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A numerical approach for Gaussian rational formulas to handle difficult poles*

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Abstract

Let f be a meromorphic function in a neighborhood V of the real interval I , such that $\{z; f(z) = \infty\} \subset V \setminus I$. Let $W(x)$ be a weight function with possibly some integrable singularities at the end points of I . The problem of evaluating the integral

$$\mathcal{I}_W(f) = \int_I f(x)W(x)dx,$$

has its own interest in applications. It is a theoretical fact that for a variety of weights $W(x)$, Gaussian quadrature formulas based on rational functions (GRQF) converge geometrically to $\mathcal{I}_W(f)$. However, the so-called difficult poles, that is, those poles which are close to $[a, b]$, produce numerical instability. W. Gautschi (1999) has developed routines to calculate nodes and coefficients for a GRQF when some poles of f are difficult. The authors and U. Fidalgo (2006) have found a method different from Gautschi's which has been successfully applied to compute simultaneous rational quadrature formulas (SRQF). This paper presents a version of the SRQF approach adapted to GRQF for evaluating $\mathcal{I}_W(f)$ efficiently even when some poles of f should be considered as difficult ones. The procedure consists in the use of smoothing transformations of $[a, b]$ to move real poles away from I , so that the modified moments of

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the measure $d\mu(x) = W(x)dx$ can be computed with accuracy. A slight variant of the method improves the numerical estimates when some poles are very difficult. Some numerical tests are shown to be compared with previous results.

Keywords: Gauss rational quadrature formula, smoothing transformation, real difficult poles, meromorphic integrand

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1 Introduction

The study of convergence properties of the Gaussian rational quadrature formulas (GRQF), and their connections with the multipoint Padé approximants was initiated by the authors in [10, 11, 12] (see also [19]). Nevertheless, [9] is possibly the first paper in presenting a suitable definition for GRQF.

Rational functions are a good choice when functions with singularities are involved in a problem whose solution must be obtained by approximation methods. We claim that the previous statement can be considered as a principle which leads to the rational approach instead of the polynomial one when, for example, we are evaluating the integral of functions which are analytic in $V \setminus \{z_1, \dots, z_m\} \supset [a, b]$, where $z_i \in V$, $i = 1, \dots, m$, are poles of f , and $I = [a, b]$ is the integration interval.

The development of the first rational procedures to calculate efficiently the integral of functions with poles close to $[a, b]$ is due to Gautschi [5, 6, 7, 8]. In the sequel we adopt Gautschi's terminology, namely, the closest poles to $[a, b]$ which besides cause instability, are called **difficult**, and the rest are **benign**. Indeed, the degree of proximity to $[a, b]$ of a given pole and the numerical problems which could be associated to it, are questions to be judged in each case. Here we introduce the notion of "very difficult pole" to be applied to those cases for which the distance from the pole to the integration interval is less than $1.0e - 03$.

Gautschi has described an algorithm to calculate the nodes and coefficients of the quadrature formula depending on which poles of the integrand are considered to be difficult. A different technique was used by Monegato [17] as an application of a result by Sloan-Smith [18]. Monegato's method involves two weight functions and two respective quadrature formulas. It consists in selecting the nodes as those of a given Gaussian quadrature formula of polynomial type associated to one of the weights. Then it calculates efficiently the coefficients for the other formula depending on the difficult poles. This technique, which has also been considered in [3] in the more general setting of the rational simultaneous rules, is mainly based on a subordination condition which one of the weight functions must fulfil with respect to the other.

Let $\{\alpha_n\}_{n=1}^{\infty}$ be a sequence of algebraic polynomials with real coefficients, such that $\deg \alpha_n \leq 2n$ and $\alpha_n(x) > 0$, for all $n \in \mathbb{N}$, $x \in [a, b]$. Let W be a positive weight function on the interval $[a, b]$ and $x_{n,j}$, $j = 1, \dots, n$, distinct points on $[a, b]$. By \mathcal{P}_n we denote the finite dimensional space of all polynomials of degree at most n . We say

that

$$\mathcal{I}_W(f) = \int_a^b f(x)W(x)dx \approx \mathcal{I}_{W,n}(f) = \sum_{j=1}^n \lambda_{n,j}f(x_{n,j}), \quad (1)$$

is a Gaussian rational quadrature formula (GRQF) with respect to α_n if equality holds in (1) for all $f = P/\alpha_n, P \in \mathcal{P}_{2n-1}$. When $\alpha_n \equiv 1$ formula (1) is the classical polynomial scheme.

The characterization of the nodes and coefficients of a rational Gaussian rule can be easily reduced to the classical case. The nodes are the zeros of the n -th orthogonal polynomial $Q_n(z) = \prod_{j=1}^n (z - x_{n,j})$ with respect to the varying measure $(\omega/\alpha_n)dx$ and the generalized Christoffel coefficients are given by

$$\lambda_{n,j} = \alpha_n(x_{n,j}) \int \left(\frac{Q_n(x)}{Q'_n(x_{n,j})(x - x_{n,j})} \right)^2 \frac{W(x)dx}{\alpha_n(x)}.$$

A typical problem is that when f is meromorphic in a neighborhood V of $[a, b]$. Under these conditions the efficiency of a numerical procedure associated with (1) can be seriously affected by the presence of difficult poles. A suitable approach consists in selecting the zeros of α_n in such a way that some of them coincide with the most difficult poles of f (cf. [5, 6, 7]).

In order to appraise the nature of this approach, consider a triangular array of complex numbers $\mathbf{A} = \{z_{n,j}; j = 1, \dots, 2n, n \in \mathbb{N}\}$, $\mathbf{A} \subset \overline{\mathbb{C}} \setminus [a, b]$, such that all its rows are symmetric with respect to the real axis (counting multiplicities). The polynomials α_n are constructed from table \mathbf{A} by

$$\alpha_n(x) = D_n \prod_{j=1}^{2n} \left(1 - \frac{x}{z_{n,j}} \right), \quad D_n \in \mathbb{R}, \quad n \in \mathbb{N}.$$

By convention, we define $x/\infty \equiv 1$.

Notice that all polynomials α_n have real coefficients. Only for numerical purposes the factor D_n scales α_n .

