terms of finite sums.

Any numerical implementation of the previous formulas is based on the following issues: i) the nodes coincide with the roots of Chebyshev polynomials, and ii) the coefficients \( \lambda_{n,k}(GW_1) \), \( 1 \leq k \leq n \), have to be calculated for every difficult factor \( G \). Moreover, the most favorable choice is one in which \( G \) does not depend on \( n \), so that the set \( \{A_m\}_{m=0}^{N} \) is calculated only once with \( N > n \), using FFT algorithm whose order is \( \mathcal{O}(N \log(N)) \).

If \( P = l_{n-1,j} \in \Pi_{n-1} \) is the \( j \)th fundamental polynomial of Lagrange interpolation, then the equations (11)–(15) correspond to the quadrature coefficient \( \lambda_{n,j}(GW) \), where \( G = K/q \) and \( W = h_1W_1 \). Moreover, \( l_{n-1,j} \) can be simulated efficiently by a routine based on its representation as a linear combination of Chebyshev polynomials of the first kind, that is,

\[
l_{n-1,j} = \frac{1}{n} \left( b_{0,n,j}T_0 + b_{1,n,j}T_1 + \cdots + b_{n-1,n,j}T_{n-1} \right),
\]

(16)

where \( b_{0,n,j} = 1 \), and \( b_{k,n,j} = 2 \cos((n-k)\pi(2j+1)/(2n)), k = 1, ..., n - 1 \).

Corollary 1 provides the simplest formulas of this section. Equation (12) can be expressed in terms of some derivatives of \( \tilde{h}_d \) at \( z = 0 \), and equation (13) only requires the knowledge of \( b_j = b_{k,n,j}, j = 1, ..., n \).

The total number of floating point operations to calculate each \( b_j \) does not depend on \( n \). Thus, when using (13), the process of calculating the \( n \)
coefficients $\lambda_{n,j}(GW)$ has a computational cost proportional to $n^2$, provided that the work of calculating $\{A_j\}_{j=0}^n$ is considered separately.

The use of (14)–(15) involves the calculation of residues of rational functions at some points of the unit disk. Let $p$ and $q$ be polynomials with $q(z_0) \neq 0$. The following algorithm can be used to estimate the residue of $r_k(z) = p(z)/q(z)/(z-z_0)^k$ at $z = z_0$, for $k = 1, 2, \cdots, \nu$.

\[
\begin{align*}
\text{If } \deg(q) &\geq 1, \text{ calculate } V = q', \ A = q(z_0) \text{ and } B = V(z_0), \\
\text{For } k = 1, 2, \ldots, \nu, \text{ do} \\
& \quad \text{Res}(r_k, z_0) = p_{k-1}(z_0)/A, \text{ where } p_0 = p, \text{ and} \\
& \quad p_{k-1} = (q p_{k-2} - (k-1)V p_{k-2})/(k-1)/A^{k-1}, \ k = 2, 3, \ldots, \nu. \\
& \text{If } q \equiv 1, \text{ then } \text{Res}(r_k, z_0) = p_{k-1}(z_0), \text{ where } p_{k-1} = p_{k-2}'/(k-1).
\end{align*}
\]

In cases that concern us, both $\deg(p)$ and $\nu$ increase with $n$. In effect, suppose that $n > m - n_2$ and $z_0 = 0$. Let $\sum \text{Res}(r_k, z_i)$ be as in (14). Then
\[
\deg(p) = 2(n + n_2), \nu = n_2 + n + 1 - m, \deg(q) = 2m \text{ and} \\
\deg(p_{k-1}) = \deg(p) + (k-1)(\deg(q)-1), \ k = 1, \ldots, \nu.
\]

If $z_0 \neq 0$, then $\nu$ is a constant that is usually not large. Note that $|q(z_0)|$ can be very small because the mapping $z \to (z + 1/z)/2$ transforms every difficult pole into two points that are very close to each other.

In general terms, let us suppose that $\deg(p) = O(n)$. We use algorithms of order $O(n)$ to carried out the calculation of $p_k'(z)$, $p_k(z_0)$ and $p_k q_i$, where $q_i$ is fixed. It follows that the previous procedure to compute $\{\text{Res}(r_k, z_0)\}_{k=1}^\nu$ is of order $O(n^3)$, provided that $\nu = O(n)$. Finally, if we apply this algorithm to (14)–(15), then the calculation of the coefficients of the $n$-point quadrature requires $O(n^3)$ operations. Moreover, if we approximate $\lambda_{n,k}(1/q)$ by the $N$th partial sum of the series expansion in (15), then the computational effort is $N$ times greater than that we make to evaluate $\lambda_{n,k}(h_1 W_1/q)$, by using (14). The range $64 \leq N \leq 512$ is suggested by Example 5, though this should vary according to the features of the integrand.

