Logo

ISSN: 1889-3066

Web site: jja.ujaen.es

Jaen J. Approx. x(x) (20xx), 1–xx

Logo

Interpolatory quadrature formulas for meromorphic integrands†

J. R. Illán González

Abstract

Let $\mathcal{I}_W(f) = \int_a^b f(x)W(x)dx$, where the integrand f is analytic on $[a, b]$ and probably meromorphic on an open set $V \supset [a, b]$. A variety of Gauss quadrature formulas based on rational functions, have been intensively applied in the last thirty years to evaluate $\mathcal{I}_W(f)$. One of the drawbacks of these procedures is that to become efficient, coefficients and nodes must depend on the poles of f. Monegato [8] presented a less costly approach based on interpolatory rules whose nodes are those common to a couple of simultaneous quadrature formulas of polynomial type. In this paper we examine a variant of Monegato's method, to estimate $\mathcal{I}_W(f)$ by means of procedures which are not of Gauss type. Our approach is mainly based upon the rational modification BW/A, which is superior to W/A, when some zeros of f lie near $[a, b]$.

Keywords: Quadrature formulas of interpolatory type, ill-scaled integrands, smoothing transformation, difficult poles, difficult zeros, meromorphic integrands..

MSC: Primary 41A55; Secondary 41A25, 42B35.

§1. Introduction

Most forms of addressing the problem of integrating functions poorly scaled are related to one of the following strategies: $\mathbf{S_1}$) *find a suitable modification of the integrand and the weight function*, $\mathbf{S_2}$) *fit a new variable into the integral.*

†This work was supported by a research grant from the Ministerio de Ciencia e Innovación, Spain, project code MTM 2008-00341.

Regarding $\mathbf{S_1}$), the problem we face after having made a modification of the weight function, is the calculation of those quadrature parameters that are associated with the new integrator, so that some additional numerical techniques are probably needed. On the other hand, the effectiveness of $\mathbf{S_2}$ depends a lot on the complexity of the integrand. In any event, our aim is to design a method which diminishes the computational effort.

Let I be a finite interval and f a real bounded Riemann integrable function on I. Given a Lebesgue integrable function $W(x)$ and a preassigned set of nodes $\{x_{n,j};\ j = 1, ..., n\}$, the following formulation corresponds to the product integration scheme.

$$\mathcal{I}_W(f) = \int_I f(x)W(x)dx \approx \mathcal{I}_{n,W}(f) = \sum_{j=1}^{n} \lambda_{n,j}(W)f(x_{n,j}). \tag{1.1}$$

We say that (1.1) is of interpolatory type when

$$\lambda_{n,j}(W) = \int_I \frac{Q_n(x)W(x)dx}{(x - x_{n,j})Q'(x_{n,j})},\quad Q_n(x) = \prod_{j=1}^{n}(x - x_{n,j}). \tag{1.2}$$

An equivalent statement for interpolatory quadrature formulas of polynomial type consists in assuming that (1.1) is exact when f is a polynomial of degree at most $n-1$. The maximum degree of exactness is $2n-1$, and it is reached by the so-called Gaussian quadrature formulas.

When f is ill-scaled, a numerical procedure based on a quadrature formula can produce a poor approximation of $\mathcal{I}_W(f)$.([1] This phenomenon occurs when some poles or zeros of f are too close to I, or f can be represented as a product of several factors and one of them varies exponentially (see [13]). Those poles of f which are the closest to I are usually called "difficult" if numerical instability shows up when a procedure like (1.1) is applied. The qualifying term "difficult" can also be applied to the zeros of f, if any.

A suitable approach we may follow, to make less harmful the effect produced by the difficult poles and zeros of f, is that which is given in terms of a suitable rational modification of W (strategy $\mathbf{S_1}$). Let $A(x)$ and $B(x)$ be two polynomials with real coefficients and such that $A(x) > 0$ and $B(x) > 0$, for all $x \in I$. The integral $\mathcal{I}_W(f)$ can be rewritten as $\mathcal{I}_{\widetilde{W}}(Af/B)$, where $\widetilde{W} = BW/A$, so that the new integrand $\widetilde{f} = Af/B$ is no longer an ill-scaled function.

Some of the techniques to make less costly the treatment of difficult poles, are due to Bultheel [4, 5], and Monegato [8]. The strategy followed by Monegato consists in selecting the nodes $\{x_{n,j}\}$ as

[1] The notion of "ill-scaled function" is established in Section 5.

those of the Gaussian rule associated to a weight $w(x)$, previously chosen, so that the main effort is addressed to compute the coefficients $\lambda_{n,j}(W/A)$.

The purpose of this paper is to describe a variant of the method of Monegato, which is based on the B/A-modification of the weight W. The theoretical part of our method, like that of Monegato, uses the technique by Sloan and Smith [10]. The following result is relevant.

Theorem 1.1. *([10]) Let $W(x)$ be an integrable positive weight function on $(-1,1)$. Let $Q_n(x)$ be the n-th degree polynomial orthogonal on $(-1,1)$ with respect to a nonnegative weight function $w(x)$, with zeros $x_{n,1}$,...,$x_{n,n}$, and*

$$\int_{-1}^{1} \frac{W(x)^2}{w(x)} dx < \infty. \tag{1.3}$$

Then, for all bounded Riemann integrable function $f(x)$, we have

$$\lim_n \sum_{j=1}^{n} |\lambda_{n,j}(W)| f(x_{n,j}) = \lim_n \sum_{j=1}^{n} \lambda_{n,j}(W) f(x_{n,j}) = \int_{-1}^{1} f(x)W(x)dx. \tag{1.4}$$

Notice that if condition (1.3) is valid for the weight W, then it also holds for any modification BW/A.

In section 2 we examine convergence when $f \in C[a,b]$ (real and continuous functions on $[a,b]$) and the approximants are constructed with respect to variant weights $\widetilde{W}_n = B_n W/A_n$. The case concerning with meromorphic integrands will be only considered in the section where the numerical method is described.

