

# Error bounds for Gauss-Kronrod quadrature formulae of analytic functions\*

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**Summary.** We consider the Gauss-Kronrod quadrature formula for the Legendre weight function. On certain spaces of analytic functions its error term is a continuous linear functional. We derive easy to compute estimates for the norm of the error functional, which lead to bounds for the error functional itself. The efficiency of these bounds is illustrated with some numerical examples.

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## 1. Introduction

The Gauss-Kronrod quadrature formula for the Legendre weight function,  $w(t) = 1$  on  $[-1, 1]$ , has the form

$$(1.1) \quad \int_{-1}^1 f(t) dt = \sum_{\nu=1}^n \sigma_{\nu} f(\tau_{\nu}) + \sum_{\mu=1}^{n+1} \sigma_{\mu}^* f(\tau_{\mu}^*) + R_n(f),$$

where  $\tau_{\nu} = \tau_{\nu}^{(n)}$  are the zeros of the  $n$ th degree Legendre polynomial, and the  $\tau_{\mu}^* = \tau_{\mu}^{*(n)}$ ,  $\sigma_{\nu} = \sigma_{\nu}^{(n)}$ ,  $\sigma_{\mu}^* = \sigma_{\mu}^{*(n)}$  are chosen such that (1.1) has maximum degree of exactness  $d_n$ , i.e.,  $R_n(f) = 0$  for all  $f \in \mathbb{P}_{d_n}$ . It is known that the  $\tau_{\mu}^*$  are simple, all contained in the interval  $(-1, 1)$  and they interlace with the  $\tau_{\nu}$ , that is,

$$(1.2) \quad \tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^*$$

(see [7]). Moreover, all weights of (1.1) are positive (the positivity of the  $\sigma_{\mu}^*$  is equivalent to the interlacing property (1.2); see [4]). These properties of the nodes

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and weights of (1.1) make it computationally useful. It has also been shown (see [6]) that the precise degree of exactness of (1.1) is

$$(1.3) \quad d_n = \begin{cases} 3n + 1 & \text{for } n \text{ even} , \\ 3n + 2 & \text{for } n \text{ odd} . \end{cases}$$

Let  $f$  be a holomorphic function in  $C_r = \{z \in \mathbb{C} : |z| < r\}$ ,  $r > 1$ . Then

$$(1.4) \quad f(z) = \sum_{k=0}^{\infty} a_k z^k, \quad z \in C_r .$$

Define

$$(1.5) \quad X_r = \{f : f \text{ holomorphic in } C_r \text{ and } |f|_r < \infty\} ,$$

where

$$(1.6) \quad |f|_r = \sup\{|a_k| r^k : k \in \mathbb{N}_0 \text{ and } R_n(t^k) \neq 0\}$$

is a seminorm on  $X_r$ . The Legendre weight function is even, and its support is symmetric with respect to the origin. Therefore, the nodes of (1.1) are symmetric with respect to the origin, and the weights corresponding to symmetric nodes are equal. It follows that

$$(1.7) \quad R_n(t^{2k+1}) = 0, \quad k \in \mathbb{N}_0 .$$

Then (1.6), in view of (1.3) and (1.7), takes the form

$$(1.8) \quad |f|_r = \sup_{k \geq [(3n+3)/2]} \{|a_{2k}| r^{2k}\} ,$$

where  $[\cdot]$  indicates the integer part of a real number. Since  $f \in C[-1, 1]$ , from (1.1) we find

$$(1.9) \quad |R_n(f)| \leq 4 \|f\|_{\infty} .$$

Thus  $R_n$  is a bounded and, equivalently, continuous linear functional on  $(C[-1, 1], \|\cdot\|_{\infty})$ . The continuity of  $R_n$ , together with the uniform convergence of the series (1.4) on  $[-1, 1]$ , implies, taking into account (1.3) and (1.7),

$$R_n(f) = \sum_{k=[(3n+3)/2]}^{\infty} a_{2k} R_n(t^{2k}) ,$$

which, by virtue of (1.8), gives

$$(1.10) \quad |R_n(f)| \leq \left[ \sum_{k=[(3n+3)/2]}^{\infty} \frac{|R_n(t^{2k})|}{r^{2k}} \right] |f|_r .$$