For the purposes of comparison, the reader is referred to [6, 1997] and the bibliography therein. More recently, Deckers et al [3, 2009] presented an algorithm of order $O(n)$ to compute rational Gauss quadrature formulas, provided that the set of poles is finite and does not depend on $n$. It is also proved in [3] that the order is $O(n^2)$ when all poles are different.
4. Examples

From the previous corollaries we can derive several integration methods. The following examples show that these procedures behave differently, depending on how we select $f$ and $G$.

Example 1. $I_\delta(k, \eta, \theta) = \int_0^\delta \frac{\sqrt{1 + 0.5\theta x}}{e^{-\eta} + e^{-x}} x^k e^{-x} dx$.

Fermi-Dirac integrals are defined as $F(k, \eta, \theta) = \lim_{\delta \to \infty} I_\delta(k, \eta, \theta)$. Further, $I_\delta(k, \eta, \theta)$ can be expressed as follows.

$I_\delta(k, \eta, \theta) = \delta^{k+1} \int_0^1 \frac{\sqrt{1 + 0.5\theta \delta x}}{e^{-\eta} + e^{-\delta x}} x^k e^{-\delta x} dx = \delta^{k+1} \int_{-1}^1 \frac{\sqrt{1 + 0.5\theta \delta (1 - x^2)}}{e^{-\eta} + e^{-\delta (1 - x^2)}} e^{-\delta (1 - x^2)} |x| \frac{(1 - x^2)^{k+1/2}}{\sqrt{1 - x^2}} dx$.  

Table 1: The integral of Example 1 is evaluated by rational Gauss quadrature ($E_G$), and by an interpolatory rule ($E$) based on formula (12), with $\theta = 10^{-4}$, $\eta = -1$, $k = 0.5$ and $m = \deg(q)$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$m$</th>
<th>$E_G$</th>
<th>$n$</th>
<th>$m$</th>
<th>$E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>5.2e-02</td>
<td>1</td>
<td>$\infty$</td>
<td>9.6e-04</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>1.3e-03</td>
<td>2</td>
<td>$\infty$</td>
<td>4.6e-04</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>2.7e-05</td>
<td>3</td>
<td>$\infty$</td>
<td>1.0e-07</td>
</tr>
<tr>
<td>4</td>
<td>8</td>
<td>2.2e-07</td>
<td>4</td>
<td>$\infty$</td>
<td>4.4e-08</td>
</tr>
<tr>
<td>5</td>
<td>10</td>
<td>4.0e-07</td>
<td>5</td>
<td>$\infty$</td>
<td>1.7e-11</td>
</tr>
<tr>
<td>7</td>
<td>14</td>
<td>1.9e-12</td>
<td>7</td>
<td>$\infty$</td>
<td>4.6e-15</td>
</tr>
</tbody>
</table>

Concerning the integrals of Fermi-Dirac, the only values of $k$ which are interesting for physics are $k = 1/2, 3/2, 5/2$. In this case, the Chebyshev weight function is $W(x) = (1 - x^2)^{k+1/2}/(\pi \sqrt{1 - x^2})$.

For comparison purposes, the values we have adopted for $\eta$ and $\theta$, correspond to examples previously studied by Gautschi [7]. Next we describe the process of calculating $F(k, \eta, \theta)$, using routines based upon Corollary 1.

The very first step is that the integration interval must be truncated conveniently. Instead of $F(1/2, -1, 10^{-4})$, we try to evaluate $I_{40}(1/2, -1, 10^{-4})$, which approximates the former up to 16 decimal figures. In turn, the new
integral on the interval \([0, 40]\) can be transformed into \(\int_{-1}^{1} f(x)G(x)W(x)dx\), where
\[
f(x) = \pi 40^{3/2}\sqrt{1 + 0.002(1 - x^2)}, \quad G(x) = \frac{E(x)}{q_{\infty}(x)},
\]
with \(E(x) = e^{-40(1-x^2)|x|}, \quad q_{\infty}(x) = e + e^{-40(1-x^2)}, \quad \text{and} \quad h_1(x) = (1 - x^2)\).

