Gaussian Quadrature Involving Einstein and Fermi Functions With an Application to Summation of Series*

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Abstract. Polynomials $\pi_k(\cdot) = \pi_k(\cdot; d\lambda)$, $k = 0, 1, 2, \ldots$, are constructed which are orthogonal with respect to the weight distributions $d\lambda(t) = (t/(e^t - 1))^r dt$ and $d\lambda(t) = (1/(e^t + 1))^r dt$, $r = 1, 2$, on $(0, \infty)$. Moment-related methods being inadequate, a discretized Stieltjes procedure is used to generate the coefficients α_k, β_k in the recursion formula $\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t)$, $k = 0, 1, 2, \ldots$, $\pi_0(t) = 1$, $\pi_{-1}(t) = 0$. The discretization is effected by the Gauss-Laguerre and a composite Fejér quadrature rule, respectively. Numerical values of α_k, β_k, as well as associated error constants, are provided for $0 \leqslant k \leqslant 39$. These allow the construction of Gaussian quadrature formulae, including error terms, with up to 40 points. Examples of n-point formulae, $n = 5(5)40$, are provided in the supplements section at the end of this issue. Such quadrature formulae may prove useful in solid state physics calculations and can also be applied to sum slowly convergent series.

1. Introduction. We are interested in Gaussian quadrature on $[0, \infty]$ relative to the weight functions $\varepsilon_r(t) = (t/(e^t - 1))^r$ and $\varphi_r(t) = (1/(e^t + 1))^r$. These functions arise, for example, in solid state physics and are referred to, when $r = 1$, as *Einstein* and *Fermi functions*, respectively. Integrals with respect to the measure $d\lambda(t) = \varepsilon_r(t) dt$, $r = 1$ and 2, are widely used in phonon statistics and lattice specific heats [7, §10], [1, §2.4], and occur also in the study of radiative recombination processes [9, §9.2]. Specifically, the average energy of a quantum harmonic oscillator of frequency ω at temperature T (representing thermal vibrations of crystal lattice atoms) is given by

$$(1.1) \qquad \overline{U} = \frac{\hbar\omega}{\exp(\hbar\omega/kT) - 1},$$

where $\hbar = h/2\pi$ (h is the Planck constant) and k is the Boltzmann constant. Therefore, $\overline{U} = kT\varepsilon_1(\hbar\omega/kT)$, where ε_1 is Einstein's function. Letting $g(\omega)$ denote the phonon density of states function, and integrating (1.1) over the entire frequency range, the total energy of thermal vibration of the crystal lattice becomes

$$(1.2) \quad U = \int_0^\infty \frac{\hbar\omega}{\exp(\hbar\omega/kT) - 1} g(\omega) \, d\omega = \frac{k^2 T^2}{\hbar} \int_0^\infty \varepsilon_1(t) g((kT/\hbar)t) \, dt.$$

Furthermore, differentiating U with respect to temperature T, yields the crystal lattice heat capacity at constant volume,

$$C_v = \frac{\partial U}{\partial T} = \int_0^\infty \frac{(\hbar\omega/kT)^2}{(\exp(\hbar\omega/kT) - 1)^2} kg(\omega) \exp(\hbar\omega/kT) \, d\omega,$$

that is,

(1.3) $$C_v = \frac{k^2 T}{\hbar} \int_0^\infty \varepsilon_2(t) f(t) \, dt \quad \text{where } f(t) = e^t g((kT/\hbar)t).$$

Similarly, integrals of the type $\int_0^\infty \varphi_1(t) f(t) \, dt$ (in fact, more generally $\int_0^\infty \varphi_1(t - t_0) f(t) \, dt$, for some parameter t_0) are encountered in the dynamics of electrons in metals, where they express the specific heat of the electron gas [8, §9.17]. For an application to heavy doped semiconductors, see also [10].

It will be shown in Section 4 that integration with respect to $d\lambda(t) = \varepsilon_1(t) \, dt$ and $d\lambda(t) = \varphi_1(t) \, dt$ is also useful in summing slowly convergent series whose general term is expressible in terms of a Laplace transform or its derivative.

Gaussian quadrature relative to the weight functions ε_r and φ_r will be particularly attractive in the case $r = 1$, since both weight functions then have poles with nonzero residues, the former at $2n\pi i$, $n = \pm 1, \pm 2, \ldots$, the latter at $(2n + 1)\pi i$, $n = 0, \pm 1, \pm 2, \ldots$. Classical integration, even based on Gauss-Laguerre quadrature, will often be too slow, but will be used to generate the desired quadrature rules, at least in the case of the weight function ε_r; see (2.3) below.

The problem, basically, amounts to generating the coefficients α_k, β_k in the recursion formula

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \qquad k = 0, 1, 2, \ldots,$$
$$\pi_{-1}(t) = 0, \qquad \pi_0(t) = 1$$

for the (monic) orthogonal polynomials $\pi_k(\cdot) = \pi_k(\cdot; d\lambda)$, $k = 0, 1, 2, \ldots$. (β_0 is arbitrary, but will be defined as $\beta_0 = \int_0^\infty d\lambda(t)$.) Once the first n of these coefficients, α_k, β_k, $k = 0, 1, \ldots, n - 1$, and β_n, are known, the m-point Gaussian quadrature formula

