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The use of rational functions in numerical quadrature

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Abstract

Quadrature problems involving functions that have poles outside the interval of integration can profitably be solved by methods that are exact not only for polynomials of appropriate degree, but also for rational functions having the same (or the most important) poles as the function to be integrated. Constructive and computational tools for accomplishing this are described and illustrated in a number of quadrature contexts. The superiority of such rational/polynomial methods is shown by an analysis of the remainder term and documented by numerical examples. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Much of numerical analysis has been dominated by polynomial approximation, i.e., approximation procedures that yield exact answers if the function to be processed were a polynomial of some appropriate degree. This is particularly true in the area of numerical quadrature. Frequently, however, the functions to be integrated are not polynomial-like. They often have poles away from the interval of integration, in which case it would be more natural to make the integration exact for rational functions having the same, or at least the more important, poles (those closest to the interval of integration). It may be desirable to still have some low-degree polynomials, e.g., constants, integrated exactly. This suggests an approximation procedure that provides exact answers for a mixture of rational functions and polynomials. The constructive and computational tools for implementing this idea are described, not only for ordinary quadrature rules, but also for more sophisticated rules such as Gauss–Kronrod and Gauss–Turán rules, and quadrature procedures for Cauchy principal value integrals.

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An idea somewhat related to our's is to require exactness for a class of Laurent polynomials, which is meaningful if the underlying measure of integration is "strong", i.e., possesses moments of positive as well as negative orders. The approach is related to two-point Padé approximation, the two points being at the origin and at infinity. For this we refer to [4–8,29–31] and to [47–49] for specific examples. For rational quadrature over the unit circle, we refer to [9] and the references cited therein. Our results in Section 6 on rational Gauss-type quadrature formulae are closely related to multipoint Padé approximation. The convergence of such approximations and of related quadrature formulae has been studied in a series of papers by López Lagomasino and others; see, e.g., [24, 35–38,25,11]. Further convergence results, also for other rational quadrature formulae, can be found in [10].

There are other approaches, essentially different from those to be described, of incorporating the influence of poles outside (and particularly near) the interval of integration. One is to construct, in some way or another, a correction term to a standard, in particular Gaussian, quadrature rule. This is an approach taken by Lether, who in [33] uses the method of subtracting the singularity, and in [34] uses the principal part of the Laurent expansion at each pole to obtain the correction term. The latter approach, however, requires the evaluation of the regular part of the integrand at the pole(s). This is avoided in a method proposed by Hunter and Okecha [28]. Another entirely different approach is discussed in [3], where expansion in sinc functions is used.

2. The principle of exactness

We begin with a quadrature rule of the simplest kind,

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{v=1}^{n} \lambda_v f(t_v) + R_n(f), \tag{2.1}$$

where $\mathrm{d}\lambda$ is a given (usually positive) measure of integration all of whose moments exist. The general *principle of exactness* can be formulated as follows. Given a linear space $\mathbb{S}_d$ of functions (integrable with respect to $\mathrm{d}\lambda$), having dimension d, determine t_v and λ_v such that formula (2.1) is exact for all functions in $\mathbb{S}_d$, i.e.,

$$R_n(g) = 0 \quad \text{for all } g \in \mathbb{S}_d. \tag{2.2}$$

Such a formula may or may not exist, and if it does, may not be unique. Classical examples are the *Newton–Cotes formulae*, where the (distinct) nodes t_v are prescribed, and one tries to determine the weights λ_v such that (2.2) holds with $d = n$ and $\mathbb{S}_n = \mathbb{P}_{n-1}$, the space of polynomials of degree $\leqslant n-1$. This determines formula (2.1) uniquely. Alternatively, one could impose conditions on the weights λ_v, for example, that they all be equal, and determine the nodes t_v so as to have polynomial degree of exactness n. This gives rise to *quadrature rules of Chebyshev type*, which may or may not exist if one insists on reality of the nodes. Among all polynomial-based quadrature rules, the optimal one is the *Gauss–Christoffel rule*, or briefly the *Gaussian rule*, where one takes $d = 2n$ and $\mathbb{S}_{2n} = \mathbb{P}_{2n-1}$. In this case, both the nodes t_v and the weights λ_v are to be determined. It is well known that they exist uniquely, that all t_v are contained in the support interval of the measure $\mathrm{d}\lambda$, and the λ_v are all positive (if the measure $\mathrm{d}\lambda$ is positive).

Here we are interested in a mixed rational/polynomial type of exactness. More precisely, given an integer parameter m with $0 \leqslant m \leqslant d$, we take $\mathbb{S}_d$ to be the direct sum of a space of rational functions and a space of polynomials,

$$\mathbb{S}_d = \mathbb{Q}_m \oplus \mathbb{P}_{d-1-m}, \quad 0 \leqslant m \leqslant d, \tag{2.3}$$

where

$$\mathbb{Q}_m = \operatorname{span}\left\{ g : g(t) = (1+\zeta_\mu t)^{-s};\ \mu = 1,2,\ldots,M; \right.$$

$$\left. s = 1,2,\ldots,s_\mu;\ \sum_{\mu=1}^{M} s_\mu = m \right\}. \tag{2.4}$$

The ζ_μ are given (in general complex) numbers satisfying

$$\zeta_\mu \neq 0, \quad 1+\zeta_\mu t \neq 0 \text{ on } \overline{\operatorname{supp}(d\lambda)}. \tag{2.5}$$

The rational component $\mathbb{Q}_m$ of $\mathbb{S}_d$ thus is made up of rational functions having poles $-1/\zeta_\mu$ of multiplicities up to s_μ outside the support of $d\lambda$. These poles are chosen to match the most important poles, if any, of the function f in (2.1). If f is an entire function, one might as well take $m = 0$, in which case $\mathbb{Q}_m$ is empty and $\mathbb{S}_d$ is a purely polynomial space. The other extreme is $m = d$, in which case $\mathbb{S}_d$ consists entirely of genuinely rational functions.