For the moment we assume: $z_{n,\nu} \in \mathbb{R} \setminus [a, b]$, if $\nu = 1, \dots, n$, and $z_{n,\nu} = \infty$ if $\nu = n + 1, \dots, 2n$, $n \in \mathbb{N}$. In addition, $z_{n,\nu} \neq z_{n,\eta}, 1 \leq \nu < \eta \leq n$, and $D_n = 1$. Choose n distinct points $x_{n,1}, \dots, x_{n,n} \subset [a, b]$. In order to obtain an interpolation formula of rational type with respect to α_n it is sufficient to solve the following linear system

$$\int_a^b \frac{W(x)dx}{(1 - x/z_{n,\nu})} = \sum_{j=1}^n \frac{\lambda_{n,j}}{(1 - x_{n,j}/z_{n,\nu})}, \quad \nu = 1, \dots, n, \quad (2)$$

with respect to the unknowns $\lambda_{n,j}$. Indeed, the polynomials $P_\nu(x) = \prod_{j \neq \nu} (x - z_{n,j}), \nu = 1, \dots, n$, form a basis in \mathcal{P}_{n-1} and $P_\nu(x)/\alpha_n(x) = (x - z_{n,\nu})^{-1}$.

Numerical testing has shown that instability is detected when $x_{n,j} - z_{n,\nu}$ is close to zero and the system (2) is solved using an arithmetic of finite precision. In case of GRQF, both nodes and coefficients must not be calculated from the non linear system

(2) but using the corresponding Jacobi matrix (see Section 3). The corresponding numerical method can be based on recursion formulas which require a suitable discrete version to evaluate accurately integrals of the form

$$\int_a^b \frac{P(x)}{\alpha_n(x)} W(x) dx, \quad (3)$$

where P is a polynomial, W possibly has integrable singularities at the end points of $[a, b]$, and some zeros of α_n are considered as difficult poles of the integrand in (3).

The paper presents a rational approach for the quadrature formula (1) when f has difficult real poles, and W has some integrable singularities at the end points of the interval $[a, b]$. By the “smoothing method” we mean the corresponding implementation of this approach. It is mainly based on the special design of the recurrence relation to be used in the algorithm, and on the technique of evaluating the integrals (3). For the latter we introduce a suitable change of variable into (3), not into $\mathcal{I}_W(f)$, to transform difficult poles into other ones practically benign.

Unlike the case in which the singularities to be annihilated are at the end points of the integration interval, the technique of changing the integrating variable does not remove the poles located around $[a, b]$. The rational transformation ϕ to be used as substitution mapping transforms poles into many more new complex poles whose effect must be taken into account. The class of functions ϕ is designed and studied in Section 2, where the problem of locating the new poles is discussed in terms of elementary results.

The smoothing method is described in Section 3. It is a Gaussian version of the procedure which is applied in [3] to simultaneous rational quadrature rules, when some real poles of the integrand must be assumed to be difficult. A smoothing transformation is only applied to modify a composite Gauss-Legendre formula of polynomial type to evaluate integrals of the form (3) which take part in the numerical procedure.

Section 4 is devoted to present a variant of the smoothing method which allows to improve the numerical estimate when the integrand has very difficult poles in the real line.

The two integrals we have selected as examples depend on a parameter ω which determines difficult poles. Both are well known nowadays because they have been considered by several authors [1, 3, 4, 5, 6, 7, 8].

2 The smoothing transformation of $[a, b]$

The technique of fitting a change of variable into an integral to increase the efficiency of some numerical procedure is not new. It seems to have been applied since 1963 (cf. [14]), and is specially recommended when the only singularities of the integrand are located at the end points of the integration interval $[a, b]$. One expects that it makes the integrand as smooth as one needs for evaluation purposes.

According to our aims, the singularities which we only consider in the paper are real poles. As for the complex poles which arise as a consequence of introducing a smoothing transformation into an integral, we expect that they are faraway in the sense that they cannot produce instability. The smoothing transformations which we plan to use also work when all the difficult poles, real and non real, are located in the region $\{z; \Re(z) \notin [a, b]\}$. A heuristic is given in Section 4 to reach such a configuration.

Let $\phi : [a, b] \rightarrow [a, b]$ be a suitable function for substituting a new variable $t = \phi(x)$, that is, ϕ is infinitely differentiable, bijective and strictly monotonically increasing. For every integrable function $f : [a, b] \rightarrow \mathbb{R}$ we have that

$$\int_a^b f(x)dx = \int_a^b f(\phi(t))\phi'(t)dt. \quad (4)$$

The integral in the left side of (4) can be approximated by a quadrature rule

$$\int_a^b f(x)dx \approx \sum_{k=1}^n \lambda_k f(x_k). \quad (5)$$

If we apply formula (5) to the integral in the right side of (4), we obtain

$$\int_a^b f(\phi(t))\phi'(t)dt \approx \sum_{k=1}^n \phi'(x_k)\lambda_k f(\phi(x_k)). \quad (6)$$

Hence, from (4–6) we derive the following new formula

$$\int_a^b f(x)dx \approx \sum_{k=1}^n \Lambda_k f(t_k), \quad (7)$$

where $t_k = \phi(x_k)$ and $\Lambda_k = \phi'(x_k)\lambda_k$.

Notice that if $\lambda_k > 0$ then $\Lambda_k > 0$, and that $\phi'(x)$ annihilates some kind of singularities at the end points of the interval $[a, b]$ provided that

$$\phi'(x) = g(x)(x - a)^{p-1}(b - x)^{q-1}, \quad (8)$$

where $p + q > 2$, and $g(x)$ does not vanish in a neighborhood of $[a, b]$.

The family of transformations to be used in this paper is given by the following formulation

$$\phi_{p,q,a,b}(x) := \frac{(b - a)(x - a)^p}{(x - a)^p + (b - x)^q} + a; \quad p, q \in \mathbb{N} \quad q, p \geq 1, \quad p + q > 2. \quad (9)$$

The derivative of $\phi_{p,q,a,b}$ has the following expression which obviously fulfils condition (8).

$$\phi'_{p,q,a,b}(x) = \frac{(b - a)(x - a)^{p-1}(b - x)^{q-1}[pb - aq + x(q - p)]}{((x - a)^p + (b - x)^q)^2} \quad (10)$$

Some especial results can be obtained by modifying (9) in some way as that described in Section 4. Other case which deserves to be mentioned is that given by Kress [15]) who applies the rational substitutions (9) with the form $\phi_{p,p,0,1}(v(s))$, where $v(s)$, $0 \leq s \leq 2\pi$, is a bijective cubic polynomial which transforms $[0, 2\pi]$ onto $[0, 1]$, to compute the solution of singular integral equations.

The technique of fitting (9) into an integral was already used by the authors and U. Fidalgo in the context of simultaneous rational quadrature formulas to treat difficult poles (cf. [3]). As for the use of different types of rational transformations to modify a non Gaussian quadrature formula of rational type we refer to [13].

