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ERROR BOUNDS FOR GAUSS-KRONROD QUADRATURE FORMULAE

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ABSTRACT. The Gauss-Kronrod quadrature formula Q_{2n+1}^{GK} is used for a practical estimate of the error R_n^G of an approximate integration using the Gaussian quadrature formula Q_n^G. Studying an often-used theoretical quality measure, for Q_{2n+1}^{GK} we prove best presently known bounds for the error constants

$$c_s(R_{2n+1}^{GK}) = \sup_{\|f^{(s)}\|_\infty \le 1} |R_{2n+1}^{GK}[f]|$$

in the case $s = 3n+2+\kappa$, $\kappa = \lfloor \frac{n+1}{2} \rfloor - \lfloor \frac{n}{2} \rfloor$. A comparison with the Gaussian quadrature formula Q_{2n+1}^G shows that there exist quadrature formulae using the same number of nodes but having considerably better error constants.

1. INTRODUCTION AND STATEMENT OF THE MAIN RESULTS

For a given nonnegative and integrable weight function w on $[-1, 1]$, a quadrature formula Q_n and the corresponding remainder R_n of (precise) degree of exactness $\deg(R_n) = s$ are linear functionals defined by

$$Q_n[f] = \sum_{\nu=1}^{n} a_{\nu,n} f(x_{\nu,n}), \qquad R_n[f] = \int_{-1}^{1} w(x) f(x)\,dx - Q_n[f],$$

$$\deg(R_n) = s \Leftrightarrow R_n[p_\nu] \begin{cases} = 0, & \nu = 0, 1, \dots, s, \\ \neq 0, & \nu = s+1, \end{cases} \qquad p_\nu(x) = x^\nu$$

with nodes $-\infty < x_{1,n} < \cdots < x_{n,n} < \infty$ and weights $a_{\nu,n} \in \mathbb{R}$. It is well known that the Gaussian quadrature formula $Q_n^G[f] = \sum_{\nu=1}^{n} a_{\nu,n}^G f(x_{\nu,n}^G)$ having the highest possible degree of exactness $\deg(R_n^G) = 2n-1$ exists uniquely under these assumptions.

In order to obtain an estimate for $R_n[f]$ in practice, often a second quadrature formula is used whose nodes, for economical reasons, include $x_{1,n}^G, \dots, x_{n,n}^G$. If there exist $n+1$ further real and distinct nodes $\xi_{1,2n+1}, \dots, \xi_{n+1,2n+1}$ and weights $\beta_{1,2n+1}^{(1)}, \dots, \beta_{n,2n+1}^{(1)}, \beta_{1,2n+1}^{(2)}, \dots, \beta_{n+1,2n+1}^{(2)}$ such that the quadrature formula

$$Q_{2n+1}^{GK}[f] := \sum_{\nu=1}^{n} \beta_{\nu,2n+1}^{(1)} f(x_{\nu,n}^G) + \sum_{\mu=1}^{n+1} \beta_{\mu,2n+1}^{(2)} f(\xi_{\mu,2n+1})$$

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satisfies $\deg(R_{2n+1}^{GK}) \geq 3n+1$, then Q_{2n+1}^{GK} is called a Gauss-Kronrod quadrature formula. Considering $Q_{2n+1}^{GK}[f]$ as a much better approximation than $Q_n^G[f]$, their difference serves as an estimate for $R_n^G[f]$.

For surveys on this method, cf. Gautschi [5] and Monegato [8], while for existence results with respect to special weight functions w cf., e.g., Szegö [14] and the recent results of Notaris [9] and Peherstorfer [10].

The Gauss-Kronrod method is basic for several practical integration routines, e.g. in QUADPACK [11], and hence one of the most often used methods for approximate integration with practical error estimate. Yet, there is still a need for a theoretical study of R_{2n+1}^{GK} which could justify the important role Gauss-Kronrod quadrature plays in practical numerical computation (cf. [8, Part II.2]).

