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The error norm of Gauss-Radau quadrature formulae for Chebyshev weight functions

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Abstract In certain spaces of analytic functions the error term of the Gauss-Radau quadrature formula relative to a (nonnegative) weight function is a continuous linear functional. We compute or estimate the norm of the error functional for any one of the four Chebyshev weight functions.

Keywords Gauss-Radau quadrature formulae · Chebyshev weight functions · Error norm

Mathematics Subject Classification (2000) 65D32

1 Introduction

We consider the Gauss-Radau quadrature formula for the (nonnegative) weight function w on $[-1, 1]$ and additional node at -1 or 1

$$\int_{-1}^{1} f(t)w(t)dt = \sum_{\nu=1}^{n} w_\nu^{(-)} f(\tau_\nu^{(-)}) + w_{n+1}^{(-)} f(-1) + R_n^{(-)}(f), \tag{1.1}$$

or

$$\int_{-1}^{1} f(t)w(t)dt = w_0^{(+)} f(1) + \sum_{\nu=1}^{n} w_\nu^{(+)} f(\tau_\nu^{(+)}) + R_n^{(+)}(f), \tag{1.2}$$

where $\tau_\nu^{(-)} = \tau_\nu^{(-)(n)}$ are the zeros of the nth degree (monic) orthogonal polynomial $\pi_n^{(-)}(\cdot) = \pi_n(\cdot; w^{(-)})$ relative to the weight function $w^{(-)}(t) = (1+t)w(t)$,

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and $\tau_\nu^{(+)} = \tau_\nu^{(+)(n)}$ the zeros of the nth degree (monic) orthogonal polynomial $\pi_n^{(+)}(\cdot) = \pi_n(\cdot; w^{(+)})$ relative to the weight function $w^{(+)}(t) = (1-t)w(t)$. It is known that the weights in (1.1) and (1.2) are all positive, and both formulae have precise degree of exactness $d = 2n$, i.e., $R_n^{(-)}(f) = 0$ and $R_n^{(+)}(f) = 0$ for all $f \in \mathbb{P}_{2n}$ (see [5, Sect. 2.1.1]).

A well-known representation for the error term $R_n^{(-)}$ of formula (1.1) can be obtained using the analysis of Markov. If $f \in C^{2n+1}[-1,1]$, then

$$R_n^{(-)}(f) = \frac{f^{(2n+1)}(\xi)}{(2n+1)!} \int_{-1}^{1} [\pi_n^{(-)}(t)]^2 w^{(-)}(t)dt, \quad -1 < \xi < 1 \tag{1.3}$$

(cf. [4, Sect. 7.4.1]). Although frequently quoted, this formula is of little practical use, mainly because of the high-order derivative that contains.

Another way of estimating $R_n^{(-)}$ is by means of Hilbert space methods. If f is a holomorphic function in $C_r = \{z \in \mathbb{C} : |z| < r\}$ with $r > 1$, then it can be written as

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

Define

$$|f|_r = \sup\{|a_k| r^k : k \in \mathbb{N}_0 \text{ and } R_n^{(-)}(t^k) \neq 0\}, \tag{1.4}$$

which is a seminorm in the space

$$X_r = \{f : f \text{ holomorphic in } C_r \text{ and } |f|_r < \infty\}. \tag{1.5}$$

The error term $R_n^{(-)}$ of (1.1) is a continuous linear functional in $(X_r, |\cdot|_r)$, and its norm is given by

$$\|R_n^{(-)}\| = \sum_{k=0}^{\infty} \frac{|R_n^{(-)}(t^k)|}{r^k} \tag{1.6}$$

(cf. [1, Sect. 1.1]). If, in addition, for an $\varepsilon \in \{-1, 1\}$,

$$\varepsilon R_n^{(-)}(t^k) \geq 0, \quad k \geq 0, \tag{1.7$_i$}$$

or

$$\varepsilon(-1)^k R_n^{(-)}(t^k) \geq 0, \quad k \geq 0, \tag{1.7$_{ii}$}$$

then the error norm can be represented by

$$\|R_n^{(-)}\| = r \left| \frac{1}{(r+1)\pi_n^{(-)}(r)} \int_{-1}^{1} \frac{\pi_n^{(-)}(t)}{r-t} w^{(-)}(t)dt \right|, \tag{1.8$_i$}$$

or

$$\|R_n^{(-)}\| = r \left| \frac{1}{(r-1)\pi_n^{(-)}(-r)} \int_{-1}^{1} \frac{\pi_n^{(-)}(t)}{r+t} w^{(-)}(t)dt \right|, \tag{1.8$_{ii}$}$$

respectively (see [1, Sect. 1.2]). The $\|R_n^{(-)}\|$ leads to bounds for $R_n^{(-)}$ itself. If $f \in X_R$, then

$$|R_n^{(-)}(f)| \le \|R_n^{(-)}\| |f|_r, \quad 1 < r \le R, \tag{1.9}$$

which, optimized as a function of r, gives

$$|R_n^{(-)}(f)| \le \inf_{1<r\le R} (\|R_n^{(-)}\| |f|_r). \tag{1.10}$$

Alternatively, $R_n^{(-)}$ can be estimated using a contour integration method. If f is a single-valued holomorphic function in a domain D containing $[-1, 1]$ in its interior, and $\bar{C}_r = \{z \in \mathbb{C} : |z| = r\}$, $r > 1$, is a contour in D surrounding $[-1, 1]$, then the error term $R_n^{(-)}(\cdot)$ of (1.1) can be represented by

$$R_n^{(-)}(f) = \frac{1}{2\pi i} \int_{\bar{C}_r} K_n^{(-)}(z) f(z) dz, \tag{1.11}$$

where the kernel $K_n^{(-)}$ is given by

$$K_n^{(-)}(z) = R_n^{(-)}\left(\frac{1}{z - \cdot}\right) = \frac{1}{(z+1)\pi_n^{(-)}(z)} \int_{-1}^{1} \frac{\pi_n^{(-)}(t)}{z - t} w^{(-)}(t) dt. \tag{1.12}$$

From (1.11), there follows that

$$|R_n^{(-)}(f)| \le r \max_{z\in\bar{C}_r} |K_n^{(-)}(z)| \max_{z\in\bar{C}_r} |f(z)|. \tag{1.13}$$

Moreover, under the additional assumption (1.7_i) or (1.7_{ii}), we have

$$\max_{z\in\bar{C}_r} |K_n^{(-)}(z)| = \begin{cases} |K_n(r)|, & \text{if } R_n^{(-)} \text{ satisfies } (1.7_i), \\ |K_n(-r)|, & \text{if } R_n^{(-)} \text{ satisfies } (1.7_{ii}) \end{cases} \tag{1.14}$$

(see [7, Sects. 2, 3 and 4]), hence, (1.13) gives, in view of (1.14), (1.12) and (1.8_i)–(1.8_{ii}),

$$|R_n^{(-)}(f)| \le \|R_n^{(-)}\| \max_{|z|=r} |f(z)|. \tag{1.15}$$

This estimate can also be obtained from (1.9) if $|f|_r$ is estimated by $\|f\|_\infty = \max_{|z|=r} |f(z)|$, which, for $f \in X_R$, exists at least for $r < R$ (cf. [1, (1.1.10)]). Consequently, (1.15) can be optimized as a function of r,

$$|R_n^{(-)}(f)| \le \inf_{1<r<R} \left(\|R_n^{(-)}\| \max_{|z|=r} |f(z)|\right). \tag{1.16}$$

The $\|R_n^{(+)}\|$ can be computed in an analogous way to that of $\|R_n^{(-)}\|$. However, if, in formula (1.2), we set $f(-t)$ in place of $f(t)$, make the change of variables $-t = \tau$ in the underlying integral, and compare the resulting formula with (1.1), we get

$$R_n^{(+)}(f(\cdot); w(\cdot)) = R_n^{(-)}(f(-\cdot); w(-\cdot)),$$

which, inserted in (1.6), implies

$$\|R_n^{(+)}(\cdot; w(\cdot))\| = \|R_n^{(-)}(\cdot; w(-\cdot))\|. \tag{1.17}$$

This can be used in order to obtain $\|R_n^{(+)}\|$ without making any direct calculations (see Sect. 2).

In the present paper, we consider formulae (1.1) and (1.2) with w being any one of the four Chebyshev weight functions

$$\begin{aligned} &w^{(1)}(t) = (1-t^2)^{-1/2}, \qquad w^{(2)}(t) = (1-t^2)^{1/2}, \quad -1 < t < 1, \\ &w^{(3)}(t) = (1-t)^{-1/2}(1+t)^{1/2}, \qquad w^{(4)}(t) = (1-t)^{1/2}(1+t)^{-1/2}, \quad -1 < t < 1. \end{aligned} \tag{1.18}$$

The error term of these formulae has been studied by Gautschi in [6] using the contour integration method described earlier. The $\max_{z\in\bar{C}_r} |K_n^{(-)}(z)|$ in (1.14), leading to bounds (1.13) and (1.15)–(1.16), has been computed explicitly for the weight functions $w^{(1)}$ and $w^{(4)}$, and it has been conjectured for the weights $w^{(2)}$ and $w^{(3)}$. In the following section, we compute $\|R_n^{(-)}\|$ for the weight functions $w^{(1)}$, $w^{(2)}$ when $1 \leq n \leq 40$, and $w^{(4)}$, while we estimate it for the weight $w^{(3)}$. This leads to bounds (1.9) and (1.10). Analogous bounds are obtained for the error term of formula (1.2), while our results are compared to those of Gautschi. Some numerical examples are given in Sect. 3.

