Gauss-type Quadrature Rules for Rational Functions*

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Abstract. When integrating functions that have poles outside the interval of integration, but are regular otherwise, it is suggested that the quadrature rule in question ought to integrate exactly not only polynomials (if any), but also suitable rational functions. The latter are to be chosen so as to match the most important poles of the integrand. We describe two methods for generating such quadrature rules numerically and report on computational experience with them.

Introduction

Traditionally, Gauss quadrature rules are designed to integrate exactly polynomials of maximum possible degree. This is meaningful for integrand functions that are "polynomial-like". For integrands having poles (outside the interval of integration) it would be more natural to include also rational functions among the functions to be exactly integrated. In this paper we consider $n$-point quadrature rules that exactly integrate $m$ rational functions (with prescribed location and multiplicity of the poles) as well as polynomials of degree $2n - m - 1$, where $0 \leq m \leq 2n$. The limit case $m = 2n$, in which only rational functions are being integrated exactly, is a rational counterpart of the classical Gauss formula; the latter corresponds to the other limit case $m = 0$.

In §1 we characterize these new quadrature rules in terms of classical (polynomial) Gauss formulae with modified weight functions. We also identify special choices of poles that are of interest in applications. The computation of the quadrature rules is discussed in §2, and numerical examples are given in §3.

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1. Gauss quadrature for rational functions

Let \( d\lambda \) be a measure on the real line having finite moments of all orders. Let \( \zeta_\mu \in \mathbb{C}, \mu = 1, 2, \ldots, M, \) be distinct real or complex numbers such that

\[
\zeta_\mu \neq 0 \quad \text{and} \quad 1 + \zeta_\mu t \neq 0 \quad \text{for} \quad t \in \text{supp}(d\lambda), \quad \mu = 1, 2, \ldots, M. \tag{1.1}
\]

For given integers \( m, n \) with \( 1 \leq m \leq 2n \), we wish to find an \( n \)-point quadrature rule that integrates exactly (against the measure \( d\lambda \)) polynomials of degree \( 2n - m - 1 \) as well as the \( m \) rational functions

\[
(1 + \zeta_\mu t)^{-s}, \quad \mu = 1, 2, \ldots, M, \quad s = 1, 2, \ldots, s_\mu, \tag{1.2}
\]

where \( s_\mu \geq 1 \) and

\[
\sum_{\mu=1}^{M} s_\mu = m. \tag{1.3}
\]

In the extreme case \( m = 2n \) (where polynomials of degree \(-1\) are understood to be identically zero) the formula integrates exactly \( 2n \) rational functions (with poles of multiplicities \( s_\mu \) at \(-1/\zeta_\mu\)), but no nontrivial polynomials. The formula, therefore, can be thought of as the rational analogue of the classical Gauss formula; the latter corresponds to the other limit case \( m = M = 0 \).

The solution of our problem is given by the following theorem.

**THEOREM 1.1.** Define

\[
\omega_m(t) = \prod_{\mu=1}^{M} (1 + \zeta_\mu t)^{s_\mu}, \tag{1.4}
\]

a polynomial of degree \( m \). Assume that the measure \( d\lambda/\omega_m \) admits a (polynomial) \( n \)-point Gaussian quadrature formula

\[
\int_{\mathbb{R}} f(t) \frac{d\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{n} w_\nu G f(t_\nu^G) + R_n^G(f), \quad R_n^G(\psi_{2n-1}) = 0, \tag{1.5}
\]

with nodes \( t_\nu^G \) contained in the support of \( d\lambda \),

\[
t_\nu^G \in \text{supp}(d\lambda). \tag{1.6}
\]

Define

\[
t_\nu = t_\nu^G, \quad \lambda_\nu = w_\nu^G \omega_m(t_\nu^G), \quad \nu = 1, 2, \ldots, n. \tag{1.7}
\]

Then

\[
\int_{\mathbb{R}} g(t) d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu g(t_\nu) + R_n(g), \tag{1.8}
\]
where

\[ R_n(g) = 0 \quad \text{if} \quad \begin{cases} 
    g(t) = (1 + \zeta_{s} t)^{-s}, & \mu = 1, 2, \ldots, M; \ s = 1, 2, \ldots, s_{\mu}, \\
    g \in \mathbb{P}_{2n-m-1}.
\end{cases} \tag{1.9} \]

Conversely, (1.8) with \( t_{\nu} \in \text{supp}(d\lambda) \) and (1.9) imply (1.5), (1.6) with \( t_{\nu}^{G}, w_{\nu}^{G} \) as defined in (1.7).

Remark. Theorem 1.1, for real \( \zeta_{s} \) and either all \( s_{\mu} = 1 \) and \( m = 2n \), or all but one \( s_{\mu} = 2 \) and \( m = 2n - 1 \), is due to Van Asche and Vanherweghen [13]. The quadrature rule (1.5), especially its convergence properties for analytic functions \( f \), has previously been studied by López and Illán [9, 10].

Proof of Theorem 1.1. Assume first (1.5), (1.6). For \( \mu = 1, 2, \ldots, M; \ s = 1, 2, \ldots, s_{\mu} \), define

\[ q_{\mu,s}(t) = \frac{\omega_{m}(t)}{(1 + \zeta_{s} t)^{s}}. \tag{1.10} \]

Since \( m \leq 2n \) and \( s \geq 1 \), we have \( q_{\mu,s} \in \mathbb{P}_{m-s} \subset \mathbb{P}_{2n-1} \), and therefore, by (1.5),

\[
\lambda^{\mathcal{S}(\mathcal{L})} \int_{\mathbb{R}} \frac{d\lambda(t)}{(1 + \zeta_{s} t)^{s}} = \int_{\mathbb{R}} q_{\nu,s}(t) \frac{d\lambda(t)}{\omega_{m}(t)} = \sum_{\nu=1}^{n} w_{\nu}^{G} q_{\mu,s}(t_{\nu}^{G})
\]

\[ = \sum_{\nu=1}^{n} w_{\nu}^{G} \frac{\omega_{m}(t_{\nu}^{G})}{(1 + \zeta_{s} t_{\nu}^{G})^{s}} = \sum_{\nu=1}^{n} \frac{\lambda_{\nu}}{(1 + \zeta_{s} t_{\nu})^{s}}, \]

where (1.7) has been used in the last step and none of the denominators on the far right vanishes by (1.6) and (1.1). This proves the assertion in the top line of (1.9). The bottom part of (1.9) follows similarly: Let \( p \) be an arbitrary polynomial in \( \mathbb{P}_{2n-m-1} \). Then, since \( p \omega_{m} \in \mathbb{P}_{2n-1} \), again by (1.5) and (1.7),

\[
\lambda^{\mathcal{S}(\mathcal{L})} \int_{\mathbb{R}} p(t) d\lambda(t) = \int_{\mathbb{R}} p(t) \frac{d\lambda(t)}{\omega_{m}(t)} = \sum_{\nu=1}^{n} w_{\nu}^{G} p(t_{\nu}^{G}) \omega_{m}(t_{\nu}^{G}) = \sum_{\nu=1}^{n} \lambda_{\nu} p(t_{\nu}).
\]