(1.4) $$\int_0^\infty f(t) \, d\lambda(t) = \sum_{\mu=1}^m \lambda_\mu f(\tau_\mu) + R_m(f),$$
$$R_m(f) = \gamma_m f^{(2m)}(\tau), \qquad 0 < \tau < \infty,$$

including the error constant γ_m, can easily be obtained for any m with $1 \leqslant m \leqslant n$. The nodes $\tau_\mu = \tau_\mu^{(m)}$, indeed, are the eigenvalues of the (symmetric tridiagonal) Jacobi matrix

$$J_m = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{m-1}} \\ 0 & & & \sqrt{\beta_{m-1}} & \alpha_{m-1} \end{bmatrix},$$

while the weights $\lambda_\mu = \lambda_\mu^{(m)}$ are given by $\lambda_\mu = \beta_0 v_{\mu,1}^2$ in terms of the first components $v_{\mu,1}$ of the corresponding normalized eigenvectors; see, e.g., [3, §5.1]. Moreover,

$$\gamma_m = \frac{\beta_0 \beta_1 \cdots \beta_m}{(2m)!}, \qquad m = 1, 2, \ldots, n.$$

A number of methods are available, and have been analyzed in [4], for computing the recursion coefficients α_k, β_k. They are either based on the moments (or modified moments) of the weight distribution $d\lambda(t)$, or else use a suitable discretization of the inner product

$$(u, v) = \int_0^\infty u(t) v(t) \, d\lambda(t), \qquad u, v \in \mathbf{P},$$

where u, v are polynomials. In the next section we discuss the relative merits of these methods for constructing the particular orthogonal polynomials at hand.

2. Generation of the Recursion Coefficients. We consider first the weight function ε_r. The classical approach (for example, the Chebyshev algorithm; see [4, §2.3]) departs from the moments of the weight function, which, in the case at hand, can be expressed in terms of the Riemann zeta function $\zeta(z)$,

(2.1)
$$\mu_k = \int_0^\infty t^k \varepsilon_r(t) \, dt$$
$$= \begin{cases} (k+1)! \zeta(k+2), & r = 1, \\ (k+2)! [\zeta(k+2) - \zeta(k+3)], & r = 2, \end{cases} \qquad k = 0, 1, 2, \ldots.$$

It is well-known, however, that the moments μ_k define the recursion coefficients α_k, β_k and the associated Gaussian quadrature formulae poorly in a numerical sense. The map G_n from the first $2n$ moments μ_k, $k = 0, 1, 2, \ldots, 2n - 1$, to the weights $\lambda_\nu^{(n)}$ and nodes $\tau_\nu^{(n)}$ of the n-point Gaussian formula, in fact becomes progressively more ill-conditioned as n increases. This is illustrated in Table 2.1, where in the second and third column the condition number of this map (in the sense of [4, Eq. (3.11)f]) is shown as a function of n for $r = 1$ and $r = 2$, respectively. (Numbers in parentheses indicate decimal exponents.)

TABLE 2.1

The numerical condition of various maps relating to the construction of orthogonal polynomials $\pi_k(\,\cdot\,; \varepsilon_r dt), r = 1, 2.$

n	cond G_n $r = 1$	cond G_n $r = 2$	cond $\tilde{G}_n$ $r = 1$	n	cond H_n $r = 1$	cond H_n $r = 2$
3	1.686(2)	7.620(1)	1.415(1)	5	7.665(0)	7.980(0)
6	1.288(5)	7.171(4)	2.934(3)	10	2.163(1)	2.161(1)
9	9.092(7)	5.820(7)	9.795(5)	15	3.299(1)	3.356(1)
12	6.334(10)	4.471(10)	4.039(8)	20	4.256(1)	4.244(1)
15	4.409(13)	3.344(13)	1.878(11)	30	6.761(1)	6.783(1)
18	3.076(16)	2.465(16)	9.441(13)	40	8.531(1)	8.556(1)

Sometimes the condition can be improved by employing modified moments $\nu_k = \int_0^\infty p_k(t)\varepsilon_r(t)\,dt$, where $\{p_k\}$ is a system of (monic) polynomials suitably chosen. If the support interval is infinite, however, as in the case at hand, the improvement is often not sufficient to make this a viable alternative. The fourth column of Table 2.1 indeed confirms this. Here, $r = 1$, and $\varepsilon_1(t) \sim te^{-t}$ as $t \to \infty$, so that the monic Laguerre polynomials with parameter $\alpha = 1$,

$$p_k(t) = (-1)^k k! L_k^{(1)}(t), \qquad k = 0, 1, 2, \ldots,$$

appear to be the most natural choices for the polynomials p_k. The corresponding modified moments can be shown to be expressible in terms of the (forward) differences, with unit step, of the Riemann zeta function at $z = 2$,

$$(2.2) \qquad \nu_k = \int_0^\infty p_k(t)\varepsilon_1(t)\,dt = (k + 1)!\Delta^k \zeta(z)\big|_{z=2}, \qquad k = 0, 1, 2, \ldots.$$

The map $\tilde{G}_n$ in Table 2.1 is the map from the first $2n$ normalized modified moments $\tilde{\nu}_k = \nu_k[\int_0^\infty p_k^2(t)te^{-t}\,dt]^{-1/2}$, $k = 0, 1, \ldots, 2n - 1$, to the weights $\lambda_\nu^{(n)}$ and nodes $\tau_\nu^{(n)}$ of the n-point Gaussian quadrature formula (1.4) (with $d\lambda(t) = \varepsilon_1(t)\,dt$). The entries in the fourth column exhibit the estimate derived in [4, Eq. (3.15)] for the condition of $\tilde{G}_n$. It can be seen that cond $\tilde{G}_n$, while somewhat smaller than cond G_n, is still growing unacceptably fast.