The zeros of \(q_{\infty}\) are much closer to \([-1, 1]\) than those of the denominator \((e + e^{-x})\), a fact which appears to be an added disadvantage.

Formula (12) allows us to obtain accurate results when calculating the integral \(I_{40}(-1, 1/2, 10^{-4})\), up to the quadrature order \(n = 512\). For purposes of comparison we have tabulated some of them in Table 1 under the label \(E\). Column \(E_G\) enumerates the relative errors reported by Gautschi [7] when rational Gauss quadrature is applied to Fermi-Dirac integrals.

**Example 2.** \(J_\delta(k, \eta, \theta) = \int_{0}^{\delta} \frac{\sqrt{1 + 0.5\theta x}}{e^{-\eta} - e^{-x}} x^k e^{-x}dx\).

*Bose-Einstein integrals are defined as* \(B(k, \eta, \theta) = \lim_{\delta \to \infty} J_\delta(k, \eta, \theta)\).

Using a procedure similar to that applied to Fermi-Dirac integrals, we have estimated the values of \(J_\delta(-1, 0.5, 10^{-4})\). The corresponding errors are shown in Table 2, to be compared with the results obtained by Gautschi [7].

**Table 2:** The integral of Example 2 is evaluated by rational Gauss quadrature \((E_G)\), and by an interpolatory rule \((E)\) based on formula (12), with \(\theta = 10^{-4}, \eta = -1, k = 0.5\) and \(\deg(q) = m\).

<table>
<thead>
<tr>
<th>(n)</th>
<th>(m)</th>
<th>(E_G)</th>
<th>(n)</th>
<th>(m)</th>
<th>(E)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2.5e-01</td>
<td>1</td>
<td>1</td>
<td>9.6e-04</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>7.8e-03</td>
<td>2</td>
<td>2</td>
<td>4.6e-04</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>1.7e-04</td>
<td>3</td>
<td>3</td>
<td>1.0e-07</td>
</tr>
<tr>
<td>4</td>
<td>7</td>
<td>2.7e-06</td>
<td>4</td>
<td>4</td>
<td>4.6e-08</td>
</tr>
<tr>
<td>5</td>
<td>9</td>
<td>6.5e-07</td>
<td>5</td>
<td>5</td>
<td>1.9e-11</td>
</tr>
<tr>
<td>6</td>
<td>11</td>
<td>2.5e-08</td>
<td>6</td>
<td>6</td>
<td>7.3e-12</td>
</tr>
</tbody>
</table>

**Example 3.** \(\int_{-1}^{1} \frac{x/\omega}{\sin(\pi x/\omega)} \sqrt{1-x^2}dx, \omega > 1\).

If \(|\omega - 1|\) is small and \(z_n = \pm n\omega, n = 1, 2, ...,\) then some points \(z_n\) could be classified as difficult poles.
Table 3 depicts the relative errors when it is used a procedure based on Corollary 2, with \( h_1(x) = (1 - x^2) \) and \( q(x) = (1 - x^2/1.001^2) \). Note that when \( n \) is large, the numerical method is fairly stable despite the presence of difficult poles. The entire process consumes less than a second when \( n = 2048 \).

Table 3: Errors when the integral of Example 3 is evaluated by an interpolatory rule based on Corollary 2, with \( \omega = 1.001 \)

<table>
<thead>
<tr>
<th>( n )</th>
<th>( E )</th>
<th>( n )</th>
<th>( E )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2.0e - 02</td>
<td>64</td>
<td>3.3e - 16</td>
</tr>
<tr>
<td>4</td>
<td>1.4e - 03</td>
<td>128</td>
<td>4.9e - 16</td>
</tr>
<tr>
<td>8</td>
<td>9.1e - 06</td>
<td>256</td>
<td>4.9e - 16</td>
</tr>
<tr>
<td>16</td>
<td>1.8e - 10</td>
<td>1024</td>
<td>9.8e - 16</td>
</tr>
<tr>
<td>32</td>
<td>1.6e - 16</td>
<td>2048</td>
<td>2.3e - 15</td>
</tr>
</tbody>
</table>

Example 4. \[
\int_{-1}^{1} \frac{\pi x/\omega}{\sinh(\pi x/\omega)} \sqrt{1 - x^2} \, dx, \, |\omega| > 1. \]