The interval $[a, b]$ divides \mathbb{R} into two regions, namely, $I_1 = (-\infty, a]$ and $I_2 = [b, +\infty)$, where we mainly assume practically all the poles under interest are located. The non-symmetric formulation of (9) (cf. [17]), that is, when $p \neq q$, corresponds with the case in which all the difficult poles of the integrand are located in one and only of the two previous regions.

In what follows we only consider the non-symmetric case when p is even and $q = 1$. We also adopt the notation ϕ instead of $\phi_{p,q,a,b}$ when they go without saying the values of the parameters.

Lemma 1 *Let $\phi = \phi_{p,q,a,b}$ and assume that one of the following conditions holds*

- i) $a \leq x \leq b$.
- ii) p is even and $x < a$.
- iii) p and q are even, and $x \in \mathbb{R}$.
- iv) q is even and $x > b$.

Then $a \leq \phi(x) \leq b$.

Proof *The equation*

$$\phi(x) = \frac{a(b-x)^q}{(x-a)^p + (b-x)^q} + \frac{b(x-a)^p}{(x-a)^p + (b-x)^q},$$

shows that each one of the conditions (i–iv) implies that $\phi(x)$ is in the convex hull of the two points set $\{a, b\}$. □

The evaluation of $\mathcal{I}_W(f)$ when f has real difficult poles and W has mild singularities is our main purpose, but it is reduced to the problem of evaluating integrals of the type (3). Thus, in the rest of the section we always refer to the rational function $R(x)$ having poles outside $[a, b]$.

The following proposition easily follows from Lemma 1.

Proposition 1 *If p (q , respectively) is even then $R(\phi(x))$ does not have real poles in $x < a$ ($x > b$, respectively). If both p and q are even then $R(\phi(x))$ does not have real poles.*

Proposition 1 ensures that the property of the exponents of being even, makes ϕ capable of removing all real poles of R in both of one of the regions I_i , in the sense that $R(\phi(x))$ no longer has real poles in it.

The proposition below asserts that every real pole x_0 of R eventually corresponds to $\max\{p, q\}$ complex poles of $R(\phi(x))$. Besides, all these complex poles can be calculated by using a formula which also allows to determine which ones are the closest.

Proposition 2 *Let p, q be even integers such that $p + q > 2$. If $x_0 \in \mathbb{R} \setminus [a, b]$ is a pole of R , then the roots of the polynomial $P(z) = (b - x_0)(z - a)^p - (x_0 - a)(b - z)^q$ are non real poles of $R(\phi(x))$.*

If $p = q$ then the roots $z_k = z_k(a, b, p, x_0)$ of $P(z)$ are exactly

$$z_k = \begin{cases} \frac{(b\rho\theta_k + a)}{(1 + \rho\theta_k)} & x_0 < a, \\ \frac{(a\rho^{-1}\theta_k + b)}{(1 + \rho^{-1}\theta_k)} & b < x_0, \end{cases}$$

where $\theta_k = e^{i\pi(1+2k)/p}$, $k = 0, \dots, p - 1$, and $\rho = |(a - x_0)/(b - x_0)|^{1/p}$.

In addition, the complex poles of ϕ yield $\max\{p, q\}$ isolated singularities of $R(\phi(x))$, which in case of $p = q$, all of them are located in the straight line $\Re(z) = (a + b)/2$.

Proof *If p, q are even then the roots of the polynomial $P(z) = (b - x_0)(z - a)^p - (x_0 - a)(b - z)^q$ are exactly the solutions of the equation $\phi_{p,q,a,b}(z) = x_0$, which are not real according to Proposition 1.*

If $p = q$ and $x_0 < a$ one finds that

$$\frac{z - a}{b - z} = e^{i\pi(1+2k)/p} \left| \frac{a - x_0}{b - x_0} \right|^{1/p}, \quad k = 0, \dots, p - 1.$$

In fact, if $x_0 < a$ and $P(z) = 0$ then

$$\left(\frac{z - a}{b - z} \right)^p = (-1) \left(\frac{a - x_0}{b - x_0} \right) = e^{i\pi} \left| \frac{a - x_0}{b - x_0} \right|.$$

The other assertions are obtained by carrying out easy calculations.

On the other hand, $d_{p,q}(x) = (x - a)^p + (b - x)^q > 0$, for all $x \in \mathbb{R}$, and any complex solution z_0 of $d_{p,p}(z) = 0$ satisfies $|z_0 - a| = |b - z_0|$, hence $\Re(z_0) = (a + b)/2$. \square

Let $z_k = z_k(a, b, p, x_0)$ be defined as that in Proposition 2, with $x_0 < a$ and $p = q$. Among all z_k , $k = 0, \dots, p - 1$, the pair of conjugated points which is formed by the two closest to $[a, b]$ is (z_0, z_{p-1}) . The rest of the conjugated pairs is easily ordered from the

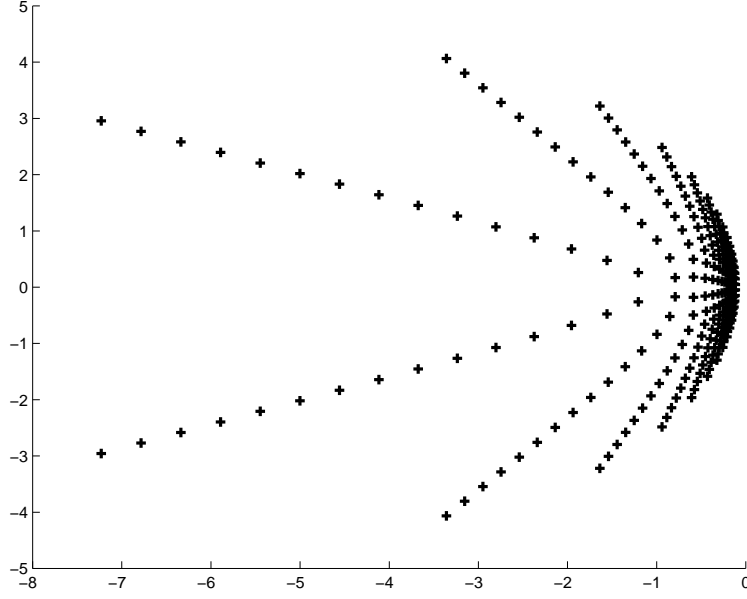


Figure 1: Poles z_k for $x_0 = -1.001$, $a = -1$, $b = 1$, $p = q = 2k + 4$, $k = 0, \dots, 14$.

closest to the farthest as $(z_1, z_{p-2}), (z_2, z_{p-3}), \dots, (z_m, z_{m-1})$, where $p = q = 2m$. It is easy to verify that $\Re(z_0) \in (a, b)$, so we must try that the following relation holds.

$$\min_k |\Im(z_k)| = \frac{(b-a)\rho |\sin(\pi/p)|}{1 + 2\rho \cos(\pi/p) + \rho^2} = \min_k d(z_k, [a, b]) > a - x_0. \quad (11)$$

Unfortunately, condition (11) not always holds. If $p \rightarrow \infty$ being the other parameters fixed, the left side of (11) tends to zero. Notice also that for a, b and x_0 fixed, $z_\infty = (a+b)/2$ is a limit point of the set $\{z_k; k = 0, \dots, p-1, p = 2, 4, 6, \dots\}$ (see Figure 1).

