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ERROR BOUNDS FOR GAUSSIAN QUADRATURE OF ANALYTIC FUNCTIONS*

WALTER GAUTSCHI† AND RICHARD S. VARGA‡

To Peter Henrici on his 60th birthday in friendship and admiration

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Abstract. For Gaussian quadrature rules over a finite interval, applied to analytic or meromorphic functions, we develop error bounds from contour integral representations of the remainder term. As in previous work on the subject, we consider both circular and elliptic contours. In contrast with earlier work, however, we attempt to determine exactly where on the contour the kernel of the error functional attains its maximum modulus. We succeed in answering this question for a large class of weight distributions (including all Jacobi weights) when the contour is a circle. In the more difficult case of elliptic contours, we can settle the question for certain special Jacobi weight distributions with parameters $\pm\frac{1}{2}$, and we provide empirical results for more general Jacobi weights. We further point out that the kernel of the error functional, at any complex point outside the interval of integration, can be evaluated accurately and efficiently by a recursive procedure. The same procedure is useful also to evaluate certain correction terms that arise when poles are present in the integrand. The error bounds obtained are illustrated numerically for two examples—an integral representation for the Bessel function of order zero, and an integral related to the complex exponential integral.

1. Introduction. We consider Gaussian quadrature with respect to some positive measure $d\lambda(t)$ on a finite interval which we normalize to be $[-1, 1]$. Thus,

$$\int_{-1}^{1} f(t)\,d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\tau_\nu^{(n)}) + R_n(f), \tag{1.1}$$

where $\tau_\nu^{(n)}$ are the zeros of the nth degree orthogonal polynomial $\pi_n(\cdot\,; d\lambda)$ and $\lambda_\nu^{(n)}$ the corresponding Christoffel numbers. If f is single-valued holomorphic in a domain D which contains $[-1, 1]$ in its interior, and Γ is a contour in D surrounding $[-1, 1]$, the remainder term $R_n(\cdot)$ can be represented as a contour integral

$$R_n(f) = \frac{1}{2\pi i}\int_\Gamma K_n(z) f(z)\,dz, \tag{1.2}$$

where the kernel K_n is given by

$$K_n(z) = R_n\left(\frac{1}{z-\cdot}\right), \tag{1.3}$$

or, alternatively, by

$$K_n(z) = \frac{\rho_n(z)}{\pi_n(z)}. \tag{1.4}$$

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Here, $\pi_n(z)$ is the orthogonal polynomial $\pi_n(\cdot\,; d\lambda)$ evaluated at z, while $\rho_n(z)$ is defined by

$$\rho_n(z) = \int_{-1}^{1} \frac{\pi_n(t)}{z-t}\, d\lambda(t); \tag{1.5}$$

see, e.g., [4, § 1.4].

There is an extensive literature using (1.2) to estimate the error R_n in (1.1); see the references cited in [4, § 4.1.1] and more recent work in [1], [11], [12]. Basically, the estimates take the form

$$|R_n(f)| \leqq \frac{l(\Gamma)}{2\pi} \max_{z\in\Gamma} |K_n(z)| \cdot \max_{z\in\Gamma} |f(z)|, \tag{1.6}$$

where $l(\Gamma)$ denotes the length of Γ. The first maximum depends only on the quadrature rule (i.e., on $d\lambda$) and not on f, while the second depends only on f. Similar estimates hold for meromorphic functions, if the contributions from the poles are separated out. In all the literature on the subject, $\max_{z\in\Gamma} |K_n(z)|$ is either bounded from above, or estimated asymptotically for large n (or large z, or both). Our objective here is to point out that for a large class of measures $d\lambda$ (including the Jacobi measure $d\lambda(t) = (1-t)^\alpha(1+t)^\beta\, dt$ for arbitrary $\alpha > -1$, $\beta > -1$), and in the case where Γ is a circle $|z| = r$, $r > 1$, this maximum can be expressed exactly as either $K_n(r)$ or $|K_n(-r)|$ (Theorem 3.1) and can be evaluated accurately and efficiently by recursion (Section 4). For elliptic contours $\Gamma = \{z : z = \frac{1}{2}(\rho e^{i\vartheta} + \rho^{-1} e^{-i\vartheta}),\ 0 \leqq \vartheta \leqq 2\pi\}$, $\rho > 1$, the problem is considerably more difficult. We are able, however, in the case of Jacobi measures with $\alpha = \beta = \pm\frac{1}{2}$ and $\alpha = -\frac{1}{2}$, $\beta = \frac{1}{2}$, to give explicit representations of the kernel K_n on Γ, and from these to determine the maximum points on the ellipse (Section 5). The latter turn out to be located on the real positive axis (Theorems 5.1 and 5.3), except when $\alpha = \beta = \frac{1}{2}$, in which case they are located on the imaginary axis, if n is odd (Theorem 5.2), or nearby, if n is even. For more general Jacobi measures we present empirical results. Section 6 contains numerical examples illustrating the quality of the error bounds obtained.

We begin by recalling a preliminary result from [7].

2. Inequalities for moment quadrature sums. Here and in the following we restrict ourselves to measures $d\lambda$ of the form

$$d\lambda(t) = w(t)\, dt, \qquad -1 < t < 1, \tag{2.1}$$

where the function w is nonnegative and integrable on $[-1, 1]$, with moments

$$\mu_k = \int_{-1}^{1} t^k\, d\lambda(t), \qquad k = 0, 1, 2, \cdots, \tag{2.2}$$

where $\mu_0 > 0$. The orthogonal polynomials associated with (2.1) are denoted by $\pi_n(\cdot) = \pi_n(\cdot\,; d\lambda)$, their zeros by $\tau_\nu^{(n)}$, and the corresponding Christoffel numbers by $\lambda_\nu^{(n)}$. The following theorem, proved in [7], shows that, for a large class of weight functions w, the Gaussian quadrature sums for approximating the moment μ_k approach this moment monotonically. (To suit our present purposes, we have slightly weakened both the assertions and the hypotheses of the theorem.)

THEOREM 2.1. *Let*

$$\mu_k^{(n)} = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} [\tau_\nu^{(n)}]^k, \qquad k = 1, 2, 3, \cdots, \quad n = 1, 2, 3, \cdots. \tag{2.3}$$

(a) *If $w(t)/w(-t)$ is nondecreasing on* $(-1, 1)$, *then*

$$0 \leqq \mu_k^{(1)} \leqq \mu_k^{(2)} \leqq \cdots \leqq \mu_k^{([k/2]+1)} = \mu_k^{([k/2]+2)} = \cdots = \mu_k. \tag{2.4}$$

(b) *If $w(t)/w(-t)$ is nonincreasing on* $(-1, 1)$, *then*

$$0 \leqq \mu_k^{(1)} \leqq \mu_k^{(2)} \leqq \cdots \leqq \mu_k^{([k/2]+1)} = \mu_k^{([k/2]+2)} = \cdots = \mu_k \tag{2.5}$$

if k is even and

$$\mu_k = \cdots = \mu_k^{([k/2]+2)} = \mu_k^{([k/2]+1)} \leqq \mu_k^{([k/2])} \leqq \cdots \leqq \mu_k^{(2)} \leqq \mu_k^{(1)} \leqq 0 \tag{2.6}$$

if k is odd.

We note, in particular, that for the Jacobi weight function $w(t) = (1-t)^\alpha(1+t)^\beta$, $\alpha > -1$, $\beta > -1$, one has

$$\frac{w(t)}{w(-t)} = \left(\frac{1+t}{1-t}\right)^{\beta-\alpha},$$

which is strictly increasing on $(-1, 1)$ if $\alpha < \beta$, equal to 1 if $\alpha = \beta$, and strictly decreasing on $(-1, 1)$ if $\alpha > \beta$. Accordingly, (2.4) holds if $\alpha \leqq \beta$, and (2.5), (2.6) if $\alpha > \beta$.