2 The error norm for Chebyshev weight functions

Our aim here is either to compute or, if this is not possible, to estimate the norm of the error term in formulae (1.1) and (1.2) when w is any one of the four Chebyshev weight functions. We do that separately for each weight, and find that the error norm can be computed explicitly in all cases, except for formula (1.1) with $w = w^{(3)}$ and formula (1.2) with $w = w^{(4)}$.

2.1 Chebyshev weight of the first kind

We consider formula (1.1) with $w = w^{(1)}$ (cf. (1.18)). Then $w^{(-)(1)}(t) = (1+t) \times w^{(1)}(t) = w^{(3)}(t)$, hence, $\tau_\nu^{(-)(1)} = \tau_\nu^{(3)}$ are the zeros of $\pi_n^{(-)(1)}(t) = \frac{1}{2^n} V_n(t)$, the nth degree (monic) Chebyshev polynomial of the third kind. This can be represented by

$$V_n(\cos\theta) = \frac{\cos(n+1/2)\theta}{\cos(\theta/2)}, \tag{2.1}$$

consequently,

$$\tau_\nu^{(-)(1)} = \cos\frac{2\nu-1}{2n+1}\pi, \quad \nu = 1, 2, \ldots, n. \tag{2.2}$$

We begin with a useful

Proposition 2.1 *The error term of formula* (1.1) *with* $w = w^{(1)}$ *satisfies*

$$\frac{1}{2}R_n^{(-)(1)}(f(\cdot)) + \frac{1}{2}R_n^{(-)(1)}(f(-\cdot)) = R_{2n}^{*(1)}(f(\cdot)), \quad n \geq 1, \tag{2.3}$$

where $R_{2n}^{*(1)}$ *is the error term of the* $(2n)$*-point Gauss-Lobatto formula for the weight function* $w^{(1)}$.

Proof Consider formula (1.1) with $w = w^{(1)}$,

$$\int_{-1}^{1} f(t)w^{(1)}(t)dt = \sum_{\nu=1}^{n} w_\nu^{(-)(1)} f(\tau_\nu^{(-)(1)}) + w_{n+1}^{(-)(1)} f(-1) + R_n^{(-)(1)}(f(\cdot)). \tag{2.4}$$

Setting $f(-t)$ in place of $f(t)$, and transforming the integral on the left-hand side of (2.4), we get

$$\int_{-1}^{1} f(t)w^{(1)}(t)dt = w_{n+1}^{(-)(1)} f(1) + \sum_{\nu=1}^{n} w_\nu^{(-)(1)} f(-\tau_\nu^{(-)(1)}) + R_n^{(-)(1)}(f(-\cdot)). \tag{2.5}$$

Multiplying each of (2.4) and (2.5) by $1/2$, and adding them, yields

$$\begin{aligned}\int_{-1}^{1} f(t)w^{(1)}(t)dt &= \frac{1}{2}w_{n+1}^{(-)(1)} f(1) + \sum_{\nu=1}^{n} \frac{1}{2}w_\nu^{(-)(1)} f(\tau_\nu^{(-)(1)}) \\ &\quad + \sum_{\nu=1}^{n} \frac{1}{2}w_\nu^{(-)(1)} f(-\tau_\nu^{(-)(1)}) + \frac{1}{2}w_{n+1}^{(-)(1)} f(-1) \\ &\quad + \frac{1}{2}R_n^{(-)(1)}(f(\cdot)) + \frac{1}{2}R_n^{(-)(1)}(f(-\cdot)).\end{aligned} \tag{2.6}$$

Let the $(2n)$th degree Chebyshev polynomial of the second kind, given by

$$U_{2n}(\cos\theta) = \frac{\sin(2n+1)\theta}{\sin\theta}. \tag{2.7}$$

Clearly, the $\tau_\nu^{(-)(1)}$, $\nu = 1, 2, \ldots, n$, are zeros of U_{2n} (cf. (2.2)), and since U_{2n} is an even polynomial, the $-\tau_\nu^{(-)(1)}$, $\nu = 1, 2, \ldots, n$, are the remaining n zeros of U_{2n}. Consequently, (2.6) is the $(2n)$-point Gauss-Lobatto formula for the weight function $w^{(1)}$, and this yields (2.3). □

Remark 2.1 The $(2n)$-point Gauss-Lobatto formula for the weight function $w^{(1)}$ is given by

$$\begin{aligned}\int_{-1}^{1} f(t)w^{(1)}(t)dt &= \frac{\pi}{2(2n+1)} f(1) + \frac{\pi}{2n+1}\sum_{\nu=1}^{2n} f(\tau_\nu^{(2)}) + \frac{\pi}{2(2n+1)} f(-1) \\ &\quad + R_{2n}^{*(1)}(f),\end{aligned} \tag{2.8}$$

where $\tau_\nu^{(2)}$ are the zeros of U_{2n} (cf. [3, (2.7.1.14)]). Comparing (2.6) with (2.8), we get, as a bi-product of Proposition 2.1, that

$$w_\nu^{(-)(1)} = \frac{2\pi}{2n+1}, \quad \nu = 1, 2, \ldots, n, \qquad w_{n+1}^{(-)(1)} = \frac{\pi}{2n+1}.$$

The following result will be used in the computation of $\|R_n^{(-)(1)}\|$.

Proposition 2.2 *The error term of formula (1.1) with $w = w^{(1)}$ satisfies*

$$(-1)^{k-1} R_n^{(-)(1)}(t^k) \geq 0, \quad k \geq 0. \tag{2.9}$$

Proof First of all,

$$R_n^{(-)(1)}(t^k) = 0, \quad k = 0, 1, \ldots, 2n. \tag{2.10}$$

Setting $f(t) = t^{2l}$ in (2.3), we get

$$R_n^{(-)(1)}(t^{2l}) = R_{2n}^{*(1)}(t^{2l}). \tag{2.11}$$

Since, for $f \in C^{4n+2}[-1, 1]$,

$$R_{2n}^{*(1)}(f) = -\frac{\pi}{2^{4n+1}(4n+2)!} f^{(4n+2)}(\xi), \quad -1 < \xi < 1$$

(cf. [3, (2.7.1.14)]), we have

$$R_{2n}^{*(1)}(t^{2l}) \begin{cases} = 0, & l = 0, 1, \ldots, 2n, \\ \leq 0, & l \geq 2n+1, \end{cases}$$

which, inserted into (2.11), yields

$$R_n^{(-)(1)}(t^{2l}) \leq 0, \quad l \geq n+1. \tag{2.12}$$

Moreover, from (1.3) with $w^{(-)} = w^{(-)(1)}$, there follows that

$$R_n^{(-)(1)}(t^{2l+1}) \geq 0, \quad l \geq n,$$

which, together with (2.10) and (2.12), proves our assertion. □

We are now in a position to compute $\|R_n^{(-)(1)}\|$ and $\|R_n^{(+)(1)}\|$.

Theorem 2.3 *Consider the Gauss-Radau formula (1.1) or (1.2) with $w = w^{(1)}$. Let $\tau = r - \sqrt{r^2 - 1}$. We have*

$$\|R_n^{(-)(1)}\| = \frac{2\pi r \tau^{2n+1}}{(1 - \tau^{2n+1})\sqrt{r^2 - 1}}, \quad n \geq 1. \tag{2.13}$$

The $\|R_n^{(+)(1)}\|$ is given by the same formula (2.13).

Proof We first compute $\|R_n^{(-)(1)}\|$. In view of (2.9) (cf. (1.7_{ii}) with $\varepsilon=-1$), (1.8_{ii}) gives

$$\|R_n^{(-)(1)}\| = r\left|\frac{1}{(r-1)\pi_n^{(-)(1)}(-r)}\int_{-1}^{1}\frac{\pi_n^{(-)(1)}(t)}{r+t}w^{(-)(1)}(t)dt\right|$$
$$= r\left|\frac{1}{(r-1)V_n(-r)}\int_{-1}^{1}\frac{V_n(t)}{r+t}w^{(3)}(t)dt\right|. \tag{2.14}$$

Making the change of variables $t=\cos\theta$, and using (2.1), the formula for the product of cosines and

$$\int_0^{\pi}\frac{\cos m\theta}{r+\cos\theta}d\theta = \frac{(-1)^m\pi\tau^m}{\sqrt{r^2-1}}, \quad m=0,1,2,\ldots \tag{2.15}$$

(cf. [10, (3.613.1)] with $a=1/r$), the integral on the right-hand side of (2.14) computes to

$$\int_{-1}^{1}\frac{V_n(t)}{r+t}w^{(3)}(t)dt = \frac{(-1)^n\pi\tau^n(1-\tau)}{\sqrt{r^2-1}}. \tag{2.16}$$

Also,

$$V_n(-r) = (-1)^n[U_n(r)+U_{n-1}(r)]$$

(cf. (2.7), with $2n$ replaced by n and $n-1$, respectively, and (2.1)), and since

$$U_m(r) = \frac{1-\tau^{2m+2}}{2\tau^{m+1}\sqrt{r^2-1}}, \quad m=0,1,2,\ldots \tag{2.17}$$

(cf. [13, p. 278]), we find

$$V_n(-r) = \frac{(-1)^n(1+\tau)(1-\tau^{2n+1})}{2\tau^{n+1}\sqrt{r^2-1}}. \tag{2.18}$$

Now, inserting (2.16) and (2.18) into (2.14), and noting that

$$\frac{1-\tau}{1+\tau} = \frac{\sqrt{r-1}}{\sqrt{r+1}}, \tag{2.19}$$

we obtain (2.13).