Figure 2 shows the location of the points z_k and the closest poles of ϕ when $p = q = 6$, $a = -1$, $b = 1$ and $x_0 = -1 - 1.0e - 03$ is the single pole of R .

Proposition 3 *Let $p \geq 2$ be an even integer. If*

$$0 < a - x_0 < p^p \left(\frac{b-a}{p-1} \right)^{p-1} (b-x_0), \quad (12)$$

then $\phi_{p,1,a,b}(z) = x_0$ does not have any real solution.

Proof *Equation $\phi_{p,1,a,b}(z) = x_0$ is equivalent to*

$$P(x) = (b-x_0)(z-a)^p - (x_0-a)(b-z) = 0.$$

Let $Q(w) = P(a+w)$. The function $Q(w)$ has a point of global minimum at $w_0 = ((a-x_0)/(p(b-x_0)))^{1/(p-1)} > 0$, and $Q(w_0) > 0$ provided that (12) holds. \square

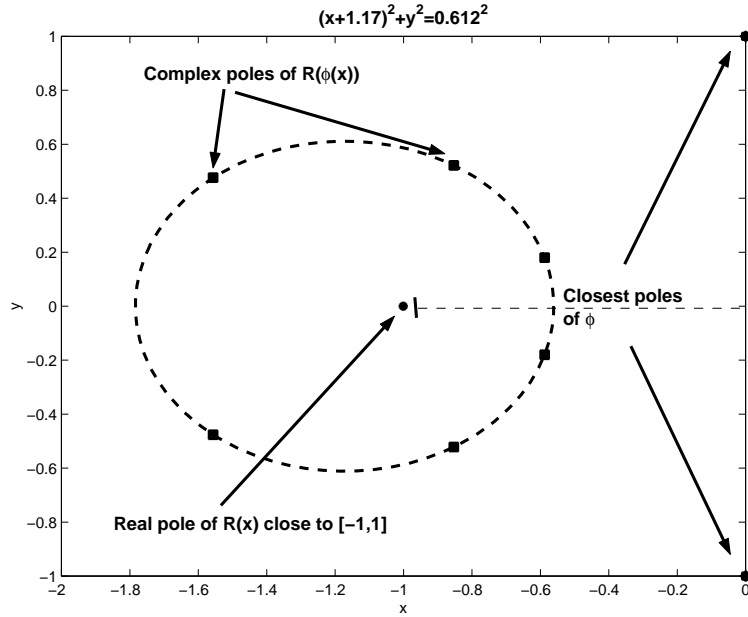


Figure 2: Pole location for $R(x)$ and $R(\phi_{6,6,-1,1}(x))$

Corollary 1 *Let p be an even integer. If*

$$b - a > (p - 1)p^{-p/(p-1)}, \tag{13}$$

then $\phi_{p,1,a,b}(z)$ does not have real poles. If, in addition, $x_0 < a$ then $\phi_{p,1,a,b}(z) = x_0$ does not have real solutions.

Proof *The denominator of $\phi_{p,1,a,b}(z)$ is $d_{p,1}(x) = (x - a)^p + b - x$. From (13) we deduce that $d_{p,1}(x) > 0$, for all $x \in \mathbb{R}$.*

Condition (13) and $x_0 < a$ imply that (12) is trivially true. Proposition 3 finishes the proof. \square

Notice that $0 < (p - 1)p^{-p/(p-1)} < 1$, for all $p > 1$. Therefore, Corollary 1 only has interest when $b - a < 1$. If $(b - a)^{p-1} < (p - 1)^{p-1}p^{-p}$ then Condition (12) establishes a particular notion of proximity to $[a, b]$, related to $\phi_{p,1,a,b}$ (see Example 1).

A similar result to Corollary 1 can be stated when q is even, $p = 1$ and $b < x_0$.

Example 1 *Let $x_0 = -0.101$, $a = -0.1$, $b = 0.1$, $p = 6$, and $q = 1$. The equation $\phi(z) = x_0$ has the real solutions $z_1 \approx 1.540879715899126e - 01$ and $z_2 \approx 1.289476182987572e - 01$, being z_2 the solution closest to $[a, b]$. Notice that $(p - 1)p^{-p/(p-1)} \approx 5.823559323096494e - 01$, for $p = 6$, whereas $b - a = 2.0e - 01$, so condition (13) does not take place.*

3 The smoothing method

In spite of the presence of difficult poles a theoretic conclusion is that convergence rate for GRQFs is geometric when the integrand is analytic on $[a, b]$. More precisely, taking into account that the stability condition

$$\sum_{j=1}^n \lambda_{n,j} = \sum_{j=1}^n |\lambda_{n,j}| = \int_a^b W(x) dx,$$

holds provided that $\deg \alpha_n \leq 2n - 1$, the proposition below can be proved with the same technique as that used in ([3], proposition 4).