To prove the converse, we first note that \( w_{\nu}^{G} \) is well defined by (1.7), since \( \omega_{m}(t_{\nu}) \neq 0 \) by the assumption on \( t_{\nu} \) and (1.1). One then easily verifies that (1.5) holds for all polynomials (1.10) (of degree \( < m \)) and all polynomials of the form \( p \omega_{m} \) where \( p \in \mathbb{P}_{2n-1-m} \). The collection of these polynomials, however, spans \( \mathbb{P}_{2n-1} \). \( \square \)

We will concentrate on six special choices of the parameters \( \zeta_{s} \) that are of interest in applications.
Case 1 (Simple real poles). All \( s_\mu = 1 \) in (1.2) (hence \( M = m \)), and all \( \zeta_{\nu} \) are real, distinct, and nonzero,
\[
\zeta_{\nu} = \xi_{\nu} \in \mathbb{R}, \quad \xi_{\nu} \neq 0, \quad \nu = 1, 2, \ldots, m.
\] (1.11a)

In this case the polynomial \( \omega_m \) has the form
\[
\omega_m(t) = \prod_{\nu=1}^{m} (1 + \xi_{\nu} t), \quad \xi_{\nu} \in \mathbb{R}.
\] (1.11b)

If the support of \( d\lambda \) is an interval, \( \omega_m \) does not change sign on it because of (1.1).

Case 2 (Simple conjugate complex poles). All \( s_\mu = 1 \) (hence \( M = m \)), \( m \) even, and the \( \zeta_{\nu} \) occur in \( m/2 \) (distinct) pairs of conjugate complex numbers (cf. [9]),
\[
\zeta_{\nu} = \xi_{\nu} + i\eta_{\nu}, \quad \zeta_{\nu+m/2} = \xi_{\nu} - i\eta_{\nu}, \quad \nu = 1, 2, \ldots, m/2,
\] (1.12a)

where \( \xi_{\nu} \in \mathbb{R} \) and \( \eta_{\nu} > 0 \). Here,
\[
\omega_m(t) = \prod_{\nu=1}^{m/2} [(1 + \xi_{\nu} t)^2 + \eta_{\nu}^2 t^2],
\] (1.12b)

which is strictly positive for real \( t \).

Case 2' (Simple conjugate complex poles plus a simple real pole). All \( s_\mu = 1 \) (hence \( M = m \)), \( m \) (odd) \( \geq 3 \), and, slightly changing the indexing of the \( \zeta \)'s,
\[
\zeta_0 \in \mathbb{R}, \quad \zeta_{\nu} = \xi_{\nu} + i\eta_{\nu}, \quad \zeta_{\nu+(m-1)/2} = \xi_{\nu} - i\eta_{\nu}, \quad \nu = 1, 2, \ldots, (m-1)/2,
\] (1.13a)

where \( \zeta_0 = \xi_0 \neq 0 \) and \( \xi_{\nu} \in \mathbb{R} \), \( \eta_{\nu} > 0 \) for \( 1 \leq \nu \leq (m-1)/2 \). Then
\[
\omega_m(t) = (1 + \xi_0 t) \prod_{\nu=1}^{(m-1)/2} [(1 + \xi_{\nu} t)^2 + \eta_{\nu}^2 t^2].
\] (1.13b)

Case 3 (Real poles of order 2). All \( s_\mu = 2 \) in (1.2) (hence \( 2M = m \)), and all \( \zeta_{\nu} \) are nonzero, real and distinct,
\[
\zeta_{\nu} = \xi_{\nu} \in \mathbb{R}, \quad \xi_{\nu} \neq 0, \quad s_{\nu} = 2, \quad \nu = 1, 2, \ldots, m/2.
\] (1.14a)

The polynomial \( \omega_m \) now has the form
\[
\omega_m(t) = \prod_{\nu=1}^{m/2} (1 + \xi_{\nu} t)^2
\] (1.14b)
and is nonnegative for real $t$, and positive on the support of $d\lambda$.

**Case 3’ (Real poles of order 2 plus a simple real pole).** Here, all $\zeta_\mu = \xi_\mu$ are nonzero, real and distinct, $s_\nu = 2$ for $\nu = 1, 2, \ldots, M - 1$ and $s_M = 1$. Thus, $m = 2M - 1$, and

$$
\omega_m(t) = (1 + \xi_M t)^{M-1} \prod_{\nu=1}^{M-1} (1 + \xi_\nu t)^2, \quad M = \frac{m + 1}{2}, \quad m \text{(odd)} \geq 3. \quad (1.15)
$$

If $M = n$, i.e., $m = 2n - 1$, the quadrature rule (1.5) is then identical with the "orthogonal quadrature rule" of [13], having as nodes the zeros of the rational function $(1 + \zeta_n t)^{-1} + \sum_{\nu=1}^{n-1} \alpha_\nu (1 + \zeta_\nu t)^{-1}$ which is orthogonal (relative to the measure $d\lambda$) to 1 and to $(1 + \zeta_\mu t)^{-1}$, $\mu = 1, 2, \ldots, n - 1$. As in Case 1, the polynomial $\omega_n$ preserves its sign on the interval on which $d\lambda$ is supported.

**Case 4 (Conjugate complex poles of order 2).** All $s_\mu = 2$ (hence $2M = m$), $m = 0 \pmod{4}$, and the $\zeta_\mu$, $\mu = 1, 2, \ldots, m/2$, occur in $m/4$ conjugate complex pairs, similarly as in Case 2. Thus,

$$
\omega_m(t) = \prod_{\nu=1}^{m/4} [(1 + \xi_\nu t)^2 + \eta_\nu^2 t^2]^2. \quad (1.16)
$$

In all six cases, the measure $d\lambda/\omega_m$ admits a Gaussian $n$-point formula for each $n = 1, 2, 3, \ldots$, so that the assumption of Theorem 1.1 is fulfilled for each $n$.

Putting $f(t) = \omega_m(t) g(t)$ in (1.5) and using (1.7), we get

$$
\int_{\mathbb{R}} g(t) d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu g(t_\nu) + R^G_n(\omega_m g), \quad (1.17)
$$

where from the well-known expression for the remainder term of Gaussian quadrature rules, one has

$$
R^G_n(\omega_m g) = \gamma_n (\omega_m g)(2n)(\tau), \quad \gamma_n = \frac{\hat{\beta}_0 \hat{\beta}_1 \cdots \hat{\beta}_n}{(2n)!}. \quad (1.18)
$$

Here, $\tau$ is some number in the smallest interval containing the support of $d\lambda$, and $\hat{\beta}_k = \beta_k (d\lambda/\omega_m)$ are the $\beta$-recursion coefficients for the measure $d\lambda/\omega_n$ (cf. (2.1) below). The latter are computed as part of the algorithms to be described in the next section.