3. The maximum of the kernel K_n on a circle and corresponding error bounds. We assume a measure $d\lambda$ of the form (2.1) and propose to find the maximum of the kernel $K_n(z)$ in (1.3) on the circle $C_r = \{z : |z| = r\}$, where $r > 1$.

THEOREM 3.1. *There holds*

$$\max_{z \in C_r} |K_n(z)| = \begin{cases} K_n(r) & \text{if } w(t)/w(-t) \text{ is nondecreasing on } (-1, 1), \\ |K_n(-r)| & \text{if } w(t)/w(-t) \text{ is nonincreasing on } (-1, 1). \end{cases} \tag{3.1}$$

Remark. If $w(t) = w(-t)$ on $(-1, 1)$ then, by symmetry, $K_n(r) = |K_n(-r)|$, and either statement in (3.1) is valid.

Proof of Theorem 3.1. By expanding $(z-t)^{-1}$ in powers of t/z, one obtains from (1.3), when $|z| > 1$, that

$$K_n(z) = \sum_{k=2n}^{\infty} \frac{R_n(t^k)}{z^{k+1}}. \tag{3.2}$$

We have used the fact that $R_n(t^k) = 0$ for $0 \leqq k < 2n$. Therefore,

$$\max_{z \in C_r} |K_n(z)| \leqq \sum_{k=2n}^{\infty} \frac{|R_n(t^k)|}{r^{k+1}}. \tag{3.3}$$

If $w(t)/w(-t)$ is nondecreasing, then, by Theorem 2.1(a), since $[k/2] \geqq n$ for $k \geqq 2n$,

$$\mu_k = \mu_k^{([k/2]+1)} \geqq \mu_k^{(n+1)} \geqq \mu_k^{(n)}, \qquad k \geqq 2n,$$

hence, by (2.2) and (2.3),

$$R_n(t^k) \geqq 0 \quad \text{for all } k \geqq 2n.$$

Therefore,

$$K_n(r) = \sum_{k=2n}^{\infty} \frac{R_n(t^k)}{r^{k+1}} = \sum_{k=2n}^{\infty} \frac{|R_n(t^k)|}{r^{k+1}}.$$

Comparison with (3.3) shows that $\max_{z \in C_r} |K_n(z)| = K_n(r)$, proving (3.1) in case (a) of Theorem 2.1.

If $w(t)/w(-t)$ is nonincreasing, one obtains from (2.5), when k is even, as before that

$$R_n(t^k) \geqq 0 \quad \text{for all } k \text{ (even)} \geqq 2n,$$

while for $k \geqq 2n+1$ odd, $\mu_k = \mu_k^{([k/2]+1)} \leqq \mu_k^{(n+1)} \leqq \mu_k^{(n)}$ by (2.6), so that

$$R_n(t^k) \leqq 0 \quad \text{for all } k \text{ (odd)} \geqq 2n+1.$$

Consequently,

$$(-1)^k R_n(t^k) \geqq 0 \quad \text{for all } k \geqq 2n,$$

and

$$|K_n(-r)| = \left| -\sum_{k=2n}^{\infty} \frac{(-1)^k R_n(t^k)}{r^{k+1}} \right| = \sum_{k=2n}^{\infty} \frac{|R_n(t^k)|}{r^{k+1}},$$

yielding $\max_{z \in C_r} |K_n(z)| = |K_n(-r)|$. □

In the situations described in Theorem 3.1, the modulus of the kernel $K_n(z)$ thus attains its maximum on the circle C_r either at $z=r$ or at $z=-r$ on the real axis. For the Jacobi weight function $w(t)=(1-t)^\alpha(1+t)^\beta$, the remark after Theorem 2.1 implies that the maximum occurs at $z=r$ if $\alpha \leqq \beta$, and at $z=-r$ if $\alpha > \beta$.

We remark that the "bound" used in [12, Eqs. (5) and (6)] for $\max_{z \in C_r} |K_n(z)|$ in the case of Gegenbauer measures is actually $K_n(r)$, hence, by Theorem 3.1, *equal* to the maximum in question. The form given in [12] for $K_n(r)$ involves infinite series and the zeros of Gegenbauer polynomials. It requires considerably more effort to evaluate than the simple recursion (Eqs. (4.3)–(4.5)) to be described below in § 4. The approach via recursion, moreover, is not restricted to Gegenbauer measures, but is valid for essentially arbitrary measures.

The error bound (1.6), in combination with, say, the first case of Theorem 3.1, now yields the final error bound

$$|R_n(f)| \leqq r \cdot K_n(r) \cdot \max_{z \in C_r} |f(z)|. \tag{3.4}$$

Whether or not this represents a realistic estimation of the error depends largely on the behavior of f on the contour C_r. If f is highly oscillatory on C_r, then (3.4) is likely to be conservative. Some improvement, for specific functions f, may be achieved by optimizing the bound on the right of (3.4) as a function of r; see § 6 for examples.

If f is meromorphic, with poles close to the interval $[-1, 1]$, the quadrature rule (1.1) will converge only very slowly. Moreover, (3.4) ceases to be applicable, since f may no longer be analytic in C_r, $r>1$. Valid error bounds can still be obtained by employing elliptic contours (see § 5), but they are of limited interest in cases of slow convergence.

It is well known, however, how the poles can be taken into account so as to restore the fast convergence one is accustomed to in the case of analytic functions. Assuming for simplicity that there are only a finite number of poles p_i in the finite complex plane, and that all are simple, then in fact (see, e.g., [10])

$$\int_{-1}^{1} f(t)\, d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} f(\tau_\nu^{(n)}) - \sum_i K_n(p_i)(\operatorname{res} f)_{p_i} + R_n(f), \tag{3.5}$$

where $\tau_\nu^{(n)}$, $\lambda_\nu^{(n)}$ are as before, and $(\operatorname{res} f)_{p_i}$ denotes the residue of f at the pole p_i. For the remainder R_n we have the same representation as before,

$$R_n(f) = \frac{1}{2\pi i} \int_\Gamma K_n(z) f(z)\, dz, \tag{3.6}$$

where Γ is a contour enclosing the interval $[-1, 1]$ as well as the poles p_i; the error bound (3.4) continues to hold if the circle C_r, $r>1$, contains all poles p_i in its interior.

As a simple example, suppose that

$$f(t)=\frac{g(t)}{t^2+\omega^2}, \qquad \omega>0, \tag{3.7}$$

with g an entire function, real-valued on the real axis. Then (3.5), by an elementary calculation, reduces to

$$\int_{-1}^{1}\frac{g(t)}{t^2+\omega^2}\,d\lambda(t)=\sum_{\nu=1}^{n}\lambda_\nu^{(n)}\frac{g(\tau_\nu^{(n)})}{[\tau_\nu^{(n)}]^2+\omega^2}-\frac{1}{\omega}\,\mathrm{Im}\,[K_n(i\omega)g(i\omega)]+R_n(f), \tag{3.8}$$

the remainder being bounded by (3.4), where $r>\max(1,\omega)$ and f is given by (3.7).