The modified Chebyshev algorithm (cf. [4, §2.4]), run in single precision on the CDC 6500 (machine precision: ca. 15 significant decimal digits), with the modified moments (2.2) computed in double precision, indeed loses accuracy very much in accordance with the growth of cond $\tilde{G}_n$; the number of correct decimal digits observed in α_k, β_k, $k = 3(3)18$, is 14, 11, 10, 6, 2, 0, respectively, not a single digit being correct for $k = 18$, not even the sign of β_{18}.

An additional complication arises in connection with the high-order differences in (2.2), which are subject to considerable cancellation errors. For $k = 40$, for example, one must expect a loss of approx. 12 decimal digits.

In contrast, methods based on discretization .appear to be incomparably more effective, particularly if one uses the natural discretization based on the Gauss-Laguerre quadrature rule,

$$(2.3) \qquad \begin{aligned} \int_0^\infty p(t)\left(\frac{t}{e^t - 1}\right)^r dt &= \frac{1}{r}\int_0^\infty p(t/r)\left(\frac{t/r}{1 - e^{-t/r}}\right)^r e^{-t}\,dt \\ &\approx \frac{1}{r}\sum_{k=1}^N \lambda_k^L p\left(\tau_k^L/r\right)\left(\frac{\tau_k^L/r}{1 - e^{-\tau_k^L/r}}\right)^r, \qquad p \in \mathbf{P}. \end{aligned}$$

Here, τ_k^L are the zeros of the Laguerre polynomial of degree N, and λ_k^L the associated Christoffel numbers. The discretized Stieltjes procedure (cf. [4, §2.2]), based on (2.3), then converges fairly rapidly as $N \to \infty$. For example, to obtain the first 12 recursion coefficients ($n = 12$) to 12 correct decimals [25 correct decimals] requires $N = 49$ [$N = 127$], when $r = 1$, and $N = 41$ [$N = 85$], when $r = 2$. The first 40 coefficients ($n = 40$) can be obtained accurately to 25 decimal digits with $N = 281$ for $r = 1$ and $N = 201$ for $r = 2$. Also the numerical stability of the procedure,

which is roughly determined (cf. [4, §3.4]) by the condition of the map

$$H_n: (\lambda_1, \ldots, \lambda_n, \tau_1, \ldots, \tau_n) \to (\alpha_0, \ldots, \alpha_{n-1}, \beta_0, \ldots, \beta_{n-1}),$$

is rather good. This can be seen from the last two columns of Table 2.1, which display the condition number of H_n in the sense of [4, Eq. (3.8)f].

One might expect that a discretization analogous to the one in (2.3) works well also for the weight function φ_r. This, however, is not the case, at least not if $r = 1$. Convergence turns out to be slow on account of the poles at $\pm i\pi$, which are twice as close to the real axis as in the case of ε_1. For example, to obtain 20 correct decimal digits (in the case $r = 1$ and for $n = 40$), requires $N = 361$. We used instead a discretization procedure based on the composite Fejér quadrature rule, decomposing the interval of integration into four subintervals, $[0, \infty] = [0, 10] \cup [10, 100] \cup [100, 500] \cup [500, \infty]$. Using $N = 201$ for $r = 1$, and $N = 281$ for $r = 2$, on each subinterval, then yields the first $n = 40$ recursion coefficients accurately to 25 decimal digits. The same procedure (with $n = 50$ and $N = 251$) was also used to check the computation based on (2.3) for ε_r, $r = 1, 2$. The maximum discrepancy observed was 1 unit in the 25th digit.

3. Numerical Results. Using the procedures outlined in the last two paragraphs of Section 2, we obtained the results shown in Tables 1–4 of the Appendix. The coefficients $\beta_0 = \zeta(2) = \pi^2/6$ in Table 1 and $\beta_0 = 2[\zeta(2) - \zeta(3)]$ in Table 2 (cf. Eq. (2.1)), agree to all 25 decimal digits with the values obtained from the 41S-table of the Riemann zeta function in [6]. Similarly, one checks the values $\beta_0 = \ln 2$ in Table 3 and $\beta_0 = \ln 2 - \frac{1}{2}$ in Table 4. Corresponding n-point Gaussian quadrature formulae, $n = 5(5)40$, for $r = 1$ and $r = 2$, can be found to 25 significant decimal digits in Tables 5–8 in the supplements section at the end of this issue.

We illustrate these formulae by computing the integrals

$$I_1 = \int_0^\infty e^{-t} \frac{t}{e^t - 1} dt = \zeta(2) - 1,$$

$$I_2 = \int_0^\infty e^{-t} \left(\frac{t}{e^t - 1} \right)^2 dt = 2[\zeta(2, 2) - 2\zeta(3, 2)],$$

$$I_3 = \int_0^\infty e^{-t} \frac{dt}{e^t + 1} = 1 - \ln 2,$$

$$I_4 = \int_0^\infty e^{-t} \frac{dt}{(e^t + 1)^2} = \frac{3}{2} - 2\ln 2,$$

where $\zeta(z, a)$ is the generalized zeta function. Table 3.1 shows the n-point approximations $I_i(n)$ to I_i, $i = 1, 2$, together with the relative errors $r_i(n)$, for $n = 5(5)25$. Similarly, $I_i(n)$ and $r_i(n)$, $i = 3, 4$, are shown in Table 3.2. In each entry the first digit in error is underlined. The error term in (1.4) yields the bounds γ_n/I_i, $i = 1, 2, 3, 4$, for the relative error, which can be computed with the help of Tables 1–4 of the Appendix and the limit values in Tables 3.1, 3.2; they are summarized in Table 3.3 for $n = 5(5)25$. The bounds for I_2, I_4 are seen to be considerably sharper than those for I_1, I_3.

