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Gaussian rational quadrature formulas for ill-scaled integrands ☆

J.R. Illán González

Departamento de Matemática Aplicada I, Universidad de Vigo, ETSI de Telecomunicación, Campus Lagoas-Marcosende s/n, 36310 Vigo, Spain

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ABSTRACT

A flexible treatment of Gaussian quadrature formulas based on rational functions is given to evaluate the integral $\int_I f(x)W(x)\mathrm{d}x$, when f is meromorphic in a neighborhood V of the interval I and $W(x)$ is an ill-scaled weight function. Some numerical tests illustrate the power of this approach in comparison with Gautschi's method.

1. Introduction

Let $\{A_m\}_{m=1}^{\infty}$ be a sequence of algebraic polynomials with real coefficients, such that $\deg A_m \leq 2m$ and $A_m(x) > 0$, $m \in \mathbb{N}$, $x \in [a, b]$. Let W be a positive, integrable weight function, on the interval $[a, b]$ and $x_{n,j}, j = 1, \ldots, n$, 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

$$\int_a^b f(x)W(x)\mathrm{d}x \approx \sum_{j=1}^{n} \lambda_{n,j} f(x_{n,j}), \tag{1}$$

is a Gaussian rational quadrature formula (GRQF) associated to $(W, \{A_m\})$ if the equality holds in (1) for $f = p/A_m$, $p \in \mathcal{P}_{2n-1}$.

The development of rational procedures to calculate efficiently the integral of functions with poles close to $[a, b]$ is mainly due to Gautschi [1,2], so we adopt his terminology, calling **difficult** those poles which are closest to $[a, b]$ and cause instability as well. Otherwise we say they are **benign**. In general, quadrature formulas of rational type are expedient for integrals which have mass concentrated on a small neighborhood of a point of the integration interval. Such an irregular distribution of mass is the main effect produced by integrable singularities at the endpoints and by difficult poles, though there are other causes. This phenomenon is clearly harmful for numerical tools and can be detected by observing very different scales for the values of the integrand (ill-scaling). A scaling procedure should be carried out by organizing the integrand in terms of the classical integration product scheme. It has been shown in previous works [3,4] that nodes and coefficients for Gauss rational formulas can be calculated using a more flexible procedure than that suggested in [1,2]. This note presents the case in which the integrand is ill-scaled and has difficult non-real poles.

In what follows, we assume that the integrand is factorized as $f(x)W(x)$, where f is analytic in $[a, b]$ ($f \in \mathcal{H}([a, b])$), and meromorphic in $V \setminus [a, b]$ and W is an ill-scaled weight function.

Let $A_m(z)$ be a polynomial having zeros carefully selected in $\mathbb{C} \setminus [a, b]$ such that they are equal to the closest poles of $f(x)$. Then we expect that $g(x) = A_m(x)f(x)$ no longer has difficult poles.

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E-mail address: jillan@uvigo.es.

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Let $H_{s,m,0} = \int_a^b P_s(x)W(x)/A_m(x)\mathrm{d}x$, where P_s is a polynomial of degree s. A stage of the process consists in calculating $H_{s,m,0}$ and it can be seriously affected by instability. We overcome this drawback by fitting a smoothing transformation ϕ into selected modified moments to diminish the adverse effect produced by the zeros of $A_m(x)$ and the singularities of W at the endpoints of the interval. We call "smoothing method" to the whole procedure of mixing Gaussian rational quadrature formulas with the technique of changing the variable.

The rational transformation ϕ to be used as a substitution mapping is presented in Section 2. The implementation of the smoothing approach is described in Section 3. For comparison, in Section 4 we include an example which had been already considered in [1,2].

2. The smoothing mapping ϕ

The smoothing transformations which we plan to use, should work when the difficult poles are in the region of the complex plane $\Omega = \mathbb{C} \setminus [a, b]$ and they are close to the endpoints of the integration interval.

Let $W_m = W/A_m$ and $\phi : [a, b] \to [a, b]$ be a suitable infinitely differentiable, bijective and strictly monotonically increasing function. For every polynomial P_s of degree s, we have that the modified moments $H_{s,m,0}$ can be approximated by a given quadrature rule with nodes $x_{n,m,k}$ and weights $\lambda_{n,m,k}$, $k = 1, \ldots, n$. If we apply such a formula after fitting ϕ into the integral in (2), we obtain

$$H_{s,m,0} = \int_a^b (P_s W_m)(\phi(t))\phi'(t)\mathrm{d}t \approx \sum_{k=1}^{n} \lambda_{n,m,k}\phi'(x_{n,m,k})(P_s W_m)(\phi(x_{n,m,k})). \tag{2}$$

Hence, we have derived a new formula with

$$t_{n,m,k} = \phi(x_{n,m,k}), \qquad \Lambda_{n,m,k} = \phi'(x_{n,m,k})\lambda_{n,m,k}.$$

Notice that if $\lambda_{n,m,k} > 0$ then $\Lambda_{n,m,k} > 0$, and that $\phi'(x)$ annihilates some kind of singularities at the endpoints of the interval $[a, b]$ provided that

$$\phi'(x) = u(x)(x-a)^{p-1}(b-x)^{q-1}, \tag{3}$$

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

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

$$\phi_{p,q,a,b}(x) := \frac{(b-a)(x-a)^p}{(x-a)^p + (b-x)^q} + a, \tag{4}$$

$p, q \in \mathbb{N}$, $q, p \geq 1$, $p + q > 2$. The derivative of $\phi_{p,q,a,b}$ fulfills condition (3).

3. The numerical method

Let $A_m(x)$ be a polynomial with degree $K_m \leq 2m$, having zeros ζ_k, $k = 1, \ldots, K_m$, in $\mathbb{C} \setminus [a, b]$, such that A_m has real coefficients and $A_m(x) > 0$, $x \in [a, b]$.

The sequence $\{Q_{m,k}\}_{k=0}^{\infty}$ of monic orthogonal polynomials associated to W_m satisfies a recurrence relation

$$Q_{m,k}(x) = (x - a_{m,k-1})Q_{m,k-1}(x) - b_{m,k-1}Q_{m,k-2}(x), \tag{5}$$

where the coefficients $a_{m,j}$, $j = 0, 1, 2, \ldots$, and $b_{m,j}$, $j = 1, 2, \ldots$, must be determined by a numerical procedure, and $b_{m,0} = \int_{[a,b]} W_m(x)\mathrm{d}x$.

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

$$P_s(x) = \prod_{k=1}^{s} \left(\frac{x - \tau_k}{h_P - \tau_k} \right), \quad s \geq 1, \tag{6}$$

where the points τ_k, $k = 1, \ldots, s$, are given complex numbers such that P_s is a polynomial with real coefficients. Moreover, $h_P \neq \tau_k$, $k = 1, \ldots, s$. The presence of the denominator $h_P - \tau_k$ in (6) is due to scaling.

Let $(H_{s,m,k})$, $s, m, k = 0, 1, \ldots$, be the array given by

$$H_{s,m,k} = \int_a^b Q_{m,k}(x)P_s(x)W_m(x)\mathrm{d}x. \tag{7}$$

From (5) and (6) we easily derive the following relation

$$H_{s,m,k} = H_{s+1,m,k-1}(h_P - \tau_{s+1}) + (\tau_{s+1} - a_{m,k-1})H_{s,m,k-1} - b_{m,k-1}H_{s,m,k-2}. \tag{8}$$

Thus, in principle, for every m, we only have to calculate $H_{s,m,0}$, $s = 0, 1, 2, \ldots$, to obtain $H_{s,m,k}$, $k \geq 1$.