4. Computation of $K_n(\pm r)$ and $K_n(z)$. For computational purposes, the second of the two expressions (1.3) and (1.4) for $K_n(z)$, that is,

$$K_n(z)=\frac{\rho_n(z)}{\pi_n(z)}, \tag{4.1}$$

is the more suitable one, as it is not subject to any loss of accuracy. (This is not sufficiently recognized in the literature; Lether [11], for example, refers to the form (4.1) as being "inconvenient".) Indeed, $\{\rho_k(z)\}$ and $\{\pi_k(z)\}$ both are solutions of the basic recurrence relation

$$y_{k+1}=(z-\alpha_k)y_k-\beta_k y_{k-1}, \qquad k=0,1,2,\cdots, \tag{4.2}$$

satisfied by the (monic) orthogonal polynomials $\pi_k(\cdot)=\pi_k(\cdot\,;d\lambda)$, whereby $y_{-1}=0$, $y_0=1$ for $\{\pi_k\}$, and $y_{-1}=1$ for $\{\rho_k\}$. (It is assumed that $\beta_0=\int_{-1}^{1}d\lambda(t)$.) If $z=\pm r$, $r>1$, so that $z\notin[-1,1]$, the solution $\{\rho_k(z)\}$ is the minimal solution of (4.2), hence uniquely determined by the single initial value $y_{-1}=1$; see [5]. It can be computed most effectively by backward recursion [5, § 5]: Let

$$r_\nu^{[\nu]}(z)=0, \qquad r_{k-1}^{[\nu]}(z)=\frac{\beta_k}{z-\alpha_k-r_k^{[\nu]}(z)}, \qquad k=\nu,\nu-1,\cdots,1,0. \tag{4.3}$$

Then, if $z\notin[-1,1]$, the limit $\lim_{\nu\to\infty}r_{k-1}^{[\nu]}(z)=r_{k-1}(z)$ exists, and

$$\rho_{-1}(z)=1, \qquad \rho_k(z)=r_{k-1}(z)\rho_{k-1}(z), \qquad k=0,1,2,\cdots,n. \tag{4.4}$$

Thus, to compute $\rho_n(z)$ to within a relative error of ε, one starts with some initial value $\nu_0>n$ of the index ν, and keeps increasing ν, say by 5, until $|r_{k-1}^{[\nu+5]}(z)-r_{k-1}^{[\nu]}(z)|\leqq\varepsilon|r_{k-1}^{[\nu+5]}(z)|$ for all $k=0,1,2,\cdots,n$. Thereafter, (4.4) is applied, with $r_{k-1}(z)$ approximated by $r_{k-1}^{[\nu+5]}(z)$ for the final index ν. The computation of $\pi_n(z)$ proceeds directly from (4.2), applied for $k=0,1,\cdots,n-1$, with $y_{-1}=0$, $y_0=1$.

In the important special case of the Jacobi weight function $w(t)=(1-t)^\alpha(1+t)^\beta$, $\alpha>-1$, $\beta>-1$, the iteration on the index ν in (4.3) can be dispensed with. An appropriate value for ν, when $z=\pm r$, $r>1$, is indeed known to be [5, Eq. (5.6′)], independently of α and β, the smallest integer ν satisfying

$$\nu\geqq n+\frac{\ln(1/\varepsilon)}{2\ln(r+\sqrt{r^2-1})}. \tag{4.5}$$

In this case, the computation of $\rho_n(z)$ by (4.3), (4.4) is particularly efficient, even for $z=\pm r$ relatively close to the interval $[-1,1]$. Some numerical values of ν/n in the case $\varepsilon=.5\times10^{-5}$ are shown in Table 4.1.

TABLE 4.1
Numerical values of ν/n for $\varepsilon = .5\times10^{-5}$, where ν is the smallest integer satisfying (4.5).

r	$n=10$	$n=20$	$n=40$	$n=80$
1.01	5.4	3.20	2.100	1.5500
1.05	3.0	2.00	1.500	1.2500
1.10	2.4	1.70	1.350	1.1750
1.50	1.7	1.35	1.175	1.0875
2.00	1.5	1.25	1.125	1.0625
5.00	1.3	1.15	1.075	1.0375

Doubling the accuracy to $\varepsilon = .25\times10^{-10}$ has the effect, essentially, of doubling $(\nu/n)-1$, as can be seen from (4.5). For the purpose of error estimation, however, five decimal digits are more than enough.

We stress the fact that the algorithm (4.3), (4.4) is valid for arbitrary complex $z\notin[-1,1]$. The estimate for ν in (4.5), when $d\lambda$ is the Jacobi measure, however, becomes a bit more complicated. We now have to take the smallest integer satisfying [5, Eq. (5.6)]

$$\nu \geqq n+\frac{\ln(1/\varepsilon)}{2\ln|z+(z-1)^{1/2}(z+1)^{1/2}|}, \tag{4.6}$$

where the principal values of $\arg(z-1)$ and $\arg(z+1)$ are to be used in evaluating the square roots. If $z=iy$ is purely imaginary, (4.6) reduces to

$$\nu \geqq n+\frac{\ln(1/\varepsilon)}{2\ln(y+\sqrt{1+y^2})}. \tag{4.7}$$

In particular, the algorithm (4.3), (4.4) may also be used to compute the numerators of $K_n(p_i)=\rho_n(p_i)/\pi_n(p_i)$ in (3.5) and of $K_n(i\omega)=\rho_n(i\omega)/\pi_n(i\omega)$ in (3.8). The denominators can be computed directly from the recursion (4.2).

5. The maximum of the kernel K_n on an ellipse and corresponding error bounds. Another frequent choice of the contour Γ is an ellipse $\mathscr{E}_\rho=\{z: z=\frac{1}{2}(u+u^{-1}), u=\rho e^{i\vartheta}, 0\leqq\vartheta\leqq2\pi\}$ with foci at $z=\pm1$ and sum of semiaxes equal to ρ, $\rho>1$. As $\rho\downarrow1$, the ellipse $\mathscr{E}_\rho$ shrinks to the interval $[-1,1]$, while with increasing ρ it becomes more and more circle-like. Since

$$\frac{1}{z-t}=\frac{2}{u}\frac{1}{u^{-2}-2tu^{-1}+1}=2\sum_{k=0}^{\infty}\frac{U_k(t)}{u^{k+1}},$$

where U_k denotes the Chebyshev polynomial of the second kind, the expansion analogous to (3.2) now reads

$$K_n(z)=2\sum_{k=2n}^{\infty}\frac{R_n(U_k)}{u^{k+1}}, \qquad z=\frac{1}{2}\left(u+\frac{1}{u}\right). \tag{5.1}$$

One has symmetry with respect to the real axis, i.e., $|K_n(\bar z)|=|K_n(z)|$, but the maximum of $|K_n(z)|$, $z\in\mathscr{E}_\rho$, is no longer always attained on the real axis.

The case of the Jacobi weight function $w(t)=(1-t)^\alpha(1+t)^\beta$, $\alpha>-1$, $\beta>-1$, is of sufficient interest to be considered in some detail, although precise results are difficult to obtain for general parameter values. Note, however, that the known identity for Jacobi polynomials, $\pi_n^{(\beta,\alpha)}(z)=(-1)^n\pi_n^{(\alpha,\beta)}(-z)$, implies $|K_n^{(\beta,\alpha)}(z)|=|K_n^{(\alpha,\beta)}(-z)|=|K_n^{(\alpha,\beta)}(-\bar{z})|$, so that an interchange of the parameters amounts to a reflection in the complex plane with respect to the imaginary axis. It suffices therefore to consider $\alpha \leqq \beta$.