As a basis of a systematic study, and as an often-used quality measure, we define the error constants $c_s(R_{2n+1}^{GK})$ by

$$c_s(R_{2n+1}^{GK}) = \sup_{\|f^{(s)}\|_\infty \leq 1} |R_{2n+1}^{GK}[f]|,$$

where $\|g\|_\infty := \sup_{x\in[-1,1]} |g(x)|$ for $g: [-1, 1] \to \mathbb{R}$. By definition, the error constants $c_s(R_{2n+1}^{GK})$ are the smallest real values independent of f satisfying the standard error bounds

$$|R_{2n+1}^{GK}[f]| \leq c_s(R_{2n+1}^{GK})\|f^{(s)}\|_\infty$$

and are well known to exist whenever $\deg(R_{2n+1}^{GK}) \geq s-1$ (cf. [1]).

Brass and Förster [2] proved

$$\frac{c_{2n}(R_{2n+1}^{GK})}{c_{2n}(R_n^G)} \leq \text{const}\,\sqrt[4]{n}\left(\frac{1}{3.493\ldots}\right)^n$$

and considered this result as a theoretical explanation for the significant superiority of Q_{2n+1}^{GK} over Q_n^G.

Only very little is known about the quality of Q_{2n+1}^{GK} itself. Rabinowitz [12] proved the existence of $c_s(R_{2n+1}^{GK})$ for $s = 1, \ldots, 3n+2+\kappa$, $\kappa = \lfloor\frac{n+1}{2}\rfloor - \lfloor\frac{n}{2}\rfloor$ and nonexistence for $s > 3n+2+\kappa$, showing that $\deg(R_{2n+1}^{GK}) = 3n+1+\kappa$; cf. also Rabinowitz [13] for a proof of the nondefiniteness of R_{2n+1}^{GK}. Brass and Förster [2], Brass and Schmeisser [3], and Monegato [7] proved upper bounds for $c_{3n+2+\kappa}(R_{2n+1}^{GK})$. In the following theorem, we give lower bounds as well as new upper bounds for $c_{3n+2+\kappa}(R_{2n+1}^{GK})$ in the case $w \equiv 1$ that improve the hitherto best-known bounds.

Theorem. *Let* $w \equiv 1$, $n \geq 4$, $\kappa = \lfloor\frac{n+1}{2}\rfloor - \lfloor\frac{n}{2}\rfloor$. *Then there holds*

$$c_{3n+2+\kappa}(R_{2n+1}^{GK}) \leq \overline{c}_{3n+2+\kappa}(R_{2n+1}^{GK}),$$

where

$$\overline{c}_{3n+2+\kappa}(R_{2n+1}^{GK}) := \frac{1}{(3n+2+\kappa)!\,2^{3n+\kappa}}\left\{\frac{17}{10\sqrt{3n-3(2+\kappa)}} + \frac{2\sqrt{2}}{\sqrt{(6n+3+2\kappa)(6n+5+2\kappa)}}\right\}.$$

Furthermore, for n *even there holds*

$$\text{(1.a)}\qquad c_{3n+2}(R_{2n+1}^{GK}) \geq \frac{1}{3e\sqrt{\pi}} \frac{2^{n+3}}{(3n+2)!} \frac{[n!]^4}{(2n)!(2n+1)!} \cdot \sqrt{\frac{3n-2}{n^2-2n} \frac{(2n+3)(5n-3)^2}{(n-2)^2(n+2)(3n-1)^3(3n+1)^2}},$$

while for n *odd there holds*

$$\text{(1.b)}\qquad c_{3n+3}(R_{2n+1}^{GK}) \geq \frac{1}{27e\sqrt{\pi}} \frac{2^{n+3}}{(3n+3)!} \frac{[n!]^4}{(2n)!(2n+1)!} \cdot \sqrt{\frac{3n-1}{n^2-3n} \frac{(2n+3)(5n^2-7n+3)^2}{(n-1)^2n^2(n+2)(n-3)^2(3n-3)(3n-2)^2}}.$$