Proposition 4 *Let $\mathcal{E}_n(f)$ be the error of a GRQF of order n for the integrand f , given by the following formula*

$$\mathcal{E}_n(f) = \left| \int_a^b f(x)W(x)dx - \sum_{j=1}^n \lambda_{n,j}f(x_{n,j}) \right|,$$

If $f \in \mathcal{H}(V)$ (f analytic in a neighborhood V of $[a, b]$), $\deg \alpha_n \leq 2n - 1$, and the zeros of α_n are in a compact set F , $F \subset \mathbb{C} \setminus [a, b]$, then there exists $\delta(V)$, $0 < \delta(V) < 1$, such that for all $f \in \mathcal{H}(V)$

$$\limsup_n |\mathcal{E}_n(f)|^{1/(2n)} \leq \delta(V). \tag{14}$$

Even though theoretic convergence is governed by (14), the size of $\delta(V)$ plays a major role in the numerical setting. From the property of $\delta = \delta(V)$ of being a decreasing function of V , we can easily show how a GRQF works making smaller $\delta(V)$. In fact, using Cauchy's integral formula and Fubini's Theorem, we derive the following equation

$$\mathcal{E}_n(f) = \frac{1}{2\pi} \left| \int_{\Gamma} f(z) (\widehat{\mu}(z) - R_n(z)) dz \right|, \tag{15}$$

where R_n is the n -th multipoint Padé approximant associated to (μ, α_n) , $d\mu(x) = W(x)dx$, $\widehat{\mu}(z)$ is the Markov's function which corresponds to μ , and Γ is a smooth Jordan curve contained in V which surrounds $[a, b]$. Equation (15), which is an essential part of the proof of proposition 4 in [3], is practically all what we need. If α_n vanishes at the most difficult poles of f , counting the respective multiplicities, then the integrand in the right of (15) is analytic in a neighborhood $V' \supset V$ because R_n interpolates $\widehat{\mu}$ at the zeros of α_n , counting multiplicities. Hence, we can improve estimate (14) by putting $\delta(V')$ in place of $\delta(V)$.

Henceforth we only concern with the numerical implementation of a GRQF, particularly when the integrand has difficult poles.

Let $W(x)$ be a positive and Riemann integrable function on $[a, b]$, with possibly some integrable singularities at the end-points on the interval. Let $\alpha(x)$ be given by

$$\alpha(x) = \prod_{k=1}^n \left(\frac{x - z_k}{h_\alpha - z_k} \right), \quad (16)$$

where the points $z_k, k = 1, \dots, n$, are complex numbers in $\mathbb{C} \setminus [a, b]$, such that α is a polynomial with real coefficients. Moreover, $h_\alpha \neq z_k, k = 1, \dots, n$.

Let Q_n be the n -th monic orthogonal polynomial associated to $d\mu(x) = W(x)dx/\alpha(x)$. Then, the sequence (Q_n) satisfies a recurrence relation

$$Q_n(x) = (x - a_{n-1})Q_{n-1}(x) - b_{n-1}Q_{n-2}(x), \quad (17)$$

where the coefficients $a_j, j = 0, 1, 2, \dots$ and $b_j, j = 1, 2, \dots$ must be determined by a numerical procedure, and

$$b_0 = \int_a^b \frac{W(x)dx}{\alpha(x)}$$

Let $P_s(x), s \geq 0$, be a polynomial defined as $P_0 \equiv 1$, and

$$P_s(x) = \prod_{k=1}^s \left(\frac{x - \zeta_k}{h_P - \zeta_k} \right), \quad s \geq 1, \quad (18)$$

where the points $\zeta_k, k = 1, \dots, n$, are given complex numbers such that P_s is a polynomial with real coefficients. Moreover, $h_P \neq \zeta_k, k = 1, \dots, n$.

The presence of the denominators $h_\alpha - z_k$ and $h_P - \zeta_k$ in (16) and (18), respectively, is due to scaling.

Let $(H_{s,n}), s, n = 0, 1, \dots$, be the array given by

$$H_{s,n} = \int_a^b Q_n(x)P_s(x) \frac{W(x)}{\alpha(x)} dx. \quad (19)$$

From (17) we easily derive the following relation

$$H_{s-1,n} = H_{s,n-1}(h_P - \zeta_s) + (\zeta_s - a_{n-1})H_{s-1,n-1} - b_{n-1}H_{s-1,n-2}. \quad (20)$$

Thus, in principle, we only have to calculate the modified moments $H_{s,0}, s = 0, 1, 2, \dots$, to obtain all $H_{s,n}$.

Different sequences of the polynomials P_s yield different numerical results, so the selection to be made of the zeros ζ_k and the constant h_P is not arbitrary. We claim that simplicity and positivity seem to be the most convenient principles in modelling P_s , and it occurs, for example, when $\zeta_k = \zeta \leq a$, where ζ is a constant, and $h_P \geq b$.

The choice of the zeros of α is made according to which poles of the integrand are considered to be the most difficult ones.

The polynomials Q_n fulfill orthogonality conditions which can be used to obtain, step by step, the recurrence coefficients $a_n, b_n, n = 0, 1, \dots$. In fact, $H_{s-1,n} = 0$ for $s \leq n$, so we get the linear system of equations given below

$$\begin{aligned} H_{n,n-1}(h_P - \zeta_s) + \zeta_s H_{n-1,n-1} &= a_{n-1} H_{n-1,n-1} + b_{n-1} H_{n-1,n-2} \\ H_{n-1,n-1}(h_P - \zeta_s) + \zeta_s H_{n-2,n-1} &= a_{n-1} H_{n-2,n-1} + b_{n-1} H_{n-2,n-2} \end{aligned} \quad (21)$$

The Jacobi matrix of order n , denoted by J_n , has the form suggested by (22).

$$J_n = \begin{pmatrix} a_0 & \sqrt{b_1} & 0 & \cdots & 0 & 0 \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & & \\ 0 & \sqrt{b_2} & a_2 & \cdots & 0 & 0 \\ 0 & 0 & \sqrt{b_3} & \cdots & 0 & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & \sqrt{b_n} & a_n \end{pmatrix} \quad (22)$$

It is well known that the nodes $x_{n,k}$ and the coefficients $\lambda_{n,k}, k = 1, \dots, n$, of the GRQF of order n are obtained from J_n . If $J_n = PDP^T$, where D is a diagonal matrix and P is an orthogonal matrix whose columns $C_i, i = 1, \dots, n$, are eigenvectors of J_n , then $x_{n,k} = D(k, k)$, and $\lambda_{n,k} = b_0 C_k(1)^2, k = 1, \dots, n$.

The accuracy to be reached by applying this method depends a lot on the calculation of the modified moments $H_{s,0}, s = 0, 1, 2, \dots$. Nevertheless, the existence of difficult poles and singularities of the weight function W at the end points of the integration interval, should produce instability. We overcome these drawbacks by changing the variable in the integrals $H_{s,0}, s = 0, 1, \dots$ with the transformation ϕ given by (9).

We show some numerical results produced by this method when it is applied to a pair of singular integrals considered by Gautschi [5, 8] (see examples 2, 3).