From (1.9),  $|R_n(t^{2k})| \leq 4$ , hence the series in (1.10) converges, and  $R_n$  is a bounded linear functional on  $(X_r, |\cdot|_r)$ . Then

$$(1.11) \quad |R_n(f)| \leq \|R_n\| |f|_r .$$

In the next section we obtain manageable estimates for  $\|R_n\|$ ,  $2 \leq n \leq 30$ , which lead to bounds for  $R_n$  of the type (1.11). The method we use was originally introduced by Hämmerlin in [3]. Even though we carry out this program for

$n = 2(1)30$ , our estimates can be applied for  $n > 30$ , after the computation of appropriate constants (cf. (2.8), (2.13) and (2.14) below). The right-hand side of (1.11) can be optimized as a function of  $r$ , that is, if  $f \in X_R$ ,

$$(1.12) \quad |R_n(f)| \leq \inf_{1 < r \leq R} (\|R_n\| |f|_r).$$

The efficiency of bounds (1.12) is demonstrated in Sect. 3 with some numerical examples.

*Remark.* For  $n = 1$ , the Gauss-Kronrod formula (1.1) is the 3-point Gauss formula for the Legendre weight function (see [1, Sect. 2]), for which a number of error bounds are available.

## 2. The error bounds

We begin with a lemma, which will be useful in the subsequent development.

**Lemma 2.1.** *The error term of the Gauss-Kronrod formula (1.1) for the Legendre weight function satisfies*

$$(2.1) \quad R_n(t^{2k}) > 0 \quad \text{for all } k \geq K_n,$$

for some constant  $K_n \geq [(3n + 3)/2]$ .

*Proof.* From (1.1) we have

$$R_n(t^{2k}) = \int_{-1}^1 t^{2k} dt - \sum_{v=1}^n \sigma_v \tau_v^{2k} - \sum_{\mu=1}^{n+1} \sigma_\mu^* \tau_\mu^{*2k}.$$

Evaluating the integral on the right-hand side, and using the interlacing property (1.2), we find

$$R_n(t^{2k}) > \frac{2}{2k+1} - \left( \sum_{v=1}^n \sigma_v + \sum_{\mu=1}^{n+1} \sigma_\mu^* \right) \tau_1^{*2k}.$$

Replacing the sum of the weights by  $\int_{-1}^1 dt$ , we get

$$R_n(t^{2k}) > 2 \left( \frac{1}{2k+1} - \tau_1^{*2k} \right).$$

Therefore, to prove (2.1), it suffices to show that

$$(2.2) \quad \frac{1}{2k+1} \geq \tau_1^{*2k} \quad \text{for all } k \geq K_n.$$

Since  $0 < \tau_1^* < 1$ , we have

$$\lim_{k \rightarrow \infty} (2k+1) \tau_1^{*2k} = 0,$$

and (2.2) follows. □

We can now derive a formula for  $\|R_n\|$ . First, (1.10) gives

$$(2.3) \quad \|R_n\| \leq \sum_{k=\lceil(3n+3)/2\rceil}^{\infty} \frac{|R_n(t^{2k})|}{r^{2k}}.$$

Letting

$$\begin{aligned} \phi(z) &= \sum_{k=\lceil(3n+3)/2\rceil}^{K_n-1} \frac{\text{sign}(R_n(t^{2k}))z^{2k}}{r^{2k+1}} + \sum_{k=K_n}^{\infty} \frac{z^{2k}}{r^{2k+1}} \\ &= \sum_{k=\lceil(3n+3)/2\rceil}^{K_n-1} \frac{\text{sign}(R_n(t^{2k}))z^{2k}}{r^{2k+1}} + \frac{z^{2K_n}}{r^{2K_n-1}(r^2-z^2)}, \quad z \in C_r, \end{aligned}$$

it is easy to see that

$$|\phi|_r = \frac{1}{r}.$$

We have

$$R_n(\phi) = \left[ \sum_{k=\lceil(3n+3)/2\rceil}^{K_n-1} \frac{\text{sign}(R_n(t^{2k}))R_n(t^{2k})}{r^{2k}} + \sum_{k=K_n}^{\infty} \frac{R_n(t^{2k})}{r^{2k}} \right] \frac{1}{r},$$

hence, by Lemma 2.1,

$$|R_n(\phi)| = \left[ \sum_{k=\lceil(3n+3)/2\rceil}^{\infty} \frac{|R_n(t^{2k})|}{r^{2k}} \right] |\phi|_r,$$

which, together with (2.3), implies

$$(2.4) \quad \|R_n\| = \sum_{k=\lceil(3n+3)/2\rceil}^{\infty} \frac{|R_n(t^{2k})|}{r^{2k}}.$$