2. Computation of the quadrature rule (1.5)

We propose essentially two methods for generating the basic quadrature rule (1.5), the first being most appropriate if the support of $d\lambda$ is a finite interval, the other more effective, though possibly slower, when the support interval of $d\lambda$ is unbounded.
2.1. Method based on partial fraction decomposition and modification algorithms. To compute the $n$-point formula (1.5), it suffices to compute the $n$th-degree orthogonal polynomial $\hat{\pi}_n(\cdot) = \pi_n(\cdot; d\hat{\lambda})$ relative to the measure $d\hat{\lambda} = d\lambda/\omega_m$, or, more precisely, the recursion coefficients $\hat{\alpha}_k = \alpha_k(d\hat{\lambda}), \hat{\beta}_k = \beta_k(d\hat{\lambda}), k = 0, 1, \ldots, n - 1$, in the three-term recurrence relation satisfied by these (monic) polynomials:

$$\hat{\pi}_{k+1}(t) = (t - \hat{\alpha}_k)\hat{\pi}_k(t) - \hat{\beta}_k\hat{\pi}_{k-1}(t),$$

$$k = 0, 1, \ldots, n - 1,$$

$$\hat{\pi}_0(t) = 1, \quad \hat{\pi}_{-1}(t) = 0.$$  \hspace{1cm} (2.1)

The nodes $t^G_\nu$ and weights $w^G_\nu$ in (1.5) can then be obtained by standard techniques via an eigensystem problem for the (symmetric, tridiagonal) Jacobi matrix of order $n$ having the $\hat{\alpha}_k, k = 0, 1, \ldots, n - 1$, on the diagonal, and $\sqrt{\hat{\beta}_k}, k = 1, 2, \ldots, n - 1$, on the side diagonals (see, e.g., [7], [4, §6]). The coefficients $\hat{\alpha}_k, \hat{\beta}_k$ in turn are expressible in terms of the orthogonal polynomials $\hat{\pi}_k$ as

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

$$\hat{\beta}_0 = (\hat{\pi}_0, \hat{\pi}_0), \quad \hat{\beta}_k = \frac{(\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_{k-1}, \hat{\pi}_{k-1})}, \quad 1 \leq k \leq n - 1,$$  \hspace{1cm} (2.2)

where $(\cdot, \cdot)$ denotes the inner product

$$(u, v) = \int_\mathbb{R} u(t)v(t)d\hat{\lambda}(t).$$  \hspace{1cm} (2.3)

(If the error constant $\gamma_n$ in (1.18) is desired, one needs to compute, in addition, $\hat{\beta}_n$.)

The basic idea of computing the coefficients in (2.2) is as follows. Suppose we can construct an $N$-point quadrature rule for $d\hat{\lambda} = d\lambda/\omega_m$, where $N > n$, which is exact for polynomials of degree $\leq 2n - 1$:

$$\int_\mathbb{R} p(t)d\hat{\lambda}(t) = \sum_{k=1}^{N} W_k p(T_k), \quad p \in \mathbb{P}_{2n-1}.$$  \hspace{1cm} (2.4)

Here the weights $W_k$ are not necessarily all positive. Denote the discrete measure implied by the sum on the right by $d\Lambda_N$:

$$\int_\mathbb{R} p(t)d\Lambda_N(t) = \sum_{k=1}^{N} W_k p(T_k).$$  \hspace{1cm} (2.5)
Then from the formulae in (2.2) one easily sees by induction that

\[ \alpha_k(d\hat{\lambda}) = \alpha_k(d\Lambda_N), \quad k = 0, 1, \ldots, n - 1. \]  

(2.6)

\[ \beta_k(d\hat{\lambda}) = \beta_k(d\Lambda_N), \]

Thus, the desired recursion coefficients are the first \( n \) of the \( \alpha \)- and \( \beta \)-coefficients belonging to the discrete measure \( d\Lambda_N \). These can be generated by Stieltjes’s procedure, which is implemented in the routine sti of [4]. (The faster routine lancz of [4], implementing the Lanczos method, would also be applicable here, even though \( d\Lambda_N \) is not necessarily a positive measure.)

We next show how a quadrature rule of type (2.4), with \( N = O(mn) \), can be constructed by means of partial fraction decomposition and suitable modification algorithms. For this, we consider separately Cases 1–3 identified in §1. The analysis of Case 4 becomes so tedious that we will not pursue it any further in this context; see, however, §2.2.

2.1.1. Simple real poles. We set up the partial fraction decomposition of \( 1/\omega_m \) in the form

\[ \frac{1}{\omega_m(t)} = \frac{1}{\prod_{\nu=1}^{m}(1 + \xi_{\nu}t)} = \sum_{\nu=1}^{m} \frac{c_{\nu}}{t + (1/\xi_{\nu})}, \]  

(2.7)

where

\[ r_{\nu} = \frac{\xi_{\nu}^{m-2}}{\prod_{\mu \neq \nu}^{m}(\xi_{\nu} - \xi_{\mu})}, \quad \nu = 1, 2, \ldots, m, \]  

(2.8)

and an empty product in (2.8) (when \( m = 1 \)) is to be taken as 1. Then, with \( d\hat{\lambda} = d\lambda/\omega_m \),

\[ \int_{\mathbb{R}} p(t)d\hat{\lambda}(t) = \sum_{\nu=1}^{m} \int_{\mathbb{R}} p(t) \frac{c_{\nu}d\lambda(t)}{t + (1/\xi_{\nu})}. \]

The integrals on the right involve measures \( c_{\nu}d\lambda \) modified by linear divisors. For such measures, the associated recursion coefficients can be obtained from those of \( c_{\nu}d\lambda \) (assumed known) by a suitable modification algorithm (cf. [4, §5]). Unless \( x_{\nu} = -1/\xi_{\nu} \) is very close to the support interval of \( d\lambda \), the most appropriate algorithm is the one embodied in the routine gchri of [4] with \( \text{iopt} = 1 \). Otherwise, the routine chri of [4] (again with \( \text{iopt} = 1 \)) is preferable. A basic ingredient of the routine gchri is the modified Chebyshev algorithm (cf. [2, §2.4]) using modified moments

\[ \int_{\mathbb{R}} \pi_{k}(t; d\lambda)c_{\nu}d\lambda(t)/(t - x_{\nu}), \quad k = 0, 1, 2, \ldots, 2n - 1. \]

These in turn are generated by backward recurrence as minimal solution of the three-term recurrence relation for the measure \( d\lambda \); cf. [1, §5].
Having obtained, in whichever way, the first \( n \) of the \( \alpha \)- and \( \beta \)-coefficients for the modified measure \( c_\nu d\lambda(t)/(t-x_\nu) \), and hence the Gaussian quadrature formula\(^{1}\)

\[
\int_{\mathbb{R}} p(t) \frac{c_\nu d\lambda(t)}{t + (1/x_\nu)} = \sum_{r=1}^{n} w^{(\nu)}_r p(t^{(\nu)}_r), \quad p \in \mathbb{P}_{2n-1}, \tag{2.9}
\]

via eigensystem techniques, we then get

\[
\int_{\mathbb{R}} p(t) \frac{d\lambda(t)}{\omega_m(t)} = \sum_{\nu=1}^{m} \int_{\mathbb{R}} p(t) \frac{c_\nu d\lambda(t)}{t + (1/x_\nu)}
\]

\[
= \sum_{\nu=1}^{m} \sum_{r=1}^{n} w^{(\nu)}_r p(t^{(\nu)}_r), \quad p \in \mathbb{P}_{2n-1},
\]

hence the desired quadrature rule (2.4), with \( N = mn \) and

\[
T_{(\nu-1)n+r} = t^{(\nu)}_r, \quad \nu = 1, 2, \ldots, m; \quad r = 1, 2, \ldots, n. \tag{2.10}
\]

\[
W_{(\nu-1)n+r} = w^{(\nu)}_r,
\]

The procedure described works best if the support of \( d\lambda \) is a finite interval. Otherwise, the modified Chebyshev algorithm underlying the procedure is likely to suffer from ill-conditioning; cf. Example 3.4. Another difficulty that may adversely affect the accuracy of the results, in particular when \( m = 2n \), is the possibility that the constants \( c_\nu \text{ sgn}_{\text{supp}(d\lambda)}(t + 1/x_\nu) \) become very large and alternate in sign; cf. Example 3.2. This will cause serious cancellation errors in evaluating inner products relative to the measure \( d\lambda_N \) (there being blocks of weights \( W_k \) which are very large positive alternating with blocks of weights which are very large negative). In such cases, either \( m \) has to be lowered, perhaps down to \( m = 1 \), or else the method discussed in §2.2 invoked, which will be more effective (but possibly more expensive).