3. Characterization of quadrature rules of rational/polynomial exactness

The basic result concerning quadrature rules (2.1) exact on the space $\mathbb{S}_d$ of (2.2)–(2.4) was proved in [16] (for $d = 2n$) and, independently, in [50] for special choices of $\mathbb{Q}_m$. We state it as the following theorem.

Theorem 3.1. *Let* $0 \leqslant m \leqslant d$ *and*

$$\omega_m(t) = \prod_{\mu=1}^{M} (1+\zeta_\mu t)^{s_\mu} \tag{3.1}$$

(a polynomial of exact degree m). *Assume there exists an n-point quadrature rule of polynomial degree of exactness* $d-1$ *for the modified measure* $d\lambda/\omega_m$:

$$\int_{\mathbb{R}} p(t) \frac{d\lambda(t)}{\omega_m(t)} = \sum_{v=1}^{n} w_v^* p(t_v^*), \quad p \in \mathbb{P}_{d-1}, \tag{3.2}$$

whose nodes t_v^* *are distinct and contained in the support of* $d\lambda$. *Define*

$$t_v = t_v^*, \quad \lambda_v = w_v^* \omega_m(t_v^*), \quad v = 1,2,\ldots,n. \tag{3.3}$$

Then

$$\int_{\mathbb{R}} g(t)\, d\lambda(t) = \sum_{v=1}^{n} \lambda_v g(t_v) + R_n(g), \tag{3.4}$$

where

$$R_n(g) = 0 \quad \textit{for all } g \in \mathbb{S}_d = \mathbb{Q}_m \oplus \mathbb{P}_{d-1-m}. \tag{3.5}$$

Conversely, if (3.4), (3.5) *hold for distinct* $t_v \in \operatorname{supp}(\mathrm{d}\lambda)$, *then so does* (3.2) *with* t_v^*, w_v^* *as obtained from* (3.3).

The (rather elementary) proof is given in [16] for $d = 2n$, but holds equally well for arbitrary d.

The theorem says nothing about the existence or uniqueness of (3.2); it merely states an implication, namely that (3.2) implies (3.4), (3.5), with t_v, λ_v as defined in (3.3), and vice versa. Specific instances of existence and uniqueness will be given later.

4. The remainder term

Assume that $\mathrm{d}\lambda$ has compact support and formula (3.2) exists. It then follows by (3.3) and (3.2) that

$$\int_{\mathbb{R}} \frac{p(t)}{\omega_m(t)}\,\mathrm{d}\lambda(t) = \sum_{v=1}^{n} \lambda_v \frac{p(t_v)}{\omega_m(t_v)}, \quad p \in \mathbb{P}_{d-1}. \tag{4.1}$$

Now define

$$\mathscr{E}_{d,m}(g) := \inf_{p\in\mathbb{P}_{d-1}} \left\| \frac{p}{\omega_m} - g \right\|_\infty = \left\| \frac{p^*}{\omega_m} - g \right\|_\infty \tag{4.2}$$

to be the best approximation of g by rational functions of the form p/ω_m in the maximum norm $\|\cdot\|_\infty$ on the support of $\mathrm{d}\lambda$. Then by a standard argument in the theory of approximation, using (4.1), we have (cf. also [45])

$$\begin{aligned} |R_n(g)| &= \left| \int_{\mathbb{R}} g(t)\,\mathrm{d}\lambda(t) - \sum_{v=1}^{n} \lambda_v g(t_v) \right| \\ &= \left| \int_{\mathbb{R}} \left[g(t) - \frac{p^*(t)}{\omega_m(t)} \right] \mathrm{d}\lambda(t) - \sum_{v=1}^{n} \lambda_v \left[g(t_v) - \frac{p^*(t_v)}{\omega_m(t_v)} \right] \right| \\ &\leqslant \mathscr{E}_{d,m}(g) \left\{ \int_{\mathbb{R}} \mathrm{d}\lambda(t) + \sum_{v=1}^{n} |\lambda_v| \right\}, \end{aligned}$$

that is,

$$|R_n(g)| \leqslant \mathscr{E}_{d,m}(g) \left\{ \int_{\mathbb{R}} \mathrm{d}\lambda(t) + \sum_{v=1}^{n} |\lambda_v| \right\}. \tag{4.3}$$

If $\lambda_v > 0$ and formula (3.4) is exact for a constant, i.e., $d - 1 - m \geqslant 0$, then (4.3) simplifies to

$$|R_n(g)| \leqslant 2\mathscr{E}_{d,m}(g) \int_{\mathbb{R}} \mathrm{d}\lambda(t), \quad m \leqslant d-1. \tag{4.4}$$

The significance of (4.3) is as follows: if g can be well approximated on $\operatorname{supp}(\mathrm{d}\lambda)$ by a function p/ω_m, where p is a polynomial, that is, $g\omega_m$ can be well approximated by a polynomial, then the

quadrature error $R_n(g)$ is small. By our choice of ω_m, multiplying g into ω_m removes the more important poles of g, and the resulting function $\omega_m g$, whose (remaining, if any) poles are now further away from the real axis, can indeed be well approximated by polynomials, certainly better than the original function g.