The estimates for  $\|R_n\|$ ,  $2 \leq n \leq 30$ , will be based on (2.4). It is then apparent that we need bounds for  $|R_n(t^{2k})|$ . Since  $f \in C^\infty[-1, 1]$ , from [5, Sect. 3, with  $\mu = 1/2$ ], we have

$$(2.5) \quad |R_n(f)| < \frac{(n!)^2}{2^{n-3}(2n)!(d_n+1)!} \max_{-1 \leq t \leq 1} |f^{(d_n+1)}(t)|,$$

with  $d_n$  given by (1.3), which yields

$$(2.6) \quad |R_n(t^{2k})| < \frac{(n!)^2 \prod_{i=0}^{d_n} (2k-i)}{2^{n-3}(2n)!(d_n+1)!}, \quad k \geq \lceil(3n+3)/2\rceil.$$

For  $2 \leq n \leq 30$ , we will show that

$$(2.7) \quad |R_n(t^{2k})| < \frac{(n!)^2 \prod_{i=0}^{d_n-t_n} (2k-i)}{2^{n-3}(2n)!(d_n+1)!}, \quad k \geq \lceil(3n+3)/2\rceil,$$

where  $\iota_n$  is a constant defined by

$$(2.8) \iota_n = \max \left\{ j: |R_n(t^{2k})| < \frac{(n!)^2 \prod_{i=0}^{d_n-j} (2k-i)}{2^{n-3}(2n)!(d_n+1)!} \text{ for all } [(3n+3)/2] \leq k < K_n \right\}.$$

Clearly, (2.7) is an improvement of (2.6) by  $\iota_n$  factors.

We first prove (2.7) for  $k \geq K_n$ . Then, in view of Lemma 2.1, we must show that

$$R_n(t^{2k}) < \frac{(n!)^2 \prod_{i=0}^{d_n-\iota_n} (2k-i)}{2^{n-3}(2n)!(d_n+1)!},$$

or equivalently, by means of (1.1),

$$\frac{(n!)^2 \prod_{i=0}^{d_n-\iota_n} (2k-i)}{2^{n-3}(2n)!(d_n+1)!} - \frac{2}{2k+1} + \sum_{\nu=1}^n \sigma_\nu \tau_\nu^{2k} + \sum_{\mu=1}^{n+1} \sigma_\mu^* \tau_\mu^{*2k} > 0,$$

which is true whenever

$$(2.9) \quad \frac{2}{2k+1} \leq \frac{(n!)^2 \prod_{i=0}^{d_n-\iota_n} (2k-i)}{2^{n-3}(2n)!(d_n+1)!}.$$

Since the left-hand side is decreasing with  $k$ , while the right-hand side is increasing, (2.9) is satisfied for all  $k \geq K_{1,n}$ , for some constant  $K_{1,n} \geq K_n$ . The values of  $K_n$ ,  $K_{1,n}$  were computed numerically for  $n = 2(1)30$ , and it was found that  $K_{1,n} = K_n$ . Thus, it remains to verify that (2.7) holds for  $[(3n+3)/2] \leq k < K_n$ . The verification was done numerically for  $n = 2(1)30$ .

It is clear that (2.7) is valid for  $n > 30$ , provided that we know  $\iota_n$ . To determine  $\iota_n$  for a fixed  $n$ , we first compute  $K_n$ . Then we start increasing  $j$  in (2.8), beginning with  $j = 1$ . For each  $j$ , we find the first  $k = K_{1,n} \geq K_n$  such that (2.9) (with  $j$  in place of  $\iota_n$ ) is satisfied, and subsequently check the inequality in (2.8) for all  $[(3n+3)/2] \leq k < K_{1,n}$ . As we already mentioned,  $K_{1,n} = K_n$ ,  $2 \leq n \leq 30$ , and we conjecture that this is the case for  $n > 30$ . The process stops when we find a  $k$ ,  $[(3n+3)/2] \leq k < K_{1,n}$ , such that the inequality in (2.8) is not satisfied. The  $\iota_n$  is then chosen to be the  $j$  of the previous step. The values of  $\iota_n$ ,  $2 \leq n \leq 30$ , are shown in Table 1. All computations in this and the following section were performed on a MicroVAX II computer in quad precision (machine precision approximately 33 decimal digits).