2.1.2. Simple conjugate complex poles. We now consider Case 2 of §1, i.e., conjugate complex parameters \( \zeta_\nu = \xi_\nu + i\eta_\nu, \zeta_{\nu+m/2} = \bar{\zeta}_\nu \), where \( \xi_\nu \in \mathbb{R}, \eta_\nu > 0 \) and \( m \) is even. In this case, an elementary computation yields the partial fraction decomposition

\[
\frac{1}{\omega_m(t)} = \sum_{\nu=1}^{m/2} \frac{c_\nu + d_\nu t}{(t + \frac{\xi_\nu}{\xi_\nu + \eta_\nu})^2 + (\frac{\eta_\nu}{\xi_\nu + \eta_\nu})^2}, \quad t \in \mathbb{R}, \tag{2.11}
\]

\(^{1}\)In order to produce positive \( \beta \)-coefficients, as required in the routine for Gauss quadrature formulae, one inputs the measure \(|c_\nu/(t-x_\nu)|d\lambda(t)\) and, if this entails a change of sign, reverses the sign of all Gauss weights after exiting from the Gauss quadrature routine.
where
\[ c_{\nu} = \frac{1}{\eta_{\nu}} \left( \frac{\xi_{\nu}}{\xi_{\nu}^{2} + \eta_{\nu}^{2}} \right) \text{Im} \, p_{\nu} + \left( \frac{\eta_{\nu}}{\xi_{\nu}^{2} + \eta_{\nu}^{2}} \right) \text{Re} \, p_{\nu} \right), \] (2.12)

\[ d_{\nu} = \frac{1}{\eta_{\nu}} \text{Im} \, p_{\nu} \]

and
\[ p_{\nu} = \prod_{\mu=1, \mu \neq \nu}^{m/2} \frac{\left( \xi_{\nu} + i\eta_{\nu} \right)^{2}}{(\xi_{\nu}^{2} - \xi_{\mu}^{2} + \eta_{\nu}^{2} - \eta_{\mu}^{2}) + 2i\eta_{\nu}(\xi_{\nu} - \xi_{\mu})} \] (2.13)

with \( p_{1} = 1 \) if \( m = 2 \). One can then proceed as in §2.1.1, except that the modification of the measure \( d\lambda \) now involves multiplication by a nonconstant linear function (if \( d_{\nu} \neq 0 \)) in addition to division by a quadratic. The former modification is handled by the routine chri of [4] with \( \text{iopt} = 1 \), the latter by the routine gchri with \( \text{iopt} = 2 \) (or, if more appropriate, by chri with \( \text{iopt} = 5 \)). The quadrature rule (2.4) so obtained has \( N = mn/2 \).

If the poles \(-1/\xi_{\nu}\) are located in conjugate pairs on a line parallel to the imaginary axis, then by an elementary calculation one can show that all \( p_{\nu} \) are real, hence \( d_{\nu} = 0 \), and there is no need to call chri.

2.1.2'. Simple conjugate complex poles plus a simple real pole. We are now in Case 2' of §1, with \( m \) odd, \( \zeta_{0} = \xi_{0} \in \mathbb{R} \) and the remaining \( \zeta_{\nu} \) conjugate complex as in Case 2. This yields
\[ \frac{1}{\omega_{m}(t)} = \frac{c'_{0}}{t + (1/\xi_{0})} + \sum_{\nu=1}^{(m-1)/2} \frac{c'_{\nu} + d'_{\nu} t}{(t + \frac{\xi_{\nu}}{\xi_{\nu}^{2} + \eta_{\nu}^{2}})^{2} + \left( \frac{\eta_{\nu}}{\xi_{\nu}^{2} + \eta_{\nu}^{2}} \right)^{2}}, \quad t \in \mathbb{R}, \] (2.14)

where
\[ c'_{0} = \frac{\xi_{0}^{m-2}}{\prod_{\nu=1}^{(m-1)/2}[(\xi_{0} - \xi_{\nu})^{2} + \eta_{\nu}^{2}]}, \]
\[ c'_{\nu} = \frac{1}{\eta_{\nu}} \left( \frac{\xi_{\nu}}{\xi_{\nu}^{2} + \eta_{\nu}^{2}} \text{Im} \, p'_{\nu} + \left( \frac{\eta_{\nu}}{\xi_{\nu}^{2} + \eta_{\nu}^{2}} \right) \text{Re} \, p'_{\nu} \right), \] (2.15)

\[ d'_{\nu} = \frac{1}{\eta_{\nu}} \text{Im} \, p'_{\nu} \]

and
\[ p'_{\nu} = \frac{\xi_{\nu} + i\eta_{\nu}}{\xi_{\nu} - \xi_{0} + i\eta_{\nu}} \, p_{\nu}, \] (2.16)

with \( p_{\nu} \) the same as in (2.13) with \( m \) replaced by \( m - 1 \). The technique called for is a combination of the one in §2.1.1, to deal with the first term in (2.14), and the one in §2.1.2, to deal with the remaining terms, and yields a quadrature rule (2.4) with \( N = (m + 1)n/2 \).
2.1.3. **Real poles of order 2.** This is Case 3 of §1, and leads to the partial fraction decomposition

\[
\frac{1}{\omega_m(t)} = \sum_{\nu=1}^{m/2} \left( \frac{c_\nu}{t + 1/\xi_\nu} + \frac{d_\nu}{(t + 1/\xi_\nu)^2} \right),
\]

(2.17)

\[
c_\nu = -\frac{2\xi_\nu^{-3} \sum_{\mu=1}^{m/2} \frac{\xi_\nu}{\xi_\nu - \xi_\mu}}{\prod_{\mu \neq \nu}^{m/2} (\xi_\nu - \xi_\mu)^2},
\]

(2.18)

\[
d_\nu = \frac{\xi_\nu^{-4}}{\prod_{\mu \neq \nu}^{m/2} (\xi_\nu - \xi_\mu)^2},
\]

(2.19)

where \(c_1 = 0, d_1 = \xi_1^{-2}\) when \(m = 2\). Here, \(N = mn\) in (2.4).