5. The rational Fejér quadrature rule

The classical Fejér quadrature rule is the interpolatory rule for $d\lambda(t) = dt$ on $[-1, 1]$,

$$\int_{-1}^{1} f(t)\,dt = \sum_{v=1}^{n} \lambda_v f(t_v) + R_n(f), \quad R_n(\mathbb{P}_{n-1}) = 0, \tag{5.1}$$

where the nodes t_v are the Chebyshev points, or, as we call them now, the *Fejér nodes*

$$t_v^{\mathrm{F}} = \cos\theta_v, \quad \theta_v = \frac{2v-1}{2n}\pi, \quad v = 1, 2, \ldots, n. \tag{5.2}$$

Fejér [13] showed that the weights λ_v in (5.1) can be computed explicitly as

$$\lambda_v = \frac{2}{n}\left(1 - 2\sum_{\mu=1}^{\lfloor n/2 \rfloor} \frac{\cos(2\mu\theta_v)}{4\mu^2 - 1}\right), \quad v = 1, 2, \ldots, n, \tag{5.3}$$

and that $\lambda_v > 0$ for all v. Similar results hold for Chebyshev points of the second kind, as was already shown by Fejér, and also for Chebyshev points of the third and fourth kind, with or without one or both of the endpoints ± 1 included, as was shown more recently in [43,44]. We consider here only Chebyshev nodes of the first kind, (5.2), and want to make the quadrature rule (5.1) exact on $\mathbb{S}_n = \mathbb{Q}_m \oplus \mathbb{P}_{n-1-m}$ (i.e., $d = n$ in (2.3)). According to our theorem (cf. (3.2), where we write $t_v^* = t_v^{\mathrm{F}}$, $w_v^* = w_v^{\mathrm{F}}$ and let $d = n$), we need to determine w_v^{F} such that

$$\sum_{v=1}^{n} w_v^{\mathrm{F}} T_k(t_v^{\mathrm{F}}) = \int_{-1}^{1} \frac{T_k(t)}{\omega_m(t)}\,dt, \quad k = 0, 1, \ldots, n-1, \tag{5.4}$$

where T_k is the Chebyshev polynomial of degree k. Letting

$$\mu_k = \int_{-1}^{1} \frac{T_k(t)}{\omega_m(t)}\,dt, \quad k = 0, 1, 2, \ldots \tag{5.5}$$

and making use of the "orthogonality" relation

$$\sum_{k=0}^{n-1}{}' T_k(t_v^{\mathrm{F}}) T_k(t_\mu^{\mathrm{F}}) = \frac{n}{2}\delta_{v\mu}, \tag{5.6}$$

which is a consequence of the Christoffel–Darboux formula for Chebyshev polynomials (the prime on the summation sign means that the first term has to be multiplied by $\frac{1}{2}$), we find from (5.4) immediately that [51]

$$w_v^{\mathrm{F}} = \frac{2}{n}\sum_{k=0}^{n-1}{}' \mu_k T_k(t_v^{\mathrm{F}}), \quad v = 1, 2, \ldots, n. \tag{5.7}$$

It is easily seen that (5.7) reduces to (5.3) when $m = 0$. The computational challenge lies in the computation of the quantities μ_k in (5.5); for these, Weideman and Laurie [51] developed recursive algorithms that allow their stable and efficient computation.

Similar techniques have been employed earlier by Monegato [41], who uses as nodes the zeros of orthogonal polynomials, and have been applied in [42] to Fredholm integral equations with rational kernels. Hasegawa and Torii [27] and Hasegawa [26], instead, use Clenshaw–Curtis nodes. Schneider [46] constructs quadrature rules by integrating rational Hermite interpolants.

6. The rational Gauss quadrature rule

Here, $d = 2n$ in (3.2), and the space of rational/polynomial gauge functions is $\mathbb{S}_{2n} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-1-m}$, where $0 \leqslant m \leqslant 2n$. The existence of the rational Gauss formula which is exact on $\mathbb{S}_{2n}$ now hinges on the existence of the (polynomial) Gauss formula

$$\int_{\mathbb{R}} p(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{v=1}^{n} w_v^{\mathrm{G}}\, p(t_v^{\mathrm{G}}), \quad p \in \mathbb{P}_{2n-1} \tag{6.1}$$

(cf. (3.2), with $t_v^* = t_v^{\mathrm{G}}$, $w_v^* = w_v^{\mathrm{G}}$ and $d = 2n$). Since the ζ_μ in (2.4) may well be complex, hence ω_m a complex-valued polynomial, the existence of (6.1) is by no means guaranteed. There are, however, a number of special cases, of interest in applications, in which the existence and uniqueness of the Gauss formula (6.1) is assured. Some of these are as follows:

(i) *Simple real poles*: Here all $s_\mu = 1$, hence $M = m$, and we write

$$\zeta_\mu = \xi_\mu \in \mathbb{R}, \quad \xi_\mu \neq 0, \quad \mu = 1, 2, \ldots, m, \tag{6.2}$$

where ξ_μ are distinct real numbers. The corresponding polynomial ω_m becomes

$$\omega_m(t) = \prod_{\mu=1}^{m}(1 + \xi_\mu t), \tag{6.3}$$

which by the assumption $1 + \xi_\mu t \neq 0$ on $\mathrm{supp}(\mathrm{d}\lambda)$ (cf. (2.5)) has constant sign on the support of $\mathrm{d}\lambda$ if the support is connected. Furthermore, if $\mathrm{d}\lambda$ has finite moments, as we assumed, then so does $\mathrm{d}\lambda/\omega_m$. Hence, the Gauss formula (6.1) exists for each n and m and is unique. According to (3.3), the nodes and weights of the rational Gauss formula (2.1) are given by

$$t_v = t_v^{\mathrm{G}}, \quad \lambda_v = w_v^{\mathrm{G}}\omega_m(t_v^{\mathrm{G}}), \quad v = 1, 2, \ldots, n. \tag{6.4}$$

Since all w_v^{G} have the same sign, namely the sign of ω_m on $\mathrm{supp}(\mathrm{d}\lambda)$, it follows that all λ_v are positive.