**Table 1.** The values of  $\iota_n$ ,  $2 \leq n \leq 30$

$n$	$\iota_n$	$n$	$\iota_n$	$n$	$\iota_n$	$n$	$\iota_n$	$n$	$\iota_n$
2	4	8	7	14	7	20	8	26	8
3	5	9	7	15	7	21	8	27	8
4	5	10	7	16	7	22	8	28	8
5	6	11	7	17	8	23	8	29	8
6	6	12	7	18	8	24	8	30	8
7	6	13	7	19	8	25	8		

Now (2.4) can be used, in conjunction with (2.7), to derive estimates for  $\|R_n\|$ ,  $2 \leq n \leq 30$ . First,

$$(2.10) \quad \|R_n\| < \frac{(n!)^2}{2^{n-3}(2n)!(d_n + 1)!} \sum_{k = [(3n + 3)/2]}^{\infty} \frac{\prod_{i=0}^{d_n - l_n} (2k - i)}{r^{2k}}.$$

Let

$$(2.11) \quad S(r) = \sum_{k = [(3n + 3)/2]}^{\infty} \frac{\prod_{i=0}^{d_n - l_n} (2k - i)}{r^{2k}}.$$

Writing  $S(r)$  explicitly, and factoring out  $(1/r)^{d_n - l_n + 1}$ , we find, after an elementary computation,

$$S(r) = \left(\frac{1}{r}\right)^{d_n - l_n + 1} \frac{d^{d_n - l_n + 1}}{d(1/r)^{d_n - l_n + 1}} \left[ \frac{(1/r)^{d_n + 1}}{1 - (1/r)^2} \right],$$

where  $d^m/d(1/r)^m$  denotes the  $m$ th derivative with respect to  $1/r$ . The division inside the brackets, and the partial fraction decomposition of  $1/[1 - (1/r)^2]$ , yield

$$S(r) = \left(\frac{1}{r}\right)^{d_n - l_n + 1} \frac{d^{d_n - l_n + 1}}{d(1/r)^{d_n - l_n + 1}} \left[ \frac{1}{2} \left( \frac{1}{1 - 1/r} + \frac{1}{1 + 1/r} \right) - 1 - \left(\frac{1}{r}\right)^2 - \dots - \left(\frac{1}{r}\right)^{d_n - 1} \right].$$

Differentiating we get, after a simple computation,

$$(2.12) \quad S(r) = (d_n - l_n + 1)! E(r),$$

where

$$(2.13) \quad E(r) = \frac{1}{2} \left[ \frac{r}{(r - 1)^{d_n - l_n + 2}} + (-1)^{l_n} \frac{r}{(r + 1)^{d_n - l_n + 2}} \right] - \left( \frac{d_n - l_n + 1 + i}{d_n - l_n + 1} \right) \frac{1}{r^{d_n - l_n + 1 + i}} - \left( \frac{d_n - l_n + 3 + i}{d_n - l_n + 1} \right) \frac{1}{r^{d_n - l_n + 3 + i}} - \dots - \left( \frac{d_n - 1}{d_n - l_n + 1} \right) \frac{1}{r^{d_n - 1}}, \quad i = \begin{cases} 0 & \text{for } l_n \text{ even,} \\ 1 & \text{for } l_n \text{ odd.} \end{cases}$$

Thus, (2.10), by virtue of (2.11) and (2.12), takes the form

$$(2.14) \quad \|R_n\| < \frac{(n!)^2 (d_n - l_n + 1)!}{2^{n-3} (2n)! (d_n + 1)!} E(r).$$

Using (2.14), we obtain bounds for  $R_n$ . First, (1.12) gives

$$(2.15) \quad |R_n(f)| \leq \frac{(n!)^2 (d_n - l_n + 1)!}{2^{n-3} (2n)! (d_n + 1)!} \inf_{1 < r \leq R} [E(r)|f|_r].$$