Smoothing method applied to the integral (23)

Example 2

$$\int_{-1}^1 \frac{(\pi x/\omega)}{\sin(\pi x/\omega)} dx, \quad \omega > 1. \quad (23)$$

The integrand in (23), where $W \equiv 1$, is analytic in a neighborhood of the interval $[-1, 1]$, and has simple real poles at $n\omega, n \in \mathbb{Z}, n \neq 0$. When $\omega \approx 1$ the most difficult poles are $\pm\omega$. All poles can be represented as the pairs $\xi_n = \pm n\omega, n = 1, \dots, d, d \geq 1$. In order to simulate the K poles closest to $[-1, 1]$ we will assume that the polynomial $\alpha(x)$ have zeros at: $\pm j\omega, j = 1, \dots, d$, hence the degree of α is $K = 2d$. The zero $\omega(d+1)$ is included when $K = 2d+1$. Thus, the polynomial α has one of the two forms given below.

$$\alpha_{2d}(x) = \prod_{k=1}^K \left(\frac{x^2 - (k\omega)^2}{1 - (k\omega)^2} \right), \quad \alpha_{2d-1}(x) = \left(\frac{x - d\omega}{1 - d\omega} \right) \alpha_{2d-2}(x).$$

The results in Table 2 suggest that this approach is superior to that reported in [3, 5, 8].

The eight poles which arise after introducing $\phi_{4,4,-1,1}$ in the integrand P_s/α when $K = 2$ and $x_0 = -\omega = -1 - 1.0e - 03$, are given below.

$$\begin{aligned} z_1 = \bar{z}_2 &\approx 1.205618632921826e + 00 + 2.607546334594217e - 01i, \\ z_3 = \bar{z}_4 &\approx 1.205618632921826e + 00 - 2.607546334594217e - 01i, \\ z_5 = \bar{z}_6 &\approx 7.923833650801722e - 01 + 1.713789321753345e - 01i, \\ z_7 = \bar{z}_8 &\approx 7.923833650801722e - 01 - 1.713789321753345e - 01i, \end{aligned}$$

which satisfy $\min_k d(z_k, [-1, 1]) = 1.713789321753345e - 01$, so they should not be considered as difficult.

We do not either expect problems in connection with the poles of $\phi_{4,4,-1,1}$ because

$$d(\{z; \phi_{4,4,-1,1}(z) = \infty\}, [-1, 1]) = 4.142135623730950e - 01.$$

Apparently, those cases for the integral (23) in which very difficult poles are present, that is, when $|\omega| < 1 + 1.0e - 03$, have not been reported so far. In this respect, Table 2 demonstrates that this approach proved to be accurate by a wide margin when it is applied to integrands with such poles.

Order	deg α	A	B	Order	deg α	A	B
1	2	4.1e-01	4.1e-01	1	4	2.7e-01	2.7e-01
2	4	8.5e-03	8.4e-03	3	4	3.4e-04	3.4e-04
3	6	1.1e-04	1.1e-04	5	4	4.1e-07	6.6e-06
4	8	8.0e-07	6.0e-07*	6	4	1.3e-08	6.1e-06
1	1	5.1e-01	4.1e-01	7	4	4.0e-10	2.5e-10*
2	2	2.9e-02	2.9e-02	3	2	2.2e-03	2.2e-03
3	3	2.1e-03	2.1e-03	4	2	1.7e-04	1.7e-04*
4	4	1.2e-05	1.2e-05*	5	2	1.2e-05	2.0e-05
5	5	4.0e-07	7.3e-06	6	2	8.8e-07	9.3e-06
6	6	9.9e-10	5.0e-06	7	2	6.3e-08	6.3e-08*

Table 1: Relative errors obtained when (23) ($\omega = 1 + 1.0e - 03$) is evaluated by a GRQF (A), using smoothing method with parameters $p = q = 4$, $h_\alpha = 0$, $\zeta_k = -1$, $h_P = 1$, compared with those obtained in ([5],1999) by a GRQF (B) using Gautschi's method. The symbol * means that the result has been reported in ([8],2004)

The need of using a GRQF when the integrand is $f(\phi(x))$, instead of a polynomial procedure, is produced by the fact that this function is still meromorphic. Table 3 is an experimental evidence of that the smoothing transformation is not enough to diminish the adverse effect of nearby poles by itself.

The comparison with [3] is not so fair because that paper deals with a rational simultaneous procedure to evaluate three integrals which have the same integrand. The common nodes and the coefficients which are used therein to calculate the integral in (23), depend on the other two integrators as well.

Order	$t = 5$	$t = 7$	$t = 9$	$t = 11$	$t = 13$	$t = 15$
2	6.2e-03	4.8e-03	3.9e-03	3.3e-03	2.6e-03	3.0e-02
3	2.4e-04	1.8e-04	1.4e-04	1.4e-04	1.2e-04	2.8e-02
4	8.5e-06	6.3e-06	5.0e-06	2.8e-05	2.2e-04	2.7e-02
5	2.8e-07	2.0e-07	1.7e-07	2.4e-05	2.2e-04	2.7e-02
6	8.8e-09	6.5e-09	9.2e-09	2.4e-05	2.2e-04	2.7e-02
7	2.7e-10	2.6e-10	4.3e-09	2.4e-05	2.2e-04	2.7e-02
8	7.9e-12	6.8e-11	4.2e-09	2.4e-05	2.2e-04	2.7e-02
9	1.2e-13	6.2e-11	4.2e-09	2.4e-05	2.2e-04	2.7e-02
10	1.3e-13	6.2e-11	4.2e-09	2.4e-05	2.2e-04	2.7e-02
11	1.2e-13	6.2e-11	4.2e-09	2.4e-05	2.2e-04	2.7e-02
12	1.4e-13	6.2e-11	4.9e-05	2.4e-05	2.2e-04	2.7e-02

Table 2: Relative errors obtained when (23) is evaluated by a GRQF, using smoothing method with $p = q = 4$, $\zeta_k = -1$, $h_P = 1$, $\deg \alpha = 4$, and $\omega = 1 + 1.0e - t$.

Smoothing method applied to the integral (24)

Example 3

$$\int_0^1 \frac{\Gamma(1+x)}{(x+\omega)\sqrt{x}} dx, \quad \omega > 0. \quad (24)$$

The integrand in (24) has poles at ω and at $x = -1 - j$, $j \in \mathbb{N}$. The factor $1/\sqrt{x}$ with a non polar singularity at $x = 0$ is assumed to be the weight function $W(x)$.