(ii) *Simple conjugate complex poles*: It is natural, in this case, to take m even, and thus

$$\zeta_\mu = \xi_v + \mathrm{i}\eta_v, \quad \zeta_{\mu+1} = \xi_v - \mathrm{i}\eta_v \quad (v = 1 + \lfloor \mu/2 \rfloor), \quad \mu\ (\mathrm{odd}) = 1, 3, \ldots, m-1. \tag{6.5}$$

Here, the polynomial

$$\omega_m(t) = \prod_{v=1}^{m/2}[(1 + \xi_v t)^2 + \eta_v^2 t^2] \tag{6.6}$$

is strictly positive on all of $\mathbb{R}$, and the Gauss formula (6.1) again exists and is unique for each n and m.

(iii) *Simple conjugate complex poles plus a real pole*: This is the case where in addition to pairs of conjugate complex poles there is one simple real pole, i.e., m is odd and

$$\zeta_\mu = \xi_\nu + \mathrm{i}\eta_\nu, \quad \zeta_{\mu+1} = \xi_\nu - \mathrm{i}\eta_\nu \quad (\nu = 1 + \lfloor \mu/2 \rfloor), \quad \zeta_m = \xi_m \in \mathbb{R}, \quad \mu \text{ (odd)} = 1, 3, \ldots, m-2. \tag{6.7}$$

The polynomial ω_m is now

$$\omega_m(t) = (1 + \xi_m t) \prod_{\nu=1}^{(m-1)/2} [(1 + \xi_\nu t)^2 + \eta_\nu^2 t^2] \tag{6.8}$$

and is of constant sign on the support of $\mathrm{d}\lambda$. Here again, formula (6.1) exists uniquely for all n and m, and is positive.

Some, or all, of the above poles could have multiplicity 2 or higher.

For rational Gauss and Gauss–Lobatto formulae on $[-1, 1]$, with $\mathrm{d}\lambda(t) = (1 - t^2)^{-1/2}\,\mathrm{d}t$, and with poles distributed as in (i) and (ii), see also [39,40].

7. Spectral characterization of the Gauss formula (6.1)

We assume that $\mathrm{d}\hat{\lambda} = \mathrm{d}\lambda/\omega_m$ is a positive measure. The connection between Gaussian quadrature and orthogonal polynomials is well known. The polynomials we need are those orthogonal with respect to $\mathrm{d}\hat{\lambda}$; we assume them to be monic and denote them by $\hat{\pi}_k(\cdot) = \pi_k(\cdot; \mathrm{d}\hat{\lambda})$, $k = 0, 1, 2, \ldots$. They satisfy a three-term recurrence relation

$$\begin{aligned} &\hat{\pi}_{k+1}(t) = (t - \hat{\alpha}_k)\hat{\pi}_k(t) - \hat{\beta}_k \hat{\pi}_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ &\hat{\pi}_{-1}(t) = 0, \quad \hat{\pi}_0(t) = 1, \end{aligned} \tag{7.1}$$

where $\hat{\alpha}_k \in \mathbb{R}$ and $\hat{\beta}_k > 0$. Associated with the recurrence relation is the *Jacobi matrix*

$$\hat{J} = J(\mathrm{d}\hat{\lambda}) = \begin{bmatrix} \hat{\alpha}_0 & \sqrt{\hat{\beta}_1} & & & \\ \sqrt{\hat{\beta}_1} & \hat{\alpha}_1 & \sqrt{\hat{\beta}_2} & & \\ & \sqrt{\hat{\beta}_2} & \hat{\alpha}_2 & \sqrt{\hat{\beta}_3} & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{7.2}$$

an infinite symmetric tridiagonal matrix. Although $\hat{\beta}_0$ is arbitrary (it multiplies $\hat{\pi}_{-1} = 0$ in (7.1)), it is customary to define it as

$$\hat{\beta}_0 = \int_{\mathbb{R}} \mathrm{d}\hat{\lambda}(t). \tag{7.3}$$

If we are interested in the n-point quadrature rule (6.1), we need only the first $n + 1$ orthogonal polynomials $\hat{\pi}_0, \hat{\pi}_1, \ldots, \hat{\pi}_n$, hence the truncated Jacobi matrix $\hat{J}_n$ — the $n \times n$ leading principal minor matrix of (7.2). The quadrature rule can then be characterized in terms of the eigenvalues and eigenvectors of $\hat{J}_n$ [23]. Indeed, the Gauss nodes t_ν^{G} are the eigenvalues of $\hat{J}_n$, and the Gauss weights

w_v^{G} expressible in terms of the first components $v_{v,1}$ of the corresponding normalized eigenvectors v_v; more precisely,

$$\hat{J}_n v_v = t_v^{\mathrm{G}} v_v, \quad v_v^{\mathrm{T}} v_v = 1,$$

$$w_v^{\mathrm{G}} = \hat{\beta}_0 v_{v,1}^2. \tag{7.4}$$

To compute the Gauss formula, it suffices therefore to solve an eigenvalue/eigenvector problem for a real symmetric tridiagonal matrix. This, nowadays, is a routine problem, and there are fast and accurate methods available for its solution, including appropriate software (cf., e.g., [18, Section 6]). The major challenge is the computation of the recursion coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$, since $\mathrm{d}\hat{\lambda} = \mathrm{d}\lambda/\omega_m$ is not a standard classical measure. For these, one can use a simple discretization procedure and special techniques for "difficult" poles, i.e., poles very close to the support interval of the measure $\mathrm{d}\lambda$. These latter techniques are somewhat technical and will not be described here in detail. Basically, one first applies the discretization procedure to the "reduced" measure $\mathrm{d}\tilde{\lambda} = \mathrm{d}\lambda/\tilde{\omega}_m$, where $\tilde{\omega}_m$ is the polynomial ω_m with the difficult poles removed, and then incorporates the difficult poles by special techniques; see [19]. The discretization procedure is described in the next section.