We can split up the ratio of two polynomials with real coefficients into a sum of ratios of polynomials with smaller degree. In principle, the technique based on the rational modification of W could be reduced to consider the following rational functions:

I) $1/(x+x_0)^m$, $x_0 \in \mathbb{R} \setminus [a,b], m \in \mathbb{N}$,

II) $1/((x-\delta)^2+\varepsilon^2)^h$, $h \in \mathbb{N}$, $\delta \in [a-\eta, b+\eta]$, $\eta > 0$,

where the distance $d(x_0,[a,b])$, $|\varepsilon|$ and η are assumed to be small for numerical purposes (see [8, 12]).

In section 3 we describe a procedure to obtain the quadrature parameters, which is mainly based on the modified moments algorithm. It is shown that both cases I-II can be considered simultaneously by using a general formulation for the quadrature weights $\lambda_{n,j}(\widetilde{W})$.

In order to calculate the first moments which appears in the algorithm, we apply a change of variable which is presented in Section 4.

Section 5 is devoted to demonstrate the superiority of the method based on the rational modification B/A by comparing with that corresponding to $1/A$. There are also listed some numerical results which show the power of the technique of changing the integration variable when it is applied in a piecewise form.

For the rest of the article we shall keep the notation and assumptions of this section.

§2. Convergence results

In this part we shall give sufficient conditions for the convergence of the quadrature formulas of polynomial type given by (1.1-1.2), but now with respect to the variant weights $\widetilde{W}_n$. In order to round off this work, we have extended this analysis to the rational quadrature formulas of interpolatory type.

Let Π_n be the space of all polynomials of degree at most n. In what follows, we shall assume that $\{A_n\}$ and $\{B_n\}$ are two sequences of polynomials with real coefficients and such that $A_n \in \Pi_n$, $A_n(x) > 0$, $B_n(x) > 0$ for all $x \in I = [a, b]$, and every $n \in \mathbb{N}$. Notice that it has not been made any assumption on the degree of B_n.

The polynomial method we consider here is similar to that examined in [8], and it can be formulated in terms of the exactness condition to be fulfilled, that is, the equality $\mathcal{I}_{n,\widetilde{W}_n}(f) = \mathcal{I}_{\widetilde{W}_n}(f)$ holds true for every $p \in \Pi_{n-1}$. We recall that the nodes $x_{n,j}$, $j = 1, ..., n$, are just the roots of the n-th orthogonal polynomial associated with w, so they do not depend on the rational modification $\widetilde{W}_n$ we have selected.

The coefficients $\widetilde{\lambda}_{n,j}(\widetilde{W}_n)$ of the rational quadrature formula of interpolatory type, associated with the trio $(W, \{A_n\}, \{B_n\})$, are given by the following expression

$$\widetilde{\lambda}_{n,j}(\widetilde{W}_n) = \frac{A_n(x_{n,j})}{B_n(x_{n,j})}\lambda_{n,j}(\widetilde{W}_n).$$

Let us adopt the notation $\widetilde{\mathcal{I}}_{n,\widetilde{W}_n}(f)$ for the quadrature sum associated with $\widetilde{\lambda}_{n,j}(\widetilde{W}_n)$. Then

$$\underbrace{\widetilde{\mathcal{I}}_{n,\widetilde{W}_n}(B_n f/A_n)}_{Rational} = \underbrace{\mathcal{I}_{n,\widetilde{W}_n}(f) = \mathcal{I}_{\widetilde{W}_n}(f)}_{Polynomial} = \underbrace{\mathcal{I}_W(B_n f/A_n)}_{Rational} \tag{2.1}$$

for every $f \in \Pi_{n-1}$.

Equation (2.1) shows something which is well known: the condition of exactness, which serves to define the rational quadrature formulas, is the same as that we use to define the quadrature formulas of polynomial type with respect to variant measures. The only fact is that they are written in a different way. The technical differences between these two approaches can be appraised by comparing the statement of Theorem 2.3 and 2.9.

2.1. Asymptotical stability

In the sequel we shall assume one of the two following conditions.

C1) $B_n(x) \leq cA_n(x)$, $x \in I$, $n \in \mathbb{N}$,

C2) $c_1 A_n(x) \leq B_n(x) \leq c_2 A_n(x)$, $x \in I$, $n \in \mathbb{N}$,

for some $c, c_1, c_2 > 0$.

Lemma 2.1. *Suppose that (1.3) takes place. Then,*

1. *Condition (C1) implies that* $\sup_n \sum_{j=1}^{n} \left|\lambda_{n,j}(\widetilde{W}_n)\right| < \infty$.

2. *Condition (C2) implies that* $\sup_n \sum_{j=1}^{n} \left|\widetilde{\lambda}_{n,j}(\widetilde{W}_n)\right| < \infty$.

Proof. The technique we apply here is a variant of [2, Theorem 2].

Let $S_{n,m}(x)$ be the m-th partial sum of the Fourier series of $B_n W/(wA_n) \in L^2(w)$. Taking into account the orthogonality condition and that $\deg(Q_n(x)/(x - x_{n,j})) = n - 1$, we can write

$$\lambda_{n,j}(\widetilde{W}_n) = \int_a^b \frac{Q_n(x)}{Q_n'(x_{n,j})(x - x_{n,j})} S_{n,n-1}(x) w(x) dx.$$

We can also apply orthogonality conditions to the polynomial

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

which has degree $n - 2$, to obtain that

$$\lambda_{n,j}(\widetilde{W}_n) = S_{n,n-1}(x_{n,j})\lambda_{n,j}(w) = S_{n,n-1}(x_{n,j})\lambda_{n,j}^{1/2}(w)\lambda_{n,j}^{1/2}(w). \tag{2.2}$$

We sum the terms in both sides of (2.2) for $j = 1, ...n$, and we apply the Cauchy-Schwartz inequality to get the following estimate

$$\sum_{j=1}^{n} \left|\lambda_{n,j}(\widetilde{W}_n)\right| \leq \left(\sum_{j=1}^{n} S_{n,n-1}^2(x_{n,j})\lambda_{n,j}(w)\right)^{1/2} \left(\sum_{j=1}^{n} \lambda_{n,j}(w)\right)^{1/2}. \tag{2.3}$$