Column \( E_1 \) of Table 4 gives the relative errors when (13) is used to compute \( \lambda_{2n+1,k} \left( G_n(x)/\sqrt{1 - x^2} \right) \), with \( G_n(x) = (1 - x^2) \prod_{k=1}^{n} (x^2/(k\omega^2) + 1)^{-1} \). Column \( E_2 \) lists the relative errors when all the poles have been moved to the weight function, i.e. \( G(x) = (1 - x^2)(\pi^2 x/\omega)/\sinh(\pi x/\omega) \). The results are compared with those obtained by using Gauss-Chebyshev quadrature formula of rational type (cf. [2, Example 5.2]). In this example, all the poles of the integrand are benign.

Table 4: Example 4 is evaluated by rational Gauss-Chebyshev quadrature (\( GCh \)), and by an interpolatory rule (\( E \)) based on (13), with \( \omega = 1.001 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( GCh )</th>
<th>( E_1 )</th>
<th>( E_2 )</th>
<th>( n )</th>
<th>( GCh )</th>
<th>( E_1 )</th>
<th>( E_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1.1e - 03</td>
<td>1.3e - 02</td>
<td>1.4e - 14</td>
<td>17</td>
<td>3.8e - 16</td>
<td>3.7e - 15</td>
<td>1.3e - 14</td>
</tr>
<tr>
<td>5</td>
<td>4.5e - 07</td>
<td>4.7e - 05</td>
<td>1.4e - 14</td>
<td>33</td>
<td>1.9e - 16</td>
<td>4.0e - 15</td>
<td>1.3e - 14</td>
</tr>
<tr>
<td>9</td>
<td>5.8e - 16</td>
<td>7.1e - 11</td>
<td>1.3e - 14</td>
<td>14</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The difficult poles of the integrand are exactly the same as those of Example 3. Let \( q(x) = \prod_{j=1}^{m}(j^2\omega^2 - x^2) \), with \( \omega > 1 \). In order to apply Corollary 3 we rewrite the integrand as \( f(x)K(x)W_1(x)/q(x) \), where \( f(x) = (\pi t/\omega)q(x)/\sin(\pi t/\omega) \) and \( K(x) = \pi \sqrt{1-x^2} \). Column \( E_G \) of Table 5 shows the errors when this integral is evaluated by a rational Gauss quadrature according to Gautschi’s approach [7]. The numbers below \( E_N \) are the relative errors produced by the interpolatory rule (4), when the coefficients are obtained from (15), and the Chebyshev series of \( \sqrt{1-x^2} \) is replaced by its \( N \)th partial sum. The errors corresponding to \( N = 64, 128, 256 \), are displayed to show that is not worth to choose \( N > 128 \).

Table 5: Errors when the integral of Example 5 is evaluated by rational Gauss quadrature \( (E_G) \) and by an interpolatory rule \( (E_N) \) based on Corollary 3, with \( \omega = 1.001 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( E_G )</th>
<th>( E_{64} )</th>
<th>( E_{128} )</th>
<th>( E_{256} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \deg(q) = 2 )</td>
<td>2</td>
<td>8.4e-02</td>
<td>1.8e-01</td>
<td>1.9e-01</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1.3e-03</td>
<td>2.7e-02</td>
<td>2.7e-02</td>
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<tr>
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<td>4</td>
<td>1.7e-04</td>
<td>1.1e-02</td>
<td>1.1e-02</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>2.0e-05</td>
<td>1.5e-03</td>
<td>1.5e-03</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>9.3e-06</td>
<td>6.4e-04</td>
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<td>7</td>
<td>7.8e-06</td>
<td>5.8e-05</td>
<td>8.1e-05</td>
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<tr>
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<td>10</td>
<td>2.0e-05</td>
<td>1.8e-06</td>
<td>1.9e-06</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>2.2e-05</td>
<td>7.1e-08</td>
<td>9.2e-08</td>
</tr>
<tr>
<td>( \deg(q) = 4 )</td>
<td>2</td>
<td>2.9e-03</td>
<td>1.1e-01</td>
<td>1.1e-01</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>3.5e-04</td>
<td>9.6e-03</td>
<td>9.6e-03</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>1.9e-05</td>
<td>3.9e-03</td>
<td>3.9e-03</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>6.6e-06</td>
<td>2.5e-04</td>
<td>2.7e-04</td>
</tr>
<tr>
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<td>9.2e-05</td>
<td>1.1e-04</td>
</tr>
<tr>
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<td>6.9e-06</td>
<td>6.9e-06</td>
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<td>10</td>
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<td>4.8e-08</td>
<td>6.9e-08</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>2.2e-05</td>
<td>1.9e-08</td>
<td>1.5e-09</td>
</tr>
</tbody>
</table>

Example 6. \( \int_{-1}^{1} \frac{e^x}{x^2 + \varepsilon^2} \, dx \).