Remark. While the upper bound in the theorem improves known results, it may still be sharpened. However, an improvement can only be obtained by a polynomial factor, since it follows that

$$\frac{\overline{c}_{3n+2+\kappa}(R_{2n+1}^{GK})}{c_{3n+2+\kappa}(R_{2n+1}^{GK})} = O(n^5)$$

if we replace $c_{3n+2+\kappa}(R_{2n+1}^{GK})$ by the lower bounds (1). A result of Brass and Schmeisser [3, Theorem 7] implies that amongst all quadrature formulae Q_m with positive weights and degree of exactness $\deg(Q_m) \geq 3n+1+\kappa$, the Lobatto formula $Q_{m^*}^{L_0}$ for $m^* = \frac{3n+2+\kappa}{2}$ is worst with respect to the error constant $c_{3n+2+\kappa}(R_{2n+1}^{GK})$, i.e. (cf. [1, p. 149])

$$c_{3n+2+\kappa}(R_m) \leq c_{3n+2+\kappa}(R_{m^*}^{L_0}) = \pi 2^{-(3n+2+\kappa)}(1+o(1)) \quad \text{as } n \to \infty.$$

The lower bounds (1) now prove that Q_{2n+1}^{GK} can be better than this upper bound only by a polynomial factor $(O(n^{5.5}))^{-1}$. Note that Brass and Schmeisser [3, Remark 4] explicitly construct a positive quadrature formula $Q_{3n+2+\kappa}^{BS}$ that satisfies

$$c_{3n+2+\kappa}(R_{3n+2+\kappa}^{BS}) = \pi 4^{-(3n+2+\kappa)}(1+o(1)) \quad \text{as } n \to \infty.$$

In the following corollary we will compare Q_{2n+1}^{GK} and Q_{2n+1}^{G} in order to show that there also exist quadrature formulae using the same number of nodes but having considerably better error constants.

Corollary. *Let* $w \equiv 1$, $n \geq 1$. *Then* $c_{3n+2+\kappa}(R_{2n+1}^{G}) \leq c_{3n+2+\kappa}(R_{2n+1}^{GK})$, *and we have equality only in the case* $n = 1$, *where the Gaussian formula and the Gauss-Kronrod formula are identical. Furthermore, for* $n \geq 15$ *there holds the sharper bound*

$$\frac{c_{3n+2+\kappa}(R_{2n+1}^{G})}{c_{3n+2+\kappa}(R_{2n+1}^{GK})} \leq 3^{-n+1},$$

while asymptotically we find

$$\lim_{n\to\infty} \sqrt[n]{\frac{c_{3n+2+\kappa}(R_{2n+1}^{G})}{c_{3n+2+\kappa}(R_{2n+1}^{GK})}} = \sqrt{\frac{6^6}{7^7}} = \frac{1}{4.2013\ldots}.$$

2. Proofs of the results

In the sequel let $m = \lfloor\frac{n+1}{2}\rfloor$, $\kappa = m - \lfloor\frac{n}{2}\rfloor$, and let $\mathscr{P}_s$ denote the space of polynomials of degree less than or equal to s.

Proof of the Theorem. We will first prove the lower bounds (1). Let $E_{n+1} \in \mathscr{P}_{n+1}$ be defined by

$$E_{n+1} = \sum_{\nu=0}^{m-1} \alpha_{\nu,n} T_{n+1-2\nu} + \begin{cases} \alpha_{m,n} T_1, & n \text{ even}, \\ \frac{1}{2}\alpha_{m,n}, & n \text{ odd}, \end{cases}$$

where T_ν denotes the νth Chebyshev Polynomial of the first kind and

$$\tag{2} \begin{gathered} \alpha_{0,n} = 1, \qquad \alpha_{\nu,n} = -f_{\nu,n} - \sum_{\mu=1}^{\nu-1} f_{\mu,n}\alpha_{\nu-\mu,n}, \quad \nu = 2, 3, \dots, \\ f_{0,n} = 1, \quad f_{\nu,n} = \sigma_{\nu,n} f_{\nu-1,n}, \quad \sigma_{\nu,n} = \left(1 - \frac{1}{2\nu}\right)\left(1 - \frac{1}{2n+2\nu+1}\right). \end{gathered}$$