Observe that $\deg(S^2_{n,n-1}) = 2n-2$, so we can use the exactness condition for the Gauss quadrature formula associated with w. In addition we apply the Bessel inequality to obtain

$$\sum_{j=1}^{n} \left|\lambda_{n,j}(\widetilde{W}_n)\right| \leq \left(\int_a^b \left(\frac{\widetilde{W}_n(x)}{w(x)}\right)^2 w(x)dx\right)^{1/2} \left(\int_a^b w(x)dx\right)^{1/2}.$$

Using condition (C1) we can derive the following inequality, which proves the first part of the lemma.

$$\sum_{j=1}^{n} \left|\lambda_{n,j}(\widetilde{W}_n)\right| \leq c_1 \mathcal{I}_W(W/w) \left(\int_a^b w(x)dx\right)^{1/2}. \tag{2.4}$$

If condition (C2) holds true then we can also obtain, by using the previous technique, the following estimate

$$\sum_{j=1}^{n} \left|\widetilde{\lambda}_{n,j}(\widetilde{W}_n)\right| \leq \frac{c_2}{c_1} \mathcal{I}_W(W/w) \left(\int_a^b w(x)dx\right)^{1/2}. \tag{2.5}$$

The lemma has been proved. ■

2.2. Polynomial rules with respect to variant weights

Lemma 2.2. *If (1.3) and condition (C1) hold true, then*

$$\lim_n (\mathcal{I}_{n,\widetilde{W}_n}(f) - \mathcal{I}_{\widetilde{W}_n}(f)) = 0,$$

for every $f \in C[a,b]$.

Proof. The approximation formula $\mathcal{I}_{n,\widetilde{W}_n}(f) \approx \mathcal{I}_{\widetilde{W}_n}(f)$ fulfils a condition of exactness which guarantees that the limit above exists and is equal to zero for every polynomial f. Lemma 2.1 allows to prove that the sequence of linear and continuous functionals $L_n(f) = \mathcal{I}_{n,\widetilde{W}_n}(f) - \mathcal{I}_{\widetilde{W}_n}(f)$, $f \in C[a,b]$, is uniformly bounded.

Every continuous function can be uniformly approximated on $[a,b]$ by means of a sequence of polynomials, so the lemma is proved. ■

Theorem 2.3. *Assume that conditions (1.3) and (C1) hold true. If $\lim_n (B_n/A_n)(x) = (B/A)(x)$, for all $x \in [a,b]$, then*

$$\lim_n \mathcal{I}_{n,\widetilde{W}_n}(f) = \mathcal{I}_{\widetilde{W}}(f), \; f \in C[a,b].$$

Proof. Lemma 2.1 and Lebesgue's theorem imply that $\widetilde{W}_n dx \xrightarrow{*} \widetilde{W} dx$. The theorem follows from Lemma 2.2 and the inequality

$$|\mathcal{I}_{n,\widetilde{W}_n}(f) - \mathcal{I}_{\widetilde{W}}(f)| \leq |\mathcal{I}_{n,\widetilde{W}_n}(f) - \mathcal{I}_{\widetilde{W}_n}(f)| + |\mathcal{I}_{\widetilde{W}_n}(f) - \mathcal{I}_{\widetilde{W}}(f)|,\ f \in C[a,b].$$

■

Remark 2.4. The assumption $\lim_n (B_n/A_n)(x) = (B/A)(x)$, for all $x \in [a,b]$, can be linked with the rounding off process suffered by data when one employs the computer.

Remark 2.5. Theorem 2.3 can be applied to modified functions Af/B, $f \in C[a,b]$, to obtain that $\lim_n \mathcal{I}_{n,\widetilde{W}_n}(Af/B) = \mathcal{I}_W(f)$. However, to meet the challenge of reconciling two points of view, the experimental and theoretical, is more realistic to adopt $\mathcal{I}_{n,\widetilde{W}_n}(A_n f/B_n)$ as quadrature approximant of $\mathcal{I}_W(f)$. We mentioned above that this method of approximation corresponds to the rational schema, a matter which is examined in Subsection 2.3.

2.3. Interpolatory rational rules

Definition 2.6. We say that $\{A_n\}$ has the **density property** with respect to the interval $[a,b]$, if for each $f \in C[a,b]$, there exists a sequence $\{p_n\}$, with $p_n \in \Pi_{n-1}$, $n \in \mathbb{N}$, such that $p_n/A_n \to f$, uniformly on $[a,b]$.

Remark 2.7. Assuming certain conditions to be fulfilled by the roots $\{\alpha_{n,k}\}$ of A_n, one can ensure that $\{1/(x-\alpha_{n,k})\}$ is dense in the sense of Definition 2.6 (see [1, 2]). One way to obtain a property similar to the previous one, this time with respect to $\{B_n p_{n-1}/A_n,\ p_{n-1} \in \Pi_{n-1}\}$, is via the following definition

Definition 2.8. The sequence $\{B_n\}$ is said to be **strongly positive** on $[a,b]$, is there exists $\kappa \in C[a,b]$, such that $B_n(x) \to e^{\kappa(x)}$, uniformly on $[a,b]$.