This integrand has difficult poles at \( \pm \varepsilon i \), when \( |\varepsilon| \) is small. We rewrite the integrand as \( fGW_1 \), where \( f(x) = e^x \) and \( G(x) = \pi \sqrt{1-x^2}/(x^2 + \varepsilon^2) \). Column \( E_1 \) of Table 6 shows the accuracy obtained when this integral is
evaluated by formula (4), and its coefficients are estimated using equation (12) of Corollary 1, with \( K(x) = G(x) \). If \( K(x) = \pi \sqrt{1-x^2} \), then we apply Corollary 3 to Example 6, with \( N = 512 \), to obtain the errors which are shown under \( E_3 \). To compare with Monegato’s method, the only three results reported in [9] appear in column \( E_M \). The results in Table 6 are relatively poor for \( n \geq 10 \), because Chebyshev nodes of the first kind seem to be inadequate for integrals whose mass is highly concentrated near \( x = 0 \). This also explains why the errors tend to be smaller when \( n \) is odd.

Table 6: Errors when the integral of Example 6 is evaluated by an interpolatory rule based on Corollary 1 (\( E_1 \)) and Corollary 3 (\( E_3 \)), with \( \varepsilon = 0.01 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( E_1 )</th>
<th>( E_3 )</th>
<th>( E_M )</th>
<th>( n )</th>
<th>( E_1 )</th>
<th>( E_3 )</th>
<th>( E_M )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.2e-03</td>
<td>3.2e-01</td>
<td></td>
<td>7</td>
<td>3.7e-09</td>
<td>3.7e-09</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2.6e-01</td>
<td>2.6e-01</td>
<td></td>
<td>8</td>
<td>1.8e-07</td>
<td>1.8e-07</td>
<td>1.3e-07</td>
</tr>
<tr>
<td>3</td>
<td>1.1e-04</td>
<td>1.1e-04</td>
<td></td>
<td>9</td>
<td>9.3e-12</td>
<td>3.1e-11</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>5.2e-03</td>
<td>5.2e-03</td>
<td>3.5e-03</td>
<td>10</td>
<td>5.0e-10</td>
<td>4.8e-10</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>8.3e-07</td>
<td>8.3e-07</td>
<td></td>
<td>11</td>
<td>6.5e-13</td>
<td>2.1e-11</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>4.2e-05</td>
<td>4.2e-05</td>
<td></td>
<td>16</td>
<td>6.3e-13</td>
<td>2.1e-11</td>
<td>2.0e-16</td>
</tr>
</tbody>
</table>

In order to provide a variant of the previous method, we use the following transformation of the integrand to move its poles to a region near the ends of the interval.

\[
\int_{-1}^{1} \frac{e^x}{x^2 + \varepsilon^2} dx = \int_{-1}^{1} \frac{\cosh(\sqrt{1-x^2}) |x| dx}{(1-x^2 + \varepsilon^2)\sqrt{1-x^2}} \tag{19}
\]

Now, let us examine Example 6 using (19). The following table depicts three different ways of choosing the integrand \( f \) and the difficult factor \( G \), with \( W(x) = 1/(\pi \sqrt{1-x^2}) \) in all cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>( f )</th>
<th>( G )</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>( \pi \cosh(\sqrt{1-x^2}) )</td>
<td>(</td>
</tr>
<tr>
<td>II</td>
<td>( \pi</td>
<td>x</td>
</tr>
<tr>
<td>III</td>
<td>( \pi )</td>
<td>( \cosh(\sqrt{1-x^2})</td>
</tr>
</tbody>
</table>