Moreover, it can be seen from (2.13) that the magnitude of  $E(r)$  is dominated by the expression inside the brackets. The remaining terms are higher-order terms with

respect to  $1/r$ , and their contribution is negligible, particularly as  $n$  increases. By omitting them, we arrive at a bound that is computationally simpler and less expensive, that is,

$$(2.16) \quad |R_n(f)| \leq \frac{(n!)^2(d_n - l_n + 1)!}{2^{n-2}(2n)!(d_n + 1)!} \cdot \inf_{1 < r \leq R} \left\{ \left[ \frac{r}{(r-1)^{d_n - l_n + 2}} + (-1)^{l_n} \frac{r}{(r+1)^{d_n - l_n + 2}} \right] |f|_r \right\}.$$

Both bounds (2.15) and (2.16) can be computed, assuming that  $|f|_r$  is available or can easily be calculated. If this is not the case,  $|f|_r$  can be estimated by  $\max_{|z|=r} |f(z)|$ , which exists at least for  $r < R$  (see [3, Eq. (4.2)]), and then (2.15) and (2.16) become

$$(2.17) \quad |R_n(f)| \leq \frac{(n!)^2(d_n - l_n + 1)!}{2^{n-3}(2n)!(d_n + 1)!} \inf_{1 < r < R} \left[ E(r) \max_{|z|=r} |f(z)| \right],$$

and

$$(2.18) \quad |R_n(f)| \leq \frac{(n!)^2(d_n - l_n + 1)!}{2^{n-2}(2n)!(d_n + 1)!} \cdot \inf_{1 < r < R} \left\{ \left[ \frac{r}{(r-1)^{d_n - l_n + 2}} + (-1)^{l_n} \frac{r}{(r+1)^{d_n - l_n + 2}} \right] \max_{|z|=r} |f(z)| \right\}.$$

### 3. Examples

#### Example 3.1

$$\int_{-1}^1 e^{-\omega t^2} dt = \sqrt{\frac{\pi}{\omega}} \Phi(\sqrt{\omega}), \quad \omega > 0,$$

where  $\Phi(t)$  is the so-called probability integral, which can be defined through a power series,

$$\Phi(t) = \frac{2}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k+1}}{(2k+1)k!}$$

(see [2, Sect. 8.25]). We shall approximate the integral using the Gauss-Kronrod formula (1.1).

Since  $f(z) = e^{-\omega z^2} = \sum_{k=0}^{\infty} \frac{(-1)^k \omega^k z^{2k}}{k!}$  is entire, we find

$$(3.1) \quad |f|_r = \begin{cases} \frac{\omega^{(d_n+1)/2} r^{d_n+1}}{[(d_n+1)/2]!}, & 1 < r \leq \sqrt{(d_n+3)/(2\omega)}, \\ \frac{\omega^{(d_n+2k+1)/2} r^{d_n+2k+1}}{[(d_n+2k+1)/2]!}, & \sqrt{(d_n+2k+1)/(2\omega)} < r \leq \sqrt{(d_n+2k+3)/(2\omega)}, \end{cases} \quad k = 1, 2, \dots,$$

under the assumption that  $d_n + 3 > 2\omega$ . In case that  $d_n + 3 \leq 2\omega$ , the formula for  $|f|_r$  starts at the branch of (3.1) for which  $d_n + 2k + 3 > 2\omega$ . Thus  $f \in X_\infty$ . Moreover, for  $|z| = r$ , we have

$$|f(z)| = |e^{-\omega r^2 \cos 2\theta - i\omega r^2 \sin 2\theta}| = e^{-\omega r^2 \cos 2\theta},$$

which implies

$$(3.2) \quad \max_{|z|=r} |f(z)| = e^{\omega r^2}.$$

Consequently, the error in approximating the integral can be estimated by means of the bounds in Sect. 2. For comparison purposes we employed all four of them: (2.15), (2.16), (2.17) and (2.18).

Our results are shown in Table 2. (Numbers in parentheses indicate decimal exponents.) The infimum for each bound was attained at the value of  $r$  given before that bound. In the last column we give the modulus of the actual error. The true value of the integral was computed from the power series expansion for the probability integral. Whenever the actual error is close to machine precision, the actual error could be larger than the error bound. In this case we enter “m.p.” (for machine precision) in the last column.