Theorem 2.9. *Suppose that both conditions (C2) and (1.3) hold true. If $\{A_n\}$ has the density property with respect to $[a,b]$, and $\{B_n\}$ is strongly positive on $[a,b]$, then*

$$\lim_n \widetilde{\mathcal{I}}_{n,\widetilde{W}_n}(f) = \mathcal{I}_W(f) \text{ for every } f \in C[a,b].$$

Proof. Let $f \in C[a,b]$, and $\{p_n\}$ be a sequence of polynomials $p_n \in \Pi_{n-1}$, $n \in \mathbb{N}$, such that $p_n(x)/A_n(x) \to e^{-\kappa(x)} f(x)$, uniformly on $[a,b]$. Then $B_n(x)p_n(x)/A_n(x) \to f(x)$, uniformly on $[a,b]$, and

$$\left|\mathcal{I}_W(f) - \widetilde{\mathcal{I}}_{n,\widetilde{W}_n}(f)\right| \leq \left(\int_a^b W(x)dx + M\right) \left\|f - \frac{B_n p_n}{A_n}\right\|_{[a,b]},$$

where $M > 0$ is the upper bound in (2.5) (Lemma 2.1). ■

§3. Procedure to compute the coefficients $\lambda_{n,j}(\widetilde{W})$

The emphasis will be put on the calculation of the coefficients $\lambda_{n,j}(\widetilde{W})$, $\widetilde{W} = BW/A$, but we are also interested in estimating the quadrature nodes by applying a traditional method, if it were necessary.

Let $W(x)$ and $\{Q_n(x)\}$ be given by (1.1-1.2). According to the assumptions of Theorem 1.1, the monic polynomials Q_n, $n = 0, 1, 2, \ldots$, must satisfy a three term recurrence relation

$$Q_{n+1}(x) = (x - a_n)Q_n(x) - b_n Q_{n-1}(x),\ n = 0, 1, \ldots \tag{3.1}$$

where $Q_{-1} \equiv 0$, $Q_0 \equiv 1$, and the coefficients $\{a_n\}$ and $\{b_n\}$ are either known data or they have to be computed.

For $n \in \mathbb{N}$ let $H_n(\widetilde{W}, z)$ be the function

$$H_n(\widetilde{W}, z) = \int_a^b \frac{Q_n(x)\widetilde{W}(x)}{x - z} dx, \tag{3.2}$$

where the integrals are defined in the Cauchy principal value sense when $z \in (a, b)$. It follows from (3.1) that (see [8])

$$H_{n+1}(\widetilde{W}, z) = m_n(\widetilde{W}) + (z - a_n)H_n(\widetilde{W}, z) - b_n H_{n-1}(\widetilde{W}, z),\ n = 0, 1, \ldots \tag{3.3}$$

where $m_n(\widetilde{W}) = \int_a^b Q_n(x)\widetilde{W}(x)dx$.

We can easily derive from (1.2) and (3.2) the following relation.

$$\lambda_{n,j}(\widetilde{W}) = \frac{H_n(\widetilde{W}, x_{n,j})}{Q_n'(x_{n,j})},\ j = 1, \ldots, n. \tag{3.4}$$

The equation $\lambda_{n,j}(\widetilde{W}) = \lambda_{n,j}(W)H_n(\widetilde{W}, x_{n,j})/H_n(W, x_{n,j})$ is mathematically equivalent to (3.4), and corresponds to the spirit of the method of Monegato. Nevertheless, we have adopted equation (3.4) which corresponds to the exact formula (1.2) and is more suitable to carry on calculations by using (3.3).

Monegato has used closed formulas for the derivatives $Q_n'(x_{n,j})$, which can be applied when dealing with classical orthogonal polynomials (see [8, 11]). Instead, we suggest the use of a general procedure to obtain the approximate values of $Q'(x_{n,j})$, whose formulation can be obtained from (3.1) by applying the differential operator.

If we use the mathematical expression $Q'(x_{n,j}) = \prod_{i\neq j}(x_{n,j} - x_{n,i})$, then we obtain acceptable results when the order is not greater than 16. The shortcoming we find using this closed formula for $Q'(x_{n,j})$, is that some factors $x_{n,j} - x_{n,i}$ can produce loss of accuracy, when n is somewhat large.

The code we need to compute $Q^{(r)}(x_{n,j})$, $r = 2, 4, ...$ can also be obtained from (3.1), though the accuracy gets worse when r is somewhat large. Such a routine may be employed as an alternative in approximating the polynomial $(Q_n(x)-Q_n(z))/(x-z)$ by means of $Q'_n(z)+\cdots+Q_n^{(h)}(z)(x-z)^{h-1}/h!$, when $x \approx z$ and $h \leq n$. Thus, we can try to calculate $H_n(\widetilde{W}, z)$ by using the expression below.

$$H_n(\widetilde{W}, z) = \int_a^b \frac{(Q_n(x) - Q_n(z))\widetilde{W}(x) + Q_n(z)(\widetilde{W}(x) - \widetilde{W}(z))}{x - z} dx + \qquad (3.5)$$

$$Q_n(z)\widetilde{W}(z) \log\left(\frac{b-z}{a-z}\right).$$

If $Q_n(z) \neq 0$ then we should find a suitable expansion for the ratio $(\widetilde{W}_n(x)-\widetilde{W}_n(z))/(x-z)$, according to the specific nature of the weight W.

The formulation given in (3.5) is well known and it is not the only to evaluate an integral given in the sense of the Cauchy principal value (see [7]).

We have not stated yet how to overcome two of the main obstacles. One is that related to the eventual presence of difficult poles in the integrand of $H_0(\widetilde{W}, z)$. The other is referred to the knowledge of the polynomials Q_n in the initial stage of the process. We can solve the first problem by applying the so-called smoothing transformation technique (see Section 4). As for the second problem, let us suppose that relation (3.1) is not known. Next we show how the first values of the sequences $\{a_n\}$ and $\{b_n\}$ can be estimated, whereas the roots of the polynomials Q_n are also calculated along the numerical procedure. The method consists in defining a suitable array $\{M_{s,n}\}$ which can be used to evaluate the terms $m_n(\widetilde{W})$ and the recurrence coefficients.