TABLE 3.1

Gaussian approximations of the integrals I_1 and I_2 and relative errors.

n	$I_1(n)$	$r_1(n)$	$I_2(n)$	$r_2(n)$
5	.644742	3.0(−4)	.4816385	4.1(−6)
10	.6449340594	1.1(−8)	.48164052105737	1.5(−12)
15	.644934066848017	3.2(−13)	.481640521058075731184	3.3(−19)
20	.64493406684822643131	8.0(−18)	.4816405210580757313458776	1.1(−25)
25	.6449340668482264364772	1.8(−22)		

TABLE 3.2

Gaussian approximations of the integrals I_3 and I_4 and relative errors.

n	$I_3(n)$	$r_3(n)$	$I_4(n)$	$r_4(n)$
5	.3068171	1.2(−4)	.113705528	9.7(−7)
10	.30685281854	2.9(−9)	.113705638880091	1.5(−13)
15	.3068528194400358	6.2(−14)	.11370563888010938116323	2.0(−20)
20	.306852819440054690208	1.2(−18)	.1137056388801093811655358	6.1(−26)
25	.3068528194400546905827607	2.3(−23)		

TABLE 3.3

Relative error bounds for $I_i(n)$, $i = 1, 2, 3, 4$.

n	$\gamma_n/I_1(n)$	$\gamma_n/I_2(n)$	$\gamma_n/I_3(n)$	$\gamma_n/I_4(n)$
5	4.8(−2)	8.3(−5)	1.2(−2)	1.3(−5)
10	1.1(−4)	3.0(−10)	1.6(−5)	1.9(−11)
15	1.9(−7)	6.7(−16)	2.0(−8)	2.3(−17)
20	2.7(−10)	1.2(−21)	2.3(−11)	2.5(−23)
25	3.6(−13)	1.8(−27)	2.5(−14)	2.7(−29)

4. Summation of Series. As an application of Gaussian integration with weight functions ε_1 and φ_1, we consider the summation of series whose general term is expressible in terms of the derivative of a Laplace transform, or in terms of the Laplace transform itself. Suppose, for example, that $a_k = -F'(k)$, where

$$(4.1) \qquad F(p) = \int_0^\infty e^{-pt} f(t)\, dt, \qquad \mathrm{Re}\, p \geqslant 1.$$

Then

$$\sum_{k=1}^\infty a_k = \sum_{k=1}^\infty \int_0^\infty t e^{-kt} f(t)\, dt = \int_0^\infty \frac{t}{e^t - 1} f(t)\, dt,$$

that is,

$$(4.2a) \qquad -\sum_{k=1}^\infty F'(k) = \int_0^\infty f(t)\varepsilon_1(t)\, dt.$$

Similarly, for "alternating" series, one obtains

$$(4.2b) \qquad -\sum_{k=1}^\infty (-1)^{k-1} F'(k) = \int_0^\infty f(t) t \varphi_1(t)\, dt$$

and

(4.2c)
$$\sum_{k=1}^{\infty} (-1)^{k-1} F(k) = \int_0^\infty f(t) \varphi_1(t)\, dt.$$

If the series on the left are slowly convergent and the respective function f on the right is smooth, then low-order Gaussian quadrature applied to the integrals on the right provides one (among many other) possible summation procedure. If f exhibits singularities, then the weight function may have to be modified if the effectiveness of the procedure is to be preserved (cf. Example 4.4). In the following examples, "(a)", "(b)", "(c)" refers to a, b, c of Eq. (4.2).

Example 4.1. (a) $\sum_{k=1}^{\infty} (k+1)^{-2} = \pi^2/6 - 1$. Here, $-F'(p) = (p+1)^{-2}$, and $F(p) = (p+1)^{-1}$, the integration constant being zero on account of $F(p) \to 0$ as $p \to \infty$. Thus, $f(t) = e^{-t}$, and the second column of Table 3.1 shows the rapid convergence of Gaussian quadrature in this case. For example, 15-point quadrature already yields 12 correct decimal digits. In contrast, 10 000 terms of the series would give only 3-digit accuracy.

(b) $\sum_{k=1}^{\infty} (-1)^{k-1} (k+1)^{-2} = 1 - \pi^2/12$. Applying Gaussian quadrature to the integral in (4.2b) yields the results shown in Table 4.1. To guarantee, on the basis of Leibniz' convergence criterion, the same accuracy as the one achieved for $n = 15$ would require the summation of approximately 690 000 terms.

(c) $\sum_{k=1}^{\infty} (-1)^{k-1} (k+1)^{-1} = 1 - \ln 2$. The convergence behavior of Gaussian quadrature applied to the integral in (4.2c) is evident from the second column of Table 3.2.

TABLE 4.1

Gaussian approximations $K(n)$ of the integral

$$K = \int_0^\infty e^{-t} t (e^t + 1)^{-1}\, dt \text{ and relative errors.}$$

n	$K(n)$	$r(n)$
5	.177753	1.2(−3)
10	.1775329780	6.5(−8)
15	.17753296657625	2.1(−12)
20	.1775329665758867915	5.5(−17)
25	.1775329665758867817640 27	1.3(−21)
30	.1775329665758867817637 92	1.4(−25)

Example 4.2. $F(p) = p^{-1} \exp(-1/p)$, $-F'(p) = (p-1)p^{-3} \exp(-1/p)$. The original function is here $f(t) = J_0(2\sqrt{t})$. This being an entire function, we expect Gaussian quadrature in (4.2) to converge rapidly. This is confirmed in Table 4.2, which shows the relative errors for the n-point formula, $n = 2(2)12$. The exact sums (to 24 significant digits), as determined by Gaussian quadrature, are, respectively,

$$\sum_{k=1}^{\infty} (k-1) k^{-3} \exp(-1/k) = .342918943844609780961838,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1} (k-1) k^{-3} \exp(-1/k) = -.044155938134083605 2736928,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1} k^{-1} \exp(-1/k) = .197107936397950656955672.$$

The first 10 000 terms of the series yield, respectively, 3, 7 and 4 correct decimal digits. The Bessel function J_0 was evaluated by means of the rational approximations in [5] indexed 5852, 6553 and 6953.