5.1. Chebyshev measures of the first and second kind. Let first $\alpha=\beta=-\frac{1}{2}$, that is, $d\lambda(t)=(1-t^2)^{-1/2}\,dt$, the orthogonal polynomials thus being the Chebyshev polynomials T_k of the first kind. From the well-known formula

$$T_n(z)=\tfrac{1}{2}[(z+\sqrt{z^2-1})^n+(z-\sqrt{z^2-1})^n], \tag{5.2}$$

putting $z=\frac{1}{2}(u+u^{-1})$, one gets

$$T_n(z)=\tfrac{1}{2}(u^n+u^{-n}), \qquad z=\tfrac{1}{2}(u+u^{-1}).$$

Furthermore, using [9, Eq. 3.613.1], one finds

$$\int_{-1}^{1}\frac{T_n(t)}{z-t}(1-t^2)^{-1/2}\,dt=\int_0^{\pi}\frac{\cos n\vartheta}{z-\cos\vartheta}\,d\vartheta=\frac{\pi}{\sqrt{z^2-1}}(z-\sqrt{z^2-1})^n, \tag{5.3}$$

hence

$$\int_{-1}^{1}\frac{T_n(t)}{z-t}(1-t^2)^{-1/2}\,dt=\frac{2\pi}{(u-u^{-1})u^n}, \qquad z=\frac{1}{2}(u+u^{-1}).$$

It follows that

$$\frac{\rho_n(z)}{\pi_n(z)}=\frac{4\pi}{(u-u^{-1})u^n(u^n+u^{-n})}, \qquad z=\frac{1}{2}(u+u^{-1}),$$

from which, in particular,

$$\begin{aligned}&|K_n(z)|=\frac{2\pi}{\rho^n}\{[a_2(\rho)-\cos 2\vartheta][a_{2n}(\rho)+\cos 2n\vartheta]\}^{-1/2},\\ &z=\tfrac{1}{2}(\rho\, e^{i\vartheta}+\rho^{-1}\,e^{-i\vartheta})\in\mathscr{E}_\rho,\end{aligned} \tag{5.4}$$

where

$$a_j(\rho)=\tfrac{1}{2}(\rho^j+\rho^{-j}), \qquad j=1,2,3,\cdots, \quad \rho>1. \tag{5.5}$$

LEMMA 5.1. *The functions in* (5.5) *satisfy*

$$\frac{a_{2n}(\rho)-1}{a_2(\rho)-1}\geqq n^2, \qquad n=1,2,3,\cdots, \quad \rho>1. \tag{5.6}$$

Proof. Multiplying numerator and denominator in (5.6) by $2\rho^{2n}$, and using (5.5), one gets

$$\frac{a_{2n}(\rho)-1}{a_2(\rho)-1}=\frac{\rho^{4n}+1-2\rho^{2n}}{\rho^{2(n-1)}(\rho^4+1-2\rho^2)}=\left\{\frac{\rho^{2n}-1}{\rho^{n-1}(\rho^2-1)}\right\}^2.$$

Observe that

$$\begin{aligned}\rho^{-(n-1)}\frac{\rho^{2n}-1}{\rho^2-1}&=\rho^{-(n-1)}[\rho^{2(n-1)}+\rho^{2(n-2)}+\cdots+1]\\&=\rho^{n-1}+\rho^{n-3}+\cdots+\rho^{-(n-3)}+\rho^{-(n-1)}.\end{aligned}$$

Since $x+x^{-1}>2$ for any $x>1$, the sum on the right is larger than $2(n/2)=n$ if n is even, and larger than $2[(n-1)/2]+1=n$ if $n \geqq 3$ is odd, hence $>n$ for any integer $n \geqq 2$, proving (5.6) with strict inequality for $n \geqq 2$. If $n=1$, (5.6) is an equality. □

THEOREM 5.1. *If* $d\lambda(t)=(1-t^2)^{-1/2}\,dt$ *on* $(-1,1)$, *then*

$$\max_{z\in\mathscr{E}_\rho} |K_n(z)| = K_n(\tfrac{1}{2}(\rho+\rho^{-1})), \tag{5.7}$$

i.e., the maximum of $|K_n(z)|$ *on* $\mathscr{E}_\rho$ *is attained on the real axis.*

Proof. By (5.4) it suffices to prove

$$(a_2-\cos 2\vartheta)(a_{2n}+\cos 2n\vartheta) \geqq (a_2-1)(a_{2n}+1), \qquad 0 \leqq \vartheta \leqq \pi/2,$$

where $a_j=a_j(\rho)$ is given by (5.5). This is equivalent to

$$(1-\cos 2\vartheta)a_{2n}-(1-\cos 2n\vartheta)a_2+1-\cos 2\vartheta\cos 2n\vartheta \geqq 0,$$

or, introducing half angles, to

$$a_{2n}+1-(a_2-1)\frac{\sin^2 n\vartheta}{\sin^2\vartheta}-2\sin^2 n\vartheta \geqq 0, \tag{5.8}$$

if $\vartheta>0$. Since

$$\left|\frac{\sin n\vartheta}{\sin\vartheta}\right| = |U_{n-1}(\cos\vartheta)| \leqq n,$$

the left-hand side of (5.8) is larger than or equal to

$$a_{2n}+1-n^2(a_2-1)-2=(a_2-1)\left\{\frac{a_{2n}-1}{a_2-1}-n^2\right\},$$

which is nonnegative by Lemma 5.1. □

For the Chebyshev measure of the second kind, $d\lambda(t)=(1-t^2)^{1/2}\,dt$, the nth degree orthogonal polynomial is

$$U_n(z)=\frac{1}{2\sqrt{z^2-1}}[(z+\sqrt{z^2-1})^{n+1}-(z-\sqrt{z^2-1})^{n+1}],$$

which yields

$$U_n(z)=\frac{u^{n+1}-u^{-(n+1)}}{u-u^{-1}}, \qquad z=\frac{1}{2}(u+u^{-1}),$$

while (cf. [9, Eq. 3.613.3])

$$\int_{-1}^{1}\frac{U_n(t)}{z-t}(1-t^2)^{1/2}\,dt=\int_0^\pi \frac{\sin(n+1)\vartheta\,\sin\vartheta}{z-\cos\vartheta}\,d\vartheta=\frac{\pi}{u^{n+1}},$$

$$z=\frac{1}{2}(u+u^{-1}).$$

Therefore,

$$|K_n(z)|=\frac{\pi}{\rho^{n+1}}\left\{\frac{a_2(\rho)-\cos 2\vartheta}{a_{2n+2}(\rho)-\cos 2(n+1)\vartheta}\right\}^{1/2},$$

$$z=\tfrac{1}{2}(\rho e^{i\vartheta}+\rho^{-1}e^{-i\vartheta})\in\mathscr{E}_\rho. \tag{5.9}$$

THEOREM 5.2. *If* $d\lambda(t)=(1-t^2)^{1/2}\,dt$ *on* $(-1,1)$, *and* n *is odd, then*

$$\max_{z\in\mathscr{E}_\rho}|K_n(z)|=\left|K_n\left(\frac{i}{2}(\rho-\rho^{-1})\right)\right|, \tag{5.10}$$

i.e., the maximum of $|K_n(z)|$ (n *odd*) *on* $\mathscr{E}_\rho$ *is attained on the imaginary axis.*

Proof. It is obvious that

$$\frac{a_2-\cos 2\vartheta}{a_{2n+2}-\cos 2(n+1)\vartheta}\le\frac{a_2+1}{a_{2n+2}-1},\quad \text{for all } \vartheta, \text{ all } n,$$

with equality holding when $\vartheta=\pi/2$ and n is odd. With (5.9), this gives the desired result. □

If, in Theorem 5.2, n is even, computation shows that the maximum of $|K_n(z)|$ on $\mathscr{E}_\rho$ is attained slightly off the imaginary axis.