It is worth noting a few things here. First, as it was already mentioned in Sect. 2, the bounds (2.15), (2.16) and (2.17), (2.18) are very close, particularly as  $\omega$  and  $n$  increase. Since (2.16) and (2.18) are computationally simpler and less expensive (in the number of arithmetic operations involved), they are a more attractive choice than (2.15) and (2.17). Also, all four bounds, which are quite sharp for small values of  $\omega$ , worsen as  $\omega$  increases, and eventually become gross overestimates of the

**Table 2.** Error bounds and actual error for Example 3.1

$\omega$	$n$	$r$	Bound (2.15)	$r$	Bound (2.16)	$r$	Bound (2.17)	$r$	Bound (2.18)	Error
0.5	5	4.472	1.074(-14)	3.166	2.797(-14)	4.343	8.439(-14)	4.034	2.775(-13)	3.469(-15)
	10	5.831	1.019(-29)	4.714	2.315(-29)	5.758	1.052(-28)	5.543	2.632(-28)	2.450(-30)
	15	7.071	6.526(-47)	7.000	1.088(-46)	7.054	8.203(-46)	6.934	1.341(-45)	m.p.
	20	8.000	1.751(-64)	7.875	2.981(-64)	7.991	2.489(-63)	7.874	4.171(-63)	m.p.
1.0	5	3.162	8.533(-12)	3.162	1.432(-11)	3.156	6.820(-11)	3.033	1.098(-10)	1.285(-12)
	10	4.243	1.216(-24)	4.123	1.653(-24)	4.160	1.280(-23)	4.088	1.711(-23)	1.229(-25)
	15	5.099	2.733(-39)	5.099	3.056(-39)	5.095	3.505(-38)	5.066	3.908(-38)	m.p.
	20	5.831	1.004(-54)	5.745	1.117(-54)	5.755	1.453(-53)	5.729	1.612(-53)	m.p.
2.0	5	2.429	1.159(-8)	2.345	1.317(-8)	2.363	9.768(-8)	2.332	1.102(-7)	3.336(-10)
	10	3.082	3.113(-19)	3.082	3.267(-19)	3.078	3.416(-18)	3.065	3.580(-18)	4.741(-21)
	15	3.808	3.416(-31)	3.800	3.453(-31)	3.753	4.560(-30)	3.751	4.603(-30)	m.p.
	20	4.243	1.944(-44)	4.243	1.959(-44)	4.218	2.923(-43)	4.216	2.944(-43)	m.p.
4.0	5	1.871	5.253(-5)	1.871	5.343(-5)	1.852	4.934(-4)	1.848	5.008(-4)	3.273(-8)
	10	2.371	3.962(-13)	2.368	3.973(-13)	2.352	4.683(-12)	2.352	4.694(-12)	1.103(-16)
	15	2.828	3.276(-22)	2.828	3.276(-22)	2.828	4.657(-21)	2.828	4.658(-21)	3.103(-27)
	20	3.162	3.615(-33)	3.162	3.615(-33)	3.153	5.738(-32)	3.153	5.738(-32)	m.p.
8.0	5	1.541	2.726(0)	1.541	2.728(0)	1.520	2.952(1)	1.520	2.954(1)	5.249(-6)
	10	1.871	9.240(-6)	1.871	9.241(-6)	1.859	1.225(-4)	1.859	1.225(-4)	1.008(-12)
	15	2.200	9.253(-12)	2.200	9.253(-12)	2.186	1.436(-10)	2.186	1.436(-10)	7.480(-21)
	20	2.424	2.676(-20)	2.424	2.676(-20)	2.411	4.590(-19)	2.411	4.590(-19)	1.646(-29)



actual error. This happens, presumably, because of  $|f|_r$  or  $\max_{|z|=r} |f(z)|$ , whose magnitude grows at a nonlinear polynomial and an exponential rate, respectively, with respect to  $\omega$  (cf. (3.1) and (3.2)). Finally, of practical importance is the fact that the bounds can also be used to determine a value of  $n$  in (1.1) guaranteeing a given accuracy, and the results are quite satisfactory. Our computations to this end usually produced an overestimation of  $n$  by just a few units.

*Example 3.2*

$$\int_{-1}^1 \frac{\cos t}{t^2 + \omega^2} dt, \quad \omega > 0.$$

We shall approximate the integral using the Gauss-Kronrod formula (1.1), without separating out the poles at  $\pm i\omega$ .