TABLE 4.2

Relative errors in Gaussian approximation of the integrals in $(4.2, a–c)$, *where* $F(p) = p^{-1} \exp(-1/p)$.

n	(a)	(b)	(c)
2	4.48(−2)	8.95(−1)	1.77(−2)
4	3.80(−6)	2.39(−4)	9.65(−7)
6	3.35(−11)	3.71(−9)	6.32(−12)
8	7.01(−17)	1.13(−14)	1.05(−17)
10	6.86(−23)	1.08(−20)	1.27(−23)
12		1.93(−23)	

Example 4.3. $F(p) = (1 + p^2)^{-1/2}$, $-F'(p) = p(1 + p^2)^{-3/2}$. Here, $f(t) = J_0(t)$—again an entire function. Convergence of Gaussian quadrature in (4.2), while still satisfactory, is not quite as fast as in Example 4.2, presumably since the argument of J_0 is now essentially squared. The relative errors are shown in Table 4.3. For reference, we list the exact values of the respective sums:

$$\sum_{k=1}^{\infty} k(1 + k^2)^{-3/2} = .900524735348125924300853,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}k(1 + k^2)^{-3/2} = .234771442466894018686113,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}(1 + k^2)^{-1/2} = .440917473865185397183787.$$

The first 10 000 terms yield 3, 8 and 4 correct decimal digits, respectively.

TABLE 4.3

Relative errors in Gaussian approximation of the integrals in $(4.2, a–c)$, *where* $F(p) = (1 + p^2)^{-1/2}$.

n	(a)	(b)	(c)
5	1.68(−3)	8.15(−3)	1.99(−4)
10	8.03(−7)	4.75(−6)	2.11(−7)
15	4.05(−10)	2.99(−9)	9.01(−12)
20	1.64(−13)	7.61(−13)	2.26(−14)
25	5.79(−17)	5.64(−16)	2.52(−19)
30	2.69(−20)	8.25(−20)	2.33(−21)
35	5.11(−24)	8.01(−23)	3.88(−25)

Example 4.4. $F(p) = 2p^{-1}(p + 1)^{-1/2}$, $-F'(p) = (3p + 2)p^{-2}(p + 1)^{-3/2}$. Here we have an example in which the original function, $f(t) = 2 \, \text{erf} \, \sqrt{t}$, is no longer smooth, having a square root singularity at $t = 0$.

TABLE 4.4

Relative errors in Gaussian approximation of the integrals in $(4.2, \text{a–c})$, *where*

$$F(p) = 2p^{-1}(p + 1)^{-1/2}, \textit{ using weight functions } t^{1/2}\varepsilon_1(t) \textit{ and } t^{1/2}\varphi_1(t).$$

n	(a)	(b)	(c)
5	2.10(−5)	4.69(−5)	9.20(−6)
10	5.47(−10)	1.54(−9)	1.58(−10)
15	1.24(−14)	3.88(−14)	2.70(−15)
20	2.62(−19)	8.78(−19)	4.61(−20)
25	5.17(−24)	1.85(−23)	4.91(−25)

This severely retards convergence of Gaussian quadrature in (4.2). When $n = 40$, for example, the relative errors are still 4.29(−4), 7.19(−6) and 4.80(−4), respectively. Better results can be obtained by integrating with respect to the measures $t^{1/2}\varepsilon_1(t) \, dt$ and $t^{1/2}\varphi_1(t) \, dt$. The recursion coefficients for the corresponding orthogonal polynomials have been computed by a discretized Stieltjes procedure [4, §2.2] involving two different discretizations, one on the interval $[0, 10]$, where a Gauss-Jacobi quadrature with parameters $\alpha = 0$, $\beta = \frac{1}{2}$ (to account for the $t^{1/2}$-singularity at $t = 0$) was used, and one on the interval $[10, \infty]$, where we used Gauss-Laguerre quadrature as before. With the special Gaussian quadrature rules thus obtained, convergence of the summation process is very satisfactory; see Table 4.4. The exact values of the sums are:

$$\sum_{k=1}^{\infty} (3k + 2)k^{-2}(k + 1)^{-3/2} = 2.5719496323104805702278028,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}(3k + 2)k^{-2}(k + 1)^{-3/2} = 1.4857615292234121110869727,$$

$$\sum_{k=1}^{\infty} (-1)^{k-1}2k^{-1}(k + 1)^{-1/2} = 1.0395265337115689829716200.$$

The error function was evaluated by a double precison version of the incomplete gamma function routine in [2], observing that $\text{erf} \, \sqrt{t} = g^*(\frac{1}{2}, t)$ in the notation of [2].

Appendix A1: Recursion coefficients α_k, β_k and error constants γ_k for orthogonal polynomials $\pi_k(\cdot\,;\varepsilon_r\,dt)$, $r = 1, 2$.