For reasons of simplicity, when no ambiguity arises, we do not indicate the dependence on n, i.e., $\alpha_\nu := \alpha_{\nu,n}$, $f_\nu := f_{\nu,n}$, and $\sigma_\nu := \sigma_{\nu,n}$. The zeros of E_{n+1} are the additionally chosen nodes $\xi_{1,2n+1}, \dots, \xi_{n+1,2n+1}$ of Q_{2n+1}^{GK} (cf. [7]). Rabinowitz [12] showed that with $g_\kappa = P_n E_{n+1} P_{n+1+\kappa}$ (P_ν denoting the νth Legendre Polynomial) there holds, for n even,

$$R_{2n+1}^{GK}[g_0] = \frac{1}{2n+2}(\alpha_m - \alpha_{m+1}),$$

while for n odd, there holds

$$R_{2n+1}^{GK}[g_1] = \frac{2n+3}{(2n+2)(2n+4)}(\alpha_{m-1} - \alpha_{m+1}).$$

From the definition of the error constants $c_s(R_{2n+1}^{GK})$ we get

$$c_s(R_{2n+1}^{GK}) \geq \frac{|R_{2n+1}^{GK}[f]|}{\|f^{(s)}\|_\infty} \quad \text{for all } f \in C^s[-1, 1]\backslash\mathscr{P}_{s-1}.$$

Defining $p_\nu(x) := x^\nu$, we conclude

$$c_{3n+2+\kappa}(R_{2n+1}^{GK}) \geq \frac{|R_{2n+1}^{GK}[p_{3n+2+\kappa}]|}{(3n+2+\kappa)!}.$$

Taking into account the leading coefficients of P_ν and E_{n+1}, one readily verifies

$$g_\kappa(x) = \frac{(2n)!}{2^n(n!)^2} 2^n \frac{(2n+2+2\kappa)!}{2^{n+1+\kappa}[(n+1+\kappa)!]^2} x^{3n+2+\kappa} + p(x), \qquad p \in \mathscr{P}_{3n+1+\kappa},$$

and, using the linearity and the degree of exactness of R_{2n+1}^{GK},

$$\tag{3} R_{2n+1}^{GK}[p_{3n+2+\kappa}] = \frac{2^{n-1-\kappa}[n!]^4}{(2n)!(2n+1)!}(\alpha_{m-\kappa} - \alpha_{m+1}).$$

We will now derive lower bounds for the difference $|\alpha_{m-\kappa} - \alpha_{m+1}|$. Szegö [14] proved that the sequence $(-\alpha_{\nu+1})$ is positive throughout, and completely monotonic, i.e.,

$$(-1)^{\nu+1}\Delta^\nu \alpha_{\nu+1} > 0, \qquad \nu = 0, 1, 2, \dots,$$

while for its sum he proved $\sum_{\nu=0}^\infty \alpha_{\nu+1} = -1$. In the following Lemma 1 we state some further properties of (α_ν) needed here; the proof of Lemma 1 will be given later.

Lemma 1. *The sequence* (α_ν) *satisfies*

$$\alpha_0 = 1\,, \quad \alpha_1 = -f_1\,, \quad \alpha_\nu = \sum_{\mu=1}^{\nu-1} \alpha_\mu f_{\nu-1-\mu}(\sigma_\nu - \sigma_{\nu-\mu})\,,\ \nu \geq 2.$$

Bounds for (α_ν) *are given by*

$$f_{\nu-1}(\sigma_\nu - \sigma_{\nu-1}) < |\alpha_\nu| < f_{\nu-1}(\sigma_\nu - \sigma_1).$$

Lower bounds for the differences of (α_ν) *are, for every* $p \in \mathbb{N}$,

$$p(\alpha_{\nu+1} - \alpha_\nu) \geq \alpha_{\nu+p} - \alpha_\nu\,,$$
$$p(\alpha_{\nu+1} - \alpha_{\nu-1}) \geq \alpha_{\nu+2p+1} - \alpha_{\nu-1}.$$