Since $w^{(1)}$ is an even weight function, by (1.17), $\|R_n^{(+)(1)}\| = \|R_n^{(-)(1)}\|$. □

In [6, Sect. 4.2], Gautschi used the contour integration method presented in the introduction, and by treating $K_n^{(-)(1)}(z)$ analytically, he showed that

$$\max_{z\in\bar{C}_r}|K_n^{(-)(1)}(z)| = \frac{4\pi}{R-R^{-1}}\frac{1}{R^{2n+1}-1}, \quad n\geq 1,$$

where $R = r + \sqrt{r^2 - 1}$. Now, combining (1.14) with (1.12) and (1.7_{ii})–(1.8_{ii}), we get, in view of (2.9),

$$\max_{z \in \bar{C}_r} |K_n^{(-)(1)}(z)| = \frac{\|R_n^{(-)(1)}\|}{r}, \quad n \geq 1,$$

which, inserting (2.13) and noting that $\tau = 1/R$, can be shown, by a simple computation, to agree with Gautschi's result.

2.2 Chebyshev weight of the second kind

We consider formula (1.1) with $w = w^{(2)}$ (cf. (1.18)). Then $w^{(-)(2)}(t) = (1 + t)w^{(2)}(t) = (1-t)^{1/2}(1+t)^{3/2}$, $-1 \leq t \leq 1$, is the Jacobi weight function with parameters $\alpha = 1/2$, $\beta = 3/2$, hence, $\tau_\nu^{(-)(2)}$ are the zeros of $\pi_n^{(-)(2)} = \pi_n^{(1/2,3/2)}$, the corresponding nth degree (monic) Jacobi polynomial. Using Christoffel's formula in [15, Theorem 2.5] for the distribution $da(t) = w^{(2)}(t)dt$ on $[-1, 1]$ with $\rho(t) = t+1$, we get

$$\pi_n^{(-)(2)}(t) = \pi_n^{(1/2,3/2)}(t) = \frac{1}{2^{n+1}} \frac{U_{n+1}(t) + \frac{n+2}{n+1} U_n(t)}{t+1}, \quad n \geq 1, \tag{2.20}$$

where U_m is the mth degree Chebyshev polynomial of the second kind.

We first examine the behavior of the error term $R_n^{(-)(2)}$ on the monomials. It is known that

$$R_n^{(-)(2)}(t^k) = 0, \quad k = 0, 1, \ldots, 2n. \tag{2.21}$$

A step further is the following

Lemma 2.4 *The error term of formula* (1.1) *with* $w = w^{(2)}$ *satisfies*

$$R_n^{(-)(2)}(t^{2l}) < 0, \quad l \geq K_n^{(-)(2)}, \tag{2.22}$$

where $K_n^{(-)(2)} \geq n + 1$.

Proof Setting $f(t) = t^{2l}$ in formula (1.1) with $w = w^{(2)}$, we have

$$\begin{aligned} R_n^{(-)(2)}(t^{2l}) &= \int_{-1}^{1} t^{2l} w^{(2)}(t)dt - \sum_{\nu=1}^{n} w_\nu^{(-)(2)} (\tau_\nu^{(-)(2)})^{2l} - w_{n+1}^{(-)(2)} \\ &< \int_{-1}^{1} t^{2l}(1-t^2)^{1/2} dt - w_{n+1}^{(-)(2)}. \end{aligned} \tag{2.23}$$

Now, since

$$\int_{-1}^{1} t^{2l}(1-t^2)^{1/2} dt = \frac{(2l)!}{2^{2l+1} l!(l+1)!}\pi, \quad l = 0, 1, 2, \ldots \tag{2.24}$$

Table 1 Values of $K_n^{(-)(2)}$, $1 \le n \le 40$

n	$K_n^{(-)(2)}$	n	$K_n^{(-)(2)}$	n	$K_n^{(-)(2)}$	n	$K_n^{(-)(2)}$
1	2	11	51	21	166	31	346
2	4	12	60	22	181	32	368
3	6	13	69	23	197	33	390
4	10	14	79	24	213	34	413
5	14	15	89	25	230	35	437
6	18	16	100	26	248	36	461
7	23	17	112	27	266	37	486
8	29	18	125	28	285	38	512
9	36	19	138	29	305	39	538
10	43	20	151	30	325	40	565

(cf. [9, p. 233] with $m = l$ and $\lambda = 1$), and

$$w_{n+1}^{(-)(2)} = \frac{3\pi}{(n+1)(n+2)(2n+3)} \tag{2.25}$$

(cf. [8, (3.10)] with $\alpha = \beta = 1/2$), (2.23) gives

$$R_n^{(-)(2)}(t^{2l}) < \frac{(2l)!}{2^{2l+1}l!(l+1)!}\pi - \frac{3\pi}{(n+1)(n+2)(2n+3)}, \tag{2.26}$$

and as the first-term on the right-hand side decreases with l, (2.26) implies (2.22) with $K_n^{(-)(2)} \ge n+1$. $\square$

The proof of Lemma 2.4 (cf. (2.26)) shows how to compute the constants $K_n^{(-)(2)}$. Their values for $1 \le n \le 40$ are given in Table 1. Examining (2.22) for the remaining values of l, we find that, when $1 \le n \le 40$, (2.22) holds true for $n+1 \le l \le K_n^{(-)(2)} - 1$. Hence, all together,

$$R_n^{(-)(2)}(t^{2l}) < 0, \quad l \ge n+1,\ 1 \le n \le 40. \tag{2.27}$$

In addition, from (1.3) with $w^{(-)} = w^{(-)(2)}$, there follows that

$$R_n^{(-)(2)}(t^{2l+1}) \ge 0, \quad l \ge n,$$

which, combined with (2.21) and (2.27), gives

$$(-1)^{k-1}R_n^{(-)(2)}(t^k) \ge 0, \quad k \ge 0,\ 1 \le n \le 40. \tag{2.28}$$

Furthermore, a computation similar to that of Lemma 2.7 in Sect. 2.3, which is too technical and lengthy in order to reproduce it here, gives

$$R_n^{(-)(2)}(t^{2n+2}) = -\frac{2n+3}{2^{2n+3}(n+1)^2}\pi, \quad n \ge 1.$$

This, together with our numerical results, suggest the following

Conjecture 2.5 *The error term of formula* (1.1) *with* $w = w^{(2)}$ *satisfies*

$$(-1)^{k-1} R_n^{(-)(2)}(t^k) \geq 0, \quad k \geq 0.$$

Now, we use (2.28) in order to compute $\|R_n^{(-)(2)}\|$ and $\|R_n^{(+)(2)}\|$.

Theorem 2.6 *Consider the Gauss-Radau formula* (1.1) *or* (1.2) *with* $w = w^{(2)}$. *Let* $\tau = r - \sqrt{r^2-1}$. *For* $1 \leq n \leq 40$, *we have*

$$\|R_n^{(-)(2)}\| = \frac{2\pi r \tau^{2n+3}(\frac{n+2}{n+1} - \tau)\sqrt{r^2-1}}{1 - \tau^{2n+4} - \frac{n+2}{n+1}\tau(1-\tau^{2n+2})}. \tag{2.29}$$

The $\|R_n^{(+)(2)}\|$, $1 \leq n \leq 40$, *is given by the same formula* (2.29).

Proof We proceed as in the proof of Theorem 2.3. In view of (2.28), we get, from (1.8$_{ii}$),

$$\|R_n^{(-)(2)}\| = r \left| \frac{1}{(r-1)\pi_n^{(1/2,3/2)}(-r)} \int_{-1}^{1} \frac{\pi_n^{(1/2,3/2)}(t)}{r+t}(1-t)^{1/2}(1+t)^{3/2} dt \right|, \tag{2.30}$$

with $\pi_n^{(1/2,3/2)}$ given by (2.20). Setting $t = \cos\theta$, and using (2.7) (with $2n$ replaced by $n+1$ or n) and (2.15), the integral on the right-hand side of (2.30) computes to

$$\int_{-1}^{1} \frac{\pi_n^{(1/2,3/2)}(t)}{r+t}(1-t)^{1/2}(1+t)^{3/2} dt = \frac{(-1)^n \pi \tau^n (1-\tau^2)(\frac{n+2}{n+1} - \tau)}{2^{n+2}\sqrt{r^2-1}}, \tag{2.31}$$

while, by means of $U_m(-t) = (-1)^m U_m(t)$, $m = 0, 1, 2, \ldots$ (cf. [15, (4.7.2) and (4.7.4)]) and (2.17), we find

$$(r-1)\pi_n^{(1/2,3/2)}(-r) = \frac{(-1)^n [1 - \tau^{2n+4} - \frac{n+2}{n+1}\tau(1-\tau^{2n+2})]}{2^{n+2}\tau^{n+2}\sqrt{r^2-1}},$$

which, inserted, together with (2.31), into (2.30), and noting that $1 - \tau^2 = 2\tau\sqrt{r^2-1}$, yields (2.29).