TABLE 1

Recursion coefficients and error constants in the case $r = 1$

k	alpha(k)	beta(k)	gamma(k)
0	1.4615259388028769974520730d+00	1.6449340668482264364724150d+00	1.6449d+00
1	3.7041914443293395135022620d+00	1.8117836906421124892896540d+00	1.4901d+00
2	5.7709986569280917921598820d+00	5.6762887062602777876808560d+00	7.0487d-01
3	7.8060807007294852726114070d+00	1.1567444086578691488445300d+01	2.7178d-01
4	9.8286605539529427839225510d+00	1.9473894450164517475665310d+01	9.4512d-02
5	1.1844779411236036491090130d+01	2.9390567089239495470498770d+01	3.0864d-02
6	1.3857039607804716524291460d+01	4.1314693297074960491414020d+01	9.6602d-03
7	1.5866775091999247411035020d+01	5.5244566808620409359188790d+01	2.9323d-03
8	1.7874750837476556733205890d+01	7.1179048000086908599819680d+01	8.6965d-04
9	1.9881441597035179376448800d+01	8.9117330865456342782596150d+01	2.5327d-04
10	2.1887159880220248717838670d+01	1.0905882037989801260149250d+02	7.2688d-05
11	2.3892121016659853800919420d+01	1.3100306239306257893473230d+02	2.0611d-05
12	2.5896478897895800245943870d+01	1.5494970090451728200253400d+02	5.7857d-06
13	2.7900346847473467191141970d+01	1.8089845069062221741000040d+02	1.6102d-06
14	2.9903810424919001925958020d+01	2.0884907903183812687006520d+02	4.4482d-07
15	3.1906935609261380606749340d+01	2.3880139309444752775495350d+02	1.2210d-07
16	3.3909774212895205488744860d+01	2.7075523096414862130375460d+02	3.3325d-08
17	3.5912367570225914859895980d+01	3.0471045511692419678421310d+02	9.0503d-09
18	3.7914749115710570754548250d+01	3.4066694756305024742953340d+02	2.4469d-09
19	3.9916946226237516603090630d+01	3.7862460616812148410539020d+02	6.5894d-10
20	4.1918981563859618461964650d+01	4.1858334182002421596274320d+02	1.7681d-10
21	4.3920874071590604525899580d+01	4.6054307621553973085872990d+02	4.7287d-11
22	4.5922639723511028295858610d+01	5.0450374010853010540186930d+02	1.2609d-11
23	4.7924292097786311023875060d+01	5.5046527190721021497163230d+02	3.3531d-12
24	4.9925842819997130009147840d+01	5.9842761653905060437525400d+02	8.8944d-13
25	5.1927301910115716740478950d+01	6.4839072453129654656713d+02	2.3539d-13
26	5.3928678056947752059104310d+01	7.0035455120724960031494940d+02	6.2163d-14
27	5.5929978837311420932028830d+01	7.5431905613012663970566530d+02	1.6384d-14
28	5.7931210892645759941793490d+01	8.1028420249278511271494210d+02	4.3103d-15
29	5.9932380072490567523374110d+01	8.6824995670931963355570932d+02	1.1320d-15
30	6.1933491551942539817105600d+01	9.2821628802743218902891690d+02	2.9682d-16
31	6.3934549928489809168100970d+01	9.9018316820452216305082580d+02	7.7711d-17
32	6.5935559302372757290084400d+01	1.0541505712298925902475710d+03	2.0317d-17
33	6.7936523343684913093391300d+01	1.1201184730852915398335400d+03	5.3049d-18
34	6.9937445348725185935930477d+01	1.1880868515375133352077144d+03	1.3834d-18
35	7.1938328287579302875456160d+01	1.2580556859579636709224520d+03	3.6032d-19
36	7.3939174844499826215966830d+01	1.3300249571650228796430430d+03	9.3747d-20
37	7.5939987452338711503869160d+01	1.4039946472857824173041670d+03	2.4365d-20
38	7.7940768322040936527864520d+01	1.4799647396343206902780910d+03	6.3263d-21
39	7.9941519468015371369499170d+01	1.5579352186041624229934920d+03	1.6410d-21