8. The discretization procedure

If the inner product underlying the measure $\mathrm{d}\hat{\lambda}$ is denoted by

$$(u, v) = \int_{\mathbb{R}} u(t) v(t)\, \mathrm{d}\hat{\lambda}(t), \quad \mathrm{d}\hat{\lambda}(t) = \frac{\mathrm{d}\lambda(t)}{\omega_m(t)}, \tag{8.1}$$

then, as is well known, the desired coefficients can be expressed in terms of this inner product and the orthogonal polynomials $\hat{\pi}_k(\cdot) = \pi_k(\cdot; \mathrm{d}\hat{\lambda})$ as

$$\hat{\alpha}_k = \frac{(t\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_k, \hat{\pi}_k)}, \quad 0 \leqslant k \leqslant n-1,$$

$$\hat{\beta}_0 = (\hat{\pi}_0, \hat{\pi}_0), \quad \hat{\beta}_k = \frac{(\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_{k-1}, \hat{\pi}_{k-1})}, \quad k = 1, 2, \ldots n-1. \tag{8.2}$$

This suggests, as already noted by Stieltjes, a simple "bootstrapping" procedure, which is now known as *Stieltjes procedure*: Since $\hat{\pi}_0 = 1$ is known, one computes $\hat{\alpha}_0$, $\hat{\beta}_0$ by (8.2) for $k = 0$. With $\hat{\alpha}_0$, $\hat{\beta}_0$ at hand, the recurrence relation (7.1), with $k = 0$, yields $\hat{\pi}_1$. This allows us to apply (8.2) with $k = 1$ to get $\hat{\alpha}_1$, $\hat{\beta}_1$, which by (7.1) for $k = 1$ yields $\hat{\pi}_2$, and so forth. The major difficulty with this procedure is the computation of the inner products in (8.2); this requires integration with respect to the measure $\mathrm{d}\hat{\lambda}$, which is not straightforward.

However, already in 1968, and later in 1994, we proposed a simple modification of Stieltjes's procedure [14,18], which consists in applying it to a discrete inner product

$$(u, v)_N = \sum_{k=1}^{N} \omega_k^{(N)} u(t_k^{(N)}) v(t_k^{(N)}), \quad N > n, \tag{8.3}$$

which approximates (u,v) in such a way that

$$\lim_{N\to\infty}(u,v)_N=(u,v)\quad\text{for all } u,v\in\mathbb{P}. \tag{8.4}$$

Here, $\mathbb{P}$ is the space of polynomials. If $\hat{\pi}_{k,N}$ denote the discrete orthogonal polynomials associated with the inner product (8.3), and $\hat{\alpha}_{k,N}$, $\hat{\beta}_{k,N}$ the respective recursion coefficients, it can be shown [14, Section 4] that for any fixed k,

$$\lim_{N\to\infty}\hat{\alpha}_{k,N}=\hat{\alpha}_k,\quad \lim_{N\to\infty}\hat{\beta}_{k,N}=\hat{\beta}_k. \tag{8.5}$$

There is no difficulty in computing the $\hat{\alpha}_{k,N}$, $\hat{\beta}_{k,N}$ by a procedure analogous to Stieltjes's procedure — now known as the *discrete Stieltjes procedure* — since all inner products required are finite sums.

A natural way of obtaining a discretization (8.3) is by applying the Gaussian quadrature rule for the measure $\mathrm{d}\lambda$ to (8.1), i.e., by taking

$$t_k^{(N)}=t_k^{(N)}(\mathrm{d}\lambda),\quad \omega_k^{(N)}=\frac{w_k^{(N)}(\mathrm{d}\lambda)}{\omega_m(t_k^{(N)})},\quad k=1,2,\ldots,N, \tag{8.6}$$

where $t_k^{(N)}(\mathrm{d}\lambda)$ and $w_k^{(N)}(\mathrm{d}\lambda)$ are the nodes and weights of the N-point Gaussian quadrature rule for $\mathrm{d}\lambda$. Since $\mathrm{d}\lambda$ is usually one of the classical measures, these quantities are easily computed; for related software, see, e.g., [18, Section 2]. Also, the procedure converges relatively fast as $N\to\infty$, unless there are poles very close to the support interval of $\mathrm{d}\lambda$. It is for this reason that special techniques are required for incorporating these "difficult" poles.

9. Examples

We present four examples for the application of rational Gauss formulae, illustrating the three configurations (i)–(iii) of poles described in Section 6 and a case of a single pole with high multiplicity. The numerical results shown were obtained with the help of software described in [19].