Since $w^{(2)}$ is even, by virtue of (1.17), $\|R_n^{(+)(2)}\|$ is given by the same formula (2.29). □

In [6, Sect. 4.2], Gautschi, using the contour integration method of the introduction, conjectured that

$$\max_{z \in \bar{C}_r} |K_n^{(-)(2)}(z)| = \frac{\pi}{R^{n+2}} \frac{(R - R^{-1})(R - \frac{n+1}{n+2})}{\frac{n+1}{n+2}(R^{n+2} - R^{-(n+2)}) - (R^{n+1} - R^{-(n+1)})}, \quad n \geq 1, \tag{2.32}$$

where $R = r + \sqrt{r^2 - 1}$. Proceeding similarly to the case of the weight function $w^{(1)}$ (cf. the end of Sect. 2.1), we get, in view of (2.28),

$$\max_{z \in \bar{C}_r} |K_n^{(-)(2)}(z)| = \frac{\| R_n^{(-)(2)} \|}{r}, \quad 1 \le n \le 40,$$

which, on account of (2.29), can be shown to agree with (2.32), thus confirming Gautschi's conjecture at least for $1 \le n \le 40$.

2.3 Chebyshev weight of the third kind

We consider formula (1.1) with $w = w^{(3)}$ (cf. (1.18)). Then, $w^{(-)(3)}(t) = (1+t) \times w^{(3)}(t) = (1-t)^{-1/2}(1+t)^{3/2} = w^{(-1/2,3/2)}(t)$, $-1 < t < 1$, is the Jacobi weight function with parameters $\alpha = -1/2$, $\beta = 3/2$, hence, $\tau_\nu^{(-)(3)}$ are the zeros of $\pi_n^{(-)(3)} = \pi_n^{(-1/2,3/2)}$, the corresponding nth degree (monic) Jacobi polynomial. Using Christoffel's formula in [15, Theorem 2.5] for the distribution $da(t) = w^{(3)}(t)dt$ on $[-1, 1]$ with $\rho(t) = t + 1$, we get

$$\pi_n^{(-)(3)}(t) = \pi_n^{(-1/2,3/2)}(t) = \frac{1}{2^{n+1}} \frac{V_{n+1}(t) + \frac{2n+3}{2n+1} V_n(t)}{t+1}, \quad n \ge 1, \tag{2.33}$$

where V_m is the mth degree Chebyshev polynomial of the third kind.

From what was said in the introduction, and subsequently demonstrated in the case of the weight functions $w^{(1)}$ and $w^{(2)}$ (cf. Sects. 2.1 and 2.2), it is clear that in order to compute $\| R_n^{(-)(3)} \|$, we need to have an assessment on the sign of $R_n^{(-)(3)}(t^k)$, $k \ge 0$. It is known that

$$R_n^{(-)(3)}(t^k) = 0, \quad k = 0, 1, \ldots, 2n. \tag{2.34}$$

The first nontrivial result is contained in the following

Lemma 2.7 *We have*

$$R_n^{(-)(3)}(t^{2n+2}) = \frac{4n^2 + 4n - 1}{2^{2n+1}(2n+1)^2} \pi, \quad n \ge 1. \tag{2.35}$$

Proof The proof is long and technical. First, setting $f(t) = t^{2n+1}(t+1)$ in (1.1) with $w = w^{(3)}$, we get

$$R_n^{(-)(3)}(t^{2n+1}(t+1)) = R_n^{GJ(-1/2,3/2)}(t^{2n+1}),$$

that is,

$$R_n^{(-)(3)}(t^{2n+2}) = R_n^{GJ(-1/2,3/2)}(t^{2n+1}) - R_n^{(-)(3)}(t^{2n+1}), \tag{2.36}$$

where $R_n^{GJ(-1/2,3/2)}$ is the error term of the Gauss formula for the Jacobi weight function $w^{(-1/2,3/2)}$. The $R_n^{GJ(-1/2,3/2)}(t^{2n+k})$, $k = 0, 1, \ldots,$ can be computed explicitly in terms of the coefficients in the series

$$\frac{1}{\pi_n^{(-1/2,3/2)}(t)} = \sum_{k=0}^{\infty} b_{nk}^{(-1/2,3/2)} t^{-n-k}, \quad n \geq 1,$$

and

$$\begin{aligned} q_n^{(-1/2,3/2)}(t) &= \int_{-1}^{1} \frac{\pi_n^{(-1/2,3/2)}(x)}{t-x} w^{(-1/2,3/2)}(x)dx \\ &= \sum_{k=0}^{\infty} c_{nk}^{(-1/2,3/2)} t^{-n-k-1}, \quad n \geq 0, \end{aligned}$$

which both converge absolutely and uniformly for $|t| \geq \mathcal{R} > 1$; in particular,

$$R_n^{GJ(-1/2,3/2)}(t^{2n+1}) = b_{n0}^{(-1/2,3/2)} c_{n1}^{(-1/2,3/2)} + b_{n1}^{(-1/2,3/2)} c_{n0}^{(-1/2,3/2)} \tag{2.37}$$

(cf. [14, Corollary 1] and [12, (3)–(8)]). Now, from [11, Theorems 1, 2 and Sect. 4], taking into account that $\pi_n^{(-1/2,3/2)}$ is a monic polynomial, we have

$$b_{n0}^{(-1/2,3/2)} = 1, \tag{2.38}$$

$$b_{n1}^{(-1/2,3/2)} = \sum_{\nu=1}^{n} \tau_\nu^{(-1/2,3/2)} = \frac{2n}{2n+1}, \tag{2.39}$$

the latter equality obtained by means of [15, Problem 14],

$$c_{n0}^{(-1/2,3/2)} = \int_{-1}^{1} \pi_n^{(-1/2,3/2)}(t) t^n w^{(-1/2,3/2)}(t)dt = \|\pi_n^{(-1/2,3/2)}\|_2^2, \tag{2.40}$$

with $\|\cdot\|_2$ denoting the L_2 norm, and

$$\begin{aligned} c_{n1}^{(-1/2,3/2)} &= \frac{n+1}{2^n k_n^{(-1/2,3/2)}} \int_{-1}^{1} t(1-t)^{n-1/2}(1+t)^{n+3/2}dt \\ &= \frac{n+1}{2^n k_n^{(-1/2,3/2)}} \int_{-1}^{1} t(1+t)^2(1-t^2)^{n-1/2}dt \\ &= \frac{n+1}{2^{n-1} k_n^{(-1/2,3/2)}} \int_{-1}^{1} t^2(1-t^2)^{n-1/2}dt = \frac{1}{k_n^{(-1/2,3/2)}} \frac{(2n)!}{2^{3n}(n!)^2}\pi, \end{aligned} \tag{2.41}$$

where $k_n^{(-1/2,3/2)}$ is the leading coefficient of the (non-monic) Jacobi polynomial $P_n^{(-1/2,3/2)}$ of degree n, and the last integral on the right-hand side of (2.41) was evaluated using [9, p. 233] with $m = 1$ and $\lambda = n$. Then (2.37), by means of (2.38)–(2.41), gives

$$R_n^{GJ(-1/2,3/2)}(t^{2n+1}) = \frac{1}{k_n^{(-1/2,3/2)}} \frac{(2n)!}{2^{3n}(n!)^2}\pi + \frac{2n}{2n+1}\|\pi_n^{(-1/2,3/2)}\|_2^2. \tag{2.42}$$

Also, from (1.3) with $w^{(-)} = w^{(-)(3)}$, there follows that

$$R_n^{(-)(3)}(t^{2n+1}) = \frac{(2n+1)!}{(2n+1)!}\int_{-1}^{1}[\pi_n^{(-)(3)}(t)]^2 w^{(-)(3)}(t)dt$$
$$= \int_{-1}^{1}[\pi_n^{(-1/2,3/2)}(t)]^2 w^{(-1/2,3/2)}(t)dt = \|\pi_n^{(-1/2,3/2)}\|_2^2. \quad (2.43)$$

Inserting (2.42) and (2.43) into (2.36), we get

$$R_n^{(-)(3)}(t^{2n+2}) = \frac{1}{k_n^{(-1/2,3/2)}}\frac{(2n)!}{2^{3n}(n!)^2}\pi - \frac{1}{2n+1}\|\pi_n^{(-1/2,3/2)}\|_2^2,$$

and since

$$k_n^{(-1/2,3/2)} = \frac{1}{2^n}\frac{(2n+1)!}{n!(n+1)!},$$
$$\|\pi_n^{(-1/2,3/2)}\|_2^2 = \frac{1}{[k_n^{(-1/2,3/2)}]^2}\frac{(2n)!(2n+4)!}{2^{4n+3}n![(n+1)!]^2(n+2)!}\pi$$

(cf. [15, (4.21.6) and (4.3.3)] with $\alpha = -1/2,\ \beta = 3/2$), a final computation gives (2.35). □

Unfortunately, the positivity of $R_n^{(-)(3)}(t^{2n+2})$ is not retained for all $R_n^{(-)(3)}(t^{2l})$, $l > n+1$.

Lemma 2.8 *The error term of formula* (1.1) *with* $w = w^{(3)}$ *satisfies*

$$R_n^{(-)(3)}(t^{2l}) \begin{cases} \geq 0, & n+1 \leq l \leq K_n^{(-)(3)} - 1, \\ < 0, & l \geq K_n^{(-)(3)}, \end{cases} \quad (2.44)$$

where $K_n^{(-)(3)} > n+1$.