We fit the transformation $\phi_{6,1,p,q}$ into the modified moments $H_k(s, 0)$, $s = 0, 1, \dots, s_0$, not into the target integral (24). After that, we apply a Gauss-Legendre rule to evaluate all of them up to $s_0 = 50$. Table 3 shows the relative error produced by a GQRF when the smoothing transformation is taken with $\omega = 1.0e - 03$, $a = 0$, $b = 1$, $p = 6$, $q = 1$, and the integrator is now modified by $1/\alpha(x)$, where

$$\alpha(x) = \begin{cases} \frac{(x+\omega)}{\omega} \prod_{j=1}^K \frac{(x+j)}{j} & n = K + 1 \\ \frac{(x+\omega)}{\omega} & n = 1. \end{cases}$$

Except for the case when the quadrature order is $r = 9$, and $\deg \alpha = 2$, the smoothing method produces better results than those obtained in [5, 8].

Notice that condition (12) is satisfied by a wide margin when $a = 0$, $b = 1$, $x_0 = -\omega = -1.0e - 03$ and $p = 6$.

The poles of the rational functions $R_\phi(x) = P_s(\phi_{6,1,0,1}(x))/\alpha(\phi_{6,1,0,1}(x))$ ($n = 1$),

Order	A	B	C	Order	A	B	C
2	6.2e-03	8.3e-01	6.7e-02	8	7.9e-12	6.1e-01	6.1e-02
3	2.4e-04	7.7e-01	1.4e-01	9	1.2e-13	5.9e-01	1.5e-02
4	8.5e-06	7.3e-01	3.0e-01	10	1.3e-13	5.7e-01	1.7e-02
5	2.8e-07	6.9e-01	9.6e-02	11	1.2e-13	5.6e-01	2.7e-02
6	8.8e-09	6.6e-01	6.0e-02	12	1.4e-13	5.4e-01	1.5e-02
7	2.7e-10	6.4e-01	9.8e-02	13	1.3e-13	5.3e-01	6.9e-03

Table 3: Relative errors obtained when (23) ($\omega = 1 + 1.0e - 05$) is evaluated by (A) a GRQF using smoothing method with parameters $p = q = 4$, $\zeta_k = 0$, $h_P = 1$, $\deg \alpha = 4$, compared with (B) a composite Gauss-Legendre rule of polynomial type applied directly to (23) and (C) after introducing $\phi_{4,4,-1,1}$ in (23).

The symbol * means that the result has been reported in ([8],2004)

Order	deg α	A	B	Order	deg α	A	B
1	1	4.3e-03	4.3e-03	1	1	4.3e-03	4.3e-03
2	2	2.8e-05	2.8e-05	2	1	1.2e-04	1.2e-04
3	3	3.5e-07	5.4e-07	3	1	3.5e-06	3.4e-06
4	4	3.2e-09	1.4e-08	4	1	1.0e-07	1.0e-07*
5	5	2.1e-11	9.3e-08	7	1	2.7e-12	2.7e-12*
1	2	2.1e-03	2.1e-03*	1	2	2.1e-03	2.1e-03*
2	4	8.0e-05	8.0e-05	2	2	2.8e-05	2.8e-05
3	6	1.7e-06	2.1e-06	4	2	1.0e-09	1.0e-09*
4	8	2.2e-08	1.4e-08	7	2	5.9e-16	2.9e-16*
5	10	2.0e-10	4.6e-07				

Table 4: Relative errors obtained when (24) ($\omega = 1.0e - 03$) is evaluated by a GRQF (column A), using smoothing method with parameters $p = 6$, $q = 1$, $h_\alpha = 0$, $\zeta_k = -0.0005$, $h_P = 1$, compared with those obtained in ([5],1999) by a GRQF (column B) using Gautschi's method .

are the following complex numbers (see formula for z_k in the proof of Proposition 3)

$$\begin{aligned}
 z_1 &\approx -2.820923896908622e - 01 + 1.713016987146600e - 01i, \\
 z_2 &\approx -2.820923896908622e - 01 - 1.713016987146600e - 01i, \\
 z_3 &\approx 1.653779452391992e - 02 + 3.174826136511961e - 01i, \\
 z_4 &\approx 1.653779452391992e - 02 - 3.174826136511961e - 01i, \\
 z_5 &\approx 2.655545951669421e - 01 + 1.422300110039108e - 01i, \\
 z_6 &\approx 2.655545951669421e - 01 - 1.422300110039108e - 01i,
 \end{aligned}$$

which yield $\min_k d(z_k, [0, 1]) = 1.422300110039108e - 01 > d(x_0, a) = 1.0e - 03$.

It has not been detected that the closest poles, z_5 and z_6 , affect adversely the evaluation of the moments $H_{s,0}$.

Even when $n > 1$ the closest poles are z_5 and $z_6 = \bar{z}_5$, which have demonstrated to

be less adverse for computing the integral of R_ϕ than $x_0 = -1.0e - 03$ with respect to the integrand is $P_s(x)/\alpha(x)$.

Finally, $d(\{z; \phi_{6,1,0,1}(z) = \infty\}, [0, 1]) = 3.005069203095515e - 01$.

4 The modified smoothing method

The “modified smoothing method” is a slight variation of the technique described in the previous section to improve the estimates of $\mathcal{I}(f)$ when some real poles are very difficult. It consists in making a substitution with $\Phi_{p,q,x_1,x_2}(x) = A\phi_{p,q,x_1,x_2}(x) + B$, where $x_1 \leq a \leq b \leq x_2 = b + a - x_1$, $A = A(p, q, x_1, x_2)$ and $B = B(p, q, x_1, x_2)$ are chosen so that $\Phi_{p,q,x_1,x_2}(a) = a$ and $\Phi_{p,q,x_1,x_2}(b) = b$. We fit Φ_{p,q,x_1,x_2} into the integrals which define the moments $H_{s,0}$, $s = 0, 1, \dots$, following the steps indicated by (4)–(7). The rest of the procedure is the same as that given in section 3, including the substitution of the new variable t : $x = \phi_{p,q,a,b}(t)$ such as the following formula indicates.

$$H_{s,0} = \int_a^b \left(\frac{P_s w}{\alpha} \right) (\Phi_{p,q,x_1,x_2}(\phi_{p,q,a,b}(t))) \Phi'_{p,q,x_1,x_2}(\phi_{p,q,a,b}(t)) \phi'_{p,q,a,b}(t) dt. \quad (25)$$

We show, using an example, how must be selected the points x_1, x_2 so that the zeros of the rational function $\alpha_\Phi(x) = \alpha(\Phi_{p,q,x_1,x_2}(x))$ are relatively far away from $[a, b]$, and the complex zeros which deserve to be considered as the closest ones are in the region $\{z; \Re(z) \notin [a, b]\}$. Here $\alpha(x)$ is a polynomial which vanishes at the closest real poles of a given integrand f . The polynomial version of α_Φ is the following

$$\alpha_\Phi(x) = \prod_{k=1}^K ((x_2 - t_k)(x - x_1)^p - (t_k - x_1)(x_2 - x)^q),$$

where $t_k, k = 1, \dots, K$ are the K most difficult poles of f in \mathbb{R} . One should take into account that if $n = \max\{p, q\}$ then the degree of $\alpha_\Phi(x)$ is n times K , which could be excessive.