Given a generic weight function k put

$$M_{s,n}(k) = \int_a^b P_s(x)Q_n(x)k(x)dx, \qquad (3.6)$$

where $\{P_s(x)\}$ is defined by a recurrence formula

$$P_{s+1}(x) = (x - \alpha_s)P_s(x) - \beta_s P_{s-1},\ s = 0, 1, ...,\ P_0 \equiv 1,\ P_{-1} \equiv 0, \qquad (3.7)$$

with preassigned coefficients $\alpha_s \in \mathbb{R}$ and $\beta_s > 0$, $s = 0, 1, ...$

The following relation follows from (3.1), (3.6) and (3.7).

$$M_{s,n+1}(k) = M_{s+1,n}(k) + \beta_s M_{s-1,n}(k) + (\alpha_s - a_n)M_{s,n}(k) - b_n M_{s,n-1}(k). \tag{3.8}$$

We observe that the terms $M_{s,0}(k) = \int_a^b P_s(x)k(x)dx$, $s = 0, 1, ...$, are the starting points of (3.8) and that $M_{0,n}(k) = m_n(k)$, $n = 0, 1, ...$ The latter sequence is used in (3.3) with $k = \widetilde{W}$.

The following diagram corresponds to the matrix $M(k) = (M_{s,n}(k))$. It indicates in a pictorial manner which steps have to be followed to obtain the entry $M_{s,n+1}(k)$. Notice that $M(w)$ has a triangular structure due to the orthogonality conditions.

$$M(k)=\left(\begin{array}{cccc|cc|c} & 0 & \cdots & n-1 & n & & n+1\\ s-1 & & & & \bullet & \searrow & \\ s & & & \bullet\longrightarrow & \bullet\longrightarrow & & \bullet \\ s+1 & & & & \bullet & \nearrow & \end{array}\right)$$

If we make $s = n$ and $s = n - 1$ in equation (3.8), then we obtain the following linear system of equations for the unknowns a_n and b_n.

$$\begin{aligned} M_{n,n+1}(k) = M_{n+1,n}(k) + \beta_n M_{n-1,n}(k) + \\ (\alpha_n - a_n)M_{n,n}(k) - b_n M_{n,n-1}(k), \\ M_{n-1,n+1}(k) = M_{n,n}(k) + \beta_{n-1} M_{n-2,n}(k) + \\ (\alpha_{n-1} - a_n)M_{n-1,n}(k) - b_n M_{n-1,n-1}(k). \end{aligned} \tag{3.9}$$

Indeed, we are employing the modified Chebyshev algorithm (MChA) to obtain $a_0, a_1, ...$ and $b_0, b_1, ...$, when still they are undetermined (see [12, Algorithm 2.1]). The MChA is based on the linear system (3.9) with $k = w$. The relevant feature is that $M_{n,n+1}(w) = M_{n-1,n+1}(w) = M_{n-1,n}(w) = M_{n-2,n}(w) = 0$.

A summary of the overall method, step by step, appears below.

1. Use (3.9) with $k = w$ to calculate a_n and b_n according to the MChA.

2. Obtain the nodes $\{x_{n,j}\}$ as the eigenvalues of the corresponding Jacobi matrices.

3. Calculate $H_0(\widetilde{W}, z)$, and $M_{s,0}(\widetilde{W})$, $s = 0, 1, ..., h$, $h > n$.

4. Apply equation (3.8) to obtain $M_{0,n}(\widetilde{W}) = m_n(\widetilde{W})$.

5. Use (3.3) to calculate $H_k(\widetilde{W}, x_{n,j})$, $k = 1, ..., n$, $j = 1, ..., n$.

6. Compute the coefficients $\lambda_{n,j}(\widetilde{W})$ using (3.4).

Remark 3.1. The computational effort in the first two steps of the method, can be reduced by making a suitable selection of the weight w. See the numerical examples in Section 5.

Step 3 is particularly special because of the presence of poles in the functions to be integrated. In order to solve this problem, we introduce a new variable into these integrals with the aim of transforming the difficult poles of the integrand into new ones which we expect are benign (see Section 4).

§4. The piecewise smoothing transformation $\Phi_{p,q}$

This section is devoted to establish the strategy $\mathbf{S_2}$ mentioned in the introduction.

Let $\phi_{a,b,p,q}(z)$ be the following rational function

$$\phi_{a,b,p,q}(z) := \frac{(b-a)(z-a)^p}{(z-a)^p + (b-z)^q} + a, \tag{4.1}$$

where $a < b$, $p, q \in \mathbb{N}$.

The derivative of $\phi_{a,b,p,q}(z)$ has the form $(z-a)^{p-1}(z-b)^{q-1}r(z)$. If $p \neq q$ then $r(x) \neq 0$, $x \in I = [a, b]$. On the other hand, it holds true that $\phi_{a,b,p,p}(z) \neq 0$ for $z \in \mathbb{C}$. A conclusion is that $u = \phi_{a,b,p,q}(x)$ can be used like a change of variable

$$\int_a^b g(x)dx = \int_a^b g(\phi_{a,b,p,q}(x))\phi'_{a,b,p,q}(x)dx,$$

which besides is able to remove singularities at the end-points of I in the sense that the new integrand should be smoother than the previous one.

The use of $\phi_{a,b,p,q}$ when the integrand has boundary singularities, has been formerly promoted by several authors. Nevertheless, we are mainly interested in using this change of variable to transform difficult poles which are close to one of the endpoints, into benign ones (see [2, 3]). The previous assertion is nothing else than a principle which is based on some elementary results and numerical tests, some of which can be seen in [3]. Further information about $\phi_{a,b,p,q}(z)$ can be found in [9] and the bibliography therein (see also [6]).

When the poles to be considered as difficult are scattered along the integration interval $I = [a, b]$, a convenient subdivision $\{I_i\}_{i=1}^m$ of I must be carried out. The aim is to transform the initial problem into another which consists in evaluating a collection of integrals, so that all the poles and zeros of the integrand are located close to the endpoints of some subinterval I_i. This point of view corresponds to the implementation of a piecewise change of variable $\Phi \in C^1[a,b]$. In general terms, Φ can be defined as follows: *given the collection of positive integers* $p_i, q_i \geq 1$, $i = 1, ..., m$, *and the intervals* $I_i = [a_i, b_i]$, $i = 1, ..., m$, *with* $b_i = a_{i+1}$, $i = 1, ..., m-1$, *and* $I = \cup_{i=1}^{m} I_i$, *we put* $\Phi(x) = \phi_{a_i, b_i, p_i, q_i}(x)$, *when* $x \in I_i$, $i = 1, ..., m$.