TABLE 2

Recursion coefficients and error constants in the case r = 2

k	alpha(k)	beta(k)	gamma(k)
0	8.1106238432719694620056717d-01	8.8575432737726430214535540d-01	8.8575d-01
1	2.0824895633609331136782997d+00	5.7219323339461376964598358d-01	2.5341d-01
2	3.1804727324923422760495140d+00	1.7599621950108990929957389d+00	3.7166d-02
3	4.2304646872325677288996590d+00	3.4523849192031173545509570d+00	4.2771d-03
4	5.2618141802225195072490160d+00	5.6467693899369006236994870d+00	4.3128d-04
5	6.2839703356414230717153380d+00	8.3443550621735235814714960d+00	3.9986d-05
6	7.3007778267374021377702570d+00	1.1545230645202395910479820d+01	3.4973d-06
7	8.3141248935361967328807210d+00	1.5249049249105138269661720d+01	2.9303d-07
8	9.3250704128598773868268310d+00	1.9455414366382882595724070d+01	2.3754d-08
9	1.0334264561796184645862380d+01	2.4163978775143915843000045d+01	1.8758d-09
10	1.1342133201330919700071013d+01	2.9374455967927655493731460d+01	1.4500d-10
11	1.2348969122257135049629721d+01	3.5086611828611050089954230d+01	1.1012d-11
12	1.3354981419873444636651210d+01	4.1300254099899015181320030d+01	8.2392d-13
13	1.4360324072034131846485650d+01	4.8015223418473265054333960d+01	6.0862d-14
14	1.5365113388088875612823130d+01	5.5231386320846917959475090d+01	4.4465d-15
15	1.6369439124062036122598340d+01	6.2948629904883895660032070d+01	3.2172d-16
16	1.7373371824546171573308160d+01	7.1166857759412578988687472d+01	2.3081d-17
17	1.8376967820178030144291210d+01	7.9885986840142133083779180d+01	1.6433d-18
18	1.9380272719125080510515648860d+01	8.9105945049022614543190770d+01	1.1621d-19
19	2.0383323902228950350940720d+01	9.8826666933905573379469390d+01	8.1686d-21
20	2.1386152341911847765082710d+01	1.0904810421493281765172810d+02	5.7101d-22
21	2.2388783951666221550086360d+01	1.1977020053480846838118370d+02	3.9715d-23
22	2.3391240603124167669163210d+01	1.3099291454352956118272540d+02	2.7497d-24
23	2.4393540903483347602881194d+01	1.4271620708557311329152320d+02	1.8958d-25
24	2.5395700797378264520627480d+01	1.5494004295888492328576660d+02	1.3020d-26
25	2.6397734038261930823843860d+01	1.6766439038022341404149070d+02	8.9102d-28
26	2.7399625256151148169598840d+01	1.8088922053952467060202510d+02	6.0775d-29
27	2.8401466782613842391705080d+01	1.9461450722592883122215300d+02	4.1327d-30
28	2.9403185837606773076216790d+01	2.0884022651194356523440110d+02	2.8022d-31
29	3.0404817778555179341344070d+01	2.2356635648511835573230200d+02	1.8950d-32
30	3.1406369733683932221743530d+01	2.3879287701881270336678760d+02	1.2783d-33
31	3.2407848039486460864384570d+01	2.5451976957534038274986830d+02	8.6024d-35
32	3.3409258350431906083860170d+01	2.7074701703608920048858380d+02	5.7764d-36
33	3.4410605730629786672603080d+01	2.8747460355422450893092687d+02	3.8708d-37
34	3.5411894730860121455464840d+01	3.0470251442655975234637700d+02	2.5888d-38
35	3.6413129453654615594387220d+01	3.2243073598124354821469680d+02	1.7282d-39
36	3.7414313608561054389190870d+01	3.4065925547957808353739400d+02	1.1516d-40
37	3.8415450559295481357773130d+01	3.5938806102925484178621870d+02	7.6617d-42
38	3.9416543364153876388221440d+01	3.7861714150777898286635180d+02	5.0892d-43
39	4.0417594810794030790824530d+01	3.9834648649454791414016590d+02	3.3754d-44

Appendix A2: Recursion coefficients α_k, β_k and error constants γ_k for orthogonal polynomials $\pi_k(\cdot\,; \varphi_r\,dt)$, $r = 1, 2$.

TABLE 3

Recursion coefficients and error constants in the case $r = 1$

k	alpha(k)	beta(k)	gamma(k)
0	1.1865691104156254528217233d+00	6.9314718055994530941723211d-01	6.9315d-01
1	3.0963542153967773858680971d+00	1.1933560457895086591789461d+00	4.1359d-01
2	5.0722272795356037485262801d+00	4.1918064245490424515900831d+00	1.4447d-01
3	7.0601226279075802377733621d+00	9.2153673854346419765449321d+00	4.4379d-02
4	9.0525619401073770633595961d+00	1.6239132448283183997839061d+01	1.2869d-02
5	1.1047275106388619531739801d+01	2.5261473216851957477380241d+01	3.6122d-03
6	1.3043313965918185241681381d+01	3.6282351051237716462310381d+01	9.9286d-04
7	1.5040204343673284236253431d+01	4.9301937719257473048112081d+01	2.6896d-04
8	1.7037679640463642149398681d+01	6.4320413060756842614069641d+01	7.2081d-05
9	1.9035577043503815723696411d+01	8.1337931068991146618837491d+01	1.9160d-05
10	2.1033790799507426836769291d+01	1.0035461812327147378443631d+02	5.0599d-06
11	2.3032248853585314508369221d+01	1.2137057733749304391791131d+02	1.3293d-06
12	2.5030900199797527167305241d+01	1.4438589330643122473411991d+02	3.4770d-07
13	2.7029707586797435879629831d+01	1.6940063606953125613434221d+02	9.0616d-08
14	2.9028643091371066700368192d+01	1.9641486420103256519956361d+02	2.3543d-08
15	3.1027685316462237145190181d+01	2.2542862717367122128790071d+02	6.1002d-09
16	3.3026817553309565986508221d+01	2.5644196716436486775657331d+02	1.5770d-09
17	3.5026026538793554654207721d+01	2.8945492044168996682388511d+02	4.0683d-10
18	3.7025301592884823916274091d+01	3.2446751844140760260028321d+02	1.0476d-10
19	3.9024634006048577790430881d+01	3.6147978860842364278815091d+02	2.6935d-11
20	4.1024016595297707349845831d+01	4.0049175506255253170225111d+02	6.9148d-12
21	4.3023443376646272047955121d+01	4.4150343913014197400313321d+02	1.7729d-12
22	4.5022909319540422004482381d+01	4.8451485977258084065933591d+02	4.5401d-13
23	4.7022410160077438245594451d+01	5.2952603393476293777085341d+02	1.1614d-13
24	4.9021942257076014995809701d+01	5.7653697683082489770386211d+02	2.9681d-14
25	5.1021502479845854437412001d+01	6.2554770218028059496560301d+02	7.5782d-15
26	5.3021088119724192603393661d+01	6.7655822240458884083768741d+02	1.9333d-15
27	5.5020696819652141364219601d+01	7.2956854879190132201781511d+02	4.9283d-16
28	5.7020326517599058473020531d+01	7.8457869163602306446864971d+02	1.2554d-16
29	5.9019975400728146240286851d+01	8.4158866035432165905308461d+02	3.1958d-17
30	6.1019641867973828152169011d+01	9.0059846358833431861604641d+02	8.1303d-18
31	6.3019324499265499639110661d+01	9.6160810929006182006445161d+02	2.0672d-18
32	6.5019022030046359841036301d+01	1.0246176047963505303172381d+03	5.2532d-19
33	6.7018733330043397658894431d+01	1.0896269568933039046555911d+03	1.3343d-19
34	6.9018457385475073081118241d+01	1.1566361718723034252406971d+03	3.3873d-20
35	7.1018193284057690197802671d+01	1.2256452555789325583329901d+03	8.5956d-21
36	7.3017940202304692382929161d+01	1.2966542134558689323332327d+03	2.1803d-21
37	7.5017697394715713791084811d+01	1.3696630505806266654642661d+03	5.5280d-22
38	7.7017464184531857309080121d+01	1.4446717716988828097633241d+03	1.4011d-22
39	7.9017239955795935855004051d+01	1.5216803812540017403820631d+03	3.5498d-23