2.1.3'. **Real poles of order 2 plus a simple real pole.** Similarly as in §2.1.3, the partial fraction decomposition has now the form

\[
\frac{1}{\omega_m(t)} = \frac{c'_M}{t + 1/\xi_M} + \sum_{\nu=1}^{M-1} \left( \frac{c'_\nu}{t + 1/\xi_\nu} + \frac{d'_\nu}{(t + 1/\xi_\nu)^2} \right), \quad M = (m+1)/2, \quad m \text{ odd},
\]

(2.20)

\[
c'_M = \frac{\xi_M^{-2}}{\prod_{\nu=1}^{M-1} (\xi_M - \xi_\nu)^2},
\]

\[
c'_\nu = -\frac{\xi_\nu^{-3}}{(\xi_\nu - \xi_M)^2 \prod_{\mu \neq \nu}^{M-1} (\xi_\nu - \xi_\mu)^2} \left( \xi_\nu + 2(\xi_\nu - \xi_M) \sum_{\mu=1}^{M-1} \frac{\xi_\mu}{\xi_\nu - \xi_\mu} \right),
\]

\[
d'_\nu = \frac{\xi_\nu^{-4}}{(\xi_\nu - \xi_M) \prod_{\mu \neq \nu}^{M-1} (\xi_\nu - \xi_\mu)^2}.
\]

Empty sums and products (when \(M = 2\)) have their conventional values 0 and 1, respectively. Again, \(N = mn\) in (2.4).

The presence of two terms in the summations of (2.17) and (2.20) complicates matters considerably, as they call for two applications of the routine gchri: First, we must generate sufficiently many of the recursion coefficients for the measure \(d\lambda(t)/(t - x_\nu)\), \(x_\nu = -1/\xi_\nu\), in order next to generate the desired recursion coefficients for \(d\lambda(t)/(t - x_\nu)^2\) by backward recursion — a recursion based on the recurrence relation generated in the first application of gchri (which in turn requires backward recursion!). The procedure nevertheless works well if the \(x_\nu\) are not too close to the support interval of \(d\lambda\); see Example 3.3.
2.2. Discretization method. In this method, the inner product (2.3) is approximated by a discrete (positive) inner product,

\[ (u, v) = \int_{\mathbb{R}} u(t)v(t) \frac{d\lambda(t)}{\omega_m(t)} \approx \sum_{k=1}^{N} \omega_k^{(N)} u(\tau_k^{(N)})v(\tau_k^{(N)}) =: (u, v)_N, \quad N > n, \]  

whereupon the formulae (2.2) are applied with the inner product \((\cdot, \cdot)\) replaced by \((\cdot, \cdot)_N\) throughout. This yields approximations

\[ \hat{\alpha}_{k,N} \approx \hat{\alpha}_k, \quad \hat{\beta}_{k,N} \approx \hat{\beta}_k, \quad k = 0, 1, \ldots, n - 1. \]  

In effect we are generating the polynomials orthogonal with respect to the discrete inner product \((\cdot, \cdot)_N\) in order to approximate the desired orthogonal polynomials.

The computation of the approximate coefficients (2.22) can be done by either Stieltjes's procedure or Lanczos's algorithm (cf., e.g., [3, §§6–7]). Both are implemented in the routine acdias of [4].

With any reasonable choice of the discretization (2.21), it will be true that the procedure converges as \(N \to \infty\),

\[ \lim_{N \to \infty} \hat{\alpha}_{k,N} = \hat{\alpha}_k, \quad \lim_{N \to \infty} \hat{\beta}_{k,N} = \hat{\beta}_k, \quad 0 \leq k \leq n - 1. \]  

A natural choice, indeed, is given by

\[ \tau_k^{(N)} = t_k^{(N)}(d\lambda), \quad \omega_k^{(N)} = \frac{u_k^{(N)}(d\lambda)}{\omega_m(t_k^{(N)})}, \quad k = 1, 2, \ldots, N, \]  

where \(t_k^{(N)}(d\lambda)\) are the zeros of the orthogonal polynomial \(\pi_N(\cdot; d\lambda)\), and \(u_k^{(N)}(d\lambda)\) the respective Christoffel numbers.

The discretization method is conceptually simpler, and sometimes more stable, than the methods of §2.1, but may become significantly more expensive, regardless of the choice of \(m\), if poles are close to the interval of integration, or if high accuracy is desired; cf. Examples 3.1 and 3.5. Note also that Case 4 that was skipped in §2.1 can easily be handled by the present method; see Example 3.6.

3. Numerical Examples

All examples in this section were computed on the Cyber 205 in both single and double precision. The respective machine precisions are \(7.11 \times 10^{-15}\) and \(5.05 \times 10^{-20}\).

Example 3.1. \(I_1(\omega) = \int_{-1}^{1} \frac{t^2}{\sin(\pi t/\omega)} \, dt, \quad \omega > 1.\)

Here, \(d\lambda(t) = dt\), and the poles of the integrand are located at the integer multiples of \(\omega\). It is natural, then, to make our quadrature rule (1.8) exact for \(m\) elementary rational functions matching the \(m\) poles closest to the origin, say those at
\[-(m/2)\omega, \ldots, -\omega, \omega, \ldots, (m/2)\omega\] when \(m\) is even. This suggests to identify \(-1/\zeta_\nu\) in (1.2) with these poles, i.e., in (1.11a) to set

\[
\xi_\nu = (-1)^\nu/\omega[(\nu + 1)/2], \quad \nu = 1, 2, \ldots, m.
\] (3.1)

Best accuracy is expected when \(m = 2n\), in which case the method described in §2.1.1 was found to work rather well, the only difficulty being the relatively slow convergence of the backward recurrence algorithm for computing the \(2n\) modified (Legendre) moments associated with the measure \(dt/(t \pm \omega)\) when \(\omega\) is very close to 1. For single-precision accuracy \(\epsilon = \frac{1}{2} \times 10^{-10}\) and double-precision accuracy \(\epsilon^d = \frac{1}{2} \times 10^{-25}\), and \(n = 20\), the respective starting indices \(k_0\) and \(k_0^d\) in the backward recursion yielding the desired accuracy are shown in Table 3.1 for selected values of \(\omega\).

<table>
<thead>
<tr>
<th>(\omega)</th>
<th>(k_0)</th>
<th>(k_0^d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>50</td>
<td>63</td>
</tr>
<tr>
<td>1.5</td>
<td>53</td>
<td>71</td>
</tr>
<tr>
<td>1.1</td>
<td>67</td>
<td>106</td>
</tr>
<tr>
<td>1.01</td>
<td>124</td>
<td>247</td>
</tr>
</tbody>
</table>

**TABLE 3.1.** Starting indices for backward recurrence when \(n = 20\)

Other than that, the method appears to be very stable and produces quadrature rules that are rapidly converging. In Table 3.2, the results of the \(n\)-point rule (1.17)

<table>
<thead>
<tr>
<th>(\omega)</th>
<th>(n)</th>
<th>(n)-point rational Gauss</th>
<th>(\gamma_n)</th>
<th>err. Gauss</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>1</td>
<td>2.1</td>
<td>3.94((-1))</td>
<td>1.43((-1))</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>2.33248722</td>
<td>3.50((-7))</td>
<td>7.18((-5))</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>2.332487232246550235</td>
<td>2.61((-15))</td>
<td>2.73((-8))</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.332487232246550241107076</td>
<td>1.48((-24))</td>
<td>1.02((-11))</td>
</tr>
<tr>
<td>1.1</td>
<td>2</td>
<td>4.43</td>
<td>1.73((-9))</td>
<td>2.60((-1))</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>4.467736367</td>
<td>2.00((-9))</td>
<td>2.09((-2))</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>4.4677364638776751</td>
<td>5.61((-18))</td>
<td>1.53((-3))</td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>4.46773646387767589236123</td>
<td>1.66((-27))</td>
<td>1.09((-4))</td>
</tr>
<tr>
<td>1.01</td>
<td>3</td>
<td>4.429</td>
<td>2.53((-4))</td>
<td>4.20((-1))</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>8.4301845803</td>
<td>6.27((-12))</td>
<td>1.85((-1))</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>8.4301845804708420582</td>
<td>7.52((-21))</td>
<td>8.37((-2))</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>8.430184580470842058971264</td>
<td>1.23((-30))</td>
<td>3.75((-2))</td>
</tr>
</tbody>
</table>