Example 1.

$$I(\omega)=\int_0^1\frac{t^{-1/2}\Gamma(1+t)}{t+\omega}\,\mathrm{d}t,\quad \omega>0.$$

Here, the appropriate measure is $\mathrm{d}\lambda(t)=t^{-1/2}\,\mathrm{d}t$, a Jacobi measure on $[0,1]$ with parameters $\alpha=0$, $\beta=-\frac{1}{2}$. The poles of the integrand are all real; those of the gamma function are located at $-1,-2,-3,\ldots$ and the remaining pole is at $-\omega$. This suggests the choices

$$\xi_\mu=\frac{1}{\mu},\quad \mu=1,2,\ldots,m-1;\quad \xi_m=\frac{1}{\omega} \tag{9.1}$$

in (6.2) and thus the polynomial ω_m in (6.3). (Note that $\xi_\mu=\xi_m$ if ω is an integer μ with $1\leqslant\mu\leqslant m-1$. In this case, $1/\omega_m$ has a pole of multiplicity 2 at $-1/\xi_\mu$.) The rational n-point Gauss formula applied to $I(\omega)$ then becomes

$$I(\omega)\approx I_n(\omega)=\sum_{\nu=1}^{n}\lambda_\nu\frac{\Gamma(1+t_\nu)}{t_\nu+\omega}. \tag{9.2}$$

Table 1
Numerical results for Example 1

$n \setminus m$	$2n$	n	1	0
2	0.995E−03	0.331E−03	0.104E−02	0.143E−01
4	0.258E−06	0.372E−07	0.877E−06	0.819E−04
6	0.153E−10	0.120E−11	0.769E−09	0.431E−06
8	0.377E−13	0.398E−13	0.571E−12	0.223E−08
13				0.419E−13

The discretization method for computing the recursion coefficients $\hat{\alpha}_k$, $\hat{\beta}_k$, and hence the nodes t_v and weights λ_v (in terms of the eigenvalues and eigenvectors of the Jacobi matrix $\hat{J}_n$) works rather well if ω is not exceptionally small. For $\omega = \frac{1}{2}$, for example, it yields essentially machine accuracy (in IEEE standard double precision) with $N = 45$ in (8.6) when $n \leqslant 10$. Some numerical results in this case are shown in Table 1, which lists the relative errors $|[I(\omega) - I_n(\omega)]/I(\omega)|$ for the choices $m = 2n, n, 1$, and 0. The last choice corresponds to applying the ordinary Gauss rule for the measure $\mathrm{d}\lambda$. Curiously, the results for $m = n$ are slightly more accurate than those for $m = 2n$, a phenomenon also observed in the subsequent examples.

For $\omega = 0.001$, the discretization method must work hard to get comparable accuracy; typically, $N = 350$ in this case.

Example 2. Generalized Fermi–Dirac integral

$$F_k(\eta, \theta) = \int_0^\infty \frac{t^k \sqrt{1 + \frac{1}{2}\theta t}}{\mathrm{e}^{-\eta + t} + 1}\, \mathrm{d}t, \quad \eta \in \mathbb{R}, \ \ \theta \geqslant 0. \tag{9.3}$$

Integrals of this type are of interest in solid-state physics, where the parameter k assumes half-integer values $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, and θ is a small parameter; cf. [17] and the literature cited therein.

To prepare the integral (9.3) for the application of our method, we write it in the form

$$F_k(\eta, \theta) = \int_0^\infty \frac{\sqrt{1 + \frac{1}{2}\theta t}}{\mathrm{e}^{-\eta} + \mathrm{e}^{-t}} t^k \mathrm{e}^{-t}\, \mathrm{d}t, \tag{9.4}$$

suggesting the integration measure $\mathrm{d}\lambda(t) = t^k \mathrm{e}^{-t}\, \mathrm{d}t$ on $[0, \infty]$ — a generalized Laguerre measure. The integrand in (9.4) has poles at $t = \eta \pm \mu \mathrm{i}\pi$, μ (odd) $= 1, 3, 5, \ldots$. The pairs of poles closest to the interval $[0, \infty]$ are captured by taking m even and

$$\zeta_\mu = -\frac{1}{\eta + \mu \mathrm{i}\pi}, \qquad \zeta_{\mu+1} = -\frac{1}{\eta - \mu \mathrm{i}\pi}, \quad \mu \text{ (odd)} = 1, 3, \ldots, m - 1. \tag{9.5}$$

The discretization method works well for all η and for θ not too large. Numerical results analogous to those in Table 1, for $k = \frac{1}{2}$, $\eta = -1$, $\theta = 10^{-4}$, are shown in Table 2.

For larger values of θ, one should include the square root $\sqrt{1 + \frac{1}{2}\theta t}$ in the measure $\mathrm{d}\lambda$ and proceed as before.

Table 2
Numerical results for Example 2

$n \setminus m$	$2n$	n	2	0
2	0.134E−02	0.414E−03	0.414E−03	0.377E−02
4	0.487E−06	0.861E−07	0.935E−06	0.241E−03
6	0.127E−09	0.374E−12	0.118E−07	0.262E−05
8	0.220E−13	0.111E−13	0.423E−09	0.250E−05
10	0.726E−14	0.669E−14	0.221E−10	0.158E−06
15			0.304E−13	0.407E−08
20			0.707E−14	0.205E−09
40				0.745E−14

Example 3. Generalized Bose–Einstein integral

$$G_k(\eta,\theta)=\int_0^\infty \frac{t^k\sqrt{1+\frac{1}{2}\theta t}}{\mathrm{e}^{-\eta+t}-1}\,\mathrm{d}t, \quad \eta<0,\ \ \theta\geqslant 0. \tag{9.6}$$

This is conveniently rewritten as

$$G_k(\eta,\theta)=\int_0^\infty \frac{t\sqrt{1+\frac{1}{2}\theta t}}{\mathrm{e}^{-\eta}-\mathrm{e}^{-t}}t^{k-1}\mathrm{e}^{-t}\,\mathrm{d}t, \tag{9.7}$$

where a factor t was split off in order for the integrand to remain regular as $t\to 0$, even if η were zero. The measure of integration therefore is $\mathrm{d}\lambda(t)=t^{k-1}\mathrm{e}^{-t}\,\mathrm{d}t$ on $[0,\infty]$. The poles of the integrand are at $t=\eta+2v\mathrm{i}\pi$, $v=0,\pm1,\pm2,\ldots$, which include a real pole at η. We thus take m odd and let

$$\zeta_\mu=-\frac{1}{\eta+(\mu+1)\mathrm{i}\pi}, \qquad \zeta_{\mu+1}=-\frac{1}{\eta-(\mu+1)\mathrm{i}\pi}, \quad \mu\ (\text{odd})=1,3,\ldots,m-2, \tag{9.8}$$

$$\zeta_m=-\frac{1}{\eta}.$$

Again, as in the preceding example, the discretization works well for $|\eta|$ not too small and θ not too large. Numerical results for $k=\frac{1}{2}$, $\eta=-1$, $\theta=10^{-4}$ are shown in Table 3.