§5. Numerical examples

Given $\int_a^b g(x)dx$, the integrand $g(x)$ is conveniently decomposed into two factors. The next step consists in deciding which of these factors should play the role of being the integrand. Afterwards, we must choose the weights w and $\widetilde{W}$, or what is the same, we must select the nodes and the rational modification of the integrand.

Next we establish the notion of ill-scaled integrand to be used in this work. Given a floating point representation of the real number N, say

$$float(N) = \pm A_1 \cdots A_m e \pm E_1 \cdots E_k,$$

the signed digit string $\pm A_1 \cdots A_m$ is known as the mantissa, and $\pm E_1 \cdots E_k$ is referred to as the characteristic or scale of $float(N)$.

We are especially interested in considering "ill-scaled" integrands, that is, those f whose range of values $\{float(|f(float(x))|);\ x \in I\}$ shows very different scales.

Suppose we have obtained the coefficients in the recurrence formula (3.1) and the roots $\{x_{n,j}\}$ of Q_n by means of some procedure, up to some value n_0 of the subscript. Many numerical evidences show that the use of (3.8) to obtain $m_n(\widetilde{W})$ appears to be less costly than the direct calculation of its integral representation.

The polynomials P_s, $s = 0, 1, ...$ are determined by the terms $\alpha_1, ...,$ and $\beta_1, ...$ whose design should be made as simple as possible. Here we have considered two choices:

1. $\alpha_s = \beta_s = 0.99$, $s = 1, ..., 60$.
2. $\alpha_s = -0.99 + 2 \times 0.99s/60$, $\beta_s = 0.1 + 0.89s/60$, $s = 0, ..., 60$.

5.1. Example: integrand with difficult poles and without zeros

The parametric integral $I_\varepsilon = \int_{-1}^{1} f_\varepsilon(x)dx$, $\varepsilon \neq 0$, we selected as example, have also been considered by Monegato in [8] for the cases $\varepsilon = 1.0$, 0.5, 0.1, 0.01.

The results we show in this subsection have been obtained when $w = 1$ (quadrature nodes of the Gauss-Legendre rule), $f_\varepsilon(x) = e^x/(x^2+\varepsilon^2)$, $\varepsilon = 1.0, 0.5, 0.1, 0.01, 0.001, 0.0001$, $W(x) = 1$ and $\widetilde{W}(x) = 1/(x^2+\varepsilon^2)$. Such a selection is made for comparison purposes. Instead, to obtain full accuracy in the results, one should put $w = 1$, $f_\varepsilon(x) = 1/(x^2+\varepsilon^2)$, $W(x) = e^x$ and $\widetilde{W}(x) = e^x/(x^2+\varepsilon^2)$.

We obtain that

$$F(x,z) = \frac{\widetilde{W}(x) - \widetilde{W}(z)}{x - z} = -\frac{x+z}{(x^2+\varepsilon^2)(z^2+\varepsilon^2)}.$$

Our approach strongly relies on a ϕ-modification of a composite Gauss-Legendre quadrature formula of low order which is described below.

Let $t_{r,j} \in (-1,1)$ and $\lambda_{r,j} > 0$, $j = 1, ..., r$, be the nodes and weights, respectively, of the r-point polynomial Gauss-Legendre formula. Let $u_{m,k} = 2k/m - 1$, $k = 0, ..., m$, and $T_k(u) = c_k u + d_k$ be such that $T_k(-1) = u_{m,k-1}$ and $T_k(1) = u_{m,k}$, $k = 1, ..., m$. We assume that $m = 2^h$, $h = 2, 3, ...$, so $u_{m,m/2} = 0$. The poles of the integrand f_ε are close to $z = 0$, hence, they are also close to one of the end-points of the sub-intervals $[-1, 0]$ and $[0, 1]$.

The following approximation formulas take place.

$$M_{s,0}(\widetilde{W}) \approx \sum_{k=0}^{m} \sum_{l=1}^{r} \Lambda_{r,l,k} P_s(\xi_{r,l,k}) \widetilde{W}(\xi_{r,l,k}), \tag{5.1}$$

$$H_0(\widetilde{W}, x_{n,j}) \approx \sum_{k=0}^{m} \sum_{l=1}^{r} \Lambda_{r,l,k,p,q} F(\xi_{r,l,k,p,q}, x_{n,j}) + \widetilde{W}(x_{n,j}) \log \left| \frac{1 - x_{n,j}}{1 + x_{n,j}} \right|, \tag{5.2}$$

where

$$\Lambda_{r,l,k,p,q} = c_k \lambda_{r,l}(\widetilde{W}) \times \begin{cases} \phi'_{-1,0,1,q}(T_k(t_{r,l})) & k \le m/2, \\ \phi'_{0,1,p,1}(T_k(t_{r,l})) & k > m/2, \end{cases}$$

and

$$\xi_{r,l,k,p,q} = \begin{cases} \phi_{-1,0,1,q}(T_k(t_{r,l})) & k \le m/2, \\ \phi_{0,1,p,1}(T_k(t_{r,l})) & k > m/2. \end{cases}$$

Formula (5.1), which employs a piecewise version $\Phi = \Phi_{p,q}$ of the smoothing transformation $\phi_{a,b,p,q}$, is called composite Gauss-Legendre formula of (Φ, m, r)-type, and it is only implemented to estimate the values $H_0(\widetilde{W}, x_{n,j})$, $j = 1, ..., n$, and $M_{s,0}(\widetilde{W})$, $s = 0, 1, ...$, when $\widetilde{W}$ possesses some difficult poles.