**TABLE 3.2.** Numerical results for \(I_1(\omega)\), error constants, and comparison with Gauss quadrature
Gauss-type quadrature rules for rational functions

applied to \( g(t) = (\pi t/\omega) / \sin(\pi t/\omega) \) in double precision are shown for \( \omega = 2, 1.1 \) and 1.01, along with the error constants \( \gamma_n \) of (1.18). Also shown in the last column are the relative errors of the \( n \)-point Gauss-Legendre rule. For \( \omega = 2 \), the exact answer is known to be \( 8C/\pi \), where \( C \) is Catalan’s constant (cf. [8, Eq. 3.747(2)]). The value shown in Table 3.2 for \( n = 10 \) agrees with it to all 25 decimal digits given. Ordinary Gauss-Legendre quadrature is seen to converge rather slowly, as \( \omega \) approaches 1. In contrast, convergence of the rational Gauss quadrature rule is fast even for \( \omega \) very close to 1. The extra effort required in this case is expended, as illustrated in Table 3.1, at the time when the rule is generated.

<table>
<thead>
<tr>
<th>( \omega )</th>
<th>( n )</th>
<th>SP</th>
<th>DP</th>
<th>method of §2.1</th>
<th>SP</th>
<th>DP</th>
<th>method of §2.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>1</td>
<td>.001</td>
<td>.004</td>
<td>.007</td>
<td>.178</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>.008</td>
<td>.036</td>
<td>.010</td>
<td>.224</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>.027</td>
<td>.125</td>
<td>.028</td>
<td>.220</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>.065</td>
<td>.296</td>
<td>.016</td>
<td>.423</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.1</td>
<td>2</td>
<td>.002</td>
<td>.014</td>
<td>.060</td>
<td>1.554</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>.013</td>
<td>.063</td>
<td>.068</td>
<td>1.649</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>.036</td>
<td>.177</td>
<td>.098</td>
<td>1.274</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>.080</td>
<td>.376</td>
<td>.104</td>
<td>1.461</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.01</td>
<td>3</td>
<td>.005</td>
<td>.037</td>
<td>.460</td>
<td>20.10</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>.020</td>
<td>.104</td>
<td>.446</td>
<td>41.51</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>.050</td>
<td>.244</td>
<td>.458</td>
<td>10.44</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>.102</td>
<td>.487</td>
<td>.525</td>
<td>12.65</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

TABLE 3.3. Timings (in seconds) of the methods in §§2.1 and 2.2 applied to Example 3.1

Identical results were obtained by the discretization method of §2.2, but with substantially greater effort, particularly for higher accuracies and for \( \omega \) close to 1. Respective timings are shown in Table 3.3, both for single-precision (SP) and double-precision (DP) accuracy requirements of \( \frac{1}{2} \times 10^{-10} \) and \( \frac{1}{2} \times 10^{-25} \), respectively.

While the choice \( m = 2n \) indeed gives best accuracy, other choices of \( m \) may be preferable if the effort and time to generate the quadrature rule is of any importance. It turns out that with the method of partial fractions, \( m = 2\lfloor (n + 1)/2 \rfloor \) gives almost the same accuracy at about half the effort, whereas \( m = 2 \) gives considerably less accuracy but requires only about one-tenth the effort. The discretization method of §2.2, on the other hand, requires essentially the same effort regardless of the choice of \( m \). Some timings required to generate the quadrature rules for various \( m \) and \( n \), and the relative errors achieved, are shown in Table 3.4.
<table>
<thead>
<tr>
<th>$\omega$</th>
<th>$n$</th>
<th>$m$</th>
<th>method of §2.1</th>
<th>method of §2.2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>SP</td>
<td>DP</td>
</tr>
<tr>
<td>2.0</td>
<td>10</td>
<td>2</td>
<td>.008</td>
<td>.037</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td></td>
<td>.033</td>
<td>.153</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td></td>
<td>.065</td>
<td>.296</td>
</tr>
<tr>
<td>1.1</td>
<td>11</td>
<td>2</td>
<td>.009</td>
<td>.047</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td></td>
<td>.045</td>
<td>.213</td>
</tr>
<tr>
<td></td>
<td>22</td>
<td></td>
<td>.080</td>
<td>.376</td>
</tr>
<tr>
<td>1.01</td>
<td>12</td>
<td>2</td>
<td>.011</td>
<td>.065</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td></td>
<td>.052</td>
<td>.258</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td></td>
<td>.102</td>
<td>.487</td>
</tr>
</tbody>
</table>

**TABLE 3.4. Timings and errors for selected $m \leq 2n$**

If $m = 2$, the values of $n$ for which full accuracy of about $10^{-25}$ is attained are 15, 21 and 22 for $\omega = 2.0$, 1.1 and 1.01, respectively. Interestingly, the timings involved are only about half those for $m = 2[(n + 1)/2]$ shown in Table 3.4.

**Example 3.2.** $I_2(\omega) = \int_0^1 \frac{t^{-1/2}(1+t)}{t+\omega} \, dt$, $0 < \omega < 1$.

Here we take $d\lambda(t) = t^{-1/2} \, dt$ on $[0,1]$. If we wish to match the first $2n - 1$ poles of the gamma function at the negative integers as well as the pole at $-\omega$, we set $m = 2n$ in

\[
\xi_1 = \frac{1}{\omega},
\]

\[
\xi_{\nu} = \frac{1}{\nu - 1}, \quad \nu = 2, 3, \ldots, m.
\]

The rational $n$-point Gauss rule (1.7), (1.17), generated by the method of §2.1.1, then produces (in double precision) results as shown in Table 3.5, where $\omega = \frac{1}{2}$. In the last column we list the absolute value of the difference between double-precision and single-precision results. In contrast to Example 3.1, we now see a case in which the accuracy reaches a limit (at about $n = 10$) and deteriorates, rather than improves, as $n$ is further increased. (When $n = 20$, the calculation even breaks down in single precision!). The last column in Table 3.5 provides a clear hint as to what is happening: a steady growth in numerical instability. Closer examination reveals the true cause of this instability. The constants $c_{\nu}$ in the partial fraction decomposition (2.7) become very large and alternate in sign. Thus, for example, $c_1 = -2.3375 \ldots \times 10^9$ and $c_{19} = 2.3336 \ldots \times 10^9$ when $n = 18$. This produces blocks of large coefficients $W_k$ in (2.10) that alternate in sign from block to block, causing severe cancellation errors in summations such as
(2.5) (which are abundant in Stieltjes’s algorithm). The phenomenon evidently is a manifestation of the asymmetric distribution of the poles of the gamma function.

| \(n\) | n-point rational Gauss | \(|DP - SP|\) |
|------|-----------------------|--------------|
| 2    | 1.746                 | 2.24(-13)    |
| 6    | 1.75012059121         | 7.05(-11)    |
| 10   | 1.750120591261335415386 | 3.36(-8)   |
| 14   | 1.75012059126133541559 | 1.52(-5)    |
| 18   | 1.75012059126133536   | 4.31(-3)     |

TABLE 3.5. Numerical results for \(I_2(\omega)\), \(\omega = .5\)

The method of §2.2, in contrast, does not suffer from any numerical instability and produces for \(n = 12\), with comparable effort, the value

\[
I_2(0.5) = 1.750120591261335415394610, \tag{3.3}
\]

believed to be correct to all 25 digits shown.