It can be seen that the rational methods here perform significantly better than the polynomial method (for $m=0$) as far as accuracy is concerned.

Example 4. A radiation transfer integral [1]

$$G_m(c)=2\int_0^1 P_m(x)[\sin(2\pi x)]^2\mathrm{e}^{-c/x}\,\mathrm{d}x, \quad c>0. \tag{9.9}$$

Here, P_m is the Legendre polynomial of degree m, and interest rests in large values of m.

[1] This example was kindly communicated to the author by Dr. Martin Gander.

Table 3
Numerical results for Example 3

$n \setminus m$	$2n-1$	$n-1$	1	0
2	0.783E−02	0.362E−02	0.362E−02	0.357E−01
4	0.317E−05	0.831E−06	0.262E−04	0.398E−02
6	0.859E−09	0.122E−10	0.720E−06	0.700E−03
8	0.197E−12	0.482E−13	0.202E−07	0.160E−03
10	0.132E−14	0.585E−15	0.115E−08	0.430E−04
15			0.837E−11	0.261E−05
20			0.924E−13	0.243E−06
40				0.154E−09
80				0.219E−14

Although the following is not necessarily the best way to proceed, it nicely illustrates the case of a pole of high multiplicity. The change of variables

$$x = \frac{1}{1+t/c}, \quad 0 \leqslant t \leqslant \infty$$

yields

$$G_m(c) = \frac{2\mathrm{e}^{-c}}{(2\pi)^2 c} \int_0^\infty P_m\left(\frac{1}{1+t/c}\right) \left[\frac{2\pi}{1+t/c} \sin \frac{2\pi}{1+t/c}\right]^2 \mathrm{e}^{-t}\, \mathrm{d}t.$$

We choose to use n-point rational Gauss quadrature with

$$n \geqslant 1 + \lfloor m/2 \rfloor,$$

$$\mathrm{d}\lambda(t) = \left[\frac{2\pi}{1+t/c} \sin \frac{2\pi}{1+t/c}\right]^2 \mathrm{e}^{-t}\, \mathrm{d}t \quad \text{on } [0,\infty]$$

and

$$\mathbb{Q}_m = \operatorname{span}\{g\colon g(t) = (1+t/c)^{-s},\ s = 1,2,\ldots,m\}.$$

Since, by the choice of n, we have

$$\mathbb{S}_{2n} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-1-m} \supset \mathbb{Q}_m \oplus \mathbb{P}_0$$

and clearly $P_m(1/(1+t/c)) \in \mathbb{Q}_m \oplus \mathbb{P}_0$, the rational Gauss formula so constructed should give the exact answer for $G_m(c)$ except for rounding errors. The latter, unfortunately, are somewhat bothersome because of the highly oscillatory behavior of the integrand $f(t) = P_m(1/(1+t/c))$ when m is large. For example, if $m = 50$ and $c = 2$, we find (in IEEE double precision)

$$G_{50}(2) = \begin{cases} \mathbf{0.29351229}600590\mathrm{E}-07 & \text{if } n = 26, \\ \mathbf{0.29351229}563622\mathrm{E}-07 & \text{if } n = 27. \end{cases}$$

Theoretically, the results should be identical, but cancellation errors in the evaluation of the quadrature sum wipe out about 5 of the 14 decimal digits.

10. Other types of integrals

Similar techniques apply, with similar success, to other types of integrals (cf. [21]).

10.1. Rational Gauss–Kronrod quadrature

The theorem of Section 3 holds also for Gauss–Kronrod quadrature, where the polynomial formula (3.2) is now

$$\int_{\mathbb{R}} p(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} w_\nu^{\mathrm{K}}\, p(t_\nu^{\mathrm{G}}) + \sum_{\mu=1}^{n+1} w_\mu^{*\mathrm{K}}\, p(t_\mu^{\mathrm{K}}), \quad p \in \mathbb{P}_{3n+1}. \tag{10.1}$$

Here, t_ν^{G} are the nodes of the n-point Gauss formula for the measure $\mathrm{d}\lambda/\omega_m$, and w_ν^{K}, $w_\mu^{*\mathrm{K}}$, t_μ^{K} are determined so as to have maximum polynomial degree of exactness $3n+1$. Assuming that this formula exists with distinct "Kronrod" nodes t_μ^{K} on the support of $\mathrm{d}\lambda$, all different from the Gauss nodes t_ν^{G}, the corresponding rational Gauss–Kronrod formula is given by

$$\int_{\mathbb{R}} g(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^{\mathrm{K}} g(\tau_\nu^{\mathrm{G}}) + \sum_{\mu=1}^{n+1} \lambda_\mu^{*\mathrm{K}} g(\tau_\mu^{\mathrm{K}}) + R_n^{\mathrm{K}}(g), \tag{10.2}$$

where

$$R_n^{\mathrm{K}}(g) = 0 \quad \text{for } g \in \mathbb{S}_{3n+2} = \mathbb{Q}_m \oplus \mathbb{P}_{3n+1-m}, \quad 0 \leqslant m \leqslant 3n+2, \tag{10.3}$$

provided that

$$\tau_\nu^{\mathrm{G}} = t_\nu^{\mathrm{G}}, \quad \tau_\mu^{\mathrm{K}} = t_\mu^{\mathrm{K}}; \quad \lambda_\nu^{\mathrm{K}} = w_\nu^{\mathrm{K}}\omega_m(t_\nu^{\mathrm{G}}), \quad \lambda_\mu^{*\mathrm{K}} = w_\mu^{*\mathrm{K}}\omega_m(t_\mu^{\mathrm{K}}). \tag{10.4}$$