Proof First of all, from Lemma 2.7, $R_n^{(-)(3)}(t^{2n+2}) > 0$. Furthermore, following the steps in the proof of Lemma 2.4, with

$$\int_{-1}^{1} t^{2l}(1-t)^{-1/2}(1+t)^{1/2}dt = \int_{-1}^{1} t^{2l}(1+t)(1-t^2)^{-1/2}dt$$
$$= \int_{-1}^{1} t^{2l}(1-t^2)^{-1/2}dt = \frac{(2l)!}{2^{2l}(l!)^2}\pi$$

(cf. [9, p. 233] with $m = l$ and $\lambda = 0$) and

$$w_{n+1}^{(-)(3)} = \frac{3\pi}{(n+1)(2n+1)(2n+3)} \quad (2.45)$$

Table 2 Values of $K_n^{(-)(3)}$, $1 \le n \le 10$

n	$K_n^{(-)(3)}$
1	32
2	390
3	2246
4	8666
5	26037
6	65898
7	147187
8	298881
9	563059
10	998360

(cf. [8, (3.10)] with $\alpha = -1/2,\ \beta = 1/2$) in place of (2.24) and (2.25), respectively, we get

$$R_n^{(-)(3)}(t^{2l}) < \frac{(2l)!}{2^{2l}(l!)^2}\pi - \frac{3\pi}{(n+1)(2n+1)(2n+3)},$$

and as $\frac{(2l)!}{2^{2l}(l!)^2}\pi$ decreases with l, we obtain (2.44) with $K_n^{(-)(3)} > n+1$. □

From

$$R_n^{(-)(3)}(t^{2l}) = \int_{-1}^{1} t^{2l} w^{(3)}(t)dt - \sum_{\nu=1}^{n} w_\nu^{(-)(3)}(\tau_\nu^{(-)(3)})^{2l} - w_{n+1}^{(-)(3)},$$

we can find the $K_n^{(-)(3)}$ in (2.44). This is the first (smallest) $l > n+1$ such that $R_n^{(-)(3)}(t^{2l}) < 0$. The values of $K_n^{(-)(3)}$ for $1 \le n \le 10$ are given in Table 2.

By (2.34) and Lemma 2.8, $R_n^{(-)(3)}(t^{2l})$ does not keep a constant sign for all $l \ge 0$, hence, $\|R_n^{(-)(3)}\|$ cannot be computed using (1.8_i)–(1.8_{ii}). The only other option is to start from formula (1.6) and try to get an estimate for the norm. First of all, from (1.3) with $w^{(-)} = w^{(-)(3)}$, there follows that

$$R_n^{(-)(3)}(t^{2l+1}) \ge 0, \quad l \ge n. \tag{2.46}$$

Then (1.6), in view of (2.34), (2.44) and (2.46), gives

$$\begin{aligned}\|R_n^{(-)(3)}\| &= \sum_{k=0}^{K_n^{(-)(3)}-1} \frac{R_n^{(-)(3)}(t^{2k})}{r^{2k}} - \sum_{k=K_n^{(-)(3)}}^{\infty} \frac{R_n^{(-)(3)}(t^{2k})}{r^{2k}} + \sum_{k=0}^{\infty} \frac{R_n^{(-)(3)}(t^{2k+1})}{r^{2k+1}} \\ &= \sum_{k=0}^{\infty} \frac{R_n^{(-)(3)}(t^{k})}{r^{k}} - 2\sum_{k=K_n^{(-)(3)}}^{\infty} \frac{R_n^{(-)(3)}(t^{2k})}{r^{2k}}.\end{aligned} \tag{2.47}$$

A comparison of the first sum on the right-hand side of (2.47) with (1.6) shows that this sum falls under the case (1.7_i) with $\varepsilon = 1$, hence, it can be computed by means of (1.8_i),

$$\sum_{k=0}^{\infty}\frac{R_n^{(-)(3)}(t^k)}{r^k}=\frac{r}{(r+1)\pi_n^{(-1/2,3/2)}(r)}\int_{-1}^{1}\frac{\pi_n^{(-1/2,3/2)}(t)}{r-t}w^{(-1/2,3/2)}(t)dt, \tag{2.48}$$

with $\pi_n^{(-1/2,3/2)}$ given by (2.33) (cf., also, either [1, Sect. 1.2, particularly, p. 16] or the more easily available [2, p. 514]). Following the proofs of Theorems 2.3 and 2.6, and using (2.33), (2.1),

$$\int_0^{\pi}\frac{\cos m\theta}{r-\cos\theta}d\theta=\frac{\pi\tau^m}{\sqrt{r^2-1}},\quad m=0,1,2,\dots \tag{2.49}$$

(cf. (2.15) and set $\pi-\theta$ in place of θ),

$$V_m(r)=U_m(r)-U_{m-1}(r),\quad m=0,1,2,\dots$$

(cf. (2.7), with $2n$ replaced by m and $m-1$, respectively, and (2.1)) and (2.17), we find

$$\int_{-1}^{1}\frac{\pi_n^{(-1/2,3/2)}(t)}{r-t}w^{(-1/2,3/2)}(t)dt=\frac{\pi\tau^n(1+\tau)(\tau+\frac{2n+3}{2n+1})}{2^{n+1}\sqrt{r^2-1}},$$

$$(r+1)\pi_n^{(-1/2,3/2)}(r)=\frac{(1-\tau)[1+\tau^{2n+3}+\frac{2n+3}{2n+1}\tau(1+\tau^{2n+1})]}{2^{n+2}\tau^{n+2}\sqrt{r^2-1}},$$

which inserted into (2.48) give, in view of (2.19),

$$\sum_{k=0}^{\infty}\frac{R_n^{(-)(3)}(t^k)}{r^k}=\frac{2\pi r\tau^{2n+2}(\tau+\frac{2n+3}{2n+1})}{1+\tau^{2n+3}+\frac{2n+3}{2n+1}\tau(1+\tau^{2n+1})}\sqrt{\frac{r+1}{r-1}}. \tag{2.50}$$

We now turn to the second sum on the right-hand side of (2.47). First,

$$\begin{aligned}-2\sum_{k=K_n^{(-)(3)}}^{\infty}\frac{R_n^{(-)(3)}(t^{2k})}{r^{2k}}&=-2R_n^{(-)(3)}\left(\sum_{k=K_n^{(-)(3)}}^{\infty}\left(\frac{t^2}{r^2}\right)^k\right)\\&=-\frac{2}{r^{2K_n^{(-)(3)}-2}}R_n^{(-)(3)}\left(\frac{t^{2K_n^{(-)(3)}}}{r^2-t^2}\right),\end{aligned}$$

and using (1.1) with $w=w^{(3)}$, we write

$$\begin{aligned}-2\sum_{k=K_n^{(-)(3)}}^{\infty}\frac{R_n^{(-)(3)}(t^{2k})}{r^{2k}}&=\frac{2}{r^{2K_n^{(-)(3)}-2}}\left[\frac{w_{n+1}^{(-)(3)}}{r^2-1}-\int_{-1}^{1}\frac{t^{2K_n^{(-)(3)}}}{r^2-t^2}w^{(3)}(t)dt\right]\\&\quad+\frac{2}{r^{2K_n^{(-)(3)}-2}}\sum_{\nu=1}^{n}w_\nu^{(-)(3)}\frac{(\tau_\nu^{(-)(3)})^{2K_n^{(-)(3)}}}{r^2-(\tau_\nu^{(-)(3)})^2}.\end{aligned} \tag{2.51}$$

The integral on the right-hand side of (2.51) can be computed if we set $t=\cos\theta$ and use (1.320.5) in [10], getting

$$\begin{aligned}
&\int_{-1}^{1}\frac{t^{2K_n^{(-)(3)}}}{r^2-t^2}w^{(3)}(t)dt\\
&\quad=\int_{-1}^{1}\frac{t^{2K_n^{(-)(3)}}}{r^2-t^2}(1-t^2)^{-1/2}dt\\
&\quad=\int_{0}^{\pi}\frac{(\cos\theta)^{2K_n^{(-)(3)}}}{r^2-\cos^2\theta}d\theta\\
&\quad=\frac{1}{2^{2K_n^{(-)(3)}}}\left[2\sum_{l=0}^{K_n^{(-)(3)}-1}\binom{2K_n^{(-)(3)}}{l}\int_0^{\pi}\frac{\cos 2(K_n^{(-)(3)}-l)\theta}{r^2-\cos^2\theta}d\theta\right.\\
&\qquad\left.+\binom{2K_n^{(-)(3)}}{K_n^{(-)(3)}}\int_0^{\pi}\frac{d\theta}{r^2-\cos^2\theta}\right],
\end{aligned}$$

where, by applying partial fractions, we find, in view of (2.49), (2.15) and $\tau=r-\sqrt{r^2-1}$,

$$\begin{aligned}
\int_0^{\pi}\frac{\cos m\theta}{r^2-\cos^2\theta}d\theta&=\frac{1}{2r}\left(\int_0^{\pi}\frac{\cos m\theta}{r-\cos\theta}d\theta+\int_0^{\pi}\frac{\cos m\theta}{r+\cos\theta}d\theta\right)\\
&=\begin{cases}\frac{4\pi\tau^{m+2}}{1-\tau^4}, & m\ (\text{even})\geq 0,\\ 0, & m\ (\text{odd})\geq 1,\end{cases}
\end{aligned}$$

so, finally,

$$\begin{aligned}
\int_{-1}^{1}\frac{t^{2K_n^{(-)(3)}}}{r^2-t^2}w^{(3)}(t)dt&=\frac{\pi\tau^2}{2^{2K_n^{(-)(3)}-2}(1-\tau^4)}\\
&\quad\times\left[2\sum_{l=0}^{K_n^{(-)(3)}-1}\binom{2K_n^{(-)(3)}}{l}\tau^{2(K_n^{(-)(3)}-l)}+\binom{2K_n^{(-)(3)}}{K_n^{(-)(3)}}\right].
\end{aligned}\tag{2.52}$$