Matching only \(n\) poles, and thus taking \(m = n\) in (3.2), stabilizes the procedure of §2.1.1 considerably, and as a consequence produces the correct result (3.3) (except for a discrepancy of 1 unit in the last decimal place) for \(n = 11\). An even more stable procedure results from taking \(m = 2\) and, amazingly, yields the correct answer (to all digits shown!) already for \(n = 13\).

**Example 3.3.** \(I_2(\omega) = \int_{-1}^{1} \left( \frac{\pi t/\omega}{\sin(\pi t/\omega)} \right)^2 dt, \quad \omega > 1.\)

Similarly as in Example 3.1, we take

\[
\xi_\nu = (-1)^\nu / (\omega \left( (\nu + 1)/2 \right)), \quad \nu = 1, 2, \ldots, m/2. \tag{3.4}
\]

We applied the procedure described in §2.1.3 for \(\omega = 2, 1.5, 1.1\) and 1.01, both in single and double precision, requesting accuracies of \(\epsilon = \frac{1}{2} \times 10^{-10}\) and \(\epsilon^d = \frac{1}{2} \times 10^{-25}\),

<table>
<thead>
<tr>
<th>(\omega)</th>
<th>(k_1)</th>
<th>(k_1^d)</th>
<th>(k_2)</th>
<th>(k_2^d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>130</td>
<td>163</td>
<td>50</td>
<td>63</td>
</tr>
<tr>
<td>1.5</td>
<td>133</td>
<td>191</td>
<td>53</td>
<td>71</td>
</tr>
<tr>
<td>1.1</td>
<td>177</td>
<td>306</td>
<td>67</td>
<td>106</td>
</tr>
<tr>
<td>1.01</td>
<td>384</td>
<td>727</td>
<td>124</td>
<td>247</td>
</tr>
</tbody>
</table>

TABLE 3.6. Starting indices for two backward recursences when \(n = 20\)
respectively. When \( m = 2n \) and \( n = 20 \), starting indices \( k_1, k_2^j \) in the first application of the backward recursion that were found to meet the accuracy requirements for the poles closest to \([-1,1]\), and the analogous starting indices \( k_2, k_2^j \) in the second application, are shown in Table 3.6 for the four values of \( \omega \). As expected, the procedure becomes laborious as \( \omega \) approaches 1. Selected double-precision results produced by the \( n \)-point rational Gauss rule, along with error constants, are shown in Table 3.7. The last column shows the relative error of results generated by the \( n \)-point Gauss-Legendre rule. For \( \omega = 2 \), the exact answer is known to be \( I_3(2) = 4 \ln 2 \) ([8, Eq. 3.837(2)]) and is correctly reproduced to 25 digits when \( n = 11 \). Note again the fast convergence of the rational Gauss quadrature rule, even for \( \omega \) very close to 1, in contrast to the relatively slow convergence of the ordinary Gauss rule, especially for \( \omega \) close to 1.

<table>
<thead>
<tr>
<th>( \omega )</th>
<th>( n )</th>
<th>( \gamma ), ( n )-point rational Gauss</th>
<th>err. Gauss</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>2</td>
<td>2.75</td>
<td>9.90(-3)</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>2.772588868</td>
<td>1.16(-9)</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>2.7725887222397811</td>
<td>3.28(-18)</td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>2.772588722239781237668928</td>
<td>9.72(-28)</td>
</tr>
<tr>
<td>1.1</td>
<td>2</td>
<td>15.5</td>
<td>3.00(-2)</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>16.5328175</td>
<td>8.54(-12)</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>16.5328177384604181</td>
<td>7.21(-24)</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>16.53281773846041830155898</td>
<td>2.35(-37)</td>
</tr>
<tr>
<td>1.01</td>
<td>2</td>
<td>184.</td>
<td>6.34(-2)</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>188.674782</td>
<td>2.20(-11)</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>188.674784224994172</td>
<td>1.88(-23)</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>188.6747842249941742708325</td>
<td>6.15(-37)</td>
</tr>
</tbody>
</table>

**TABLE 3.7. Numerical results for** \( I_3(\omega) \), **error constants, and comparison with Gauss quadrature**

While the choice \( m = 2[\left( (n+1)/2 \right) \] produced similar advantages as in Example 3.1 — an increase of speed by a factor of about 2 at only a slight loss of accuracy — the choice \( m = 2 \) offered no significant gains in accuracy over the Gauss-Legendre rule, unlike \( m = 4 \), which did (since a symmetric pair of double poles is now accounted for).

We also applied the discretization method of §2.2 and obtained identical results with somewhat less effort in the case \( \omega = 2 \), and about the same effort in the case \( \omega = 1.1 \). For \( \omega = 1.01 \), however, we were unable to attain the requested double-precision accuracy with a discretization parameter \( N \leq 800 \) (in (2.21)).

**Example 3.4.** \( I_4 = \int_0^\infty \frac{t}{e^{t-1}} e^{-t}dt \).

The appropriate measure here is \( d\lambda(t) = e^{-t}dt \) on \([0,\infty)\). Since the integrand has poles at the integer multiples of \( 2\pi i \), we let \( \zeta = -1/(2\nu \pi i) = i/(2\nu \pi) \), and thus in
(1.12) take
\[ \xi_\nu = 0, \quad \eta_\nu = \frac{1}{2\nu r}, \quad \nu = 1, 2, \ldots, m/2. \] (3.5)
The quantity \( p_\nu \) in (2.13) being real, and thus \( d_\nu = 0 \) in (2.12), there is no nonconstant linear factor in the numerators of (2.11). This simplifies somewhat the procedure in §2.1.2, as it obviates the need to apply the routine \texttt{chri}.

In Table 3.8 we compare the performance (in double precision and for \( m = 2n \)) of our rational quadrature routine with Gauss-Laguerre quadrature (applied to \( f(t) = t/(e^t - 1) \)) and the Gaussian quadrature rule (applied to \( f(t) = e^{-t} \)) associated with "Einstein's weight function" \( t/(e^t - 1) \); for the latter see [6]. The respective relative errors are shown in the last two columns. It can be seen that the Gauss-Laguerre and Gauss-Einstein quadratures are comparable in accuracy, the former being somewhat more accurate for small values of \( n \), the latter for larger values of \( n \). Both quadrature rules, however, are incomparably inferior to the rational Gauss formula, which for \( n = 15 \) produces the true value of the integral, \( \zeta(2) - 1 = (\pi^2/6) - 1 \), to 25 correct decimal digits. (Actually, the last digit is off by one unit.) The results become even slightly more accurate when we choose \( m = 2[(n+1)/2] \), and are still better, by several orders of magnitude, than those for Gauss-Laguerre and Gauss-Einstein quadrature when \( m = 2 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( n )-point rational Gauss</th>
<th>err GL</th>
<th>err GE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>.59</td>
<td>9.76(-2)</td>
<td>4.09(-1)</td>
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<td>5</td>
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<td>1.50(-5)</td>
<td>2.97(-4)</td>
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<td>2.22(-8)</td>
<td>1.15(-8)</td>
</tr>
<tr>
<td>15</td>
<td>.6449340668482264364724151</td>
<td>1.59(-11)</td>
<td>3.25(-13)</td>
</tr>
</tbody>
</table>

TABLE 3.8. Numerical results for \( I_4 \) and comparison with Gauss-Laguerre and Gauss-Einstein quadrature

The high accuracy of our rational quadrature rules in this example is all the more remarkable as the routine \texttt{chri}, used in their construction (by the methods of §2.1.2), is subject to ill-conditioning, causing the recursion coefficients for the relevant orthogonal polynomials to gradually lose accuracy (by as much as 10 decimals, when \( n = 15 \) and \( m = 2n \)).