Order	A	B	Order	A	B
2	2.6e-03	1.1e-02	8	2.2e-04	9.3e-06
3	1.2e-04	7.0e-04	9	2.2e-04	9.3e-06
4	2.2e-04	5.8e-05	10	2.2e-04	9.3e-06
5	2.2e-04	1.3e-05	11	2.2e-04	9.3e-06
6	2.2e-04	9.6e-06	12	2.2e-04	9.3e-06
7	2.2e-04	9.4e-06	13	2.2e-04	2.1e-02

Table 5: Relative errors when (23) with $\omega = 1 + 1.0e - 13$ is evaluated by the smoothing method of Section 3 (**A**), and the corresponding modification (**B**)

Example 4 Assume that $p = q = 4$, $a = -1$, $b = 1$ and $x_0 = -1 - 1.0e - 13$. Let x_1, x_2 be two real numbers such that $x_2 = -x_1$ and $x_1 < x_0 < a$. When we try to solve the equations $\Phi_{p,p,x_1,x_2}(x) = \pm x_0$, where $\pm x_0$ are the only points to be considered as difficult poles, we derive the following relation (the cases $\pm x_0$ are symmetric with respect to $\Re(z) = 0$)

$$\left(\frac{x - x_1}{x_2 - x}\right)^4 = -\frac{Ax_1 + B - x_0}{Ax_2 + B - x_0}. \quad (26)$$

The solution of (26) contains real numbers if and only if

$$C(x_0, x_1) = (Ax_1 + B - x_0)/(Ax_2 + B - x_0) < 0.$$

Using Matlab tools we can find the value $x_1 = -1.001001365076944$, such that $C(x_0, x_1) < 0$ and x_1 is close enough to the point x_1^0 which fulfils $C(x_0, x_1^0) = 0$. If we restrict our attention to the only difficult poles $\pm x_0$, then

$$\alpha_\Phi(x) = D_1(\Phi_{4,4,x_1,x_2}(x)^2 - x_0^2), \quad (27)$$

where D_1 is a constant for scaling.

The equation $\alpha_\Phi(z) = 0$ has eight roots, four of them real and the rest complex in the region $\{z; \Re(z) \notin [a, b]\}$. Besides, the closest poles of $1/\alpha_\Phi$ to the points $x = \pm 1$ are real and considerably less difficult than $\pm x_0$ when the latter are seen as poles.

The eight zeros of α_Φ are approximately

$$\begin{aligned} z_1 &\approx 1.001673003797011e + 00, \\ z_3 &\approx 1.001001139434780e + 00 + 6.714129262901433e - 04i, \\ z_5 &\approx 1.001001139434780e + 00 - 6.714129262901433e - 04i, \\ z_7 &\approx 1.000330177641305e + 00, \\ z_2 &= -z_1, \quad z_4 = -z_3, \quad z_6 = -z_5, \quad z_8 = -z_7, \end{aligned}$$

and all of them are in $\{z; \Re(z) < -1\} \cup \{z; \Re(z) > 1\}$. Besides,

$$\min_{1 \leq k \leq 8} d(z_k, [a, b]) = 3.301776413047186e - 04, \quad (28)$$

which is very large in comparison with $1.0e - 13$.

Section 2 says nothing about the location of the solutions of $\phi_{4,4,-1,1}(z) = z_k$, when z_k is non-real, $k = 1, \dots, 8$. It means that formula (25) does not guarantee accuracy. Nevertheless, the especial location of the points z_k seems to be the reason for which the following result takes place

$$\min_{1 \leq k \leq 8} d(\{z; \phi_{4,4,-1,1}(z) = z_k\}, [-1, 1]) = 1.366390345627513e - 01,$$

which represents a result much more favorable than that given by (28).

The integrand in (23) with $\omega = -x_0$ has the only difficult poles $\pm(1 + 1.0e - 13)$. For the purposes of comparison Table 4 organizes the relative errors yielded by **(A)**: the smoothing method of Section 3 (see Table 2), and **(B)**: the modified smoothing method with α_Φ given by (27).

5 Conclusions

The theory in Section 2 points out that the problem of integrating a function with only a difficult real pole can be transformed into another problem which only have complex poles, possibly non difficult. On the other hand, the real poles x_0 which should be considered as difficult ones are those which not only are apparently close to $[a, b]$, but those which in addition fulfil condition (12) (Proposition 3), especially when $b - a < 1$. The previous statement is valid when p is even and $q = 1$, or when q is even and $p = 1$. The examples which we have examined, integral (23) and (24), satisfy $b - a \geq 1$.

If Condition (13) holds then Corollary 1 assures that all real poles of f are removed by the transformation ϕ , including those to be considered as benign. Then the problem consists in finding out whether the complex poles of $f(\phi)$ are difficult or not. It seems to be one of the main reasons for which the change of variable is not so effective when it is fitted into the target integral which in turn is evaluated by a polynomial quadrature rule.

In principle, the smoothing transformation method is effective enough when the difficult poles are real or complex in the region $\{z; \Re(z) \notin [a, b]\}$. For known difficult poles in $\{z; \Re(z) \in [a, b]\}$ the interval have to be conveniently divided into several subintervals.

The modified method described in Section 4 can improve the accuracy of a GRQF but not its rate of convergence which is very slow (see Table 2 and 4).

The technique of fitting a smoothing transformation $\phi_{p,q,a,b}$ has different effects depending on whether we are dealing with close poles or integrable singularities at the end points of the integration interval $[a, b]$. In case of the former, $\phi_{p,p,a,b}$ transforms k poles in $k \times p$ complex poles which can be too near $[a, b]$. It means that $f(\phi_{p,p,a,b})$ is also meromorphic and its complex poles cannot be annihilated by any mapping of ϕ -type when they lie in $a < \Re(z) < b$.

An open problem is to obtain an estimate for the quadrature error of a GRQF as that given in [13] which depends explicitly on the smoothing transformation.

All the calculations have been carried out by running Matlab[®] tools on a computer with an Intel Pentium 4 processor, 2.0 GHz and 512 Mb RAM.

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