The last quantity on the right-hand side of (2.51),

$$\frac{2}{r^{2K_n^{(-)(3)}-2}}\sum_{\nu=1}^{n}w_\nu^{(-)(3)}\frac{(\tau_\nu^{(-)(3)})^{2K_n^{(-)(3)}}}{r^2-(\tau_\nu^{(-)(3)})^2},\tag{2.53}$$

cannot be computed explicitly, so we shall try to estimate it. First, setting $t = \cos \frac{2\nu-1}{2n+2}\pi,\ \nu = 1, 2, \ldots, n+1$, in (2.33), we find

$$\pi_n^{(-)(3)}\left(\cos\frac{2\nu-1}{2n+2}\pi\right)$$
$$= (-1)^{\nu-1}\frac{\sin\frac{2\nu-1}{2n+2}\frac{\pi}{2}}{2^n(2n+1)\cos\frac{2\nu-1}{2n+2}\frac{\pi}{2}(1+\cos\frac{2\nu-1}{2n+2}\pi)}, \quad \nu = 1, 2, \ldots, n+1,$$

hence,

$$\operatorname{sign}\pi_n^{(-)(3)}\left(\cos\frac{2\nu-1}{2n+2}\pi\right) = (-1)^{\nu-1}, \quad \nu = 1, 2, \ldots, n+1, \tag{2.54}$$

i.e., the $\tau_\nu^{(-)(3)},\ \nu = 1, 2, \ldots, n$, interlace with the $\cos\frac{2\nu-1}{2n+2}\pi,\ \nu = 1, 2, \ldots, n+1$, which, incidentally, are the zeros of the $(n+1)$th degree Chebyshev polynomial of the first kind. In addition,

$$\pi_n^{(-)(3)}\left(\cos\frac{\pi}{2n+1}\right) = -\frac{\sin\frac{\pi}{2n+1}}{2^{n+1}\cos\frac{\pi}{2(2n+1)}(1+\cos\frac{\pi}{2n+1})},$$
$$\pi_n^{(-)(3)}\left(\cos\frac{2n\pi}{2n+1}\right) = (-1)^n\frac{\frac{2n+3}{2n+1}+\cos\frac{2n\pi}{2n+1}}{2^{n+1}\cos\frac{n\pi}{2n+1}(1+\cos\frac{2n\pi}{2n+1})},$$

that is,

$$\pi_n^{(-)(3)}\left(\cos\frac{\pi}{2n+1}\right) < 0,$$
$$\operatorname{sign}\pi_n^{(-)(3)}\left(\cos\frac{2n\pi}{2n+1}\right) = (-1)^n,$$

which, together with (2.54), give

$$\cos\frac{\pi}{2n+1} < \tau_1^{(-)(3)} < \cos\frac{\pi}{2n+2}, \tag{2.55}$$
$$-\cos\frac{\pi}{2n+1} = \cos\frac{2n\pi}{2n+1} < \tau_n^{(-)(3)} < \cos\frac{2n-1}{2n+2}\pi. \tag{2.56}$$

Now, combining (2.54)–(2.56), we get

$$|\tau_\nu^{(-)(3)}| < \tau_1^{(-)(3)}, \quad \nu = 2, 3, \ldots, n.$$

Based on that, (2.53) takes the form

$$\frac{2}{r^{2K_n^{(-)(3)}-2}}\sum_{\nu=1}^{n} w_\nu^{(-)(3)}\frac{(\tau_\nu^{(-)(3)})^{2K_n^{(-)(3)}}}{r^2-(\tau_\nu^{(-)(3)})^2} < \frac{2}{r^{2K_n^{(-)(3)}-2}}\frac{(\tau_1^{(-)(3)})^{2K_n^{(-)(3)}}}{r^2-(\tau_1^{(-)(3)})^2}\sum_{\nu=1}^{n} w_\nu^{(-)(3)},$$

Table 3 Actual values of the quantity in (2.53) for $1 \le n \le 5$ and certain values of r

n	r	Quantity (2.53)	n	r	Quantity (2.53)	n	r	Quantity (2.53)
1	1.1	1.077(−13)	3	1.1	2.950(−345)	5	1.1	1.719(−2950)
	1.5	2.034(−22)		1.5	1.214(−950)		1.5	m.u.
	2.0	1.853(−30)		2.0	5.719(−1512)		2.0	m.u.
	5.0	5.705(−56)		5.0	1.325(−3299)		5.0	m.u.
	10.0	3.052(−75)		10.0	7.659(−4652)		10.0	m.u.
2	1.1	8.838(−84)	4	1.1	9.404(−1103)			
	1.5	4.427(−189)		1.5	1.012(−3437)			
	2.0	1.288(−286)		2.0	m.u.			
	5.0	4.380(−597)		5.0	m.u.			
	10.0	6.734(−832)		10.0	m.u.			

and using (2.55) and

$$\sum_{\nu=1}^{n} w_\nu^{(-)(3)} = \int_{-1}^{1} w^{(3)}(t)dt - w_{n+1}^{(-)(3)}$$
$$= \pi - \frac{3\pi}{(n+1)(2n+1)(2n+3)}$$
$$= \frac{\pi n(4n^2+12n+11)}{(n+1)(2n+1)(2n+3)}$$

(cf. (1.1), with $w = w^{(3)}$ and $f(t) = 1$, and (2.45)), there finally becomes

$$\frac{2}{r^{2K_n^{(-)(3)}-2}} \sum_{\nu=1}^{n} w_\nu^{(-)(3)} \frac{(\tau_\nu^{(-)(3)})^{2K_n^{(-)(3)}}}{r^2 - (\tau_\nu^{(-)(3)})^2}$$
$$< \frac{2\pi n(4n^2+12n+11)}{(n+1)(2n+1)(2n+3)} \frac{(\cos\frac{\pi}{2n+2})^{2K_n^{(-)(3)}}}{r^{2K_n^{(-)(3)}-2}(r^2 - \cos^2\frac{\pi}{2n+2})}. \tag{2.57}$$

Therefore, the quantity in (2.53) is dominated by $\left(\frac{\cos\frac{\pi}{2n+2}}{r}\right)^{2K_n^{(-)(3)}}$, which, due to the rapidly increasing values of $K_n^{(-)(3)}$ with n (cf. Table 2), decays very fast. In Table 3, we give the actual value of this quantity for $1 \le n \le 5$ and certain values of r. For $n = 4,\ r = 2.0,\ 5.0$ or 10.0 and $n = 5,\ r = 1.5,\ 2.0,\ 5.0$ or 10.0, the quantity in (2.53) is below the smallest positive machine number, i.e., we have a case of underflow and the machine returns a 0; this is indicated by "m.u." for "machine underflow". Given that all computations were performed on a SUN Ultra 5 computer in quad precision, the underflow threshold is 3.362×10^{-4932}. The underflow was also the reason for not computing the quantity in (2.53) for values of $n > 5$.

Inserting (2.50) and (2.51), in view of (2.45), (2.52), $r^2 - 1 = \frac{(1-\tau^2)^2}{4\tau^2}$ and (2.57), into (2.47), we obtain

Theorem 2.9 *Consider the Gauss-Radau formula* (1.1) *with* $w = w^{(3)}$. *Let* $\tau = r - \sqrt{r^2 - 1}$. *There holds*

$$\begin{aligned}
\|R_n^{(-)(3)}\| &< \frac{2\pi r \tau^{2n+2}(\tau + \frac{2n+3}{2n+1})}{1 + \tau^{2n+3} + \frac{2n+3}{2n+1}\tau(1+\tau^{2n+1})}\sqrt{\frac{r+1}{r-1}} \\
&\quad + \frac{2\pi}{r^{2K_n^{(-)(3)}-2}(r^2-1)}\left\{\frac{3}{(n+1)(2n+1)(2n+3)}\right. \\
&\quad - \frac{1-\tau^2}{2^{2K_n^{(-)(3)}}(1+\tau^2)}\left[2\sum_{l=0}^{K_n^{(-)(3)}-1}\binom{2K_n^{(-)(3)}}{l}\tau^{2(K_n^{(-)(3)}-l)}\right. \\
&\quad \left.\left. + \binom{2K_n^{(-)(3)}}{K_n^{(-)(3)}}\right]\right\} \\
&\quad + \frac{2\pi n(4n^2+12n+11)}{(n+1)(2n+1)(2n+3)} \frac{(\cos\frac{\pi}{2n+2})^{2K_n^{(-)(3)}}}{r^{2K_n^{(-)(3)}-2}(r^2 - \cos^2\frac{\pi}{2n+2})}, \quad n \geq 1.
\end{aligned} \tag{2.58}$$

Also, from (1.17) with $w = w^{(3)}$, we get $\|R_n^{(+)(3)}\| = \|R_n^{(-)(4)}\|$, and using Theorem 2.13 in Sect. 2.4, we obtain

Theorem 2.10 *Consider the Gauss-Radau formula* (1.2) *with* $w = w^{(3)}$. *Then* $\|R_n^{(+)(3)}\|$ *is given by formula* (2.69).