We recall (see, e.g., [15]) that t_ν^{G} in (10.1) are the zeros of $\hat{\pi}_n(\,\cdot\,) = \pi_n(\cdot; \mathrm{d}\lambda/\omega_m)$, and t_μ^{K} the zeros of $\pi_{n+1}^*(\,\cdot\,) = \pi_{n+1}(\cdot; \hat{\pi}_n\,\mathrm{d}\lambda/\omega_m)$. Constructive procedures for computing Gauss–Kronrod formulae that, like the Golub–Welsch procedure, are based on eigenvalues and eigenvectors of a Jacobi-like matrix of order $2n+1$, have recently been developed by Laurie [32], Ammar et al. [1], and Calvetti et al. [12]; see also [20]. Rational Gauss–Kronrod rules are also considered in [2, Section 4.2], where an asymptotic error estimate is given for analytic functions.

10.2. Rational Gauss–Turán quadrature

These are Gauss-type formulae in which not only function values, but also derivative values up to some even order, occur in the quadrature sum. The polynomial formula (analogous to (3.2)) has the form

$$\int_{\mathbb{R}} p(t)\frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n}\sum_{\sigma=0}^{2s} w_\nu^{(\sigma)\mathrm{T}}\, p^{(\sigma)}(t_\nu^{\mathrm{T}}), \quad p \in \mathbb{P}_{2(s+1)n-1}, \tag{10.5}$$

whereas the rational counterpart is

$$\int_{\mathbb{R}} g(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n}\sum_{\sigma=0}^{2s} \lambda_\nu^{(\sigma)} g^{(\sigma)}(\tau_\nu) + R_n^{\mathrm{T}}(g) \tag{10.6}$$

with the exactness property

$$R_n^{\mathrm{T}}(g) = 0 \quad \text{for } g \in \mathbb{S}_{2(s+1)n} = \mathbb{Q}_m \oplus \mathbb{P}_{2(s+1)n-m-1}, \quad 0 \leqslant m \leqslant 2(s+1)n, \tag{10.7}$$

provided that

$$\tau_v = t_v^{\mathrm{T}}, \quad v = 1, 2, \ldots, n,$$

$$\lambda_v^{(\sigma)} = \sum_{\rho=\sigma}^{2s} w_v^{(\rho)\mathrm{T}} \binom{\rho}{\sigma} \omega_m^{(\rho-\sigma)}(t_v^{\mathrm{T}}), \quad v = 1, 2, \ldots, n, \ \ \sigma = 0, 1, \ldots, 2s. \tag{10.8}$$

We recall that t_v^{T} in (10.5) are the zeros of the nth-degree s-orthogonal polynomial $\pi_{n,s}$ for the measure $\mathrm{d}\lambda/\omega_m$, i.e., the polynomial of degree n which satisfies the power orthogonality relation

$$\int_{\mathbb{R}} [\pi_{n,s}(t)]^{2s+1} p(t) \frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = 0 \quad \text{for all } p \in \mathbb{P}_{n-1}. \tag{10.9}$$

Constructive procedures for generating Gauss–Turán formulae (10.5) are discussed in [22].

10.3. Rational Cauchy principal value quadrature

Here the object is to construct a quadrature rule of the form

$$\int_{\mathbb{R}} \frac{g(t)}{t-x} \, \mathrm{d}\lambda(t) = \sum_{v=1}^{n} \frac{\lambda_v}{\tau_v - x} g(\tau_v) + \lambda_0(x) g(x) + R_n^{\mathrm{C}}(g), \tag{10.10}$$

where

$$\lambda_0(x) = \int_{\mathbb{R}} \frac{\mathrm{d}\lambda(t)}{t-x} - \sum_{v=1}^{n} \frac{\lambda_v}{\tau_v - x} \tag{10.11}$$

and where we require the exactness condition

$$R_n^{\mathrm{C}}(g) = 0 \quad \text{for all } g \in \mathbb{S}_{2n+1} = \mathbb{Q}_m \oplus \mathbb{P}_{2n-m}, \quad 0 \leqslant m \leqslant 2n. \tag{10.12}$$

Note that x is assumed to be inside the support of $\mathrm{d}\lambda$, so that the integrals in (10.10) and (10.11) are Cauchy principal value integrals.

It turns out that the exactness property (10.12) can be achieved for the formula (10.10) if we choose

$$\tau_v = t_v^{\mathrm{G}}, \quad \lambda_v = w_v^{\mathrm{G}} \omega_m(t_v^{\mathrm{G}}), \quad v = 1, 2, \ldots, n, \tag{10.13}$$

where t_v^{G} and w_v^{G} are the Gauss nodes and weights for the measure $\mathrm{d}\lambda/\omega_m$,

$$\int_{\mathbb{R}} p(t) \frac{\mathrm{d}\lambda(t)}{\omega_m(t)} = \sum_{v=1}^{n} w_v^{\mathrm{G}} p(t_v^{\mathrm{G}}), \quad p \in \mathbb{P}_{2n-1}, \tag{10.14}$$

provided that none of the t_v^{G} equals x. Formula (10.14) can be constructed as described in Sections 7 and 8.

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