Table 7 lists the relative errors for the three cases, when the procedure is based upon equation (13). The results for case II are affected by the presence of \( |x| \) in the integrand. To increase accuracy, we have calculated \( 5 \times 10^7 \) coefficients \( A_j \). Case III of Table 7 indicates that, for \( n \leq 15 \), the procedure based on (19) can provide higher precision than Monegato’s method.
Table 7: The integral of Example 6 is evaluated using (19), with $\varepsilon = 0.01$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$I$</th>
<th>$II$</th>
<th>$III$</th>
<th>$n$</th>
<th>$I$</th>
<th>$II$</th>
<th>$III$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$2.6e-01$</td>
<td>$2.9e-01$</td>
<td>$6.0e-15$</td>
<td>64</td>
<td>$6.9e-15$</td>
<td>$6.0e-06$</td>
<td>$8.0e-15$</td>
</tr>
<tr>
<td>4</td>
<td>$5.2e-03$</td>
<td>$3.5e-02$</td>
<td>$6.0e-15$</td>
<td>128</td>
<td>$1.2e-14$</td>
<td>$5.8e-07$</td>
<td>$1.0e-14$</td>
</tr>
<tr>
<td>8</td>
<td>$1.8e-07$</td>
<td>$4.4e-03$</td>
<td>$6.4e-15$</td>
<td>256</td>
<td>$1.0e-14$</td>
<td>$7.3e-08$</td>
<td>$1.0e-14$</td>
</tr>
<tr>
<td>16</td>
<td>$6.9e-15$</td>
<td>$5.3e-04$</td>
<td>$7.1e-15$</td>
<td>512</td>
<td>$1.4e-14$</td>
<td>$1.6e-08$</td>
<td>$1.2e-14$</td>
</tr>
<tr>
<td>32</td>
<td>$5.1e-15$</td>
<td>$5.9e-05$</td>
<td>$5.3e-15$</td>
<td>1024</td>
<td>$1.2e-14$</td>
<td>$3.9e-09$</td>
<td>$1.0e-14$</td>
</tr>
</tbody>
</table>

5. Note on the coefficients $A_j$

Both formulas (12) and (13) have shown to be a good reference to develop routines in any programming language. They depend on the first $d + n + 1$ coefficients of the Chebyshev series expansion $K(x) = \sum_{j=0}^{\infty} A_j T_j(x)$, which in turn could depend on other parameters. For example, the previous schema for Fermi-Dirac integrals refers to $q_{\infty}(x) = e^{-\eta} + e^{-40(1-x^2)}$, hence $A_j = A_j(\eta)$. A physical fact is that the parameter $\eta$ depends on temperature, so the coefficients $A_j$ are often calculated and the procedure becomes more costly. In such case it seems to be more convenient to put $q_{\infty} \equiv 1$, namely

$$f(x) = \pi 40^{3/2} \frac{\sqrt{1 + 0.002(1 - x^2)}}{e^{-\eta} + e^{-40(1-x^2)}}, \quad G(x) = e^{-40(1-x^2)}|x|. \quad (20)$$

Table 8 enumerates relative errors for different values of $\eta$ when both the integrand and the weight function are selected according to (20). Despite of the convergence being slower, it is quite easy to reach a precision of 14 decimal figures. The advantage of this variant is that the coefficients are calculated only once.

Table 8: Errors when the integral of Example 1 is evaluated for several values of $\eta$, with $\theta = 10^{-4}$, $k = 0.5$, $q_{\infty} \equiv 1$.

<table>
<thead>
<tr>
<th>$\eta$</th>
<th>$n = 4$</th>
<th>$n = 16$</th>
<th>$n = 32$</th>
<th>$n = 64$</th>
<th>$n = 80$</th>
<th>$n = 128$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-10^{-2}$</td>
<td>$3.0e-01$</td>
<td>$1.1e-02$</td>
<td>$8.5e-05$</td>
<td>$1.3e-10$</td>
<td>$1.8e-13$</td>
<td>$5.0e-16$</td>
</tr>
<tr>
<td>$-1$</td>
<td>$1.2e-01$</td>
<td>$1.0e-02$</td>
<td>$2.2e-05$</td>
<td>$1.4e-12$</td>
<td>$1.3e-14$</td>
<td>$9.6e-16$</td>
</tr>
<tr>
<td>$-5$</td>
<td>$2.4e-03$</td>
<td>$3.0e-04$</td>
<td>$1.5e-07$</td>
<td>$2.0e-15$</td>
<td>$1.6e-14$</td>
<td>$7.3e-16$</td>
</tr>
<tr>
<td>$-10$</td>
<td>$1.6e-05$</td>
<td>$2.0e-06$</td>
<td>$1.3e-09$</td>
<td>$6.9e-15$</td>
<td>$2.1e-14$</td>
<td>$4.7e-15$</td>
</tr>
</tbody>
</table>
The coefficient $A_j$ is the integral of $K$ with respect to the weight $2T_jW_1$, so we can construct a low cost procedure from the following formula.

$$A_j \approx \sum_{k=1}^{n} \lambda_{n,k}(2T_jW_1)K(x_{n,k}), \ j = 1, 2, \ldots, \ (21)$$

and $A_0 \approx \sum_{k=1}^{n} \lambda_{n,k}(W_1)K(x_{n,k})$.