5.2. Jacobi measure with $\alpha=-\frac{1}{2}$ and $\beta=\frac{1}{2}$. The orthogonal polynomials in this case are those with respect to $d\lambda(t)=\sqrt{(1+t)/(1-t)}\,dt$, and are given by

$$p_n(z)=\frac{T_{2n+1}(\sqrt{\frac{1}{2}(z+1)})}{\sqrt{\frac{1}{2}(z+1)}},$$

where T_{2n+1} is the Chebyshev polynomial of degree $2n+1$. With $z=\frac{1}{2}(u+u^{-1})$, so that $\sqrt{\frac{1}{2}(z+1)}=(u+1)/(2\sqrt{u})$, we find by (5.2), after a little computation,

$$p_n(z)=\frac{u^{n+1}+u^{-n}}{u+1},\qquad z=\frac{1}{2}(u+u^{-1}).$$

Furthermore,

$$\int_{-1}^{1}\frac{p_n(t)}{z-t}\sqrt{\frac{1+t}{1-t}}\,dt=\int_0^\pi\frac{2\cos(2n+1)\vartheta/2\cos\vartheta/2}{z-\cos\vartheta}\,d\vartheta$$
$$=\int_0^\pi\frac{\cos(n+1)\vartheta+\cos n\vartheta}{z-\cos\vartheta}\,d\vartheta,$$

hence, using (5.3),

$$\int_{-1}^{1}\frac{p_n(t)}{z-t}\sqrt{\frac{1+t}{1-t}}\,dt=\frac{2\pi(u+1)}{(u-u^{-1})u^{n+1}},\qquad z=\frac{1}{2}(u+u^{-1}).$$

There follows

$$\frac{\rho_n(z)}{\pi_n(z)}=\frac{2\pi(u+1)^2}{(u-u^{-1})u^{n+1}(u^{n+1}+u^{-n})},$$

and, by an elementary computation,

$$|K_n(z)|=\frac{2\pi}{\rho^{n+1/2}}\frac{a_1(\rho)+\cos\vartheta}{\{[a_2(\rho)-\cos 2\vartheta][a_{2n+1}(\rho)+\cos(2n+1)\vartheta]\}^{1/2}}, \tag{5.11}$$
$$z=\frac{1}{2}(\rho e^{i\vartheta}+\rho^{-1}e^{-i\vartheta})\in\mathscr{E}_\rho,$$

where $a_j(\rho)$ is again given by (5.5).

LEMMA 5.2. *There holds*

$$\frac{a_1(\rho)a_{2n+1}(\rho)-1}{a_2(\rho)-1}>\left(n+\frac{1}{2}\right)^2,\qquad n=1,2,3,\cdots,\quad \rho>1. \tag{5.12}$$

Proof. A simple computation based on the definition (5.5) of $a_j(\rho)$ yields

$$\frac{a_1(\rho)a_{2n+1}(\rho)-1}{a_2(\rho)-1}=\frac{1}{2}\left\{\frac{\rho^{2n+2}-1}{\rho^n(\rho^2-1)}\right\}^2+\frac{1}{2}\left\{\frac{\rho^{2n}-1}{\rho^{n-1}(\rho^2-1)}\right\}^2.$$

Applying to each of the two squares on the right the reasoning used in the proof of Lemma 5.1 produces the lower bound $\frac{1}{2}[(n+1)^2+n^2]=n^2+n+\frac{1}{2}>n^2+n+\frac{1}{4}=(n+\frac{1}{2})^2$. □

THEOREM 5.3. *If* $d\lambda(t)=\sqrt{(1+t)/(1-t)}\,dt$ *on* $(-1,1)$, *then*

$$\max_{z\in\mathscr{E}_\rho}|K_n(z)|=K_n(\tfrac{1}{2}(\rho+\rho^{-1})), \tag{5.13}$$

i.e., the maximum of $|K_n(z)|$ *on* $\mathscr{E}_\rho$ *is attained on the positive real axis.*

Proof. We shall show that the expression on the right of (5.11), considered as a function of ϑ on $[0,\pi]$, attains its maximum only at $\vartheta=0$. Using

$$a_2(\rho)=2[a_1(\rho)]^2-1,$$

we can write this assertion in the form

$$\frac{a_1+\cos\vartheta}{(a_1-\cos\vartheta)(a_{2n+1}+\cos(2n+1)\vartheta)}<\frac{a_1+1}{(a_1-1)(a_{2n+1}+1)},\qquad 0<\vartheta\leqq\pi,$$

where $a_j=a_j(\rho)$. Clearing the denominators, and multiplying out everything, produces an aggregate of terms that can be combined to suggest the introduction of half angles, and then yields the equivalent inequality

$$\frac{a_1(a_{2n+1}+1)}{a_1+1}-\frac{1}{2}(a_1-1)\frac{\sin^2((2n+1)\vartheta/2)}{\sin^2(\vartheta/2)}-\sin^2(2n+1)\frac{\vartheta}{2}>0.$$

Now the left-hand side is larger than or equal to

$$\frac{a_1(a_{2n+1}+1)}{a_1+1}-\frac{1}{2}(a_1-1)(2n+1)^2-1=2(a_1-1)\left\{\frac{a_1a_{2n+1}-1}{a_2-1}-\left(n+\frac{1}{2}\right)^2\right\},$$

which is strictly positive by Lemma 5.2. □

5.3. Gegenbauer measure. In the case $\alpha=\beta$ we have only empirical results based on computation. These seem to indicate the following. If $-1<\alpha\leqq-\frac{1}{2}$, we have the behavior exhibited by the Chebyshev polynomials of the first kind: The maximum of $|K_n^{(\alpha,\alpha)}(z)|$ on $\mathscr{E}_\rho$ is attained on the real axis, i.e., we have (5.7). If $-\frac{1}{2}<\alpha<0$, the maximum is attained on the imaginary axis if $n=1$; as n becomes larger, the maximum point moves along $\mathscr{E}_\rho$ to the real axis, more rapidly so, the larger ρ is. If $0\leqq\alpha$, the maximum is attained on the imaginary axis, except when n is even and ρ not too large, in which case it is assumed slightly off the imaginary axis. Thus, the Chebyshev polynomials of the second kind (cf. Theorem 5.2) are a prototype for the case $\alpha\geqq0$.

Another interesting empirical observation is the apparent monotonic decrease of $\max_{z\in\mathscr{E}_\rho}|K_n^{(\alpha,\alpha)}(z)|$ as a function of α, $\alpha>-1$, for fixed ρ and n.

5.4. General Jacobi measure. For arbitrary $-1<\alpha<\beta$ we again have only empirical information, the extent of computational experimentation being of necessity more limited. What appears to be happening, nevertheless, is the following: For all $-1<\alpha\leqq-\frac{1}{2}$, $\alpha<\beta$, we have (5.7), i.e., the maximum occurs on the positive real axis. For $-\frac{1}{2}<\alpha<\beta$, the maximum point for $|K_n^{(\alpha,\beta)}(z)|$ on $\mathscr{E}_\rho$ is located to the right of the imaginary axis and is moving toward the positive real axis as both ρ and n increase.