According to the lower bounds for the differences in Lemma 1, we are now looking for $p = p(n)$ such that the right-hand sides of

$$|\alpha_m - \alpha_{m+1}| \geq \frac{1}{p(n)}(f_{m-1}(\sigma_m - \sigma_{m-1}) - f_{m+p(n)-1}(1 - \sigma_1))$$

for n even, and

$$|\alpha_{m-1} - \alpha_{m+1}| \geq \frac{1}{p(n)}(f_{m-2}(\sigma_{m-1} - \sigma_{m-2}) - f_{m+2p(n)}(1 - \sigma_1))$$

for n odd, be positive and as big as possible. (Recall the definition of m at the beginning of this section.) By (2) we calculate $1 - \sigma_1 = \frac{n+2}{2n+3}$, and for even $n > 2$,

$$\sigma_m - \sigma_{m-1} = \frac{4(5n-3)}{(n-2)(3n-1)(3n+1)}$$

while for odd $n > 3$,

$$\sigma_{m-1} - \sigma_{m-2} = \frac{4(5n^2 - 7n + 3)}{3n(n-3)(n-1)(3n-2)}.$$

Now let n be even. The following representation of the f_ν can easily be proved by induction:

$$f_\nu = \frac{(2\nu)!}{[\nu!]^2}\left[\frac{(n+\nu)!}{n!}\right]^2 \frac{(2n+1)!}{(2n+2\nu+1)!}. \tag{4}$$

We determine $p = p(n)$ such that

$$f_{m-1}\frac{4(5n-3)}{(n-2)(3n-1)(3n+1)} - f_{m+p(n)-1}\frac{n+2}{2n+3} > 0$$

holds, which is equivalent to

$$\begin{aligned} &\frac{4(2n+3)(5n-3)}{(n-2)(n+2)(3n-1)(3n+1)} \\ &\qquad > \frac{(2m+2p(n)-2)!}{[(m+p(n)-1)!]^2}\frac{((m-1)!)^2}{(2m-2)!}\frac{(2n+2m-2)!}{((n+m-1)!)^2} \\ &\qquad \cdot \frac{((n+m+p(n)-1)!)^2}{(2n+2m+2p(n)-2)!}. \end{aligned} \tag{5}$$

For the right side of the inequality we find by some elementary calculation, using Stirling's formula,

$$\frac{(2m+2p(n)-2)!}{[(m+p(n)-1)!]^2}\frac{((m-1)!)^2}{(2m-2)!}\frac{(2n+2m-2)!}{((n+m-1)!)^2}\frac{((n+m+p(n)-1)!)^2}{(2n+2m+2p(n)-2)!} < \sqrt{e}\frac{2n+2m-1}{2n+2m+2p(n)-1}.$$

Replacing the right side of (5) by this simpler estimate, the following condition for $p(n)$ arises:

$$2p(n) \geq \frac{\sqrt{e}(n-2)(n+2)(3n-1)^2(3n+1)}{4(5n-3)(2n+3)} - (3n-1).$$

We may now choose $p(n)$ for n even as

$$p(n) := \left\lceil c \cdot \frac{\sqrt{e}(n-2)(n+2)(3n-1)^2(3n+1)}{8(2n+3)(5n-3)} - \frac{3n-1}{2}\right\rceil, \qquad c \geq 1,$$

leading to

$$|\alpha_m - \alpha_{m+1}| > \frac{1}{p(n)} f_{m-1} \frac{4(5n-3)}{(n-2)(3n-1)(3n+1)}\left(1 - \frac{1}{c}\right),$$

where for $n \geq 4$ from (4), using Stirling's formula, we can show

$$f_{m-1} \geq \frac{2}{3\sqrt{e\pi}}\sqrt{\frac{3n-2}{n(n-2)}}.$$

Since by definition of $p(n)$,

$$p(n) \leq c \cdot \frac{\sqrt{e}(n-2)(n+2)(3n-1)^2(3n+1)}{8(5n-3)(2n+3)},$$

we readily conclude

$$|\alpha_m - \alpha_{m+1}| > \frac{64}{3e\sqrt{\pi}}\sqrt{\frac{3n-2}{n(n-2)}}\frac{(2n+3)(5n-3)^2}{(n-2)(n+2)(3n-1)^3(3n+1)^2}\left(\frac{c-1}{c^2}\right).$$