The mapping $\Phi_{p,q}$ is defined as

$$\Phi_{p,q}(x) = \begin{cases} \phi_{-1,0,1,q}(x), & x \leq 0, \\ \phi_{0,1,p,1}(x), & x > 0. \end{cases}$$

The columns headed by $E(L)$, $E(G)$ and $E(M)$ in Tables 1-4 correspond to the results reported in [8] when the integral I_ε is estimated by different procedures. The relative errors obtained by applying the Gauss-Legendre rule are listed in column $E(L)$. The errors that appear in column $E(G)$, are due to the method of Gautschi, applied to Gauss quadrature formulas of $1/A$-rational type. The numerical results which correspond to the interpolatory quadrature rule of Monegato [8], are shown in column $E(M)$. We are mainly interested in comparing $E(M)$ with our results listed in the columns E_m, $m = 8, 128, 1024$.

The symbol $E_{m=\mu}$ indicates that the quadrature errors have been estimated when it is used a composite Gauss-Legendre formula of $(\Phi, \mu, 5)$-type.

The condition $p = q = 1$ means that the transformation Φ has not been introduced into the integral. Hence, the results which are enumerated in tables 1–2 have been obtained without using any change of variable. The reason of doing so is that the poles $\pm i$ and $\pm 0.5i$ are sufficiently far away from $I = [-1, 1]$, and instability is not detected.

Table 5 illustrates the power of the smoothing method, even when the values of ε are much smaller than those considered in [8].

5.2. Example: integrand with difficult poles and difficult zeros

Let $\mathcal{I}_W(f_\varepsilon) = \int_{-1}^{1} f_\varepsilon(x)W(x)dx$, with

$$f_\varepsilon(x) = \frac{((x+1)^2+\varepsilon^2)((x-1)^2+\varepsilon^2)e^x}{x^2+\varepsilon^2}, \; \varepsilon \neq 0.$$

n	$E(L)$	$E(G)$	$E(M)$	$E_{m=8}$	$E_{m=128}$	$E_{m=1024}$
2	2.1e-02			2.5e-02	2.5e-02	2.5e-02
4	6.5e-04	1.1e-07	9.7e-05	9.7e-05	9.7e-05	9.7e-05
8	5.8e-07	3.2e-15	1.1e-10	1.1e-10	1.1e-10	1.1e-10
16	4.1e-13	3.2e-14	8.8e-16	3.8e-15	3.5e-15	2.0e-15

Table 1: Integral I_1, $p = q = 1$

n	$E(L)$	$E(G)$	$E(M)$	$E_{m=8}$	$E_{m=128}$	$E_{m=1024}$
2	1.8e-01			6.0e-02	6.0e-02	6.0e-02
4	2.9e-02	9.1e-08	5.0e-04	5.0e-04	5.0e-04	5.0e-04
8	6.2e-04	8.8e-16	2.8e-09	3.0e-09	2.8e-09	2.8e-09
16	2.8e-07	5.0e-16	5.7e-16	2.4e-10	1.6e-15	1.1e-15

Table 2: Integral $I_{0.5}$, $p = q = 1$.

n	$E(L)$	$E(G)$	$E(M)$	$E_{m=8}$	$E_{m=128}$	$E_{m=1024}$
2	7.7e-01			1.4e-01	1.4e-01	1.4e-01
4	5.9e-01	3.1e-08	2.4e-03	2.4e-03	2.4e-03	2.4e-03
8	3.2e-01	1.2e-16	6.1e-08	7.9e-06	6.1e-08	6.1e-08
16	7.4e-02		2.1e-16	7.9e-06	2.2e-15	1.6e-15

Table 3: Integral $I_{0.1}$, $p = q = 3$.

n	$E(L)$	$E(G)$	$E(M)$	$E_{m=8}$	$E_{m=128}$	$E_{m=1024}$
2	9.8e-01			1.7e-01	1.7e-01	1.7e-01
4	9.6e-01	3.6e-09	3.5e-03	4.5e-03	3.5e-03	3.5e-03
8	9.2e-01	1.6e-16	1.3e-07	9.6e-04	1.3e-07	1.3e-07
16	8.4e-01		2.0e-16	1.7e-04	4.4e-15	4.4e-15

Table 4: Integral $I_{0.01}$, $p = q = 4$.

	$\varepsilon = 0.01$		$\varepsilon = 0.001$		$\varepsilon = 0.0001$	
n	$p, q = 1$	$p, q = 4$	$p, q = 1$	$p, q = 5$	$p, q = 1$	$p, q = 6$
2	1.7e-01	1.7e-01	2.2e-01	1.7e-01	7.1e-01	1.7e-01
4	3.5e-03	3.5e-03	4.1e-02	3.7e-03	7.6e-01	3.7e-03
6	3.5e-05	2.9e-05	4.5e-02	3.1e-05	7.6e-01	3.1e-05
8	6.2e-06	1.3e-07	4.5e-02	1.4e-07	7.6e-01	1.4e-07
12	6.3e-06	6.4e-13	4.5e-02	7.2e-13	7.6e-01	7.7e-13
16	6.3e-06	4.4e-15	4.5e-02	5.6e-15	7.6e-01	4.4e-14

Table 5: Integral I_ε, $m = 128$

	$E_{m=8}$		$E_{m=128}$		$E_{m=1024}$	
n	$1/A$	B/A	$1/A$	B/A	$1/A$	B/A
2	4.8e-01	1.7e-01	4.8e-01	1.7e-01	4.8e-01	1.7e-01
4	3.7e-02	4.0e-03	3.6e-02	3.7e-03	3.6e-02	3.7e-03
6	9.9e-03	2.9e-04	1.0e-02	3.1e-05	1.0e-02	3.1e-05
8	5.4e-04	3.2e-04	2.2e-04	1.4e-07	2.2e-04	1.4e-07
12	3.2e-04	3.2e-04	8.5e-09	7.2e-13	8.5e-09	7.2e-13
16	3.2e-04	3.2e-04	5.0e-14	5.5e-15	5.3e-14	5.1e-15

Table 6: Example 5.2 with $\varepsilon = 0.001$, and $p = q = 5$

In addition to the poles already considered in Example 5.1, the integrand f_ε also has difficult zeros when $|\varepsilon|$ is small enough. The effectiveness of the method based upon the modification B/A, is compared in Table 6 with that which is produced by $1/A$, when $\varepsilon = 0.001$.