This weakness is accentuated when one tries to deal with more difficult integrals, for example,

\[ I(\theta) = \int_0^\infty \frac{t}{e^t - 1} \sqrt{1 + \frac{1}{2} \theta t} \ dt = \int_0^\infty \frac{t}{1 - e^{-t}} \sqrt{1 + \frac{1}{2} \theta t} \cdot e^{-t} \ dt, \quad \theta > 0, \] (3.6)

which has an additional branch point singularity at \( t = -2/\theta \). Here, when \( \theta = .75 \), the \( n \)-point rational Gauss formula (in double precision and for \( m = 2n \)) gives only about
13 correct decimal places for $n = 15$, and 18 for $n = 30$. By the time $n$ reaches 33, the ill-conditioning in the routine gchri has built up to such a level that the method fails (by producing a negative $\beta$-recursion coefficient). To get higher accuracy, one needs to apply the discretization method of §2.2, which is more stable, but becomes fairly expensive if pushed much beyond $n = 30$. Using $d\lambda(t) = e^{-t}dt$, and hence the $N$-point Gauss-Laguerre formula, to effect the discretization in (2.21), and requesting an accuracy of $\frac{1}{2} \times 10^{-25}$ for the desired recursion coefficients, we have observed timings of the order 12–16 seconds, and discretization parameters $N$ as large as $N = 370$, for $33 \leq n \leq 40$. The rational Gauss formula so produced then yields relative errors of $4.26 \times 10^{-21}$ for $n = 35$, and $9.65 \times 10^{-23}$ for $n = 40$. This is still better, by about 4 decimal orders of accuracy, than Gauss-Laguerre quadrature applied to the second form of the integral in (3.6), and Gauss-Einstein quadrature applied to the first form.

Generalized Fermi-Dirac integrals (cf. [12]) are similar to $I(0)$ except that $t/(e^t - 1)$ is replaced by $t^k/(e^{-\nu t} + 1)$, where $\eta$ is a real parameter and $k = 1/2, 3/2$ or $5/2$. The poles are now located at $\eta \pm (2\nu - 1)i\pi, \nu = 1, 2, 3, \ldots$. The use of rational Gauss quadrature to compute such integrals is dealt with elsewhere [5].

**Example 3.5.** $I_5(\eta) = \int_0^\infty \frac{t}{e^{-\eta t + 1}} e^{-t}dt, \quad \eta < 0$.

Again, we take $d\lambda(t) = e^{-t}dt$ and note that the poles are now at $\eta \pm 2\nu\pi i, \nu = 0, 1, 2, \ldots$. Accordingly, in (1.13) we take

$$
\xi_0 = -\frac{1}{\eta}, \quad \xi_\nu = -\frac{\eta}{\eta^2 + 4\nu^2\pi^2}, \quad \eta_\nu = \frac{2\nu\pi}{\eta^2 + 4\nu^2\pi^2}, \quad \nu = 1, 2, \ldots ,(m - 1)/2, \quad (3.7)
$$

and use the procedure of §2.1.2'. Selected results (for $m = 2n - 1$), comparing rational Gauss formulae with Gauss-Laguerre formulae, are shown in Table 3.9. In the case

<table>
<thead>
<tr>
<th>$\eta$</th>
<th>$n$</th>
<th>$n$-point rational Gauss</th>
<th>err GL</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-1.0$</td>
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<td>.113</td>
<td>2.14(-1)</td>
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<td></td>
<td>6</td>
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<td>5.07(-3)</td>
</tr>
<tr>
<td></td>
<td>11</td>
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<td>1.81(-4)</td>
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<td></td>
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<td>1.26(-5)</td>
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<td>2</td>
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<td>1.79(-1)</td>
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<tr>
<td></td>
<td>6</td>
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<td>1.57(-4)</td>
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<td></td>
<td>11</td>
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<td>7.31(-9)</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>.1135021146353905701870968(-4)</td>
<td>1.20(-12)</td>
</tr>
</tbody>
</table>

**TABLE 3.9.** Numerical results for $I_5$ and comparison with Gauss-Laguerre quadrature
Gauss-type quadrature rules for rational functions

\[ \eta = -1, \] we were able to go only up to \( n = 13 \); when \( n = 14 \), our procedure failed by producing a negative \( \beta \)-coefficient in (2.2). The difficulty is caused by the ill-conditioning (mentioned after (2.10)) affecting the modified Chebyshev procedure. Even though our procedure was successful for \( n = 13 \), it had to work hard to take care of the pole at \( \eta = -1 \): Backward recursion to compute modified moments had to start at \( \nu = 584 \) to get single-precision accuracy \( \frac{1}{2} \times 10^{-10} \), and at \( \nu = 2650 \) to get double-precision accuracy \( \frac{1}{2} \times 10^{-25} \).

Replacing the numerator \( te^{-t} \) in the integrand by \( t^k \), where \( k = 1/2, 3/2 \) or \( 5/2 \), and adding a factor \( \sqrt{1 + \frac{1}{2} \beta t} \) as in (3.6), produces the Bose-Einstein integral whose computation by rational Gauss quadrature is discussed in [5].

**Example 3.6.** \( I_5 = \int_0^\infty \left( \frac{t}{e^t - 1} \right)^2 e^{-t} dt \).

Here, as in Example 3.4, we take \( d\lambda(t) = e^{-t} dt \) and parameters \( \xi, \eta \) as in (3.5), except that there are only \( m/4 \) of them, \( m \) being divisible by 4. In Table 3.10 we give

<table>
<thead>
<tr>
<th>( n )</th>
<th>( n )-point rational Gauss</th>
<th>err GL</th>
<th>err GE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
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<td>3.71(−2)</td>
<td>1.61(−2)</td>
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<tr>
<td>8</td>
<td>.4816405209</td>
<td>1.16(−6)</td>
<td>5.99(−10)</td>
</tr>
<tr>
<td>14</td>
<td>.4816405210580757311</td>
<td>4.36(−9)</td>
<td>7.26(−18)</td>
</tr>
<tr>
<td>20</td>
<td>.4816405210580757313458777</td>
<td>2.80(−11)</td>
<td>1.09(−25)</td>
</tr>
</tbody>
</table>

**Table 3.10. Numerical results for \( I_5 \) and comparison with Gauss-Laguerre and Gauss-Einstein quadrature**

the results for \( m = 2n \) (\( n \) even) obtained by the discretization method of §2.2, analogous to those of Table 3.8 but using the square of the Einstein function as weight function in GE. (The method of §2.1, as mentioned earlier, was not implemented.) What is remarkable in this example is the competitiveness of the Gauss-Einstein quadrature rule vis-à-vis the rational Gauss rule.

**References**


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