As a practical matter, it was determined that a generally good *estimate* of the maximum of $|K_n^{(\alpha,\beta)}(z)|$ on $\mathscr{E}_\rho$ can be found as follows, if $\alpha \leqq \beta$:

$$\max_{z\in\mathscr{E}_\rho} |K_n^{(\alpha,\beta)}(z)| \approx \begin{cases} K_n^{(\alpha,\beta)}(\tfrac{1}{2}(\rho+\rho^{-1})), & \text{if } -1<\alpha\leqq -\tfrac{1}{2}, \\ \max\left\{K_n^{(\alpha,\beta)}(\tfrac{1}{2}(\rho+\rho^{-1})), \left|K_n^{(\alpha,\beta)}\left(\frac{i}{2}(\rho-\rho^{-1})\right)\right|\right\}, & \text{otherwise.} \end{cases} \tag{5.14}$$

If $\alpha>\beta$, the estimate (5.14), by symmetry, continues to hold if $K_n^{(\alpha,\beta)}(\frac{1}{2}(\rho+\rho^{-1}))$ is replaced by $|K_n^{(\alpha,\beta)}(-\frac{1}{2}(\rho+\rho^{-1}))|$. The value of the kernel $K_n^{(\alpha,\beta)}(z)$ on the imaginary axis, $z=iy$, $y>0$, can be computed to a relative accuracy of ε as in (4.3), (4.4), where $z=iy$, and where ν may be taken to be the smallest integer satisfying (4.7).

5.5. Error bound. To obtain the error bound in final form, assume, for definiteness, that (5.7) holds. Since the ellipse $\mathscr{E}_\rho$ has length $l(\mathscr{E}_\rho)=4\varepsilon^{-1}E(\varepsilon)$, where

$$\varepsilon=\frac{2}{\rho+\rho^{-1}} \tag{5.15}$$

is the eccentricity of $\mathscr{E}_\rho$ and

$$E(\varepsilon)=\int_0^{\pi/2}\sqrt{1-\varepsilon^2\sin^2\vartheta}\,d\vartheta \tag{5.16}$$

the complete elliptic integral of the second kind, we obtain from (1.6)

$$|R_n(f)|\leqq\frac{2}{\pi}\varepsilon^{-1}E(\varepsilon)\cdot K_n(\varepsilon^{-1})\cdot\max_{z\in\mathscr{E}_\rho}|f(z)|, \qquad \varepsilon=\frac{2}{\rho+\rho^{-1}}. \tag{5.17}$$

Again it is possible to optimize the bound on the right as a function of ρ. Also, the bound (5.17) can be used in connection with the modified quadrature rule (3.5) if $\mathscr{E}_\rho$ contains all the poles p_i.

6. Examples.

Example 6.1.

$$\int_{-1}^{1}\frac{\cos[\omega(t+1)]}{\sqrt{(3+t)(1-t)}}\,dt=\frac{\pi}{2}J_0(2\omega), \qquad \omega>0.$$

We take for $d\lambda$ the Jacobi measure $d\lambda(t)=(1-t)^{-1/2}\,dt$ with parameters $\alpha=-\frac{1}{2}$, $\beta=0$. Accordingly,

$$f(z)=\frac{\cos[\omega(z+1)]}{\sqrt{3+z}}, \tag{6.1}$$

the square root being understood in the sense of the principal value. We first illustrate the error bounds based on circular contours.

The singularity closest to the origin is the branch point at $z=-3$; hence all circles C_r with $1<r<3$ are admissible. To bound f on C_r, we note

$$|\cos[\omega(z+1)]|=\tfrac{1}{2}|e^{-\omega y}e^{i\omega(x+1)}+e^{\omega y}e^{-i\omega(x+1)}|$$
$$\leqq\tfrac{1}{2}(e^{-\omega y}+e^{\omega y}), \qquad z=x+iy,$$

and

$$|\sqrt{3+z}|=\sqrt{|3+z|}\geqq\sqrt{3-|z|},$$

so that

$$|f(z)| \leqq \frac{\cosh(\omega r)}{\sqrt{3-r}}, \qquad z \in C_r. \tag{6.2}$$

Since we are in the first case of Theorem 3.1, we obtain, according to (3.4),

$$|R_n(f)| \leqq r \cdot K_n(r) \cdot \frac{\cosh(\omega r)}{\sqrt{3-r}}, \qquad 1 < r < 3. \tag{6.3}$$

The bound on the right of (6.3) may be optimized as a function of r by using a simple dichotomous search procedure in combination with the recursive algorithm (4.3)–(4.5) for evaluating $K_n(r)$. A few optimal values r_{opt} of r thus computed, and corresponding optimal bounds, are shown in Table 6.1, together with the modulus of

TABLE 6.1
Optimal error bound (6.3) *and actual error.*

ω	n	r_{opt}	bound	error	ω	n	r_{opt}	bound	error
.5	5	2.853	1.19 (−6)	3.93 (−9)	8.0	5	1.628	3.29 (1)	1.05 (−1)
	10	2.928	3.83 (−14)	6.73 (−17)		10	2.481	4.90 (−5)	3.01 (−7)
	15	2.952	1.05 (−21)	1.25 (−24)		15	2.851	3.19 (−12)	3.50 (−15)
	20	2.964	2.68 (−29)	m.p.		20	2.925	1.03 (−19)	1.27 (−24)
1.0	5	2.828	4.69 (−6)	4.36 (−9)		25	2.951	2.83 (−27)	m.p.
	10	2.922	1.57 (−13)	6.33 (−17)	16.0	5	1.224	1.94 (6)	3.82 (−1)
	15	2.950	4.36 (−21)	1.10 (−24)		10	1.615	3.41 (2)	3.10 (−2)
	20	2.963	1.13 (−28)	m.p.		15	2.095	1.69 (−3)	9.38 (−7)
2.0	5	2.752	7.63 (−5)	3.88 (−7)		20	2.558	5.78 (−10)	5.22 (−13)
	10	2.908	2.89 (−12)	7.04 (−17)		25	2.832	3.70 (−17)	1.90 (−20)
	15	2.944	8.28 (−20)	1.38 (−24)		30	2.917	1.25 (−24)	3.64 (−27)
	20	2.960	2.17 (−27)	2.27 (−28)	32.0	5	1.074	1.33 (14)	5.21 (−1)
4.0	5	2.380	1.37 (−2)	7.69 (−5)		10	1.203	8.56 (11)	1.63 (−1)
	10	2.860	9.32 (−10)	5.98 (−14)		20	1.608	3.62 (4)	2.14 (−3)
	15	2.929	2.94 (−17)	4.92 (−25)		30	2.109	8.57 (−7)	3.05 (−12)
	20	2.952	8.02 (−25)	2.35 (−27)		40	2.612	7.48 (−20)	1.21 (−24)

the actual errors. (Numbers in parentheses indicate decimal exponents. Close to machine precision, the actual error may be larger than the bound; this is indicated by "m.p." for "machine precision".) The actual error was computed in double precision on the CDC 6500 computer (machine precision of approx. 29 decimal digits), using software for Gaussian quadrature rules currently under development and a well-known recursive procedure (see, e.g., [3]) for evaluating the Bessel function J_0.

Several interesting features are worth noting: The optimal radius r_{opt} increases with n, approaching the radius of convergence $r = 3$ rather quickly when ω is small or moderately large. This is so, presumably, because of the "weak" nature of the singularity. Increasing ω, on the other hand, has the effect of reducing r_{opt}. The bounds are seen to overestimate the error by several orders of magnitude, becoming ludicrously large when ω is large and n relatively small. The latter is caused by the highly oscillatory behavior of f on the circle C_r. The use of ellipses, snuggling closely around the interval $[-1, 1]$, improves the matter considerably; see Table 6.3. While it is true that the bounds are excessively conservative, it must also be noted that the actual errors decrease rapidly with increasing n. Using the bounds to estimate not the error, but the appropriate value of n to be used, yields an overestimation of n by only a few units (1–2 in most cases, as was determined by additional computation). In this sense, therefore, the bounds obtained are not without practical interest.