Here we also assume that $w = 1$ (quadrature nodes of the Gauss-Legendre rule), and $W = 1$. Now, the zeros and poles of the new weight function $\widetilde{W}$, are equal to those of f_ε, namely, $\widetilde{W}(x) = ((x+1)^2 + \varepsilon^2)((x-1)^2 + \varepsilon^2)/(x^2 + \varepsilon^2)$.

Figure 1 makes special emphasis on those differences which can be appraised in the scale, when $f_{0.001}$ is compared with $Af_{0.001}/B = e^x$. For a sake of clarity we have plotted the graph of $f_{0.001}$ on the subinterval $[-0.06, 0.04]$.

§6. Conclusions and remarks

This work has tried to present an approach more general than that of Monegato [8], keeping the effectiveness of the original method. In order to accomplish this goal we have linked two approaches formerly treated in [8, 9]. One is the smoothing transformation ϕ, whose piecewise version $\Phi_{p,q}$ is a novelty. The other technical feature of this work, which deserves to be mentioned, is that which is based on the theory of Sloan and Smith (Theorem A). In this context, we have introduced conditions (C1) and (C2) to guarantee the convergence of a procedure associated with a sequence of rational modifications.

The approach we have presented relies basically in assuming that the zeros of the integrand can also produce instability. We have represented briefly this technique by the symbol B/A. The experimental conclusion is that B/A is quite superior to $1/A$ when the integrand has difficult zeros.

Theorem 2.3 is a manner of supporting the assertion of W. Gautschi, in the sense that it is sufficient

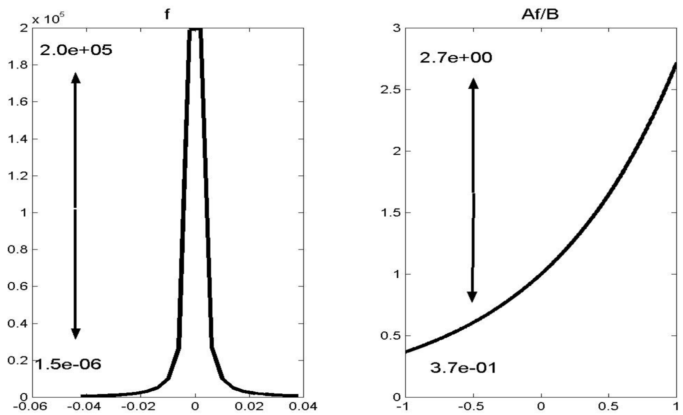

Figure 1: The integrand $f = f_{0.001}$ before and after the modification.

that the roots of $A(x)$ lie near the poles of the integrand. Indeed, Gautschi does not precise what should be the degree of proximity between these points in order to guarantee numerical stability. We either. Our result only tries to explain how the numerical process performs.

The precision of the results for $n = 16$ in the tables 1-4, which have been reached using Matlab© tools, is one figure smaller than that obtained by Monegato's method. This loss of digits is basically due to the numerical behavior of the routine we have derived from the recursion formula (3.1).

Nowadays, in light of current knowledge, we can assert that Theorem A belongs to the theory of simultaneous quadrature formulas. The conditions (C1) and (C2), which have been imposed to the polynomials A_n and B_n in Lemma 2.1, are inspired in [2], where it is studied the convergence of a couple of simultaneous quadrature formulas associated with the $1/A$-rational modification.

References

[1] N. I. Achieser (1992)
Theory of Approximation, New York: Dover.

[2] U. Fidalgo Prieto, J. R. Illán González and G. López Lagomasino (2007)

Convergence and computation of simultaneous rational quadrature formulas, Numer. Math. 106, 99–128.

[3] J. R. Illán González and G. López Lagomasino (2006)
A numerical approach for Gaussian rational formulas to handle difficult poles, in: B.H.V. Topping, G. Montero & R. Montenegro, (eds.), Fifth International Conference on Engineering Computational Technology, Civil-Comp Press, Stirlingshire, Scotland, paper 31.

[4] J. Van Deun, A. Bultheel and P. González-Vera (2006)
On computing rational Gauss-Chebyshev quadrature formulas, Math. Comp., 75, 307–326.

[5] K. Deckers, J. Van Deun and A. Bultheel (2006)
Computing rational Gauss-Chebyshev quadrature formulas with complex poles: the algorithm, in: B.H.V. Topping, G. Montero & R. Montenegro, (eds.), Fifth International Conference on Engineering Computational Technology, Civil-Comp Press, Stirlingshire, Scotland.

[6] R. Kress (1990)
A Nyström method for boundary integral equations in domains with corners, Numer. Math. 58, 145–161.

[7] G. Monegato (1982)
The numerical evaluation of one-dimensional Cauchy principal value integrals, Computing 29, 337–354.

[8] G. Monegato (1986) Quadrature formulas for functions with poles near the interval of integration, Math. Comp. 47, 301-312.

[9] G. Monegato, and L. Scuderi (1999)
Numerical integration of functions with boundary singularities, J. Comput. Appl. Math. 112, 201–214.

[10] I. H. Sloan and W. E. Smith (1982)
Properties of interpolatory product integration rules, SIAM J. Numer. Anal. 19, 427–442.

[11] G. Szegö (1939)
Orthogonal polynomials, American Mathematical Society. Colloquium Publications. Vol. XXIII, Providence, Rhode Island.

[12] W. Gautschi (2004)
Orthogonal Polynomials. Computation and Approximation, Numerical Mathematics and Scientific Computation, Oxford University Press, New York.

[13] W. Van Assche, and I. Vanherwegen (1993)
Quadrature formulas based on rational interpolation, Math. Comput. 61, (204), pp. 765–783.

J. R. Illán González,
Departamento de Matemática Aplicada I, Universidad de Vigo,
Campus Lagoas-Marcosende, 36200 Vigo, Spain.
jillan@uvigo.es