Both  $\cos z$  and  $1/(z^2 + \omega^2)$  have a Maclaurin series expansion for  $z \in \mathbb{C}$  and  $z \in C_\omega$ , respectively. From the series multiplication theorem we find

$$f(z) = \frac{\cos z}{z^2 + \omega^2} = \sum_{k=0}^{\infty} (-1)^k \left[ 1 + \frac{\omega^2}{2!} + \dots + \frac{\omega^{2k}}{(2k)!} \right] \frac{z^{2k}}{\omega^{2k+2}}, \quad z \in C_\omega.$$

The bounds of Sect. 2 can be used, to estimate the error in approximating the integral, only if  $\omega > 1$ . The calculation of  $|f|_r$ ,  $1 < r \leq \omega$ , is quite cumbersome, hence  $|f|_r$  was estimated by  $\max_{|z|=r} |f(z)|$ . By setting  $\cos z = \frac{1}{2}(e^{iz} + e^{-iz})$ , we compute, for  $|z| = r$ ,

$$\begin{aligned} |f(z)| &= \frac{1}{2} \left| \frac{e^{-r \sin \theta + ir \cos \theta} + e^{r \sin \theta - ir \cos \theta}}{r^2 \cos 2\theta + \omega^2 + ir^2 \sin 2\theta} \right| \\ &\leq \frac{1}{2} \frac{e^{r \sin \theta} + e^{-r \sin \theta}}{\omega^2 - r^2} = \frac{\cosh(r \sin \theta)}{\omega^2 - r^2}, \end{aligned}$$

from which it follows that

$$\max_{|z|=r} |f(z)| \leq \frac{\cosh r}{\omega^2 - r^2}.$$

Since for  $\theta = \pi/2$ , we have

$$|f(z)| = \frac{1}{2} \frac{e^r + e^{-r}}{\omega^2 - r^2} = \frac{\cosh r}{\omega^2 - r^2},$$

we finally get

$$(3.3) \quad \max_{|z|=r} |f(z)| = \frac{\cosh r}{\omega^2 - r^2}, \quad 1 < r < \omega.$$

Thus  $f \in X_\omega$ .

The error bounds resulting from (2.17) and (2.18), together with the modulus of the actual error are shown in Table 3. The true value of the integral was computed using the Maclaurin expansion for  $f(z)$ ,

$$\int_{-1}^1 \frac{\cos t}{t^2 + \omega^2} dt = 2 \sum_{k=0}^{\infty} (-1)^k \left[ 1 + \frac{\omega^2}{2!} + \dots + \frac{\omega^{2k}}{(2k)!} \right] \frac{1}{(2k+1)\omega^{2k+2}}.$$

**Table 3.** Error bounds and actual error for Example 3.2

$\omega$	$n$	$r$	Bound (2.17)	$r$	Bound (2.18)	Error
2.0	5	1.923	2.286(-9)	1.922	2.339(-9)	6.719(-13)
	10	1.961	1.613(-16)	1.961	1.613(-16)	1.181(-22)
	15	1.976	4.478(-22)	1.976	4.478(-22)	9.196(-33)
	20	1.982	5.636(-29)	1.982	5.636(-29)	m.p.
3.0	5	2.844	2.497(-13)	2.831	3.490(-13)	1.281(-15)
	10	2.920	2.985(-24)	2.919	3.077(-24)	9.970(-28)
	15	2.951	1.326(-34)	2.951	1.326(-34)	m.p.
	20	2.963	2.050(-45)	2.963	2.051(-45)	m.p.
4.0	5	3.764	1.213(-15)	3.725	2.958(-15)	1.488(-17)
	10	3.878	1.135(-28)	3.874	1.407(-28)	2.322(-31)
	15	3.925	9.253(-42)	3.924	9.391(-42)	m.p.
	20	3.943	7.485(-55)	3.943	7.508(-55)	m.p.

Here, there seems to be almost no difference between bounds (2.17) and (2.18), which stresses once more the point made in Sect. 2 and Example 3.1. Also, both bounds worsen as  $\omega$  decreases, and become gross overestimates of the actual error when  $\omega$  drops below 2. In fact, for a fixed value of  $\omega$ , the bounds are worse for higher values of  $n$ . The reason for all this is the term  $r/(r-1)^{d_n - \iota_n + 2}$  contained in both bounds. The magnitude of this term gets large for  $r < 2$ , and even larger when  $d_n - \iota_n + 2$  is high (both of which happen when  $\omega < 2$  and  $n$  is high).

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