For purposes of reference, we list the true values of the integral (to 27 decimals) in Table 6.2.

TABLE 6.2
True values of the integral in Example 6.1.

ω	$(\pi/2)J_0(2\omega)$
.5	1.20196 97153 17206 49913 66624 46
1.0	.35168 68134 78300 44589 24008 93
2.0	−.62384 14625 21423 05380 16654 91
4.0	.26962 84573 43048 89859 64559 11
8.0	−.27473 08229 73313 59029 11052 65
16.0	.21689 40013 17366 77422 90002 39
32.0	.14544 00510 86862 98391 53851 72

Using elliptic contours, we have in place of (6.2),

$$|f(z)| \leqq \frac{\cosh\left(\frac{1}{2}\omega(\rho-\rho^{-1})\right)}{\sqrt{3-\frac{1}{2}(\rho+\rho^{-1})}}, \qquad z \in \mathscr{E}_\rho. \tag{6.4}$$

The empirical information mentioned in § 5.4 suggests the use of (5.17), giving

$$|R_n(f)| \leqq \frac{2}{\pi}\varepsilon^{-1}E(\varepsilon)\cdot K_n(\varepsilon^{-1})\cdot\frac{\cosh\left(\frac{1}{2}\omega(\rho-\rho^{-1})\right)}{\sqrt{3-\varepsilon^{-1}}}, \tag{6.5}$$
$$\varepsilon = 2/(\rho+\rho^{-1}), \quad 1<\rho<3+\sqrt{8}=5.828\cdots.$$

We have also optimized this bound as a function of ρ, using the polynomial approximations in [2] to evaluate $E(\varepsilon)$. The results are similar to those in Table 6.1, for relatively small ω, with the bounds being consistently somewhat smaller. The improvement becomes more pronounced with increasing ω, and is quite dramatic for $\omega = 16$ and $\omega = 32$, as is shown in Table 6.3.

TABLE 6.3
Optimal error bound (6.5) *and actual error.*

ω	n	ρ_{opt}	bound	error
16.0	5	1.138	2.64 (1)	3.82 (−1)
	10	2.116	5.15 (−1)	3.10 (−2)
	15	3.425	2.05 (−5)	9.38 (−7)
	20	4.589	1.91 (−11)	5.22 (−13)
	25	5.367	1.88 (−18)	1.90 (−20)
	30	5.625	7.11 (−26)	3.64 (−27)
32.0	5	1.046	7.65 (1)	5.21 (−1)
	10	1.068	5.28 (1)	1.63 (−1)
	20	2.063	8.09 (−2)	2.14 (−3)
	30	3.442	1.44 (−10)	3.05 (−12)
	40	4.678	9.87 (−23)	1.21 (−24)

Example 6.2.

$$I(\omega)=\int_{-1}^{1}\frac{e^{-t}}{t^2+\omega^2}\,dt, \qquad \omega>0.$$

The integral could be expressed in terms of the complex exponential integral $E_1(z)$ as

$$I(\omega)=\frac{1}{\omega}\{\mathrm{Im}\,[e^{i\omega}E_1(1+i\omega)]-\mathrm{Im}\,[e^{i\omega}E_1(-1+i\omega)]\}$$

(cf. [8, Eq. 5.1.43]). However, it is much simpler to evaluate it by the modified Gauss–Legendre quadrature rule (3.8) (where $g(t)=e^{-t}$).

We illustrate the use of ordinary Gaussian quadrature (i.e., without separating out the poles $\pm i\omega$), and compare error bounds based on circular and elliptic contours.

Circular contours C_r can be used only if $\omega>1$ and require $1<r<\omega$. If we take $d\lambda(t)=dt$, hence

$$f(z)=\frac{e^{-z}}{z^2+\omega^2},$$

we find

$$|f(z)|=\frac{e^{-r\cos\vartheta}}{\{(r^2\cos 2\vartheta+\omega^2)^2+r^4\sin^2 2\vartheta\}^{1/2}}, \qquad z=re^{i\vartheta}\in C_r.$$

An elementary calculation shows that the denominator attains its minimum at $\vartheta=\pi/2$, so that

$$|f(z)|\leqq\frac{e^r}{\omega^2-r^2}, \qquad z\in C_r, \quad 1<r<\omega, \quad d\lambda(t)=dt. \tag{6.6}$$

We will also consider $d\lambda(t)=e^{-t}\,dt$ on $[-1,1]$, a measure for which part (b) of Theorem 2.1, hence the second statement in (3.1), is applicable. In this case

$$f(z)=\frac{1}{z^2+\omega^2},$$

and (6.6) is to be replaced by

$$|f(z)|\leqq\frac{1}{\omega^2-r^2}, \qquad z\in C_r, \quad 1<r<\omega, \quad d\lambda(t)=e^{-t}\,dt. \tag{6.7}$$

If ω and r are large, one expects the error bound based on (1.6) and (3.1) to be more realistic in the case $d\lambda(t)=e^{-t}\,dt$ than in the case $d\lambda(t)=dt$, on account of the absence of the exponential e^r in the bound of (6.7). Some selected numerical examples of error bounds that result from (1.6), (3.1) and (6.6), (6.7), after optimization in r, are shown in Table 6.4, together with the true errors. The true values of the integral were computed by the modified Gauss–Legendre formula (3.8), which converges quite rapidly, even for very small values of ω. We quote as typical the error bounds 1.59(−3), 5.45(−11), 3.11(−26) for $n=2$, 5 and 10, respectively, with associated optimal radii 6.066, 12.038, 22.022, which hold when $\omega=.1$. Some reference values for the integral $I(\omega)$ are given in Table 6.5.

Before turning to error bounds based on elliptic contours, we digress briefly to explain how the Gauss formulae with measure $d\lambda(t)=e^{-t}\,dt$ on $[-1,1]$ were obtained.

TABLE 6.4
Optimal error bounds for Example 6.2, based on circular contours, and actual errors.

ω	n	$d\lambda(t)=dt$ r_{opt}	bound	$d\lambda(t)=e^{-t}\,dt$ r_{opt}	bound	error
1.6	5	1.414	3.20 (−3)	1.498	1.06 (−3)	1.19 (−7)
	10	1.540	1.86 (−7)	1.544	5.76 (−8)	4.57 (−13)
	15	1.559	7.99 (−12)	1.561	2.41 (−12)	1.73 (−18)
	20	1.569	3.04 (−16)	1.570	9.06 (−17)	6.54 (−24)
3.2	5	2.858	9.63 (−7)	2.941	6.32 (−8)	1.97 (−9)
	10	3.037	2.43 (−14)	3.060	1.37 (−15)	1.37 (−17)
	15	3.094	4.26 (−22)	3.104	2.26 (−23)	9.47 (−26)
6.4	5	5.379	2.87 (−9)	5.854	1.10 (−11)	4.45 (−12)
	10	5.995	7.54 (−20)	6.107	1.92 (−22)	4.70 (−24)

TABLE 6.5
True values of the integral in Example 6.2.