In [6, Sect. 4.2], Gautschi estimated $R_n^{(-)(3)}$ using the contour integration method presented in the introduction and conjectured that

$$\max_{z \in \bar{C}_r} |K_n^{(-)(3)}(z)| = K_n^{(-)(3)}(r), \quad n \geq 1. \tag{2.59}$$

Now, although (1.14) gives only a sufficient condition for the maximum of $|K_n^{(-)(3)}(z)|$ on $\bar{C}_r$, the fact that (1.7_i) with $\varepsilon = 1$ does not hold for $w = w^{(3)}$ gives sufficient ground for investigating (2.59) further. Indeed, for $n = 1$, an explicit, and rather tedious, computation shows that

$$K_1^{(-)(3)}(r) \geq K_1^{(-)(3)}(-r) \quad \text{if } r \geq \frac{8\sqrt{7}}{21} = 1.0079052\ldots,$$

and, similarly, for $n = 2$,

$$K_2^{(-)(3)}(r) \geq K_2^{(-)(3)}(-r) \quad \text{if } r \geq \frac{\sqrt{23(1151 + 24\sqrt{2301})}}{230} = 1.0004889\ldots.$$

Consequently, (2.59) is not true for $n = 1$ and $n = 2$, and this throws some doubt upon its validity in general.

2.4 Chebyshev weight of the fourth kind

We consider formula (1.1) with $w = w^{(4)}$ (cf. (1.18)). Then $w^{(-)(4)}(t) = (1+t)w^{(4)}(t) = w^{(2)}(t)$, hence, $\tau_\nu^{(-)(4)} = \tau_\nu^{(2)}$ are the zeros of $\pi_n^{(-)(4)}(t) = \frac{1}{2^n}U_n(t)$, the nth degree (monic) Chebyshev polynomial of the second kind.

The following results will be useful for the computation of $\|R_n^{(-)(4)}\|$.

Proposition 2.11 *The error term of formula* (1.1) *with $w = w^{(4)}$ satisfies*

$$(-1)^{k-1}R_n^{(-)(4)}(t^k) \ge 0, \quad k \ge 0. \tag{2.60}$$

Proof First of all,

$$R_n^{(-)(4)}(t^k) = 0, \quad k = 0, 1, \ldots, 2n. \tag{2.61}$$

Also, if in formula (1.1) with $w = w^{(4)}$, we set $(1+t)f(t)$ in place of $f(t)$, we get

$$\int_{-1}^{1} f(t)w^{(2)}(t)dt = \sum_{\nu=1}^{n}(1+\tau_\nu^{(2)})w_\nu^{(-)(4)}f(\tau_\nu^{(2)}) + R_n^{(-)(4)}((1+\cdot)f(\cdot)),$$

i.e., the Gauss formula for the weight function $w^{(2)}$, hence,

$$R_n^{(-)(4)}((1+\cdot)f(\cdot)) = R_n^{(2)}(f(\cdot)), \tag{2.62}$$

where $R_n^{(2)}$ is the error term of the Gauss formula in question. Setting $f(t) = t^{2l-1}$ in (2.62), we have

$$R_n^{(-)(4)}((1+t)t^{2l-1}) = R_n^{(2)}(t^{2l-1}), \tag{2.63}$$

and since, by symmetry, $R_n^{(2)}(t^{2l-1}) = 0$, (2.63) implies

$$R_n^{(-)(4)}(t^{2l}) = -R_n^{(-)(4)}(t^{2l-1}). \tag{2.64}$$

Now, from (1.3) with $w^{(-)} = w^{(-)(4)}$, there follows that

$$R_n^{(-)(4)}(t^{2l-1}) \ge 0, \quad l \ge n+1,$$

which, together with (2.61) and (2.64), proves our assertion. □

Proposition 2.12 *The error norm of formula* (1.1) *with $w = w^{(4)}$ satisfies*

$$\|R_n^{(-)(4)}\| = \frac{1}{r-1}\|R_n^{(2)}\|, \tag{2.65}$$

where $R_n^{(2)}$ is the error term of the Gauss formula for the weight function $w^{(2)}$.

Proof From [1, (1.1.5)], in view of $R_n^{(2)}(t^{2k}) \ge 0,\ k \ge 0$, and $R_n^{(2)}(t^{2k-1}) = 0,\ k \ge 1$ (cf. [5, (1.18)]), we have

$$\|R_n^{(2)}\| = \sum_{k=0}^{\infty}\frac{R_n^{(2)}(t^{2k})}{r^{2k}}. \tag{2.66}$$

Setting $f(t)=t^{2k}$ in (2.62), we get

$$R_n^{(2)}(t^{2k}) = R_n^{(-)(4)}(t^{2k}) + R_n^{(-)(4)}(t^{2k+1}), \quad k \geq 0, \tag{2.67}$$

while, (2.64), with $l=k+1$, reads

$$R_n^{(-)(4)}(t^{2k+2}) + R_n^{(-)(4)}(t^{2k+1}) = 0, \quad k \geq 0. \tag{2.68}$$

Inserting (2.67) and (2.68) into (2.66), gives, in view of (2.60) and (1.6),

$$\begin{aligned}
\|R_n^{(2)}\| &= \sum_{k=0}^{\infty} \frac{R_n^{(-)(4)}(t^{2k}) + R_n^{(-)(4)}(t^{2k+1})}{r^{2k}} - \sum_{k=0}^{\infty} \frac{R_n^{(-)(4)}(t^{2k+1}) + R_n^{(-)(4)}(t^{2k+2})}{r^{2k+1}} \\
&= r\left[\sum_{k=0}^{\infty} \frac{-R_n^{(-)(4)}(t^{2k+2})}{r^{2k+2}} + \sum_{k=0}^{\infty} \frac{R_n^{(-)(4)}(t^{2k+1})}{r^{2k+1}}\right] \\
&\quad - \left[\sum_{k=0}^{\infty} \frac{-R_n^{(-)(4)}(t^{2k})}{r^{2k}} + \sum_{k=0}^{\infty} \frac{R_n^{(-)(4)}(t^{2k+1})}{r^{2k+1}}\right] \\
&= (r-1)\sum_{k=0}^{\infty} \frac{|R_n^{(-)(4)}(t^{k})|}{r^{k}} = (r-1)\|R_n^{(-)(4)}\|,
\end{aligned}$$

which implies (2.65). □

We can now compute $\|R_n^{(-)(4)}\|$ and $\|R_n^{(+)(4)}\|$.

Theorem 2.13 *Consider the Gauss-Radau formula* (1.1) *with* $w=w^{(4)}$. *Let* $\tau = r-\sqrt{r^2-1}$. *We have*

$$\|R_n^{(-)(4)}\| = \frac{2\pi r \tau^{2n+2}}{1-\tau^{2n+2}}\sqrt{\frac{r+1}{r-1}}, \quad n \geq 1. \tag{2.69}$$

Proof Theorem 3.2 in [13], with $\alpha=1,\ \beta=2$ and $\delta=0$, gives

$$\|R_n^{(2)}\| = \frac{2\pi r \tau^{2n+2}\sqrt{r^2-1}}{1-\tau^{2n+2}}, \quad n \geq 1,$$

which, inserted into (2.65), yields (2.69). □

Theorem 2.14 *Consider the Gauss-Radau formula* (1.2) *with* $w=w^{(4)}$. *Then* $\|R_n^{(+)(4)}\|$ *is given by formula* (2.58).

Proof By (1.17) with $w=w^{(4)}$, we get $\|R_n^{(+)(4)}\| = \|R_n^{(-)(3)}\|$, and the assertion follows. □

In [6, Sect. 4.2], Gautschi, using the contour integration method of the introduction and treating $K_n^{(-)(4)}(z)$ analytically, showed that

$$\max_{z\in\bar{C}_r}|K_n^{(-)(4)}(z)| = 2\pi\frac{R+1}{R-1}\frac{1}{R^{2n+2}-1}, \quad n\geq 1,$$

where $R = r+\sqrt{r^2-1}$. Like in the case of the weight function $w^{(1)}$ (cf. the end of Sect. 2.1), we find, in view of (2.60),

$$\max_{z\in\bar{C}_r}|K_n^{(-)(4)}(z)| = \frac{\|R_n^{(-)(4)}\|}{r}, \quad n\geq 1,$$

which, on account of (2.69), can be shown to agree with Gautschi's result.

3 Examples

Example 3.1

$$\int_{-1}^{1} e^{-t^2}\sqrt{1-t^2}dt. \tag{3.1}$$

The integral will be approximated using formula (1.1) with $w = w^{(2)}$ (cf. (1.18)).