TABLE 4

Recursion coefficients and error constants in the case r = 2

k	alpha(k)	beta(k)	gamma(k)
0	6.69540463853843823238 7227d-01	1.93147180559945309417 2321d-01	1.9315d-01
1	1.66468613300982968001 1075d+00	3.70527871085168485680 6622d-01	3.5783d-02
2	2.61943184101575847660 4192d+00	1.15490785365260136536 5824d+00	3.4439d-03
3	3.59386536697407229975 6279d+00	2.41678287193756902772 3998d+00	2.7744d-04
4	4.57956061124442250923 1409d+00	4.17898336359948107116 6374d+00	2.0704d-05
5	5.57039324488908101318 3465d+00	6.44237334182313934233 8233d+00	1.4820d-06
6	6.56386385646327482128 2662d+00	9.20582454373696897223 6729d+00	1.0336d-07
7	7.55889043571058239101 7287d+00	1.24688599041073718623 2674d+01	7.0810d-09
8	8.55493150694510173535 0174d+00	1.62313604104084499222 8737d+01	4.7889d-10
9	9.55168042407351284402 5433d+00	2.04933282758509899839 084d+01	3.2072d-11
10	1.05489474942684973675 8553d+01	2.52548003830609252223 979d+01	2.1315d-12
11	1.15466077449982794940 0336d+01	3.05158205689630751679 3924d+01	1.4079d-13
12	1.25445748719504500792 1430d+01	3.62764310278857077257 8227d+01	9.2524d-15
13	1.35427870359185112255 0789d+01	4.25366698803941543418 8650d+01	6.0549d-16
14	1.45411985846388167319 0978d+01	4.92965707916051973434 4687d+01	3.9482d-17
15	1.55397749704140948072 2936d+01	5.65561632661262475600 2118d+01	2.5666d-18
16	1.65384894959772310588 5520d+01	6.43154731343523431708 1962d+01	1.6640d-19
17	1.75373211570112602326 8357d+01	7.25745230546481570736 3551d+01	1.0764d-20
18	1.85362531688566647125 1907d+01	8.13333297094291496385 707d+01	6.9479d-22
19	1.95352719345285255182 4561d+01	9.05919205090994107419 572d+01	4.4767d-23
20	2.05343663056676925886 4606d+01	1.00350301315548550875 4740d+02	2.8797d-24
21	2.15335270428624100991 3773d+01	1.10608489336027848003 3078d+02	1.8497d-25
22	2.25327464146852066733 2283d+01	1.21366497056645412086 5567d+02	1.1865d-26
23	2.35320178951521043637 3844d+01	1.32624335700416860219 7873d+02	7.6022d-28
24	2.45313359322501878801 3906d+01	1.44382015394487871329 8334d+02	4.8653d-29
25	2.55306957685986648380 9419d+01	1.56639545310722693349 0024d+02	3.1106d-30
26	2.65300933009043351995 3643d+01	1.69396933784657406974 8673d+02	1.9869d-31
27	2.75295249686663714919 31937d+01	1.82654188416572333905 5932d+02	1.2681d-32
28	2.85289876651779462679 2057d+01	1.96411316157743525955 8123d+02	8.0864d-34
29	2.95284786657776107376 0216d+01	2.10668323384365569164 1098d+02	5.1529d-35
30	3.05279955569455945779 10743d+01	2.25425215961178175356 0632d+02	3.2813d-36
31	3.15275362510464093015 7417d+01	2.40681999296458230478 6437d+02	2.0882d-37
32	3.25270988217642175770 3103d+01	2.56438678389740217480 5713d+02	1.3281d-38
33	3.35266815964358382359 4838d+01	2.72695257873387010668 8784d+02	8.4422d-40
34	3.45262830661164662197 5720d+01	2.89451742048938337922 9000d+02	5.3635d-41
35	3.55259018750786819483 2644d+01	3.06708134919006400574 6629d+02	3.4059d-42
36	3.65255368013707082955 7449d+01	3.24464440215359801741 6908d+02	2.1617d-43
37	3.75251867403076768726 2801d+01	3.42720661423732173950 8610d+02	1.3715d-44
38	3.85248506903868371384 6996d+01	3.61476801805806053751 9819d+02	8.6975d-46
39	3.95245277412169598056 5398d+01	3.80732864418751931924 5180d+02	5.5135d-47

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