Let $P_{n-1,K}$ be the Lagrange polynomial of degree $n-1$, which interpolates $K$ at the Chebyshev points \{x_{n,k}\}. Then $P_{n-1,K}(x) = \sum_{j=0}^{n-1} d_{n,j}T_j(x)$, where

$$d_{n,j} = \frac{2}{n} \Re \left( \sum_{k=0}^{n-1} K(x_{n,k}) \exp\left( \frac{i\pi j (2k + 1)}{2n} \right) \right), \ j \geq 1, \ (22)$$

and $d_{n,0} = \sum_{k=0}^{n-1} K(x_{n,k})/n$.

We use orthogonality and Proposition 2 to prove that (21) is exact in the limit, i.e. $\lim_n d_{n,j} = A_j$.

From the above we deduce the following formulas for $A_j$.

If $K$ is even, then $A_{2j} \approx 2\Re(A^{(1)}_{j,n})$, where

$$A^{(1)}_{j,n} = \frac{e^{-j\pi i/n}}{n} \sum_{k=0}^{n-1} K(x_{n,k}) \exp\left( -\frac{2kj\pi i}{n} \right), \ (23)$$

and $A_0$ must be halved.

If $K$ is odd, then $A_{2j+1} \approx 2\Re(A^{(2)}_{j,n})$, where

$$A^{(2)}_{j,n} = \frac{e^{-j\pi i/n}}{n} \sum_{k=0}^{n-1} K(x_{n,k})e^{-i\pi (2k+1)/(2n)} \exp\left( -\frac{2kj\pi i}{n} \right). \ (24)$$

Both expressions (23) and (24) can be computed efficiently by means of any FFT algorithm. The larger the value of $n$, the better the approximation of the coefficients $A_j$. Nevertheless, the convergence of both formulas (23) and (24), is not uniform with respect to $j$, as $n \to \infty$. The size of $n$ in formulas (23) and (24) depends on the code we use to simulate $K$, as well as the mathematical complexity of the latter.

In the experimental stage of this work, we have used Matlab® tools to carry on the calculations with a precision of 15 decimal figures. The programs have been run using a 64-bit CPU, with frequency of 3.3 GHz.
6. Concluding remarks

Formulation (4)–(5) and the theory in Section 2 attempt to go beyond the well known rational approach, although the discretization process is mainly established in terms of rational functions, as shown in Section 3. The non-rational focus we want to introduce is given by Corollary 1. Using the latter we have shown that, in some cases, a modified interpolatory rule can provide superior accuracy to that obtained by rational Gauss formula. Besides, Corollary 1 allows to remove one of the worst drawbacks of the rational methods, namely, the need of calculating all the difficult poles of the integrand. Likewise, the calculation of the coefficients can be done in a way much simpler for some special cases.

An objection to the results of Section 3 is that some of them contemplate the calculation of residues of rational functions at some poles, which is an ill-conditioned problem when the denominator is near a polynomial with multiple roots. That is why we have suggested a very simple algorithm in Section 4. On the other hand, equation (12) of Corollary 1 is established solely in terms of residues at the point \( z = 0 \), that are fairly easy to calculate in terms of the derivatives of a polynomial. In principle, all cases can be reduced to formula (13), which requires little coding effort.

We have implemented our approach for a type of integral which includes the four kinds of Chebyshev weight functions. Any definite integral on a bounded interval can be transformed into another integral in which appears one of the four Chebyshev weight functions. The following equation differs from (19) and corroborates the above statement.

\[
\int_a^b Z(x)dx = \frac{b - a}{2} \int_{-1}^1 \frac{Z((b - a)\sqrt{1 - x^2} + a)\sqrt{1 - x^2}}{\sqrt{1 - x^2}} |x|dx. \tag{25}
\]

However, no formula is appropriate for all cases, and (25) is no exception.

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References