The function $f(z) = e^{-z^2} = \sum_{k=0}^{\infty}\frac{(-1)^k z^{2k}}{k!}$ is entire. Applying (1.4), and taking into account that formula (1.1) has degree of exactness $2n$, we find

$$|f|_r = \begin{cases} \frac{r^{2n+2}}{(n+1)!}, & 1 < r \leq \sqrt{n+2}, \\ \frac{r^{2n+2k+2}}{(n+k+1)!}, & \sqrt{n+k+1} < r \leq \sqrt{n+k+2},\ k = 1,2,\ldots, \end{cases}$$

hence, $f \in X_\infty$ (cf. (1.5)). Then, from (1.10),

$$|R_n^{(-)(2)}(f)| \leq \inf_{1<r<\infty}(\|R_n^{(-)(2)}\||f|_r), \tag{3.2}$$

with the $\|R_n^{(-)(2)}\|$ given by (2.29). Moreover, estimating $|f|_r$ by

$$\max_{|z|=r}|f(z)| = e^{r^2},$$

we get from (1.16),

$$|R_n^{(-)(2)}(f)| \leq \inf_{1<r<\infty}(\|R_n^{(-)(2)}\|e^{r^2}). \tag{3.3}$$

Our results are summarized in Table 4. (Numbers in parentheses indicate decimal exponents.) All computations were performed on a SUN Ultra 5 computer in quad precision (machine precision 1.93×10^{-34}). The value of r, at which the infimum in each of bounds (3.2) and (3.3) was attained, is given in the column headed r_{opt}, which is placed immediately before the column of the corresponding bound. In the

Table 4 Error bounds and actual error in approximating the integral (3.1) using formula (1.1) with $w = w^{(2)}$

n	r_{opt}	Bound (3.2)	r_{opt}	Bound (3.3)	Error
5	2.618	5.367(−6)	2.464	3.357(−5)	1.204(−7)
10	3.412	1.147(−13)	3.321	9.620(−13)	1.106(−15)
15	4.069	2.482(−22)	4.002	2.503(−21)	1.389(−24)
20	4.638	1.116(−31)	4.584	1.287(−30)	7.704(−34)

last column we give the modulus of the actual error. The true value of the integral was computed by means of Gaussian quadrature for the Chebyshev weight function of the second kind.

Both bounds are seen to overestimate the actual error by a few orders of magnitude. In view of the series representation for f, this is due to the high value of $|f|_r$ and of $\max_{|z|=r}|f(z)|$ at $r = r_{opt}$. However, as the actual error decreases rapidly with n, the bounds could be used in order to estimate, not the error itself, but the appropriate value of n which gives rise to that error. An independent computation yields an overestimation of n by at most 2 units, hence, the bounds under consideration are also of practical interest.

Example 3.2

$$\int_{-1}^{1} \frac{t^2}{2(2+t)}\sqrt{\frac{1+t}{1-t}}\,dt = \frac{15-8\sqrt{3}}{12}\pi. \tag{3.4}$$

The integral will be approximated using formula (1.1) with $w = w^{(3)}$ (cf. (1.18)).

The function $f(z) = \frac{z^2}{2(2+z)} = \sum_{k=2}^{\infty} \frac{(-1)^k z^k}{2^k}$ is holomorphic in $C_2 = \{z \in \mathbb{C} : |z| < 2\}$, and

$$|f|_r = \frac{r^{2n+1}}{2^{2n+1}}, \quad 1 < r \le 2,$$

hence $f \in X_2$ (cf. (1.4)–(1.5)). In addition,

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

Thus, (1.10) and (1.16) give

$$|R_n^{(-)(3)}(f)| \le \inf_{1<r\le 2} (\|R_n^{(-)(3)}\| |f|_r), \tag{3.5}$$

$$|R_n^{(-)(3)}(f)| \le \inf_{1<r<2} \left[\|R_n^{(-)(3)}\| \frac{r^2}{2(2-r)} \right], \tag{3.6}$$

with the $\|R_n^{(-)(3)}\|$ given by (2.58). Unfortunately, due to the exceedingly high values of $K_n^{(-)(3)}$ for $n > 2$ (cf. Table 2), the computation of $\binom{2K_n^{(-)(3)}}{l}$, as l approaches $K_n^{(-)(3)}$ (cf. (2.58)), leads to a numerical overflow. To treat this, we first note that, as

Table 5 Error bounds and actual error in approximating the integral (3.4) using formula (1.1) with $w = w^{(3)}$

n	r_{opt}	Bound (3.5)	r_{opt}	Bound (3.6)	Error
1	2.000	1.490(−1)	1.513	1.230(0)	9.331(−2)
2	2.000	9.766(−3)	1.679	1.411(−1)	4.861(−3)
5	2.000	3.283(−6)	1.846	1.089(−4)	1.329(−6)
10	2.000	5.994(−12)	1.918	3.868(−10)	2.220(−12)

$\tau = r - \sqrt{r^2 - 1}$ decreases with r, the same does $2\sum_{l=0}^{K_n^{(-)(3)}-1} \binom{2K_n^{(-)(3)}}{l} \tau^{2(K_n^{(-)(3)}-l)}$, and that way it becomes and remains smaller than $\binom{2K_n^{(-)(3)}}{K_n^{(-)(3)}}$ for all $r \geq r_n > 1$; so, we omit the term $2\sum_{l=0}^{K_n^{(-)(3)}-1} \binom{2K_n^{(-)(3)}}{l} \tau^{2(K_n^{(-)(3)}-l)}$, and, using Stirling's asymptotic formula (cf. [10, (8.327)]), we write

$$\binom{2K_n^{(-)(3)}}{K_n^{(-)(3)}} \simeq \frac{2^{2K_n^{(-)(3)}}}{\sqrt{\pi K_n^{(-)(3)}}},$$

where $a_n \simeq b_n$ has the meaning that $a_n/b_n \to 1$ as $n \to \infty$. Then, $\|R_n^{(-)(3)}\|$ is estimated by

$$\frac{2\pi r \tau^{2n+2}(\tau + \frac{2n+3}{2n+1})}{1 + \tau^{2n+3} + \frac{2n+3}{2n+1}\tau(1 + \tau^{2n+1})} \sqrt{\frac{r+1}{r-1}}$$
$$+ \frac{2\pi}{r^{2K_n^{(-)(3)}-2}(r^2 - 1)} \left[\frac{3}{(n+1)(2n+1)(2n+3)} - \frac{1-\tau^2}{(1+\tau^2)\sqrt{\pi K_n^{(-)(3)}}} \right]$$
$$+ \frac{2\pi n(4n^2 + 12n + 11)}{(n+1)(2n+1)(2n+3)} \frac{(\cos\frac{\pi}{2n+2})^{2K_n^{(-)(3)}}}{r^{2K_n^{(-)(3)}-2}(r^2 - \cos^2\frac{\pi}{2n+2})}. \tag{3.7}$$

Our results are summarized in Table 5.

Estimate (3.7) for $\|R_n^{(-)(3)}\|$ is quite reasonable. Indeed, if, for $n = 1$ and $n = 2$, $\|R_n^{(-)(3)}\|$ is estimated by (2.58), as in these two cases there is no overflow, then the bounds obtained by (3.5) and (3.6) are precisely the same with those shown in Table 5. Furthermore, the bounds in Table 5 remain unchanged if $\|R_n^{(-)(3)}\|$ is estimated by only the first term in (3.7); this is quite interesting as in this case the bounds can easily be computed for all values of n.

References

1. Akrivis, G.: Fehlerabschätzungen bei der numerischen Integration in einer und mehreren Dimensionen. Doctoral Dissertation, Ludwig-Maximilians-Universität, München (1982)

2. Akrivis, G.: The error norm of certain Gaussian quadrature formulae. Math. Comput. **45**, 513–519 (1985)
3. Davis, P.J., Rabinowitz, P.: Methods of Numerical Integration, 2nd edn. Academic Press, San Diego (1984)
4. Engels, H.: Numerical Quadrature and Cubature. Academic Press, San Diego (1980)
5. Gautschi, W.: A survey of Gauss-Christoffel quadrature formulae. In: Butzer, P.L., Fehér, F. (eds.) EB Christoffel: The Influence of His Work in Mathematics and the Physical Sciences, pp. 72–147. Birkhäuser, Basel (1981)
6. Gautschi, W.: On the remainder term for analytic functions of Gauss-Lobatto and Gauss-Radau quadratures. Rocky Mt. J. Math. **21**, 209–226 (1991)
7. Gautschi, W.: Remainder estimates for analytic functions. In: Espelid, T.O., Genz, A. (eds.) Numerical Integration: Recent Developments, Software and Applications. NATO ASI Series, Series C: Mathematical and Physical Sciences, vol. 357, pp. 133–145. Kluwer Academic, Dordrecht (1992)
8. Gautschi, W.: Gauss-Radau formulae for Jacobi and Laguerre weight functions. Math. Comput. Simul. **54**, 403–412 (2000)
9. Gautschi, W., Notaris, S.E.: An algebraic study of Gauss-Kronrod quadrature formulae for Jacobi weight functions. Math. Comput. **51**, 231–248 (1988)
10. Gradshteyn, I.S., Ryzhik, I.M.: Table of Integrals, Series, and Products, 4th edn. Academic Press, San Diego (1980)
11. Hunter, D.B.: Some properties of orthogonal polynomials. Math. Comput. **29**, 559–565 (1975)
12. Hunter, D.B., Smith, H.V.: Some problems involving orthogonal polynomials. In: Brass, H., Hämmerlin, G. (eds.) Numerical Integration IV. International Series of Numerical Mathematics, vol. 112, pp. 189–197. Birkhäuser, Basel (1993)
13. Notaris, S.E.: The error norm of Gaussian quadrature formulae for weight functions of Bernstein-Szegö type. Numer. Math. **57**, 271–283 (1990)
14. Stenger, F.: Bounds on the error of Gauss-type quadratures. Numer. Math. **8**, 150–160 (1966)
15. Szegö, G.: Orthogonal Polynomials, 4th edn. Colloquium Publications, vol. 23. American Mathematical Society, Providence (1975)