ω	$I(\omega)$
.1	30.30306 13396 82348 89801 1277
.2	14.48521 60752 92332 62573 9000
.4	6.49657 69543 56769 22643 33955
.8	2.53625 92876 02957 26987 44666
1.6	.80972 41454 64440 32089 68500 1
3.2	.22163 00516 42300 12649 17735 9
6.4	.05686 69117 77072 55597 11571 19

We found it expedient to employ the modified Chebyshev algorithm [6, § 2.4] to generate the recursion coefficients for the required orthogonal polynomials from "modified moments". For the latter we chose Legendre moments,

$$\int_{-1}^{1} P_n(t)\,e^{-t}\,dt=\sqrt{2\pi}\,i^{n-1/2}J_{n+1/2}(i),\qquad n=0,1,2,\cdots \tag{6.8}$$

(cf. [9, Eq. 7.321]), where P_n is the Legendre polynomial. (Actually, they have to be normalized to correspond to the monic Legendre polynomials, which requires division by $k_n=(2n)!/(2^n n!^2)$.) Being expressible in terms of Bessel functions, these moments can be readily computed as minimal solution of the recurrence relation

$$y_{n+1}-(2n+1)y_n-y_{n-1}=0,\qquad n=1,2,3,\cdots, \tag{6.9}$$

especially since the initial value is simply

$$y_0=e-e^{-1}. \tag{6.10}$$

Once the recursion coefficients for the orthogonal polynomials $\pi_n(\cdot\,;e^{-t}\,dt)$ are found, the corresponding Gauss formulae can be obtained from the associated Jacobi matrix by well-known procedures (cf., e.g., [4, § 5.1]).

Returning now to elliptic contours $\mathscr{E}_\rho$, where ρ is to be constrained by $1<\rho<\omega+\sqrt{\omega^2+1}$, we have in place of (6.6),

$$|f(z)|\le\frac{\exp\left(-\frac{1}{2}(\rho+\rho^{-1})\cos\vartheta\right)}{\{[\frac{1}{4}(\rho^2+\rho^{-2})\cos 2\vartheta+\omega^2+\frac{1}{2}]^2+\frac{1}{16}(\rho^2-\rho^{-2})^2\sin^2 2\vartheta\}^{1/2}},$$
$$z=\tfrac{1}{2}(\rho\,e^{i\vartheta}+\rho^{-1}e^{-i\vartheta})\in\mathscr{E}_\rho,\qquad d\lambda(t)=dt. \tag{6.11}$$

The derivative with respect to ϑ of the radicand in the denominator of (6.11) computes to

$$-\sin 2\vartheta\{\cos 2\vartheta + (\rho^2+\rho^{-2})(\omega^2+\tfrac{1}{2})\},$$

and hence can only vanish at $\vartheta = 0$ and $\vartheta = \pi/2$ (modulo π). The value of the radicand at $\vartheta = \pi/2$ is clearly the smaller of the two, so that

$$(6.12)\qquad |f(z)| \leq \frac{\exp(\frac{1}{2}(\rho+\rho^{-1}))}{\omega^2+\frac{1}{2}-\frac{1}{4}(\rho^2+\rho^{-2})}, \qquad z \in \mathscr{E}_\rho, \quad 1<\rho<\omega+\sqrt{\omega^2+1}, \quad d\lambda(t)=dt.$$

(The denominator in (6.12) is positive under the constraint imposed on ρ and ω.) A similar bound, without the exponential in the numerator, holds in the case $d\lambda(t) = e^{-t}\,dt$. Neither in the case $d\lambda(t) = dt$, nor in the case $d\lambda(t) = e^{-t}\,dt$ do we have any theoretical basis upon which to evaluate $\max_{z\in\mathscr{E}_\rho} |K_n(z)|$. Nevertheless, empirical work alluded to in § 5.3 suggests the use of the approximation $\max_{z\in\mathscr{E}_\rho}|K_n(z)| \approx |K_n((i/2)(\rho-\rho^{-1}))|$ in the case $d\lambda(t) = dt$. When $d\lambda(t) = e^{-t}\,dt$ on $[-1, 1]$, it was found

TABLE 6.6

Optimal error bounds for Example 6.2, based on elliptic contours, and actual errors.

		$d\lambda(t)=dt$		$d\lambda(t)=e^{-t}dt$		
ω	n	ρ_{opt}	bound	ρ_{opt}	bound	error
.1	5	1.066	1.81 (3)	1.052	6.23 (2)	3.11 (1)
	10	1.056	3.77 (2)	1.065	3.45 (2)	6.83 (0)
	15	1.078	2.74 (2)	1.074	1.83 (2)	2.96 (0)
	20	1.081	1.11 (2)	1.081	9.00 (1)	1.02 (0)
	40	1.092	3.98 (0)	1.092	3.39 (0)	1.94 (−2)
	80	1.098	2.61 (−3)	1.098	2.30 (−3)	6.54 (−6)
.2	5	1.148	1.52 (2)	1.136	7.87 (1)	3.86 (0)
	10	1.167	2.70 (1)	1.169	2.04 (1)	4.65 (−1)
	15	1.184	5.53 (0)	1.184	4.20 (0)	6.50 (−2)
	20	1.192	9.82 (−1)	1.192	7.68 (−1)	8.90 (−3)
	40	1.205	6.71 (−4)	1.205	5.38(−4)	3.15 (−6)
	80	1.212	1.65 (−10)	1.212	1.34 (−10)	3.94 (−13)
.4	5	1.359	7.27 (0)	1.360	4.45 (0)	1.98 (−1)
	10	1.410	2.66 (−1)	1.412	1.76 (−1)	3.97 (−3)
	15	1.431	7.93 (−3)	1.432	5.27 (−3)	8.07 (−5)
	20	1.442	2.12 (−4)	1.443	1.41 (−4)	1.63 (−6)
	40	1.459	6.99 (−11)	1.459	4.68 (−11)	2.75 (−13)
	80	1.468	3.90 (−24)	1.468	2.61 (−24)	3.51 (−26)
.8	5	1.892	1.02 (−1)	1.909	4.85 (−2)	1.68 (−3)
	10	1.981	1.32 (−4)	1.987	6.16 (−5)	1.12 (−6)
	15	2.013	1.30 (−7)	2.016	5.99 (−8)	7.41 (−10)
	20	2.030	1.14 (−10)	2.031	5.22 (−11)	4.89 (−13)
	40	2.055	4.26 (−23)	2.055	1.93 (−23)	9.46 (−26)
1.6	5	3.142	3.22 (−4)	3.191	7.62 (−5)	1.19 (−7)
	10	3.313	2.53 (−9)	3.327	5.54 (−10)	4.57 (−13)
	15	3.370	1.45 (−14)	3.377	3.09 (−15)	1.73 (−18)
	20	3.400	7.33 (−20)	3.403	1.54 (−20)	6.54 (−24)
3.2	5	5.796	5.96 (−7)	5.990	3.38 (−8)	1.97 (−9)
	10	6.198	9.34 (−15)	6.250	4.49 (−16)	1.37 (−17)
	15	6.322	1.00 (−22)	6.346	4.57 (−24)	9.47 (−26)
6.4	5	10.773	2.62 (−9)	11.764	9.38 (−12)	4.45 (−12)
	10	12.047	6.16 (−20)	12.281	1.46 (−22)	4.70 (−24)

by computation that the maximum is attained close to, or on the negative real axis, thus suggesting the approximation $\max_{z\in\mathscr{E}_\rho}|K_n(z)|\approx|K_n(-\frac{1}{2}(\rho+\rho^{-1}))|$ in the case $d\lambda(t)=e^{-t}\,dt$. With these approximations replacing $K_n(\varepsilon^{-1})$ in (5.17), the error estimate (5.17), when optimized as a function of ρ, yields the bounds shown in Table 6.6. It can be seen that the bounds in the case $d\lambda(t)=e^{-t}\,dt$ are consistently better than those for $d\lambda(t)=dt$, appreciably so, if ω is large.

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