Maximizing the right side with respect to $c \geq 1$ leads to $c = 2$ and therefore to the asserted inequality for n even. For the proof of the lower bound for $|\alpha_{m-1} - \alpha_{m+1}|$, n odd, we can proceed in an analogous way. This time, a sufficient condition for the $p(n)$ is

$$\frac{4(2n+3)(5n^2-7n+3)}{3(n-3)(n-1)n(n+2)(3n-2)} > \sqrt{e}\frac{2n+2m-4}{2n+2m+4p(n)+1}.$$

For n odd, we then choose

$$p(n) := \left\lceil c \cdot \frac{3\sqrt{e}(n-3)(n-1)n(n+2)(3n-3)(3n-2)}{16(2n+3)(5n^2-7n+3)} - \frac{3n+2}{4}\right\rceil, \qquad c \geq 1.$$

Using the inequality

$$f_{m-2} \geq \frac{2}{3\sqrt{e\pi}}\sqrt{\frac{3n-1}{n(n-3)}}$$

leads again, after maximization with respect to c, to the lower bound for n odd.

We will now prove the upper bounds stated in the Theorem with the help of the following lemma, which is contained in [2, Theorem 1].

Lemma 2. *Let* R *be a continuous, linear functional on* $C[-1, 1]$ *satisfying* $R[\mathscr{P}_{m-1}] = 0$, *and let*

$$K_{m,s}(x) := \frac{2}{\pi}\frac{m!2^m}{(2m)!}\sum_{\mu=0}^{s-1}(1-x^2)^{m-1/2}R[T_{m+\mu}]\frac{P_\mu^{(m)}(x)}{P_\mu^{(m)}(1)},$$

where $P_\mu^{(m)}$ *denotes the* μ*th ultraspherical polynomial of order* m. *The limit*

$$K_m(x) := \lim_{s\to\infty} K_{m,s}(x), \qquad x \in [-1, 1],$$

exists. If $f \in C^m[-1, 1]$, *then*

$$R[f] = \int_{-1}^{1} f^{(m)}(x)K_m(x)\,dx.$$

If $s = 0, 1, 2, \ldots$, *then*

$$c_m(R) = \int_{-1}^{1} |K_{m,s}(x)|\,dx + \rho_s,$$

where

$$|\rho_s| \le \frac{1}{m!2^{m-1}}\left\{\frac{(2m)!s!}{(2m+s)!}\frac{2m+s}{2m-1}\right\}^{1/2}\sup_{\mu\ge s}|R[T_{\mu+m}]|.$$

Using (3) and $T_\nu(x) = 2^{\nu-1}x^\nu + p(x)$, $p \in \mathscr{P}_{\nu-1}$, we find

$$R_{2n+1}^{GK}[T_{3n+2+\kappa}] = \frac{2^{4n}[n!]^4}{(2n)!(2n+1)!}(\alpha_{m-\kappa} - \alpha_{m+1}). \tag{6}$$

Taking advantage of the monotonicity of $(-\alpha_{\nu+1})$, from Lemma 1 we get

$$|\alpha_{m-\kappa} - \alpha_{m+1}| < |\alpha_{m-\kappa}| < f_{m-1-\kappa}(\sigma_{m-\kappa} - \sigma_1). \tag{7}$$

Using (4), we obtain by the use of Stirling's formula

$$f_{m-1-\kappa} \le \frac{2n+2-\kappa}{3n}\sqrt{\frac{3n-2+\kappa}{n(n-2-\kappa)}}. \tag{8}$$

According to (2) we get for n even

$$\sigma_m - \sigma_1 = \frac{3n^2-n-10}{(2n+3)(3n+1)} \tag{9}$$

and for n odd

$$\sigma_{m-1} - \sigma_1 = \frac{3n^3-5n^2-14n+6}{(n-1)(2n+3)(3n-2)}. \tag{10}$$

Lemma 2 implies for $R = R_{2n+1}^{GK}$, $s = 1$, and $m = 3n+2+\kappa$

$$\begin{aligned} &c_{3n+2+\kappa}(R_{2n+1}^{GK}) \\ &\quad\le |R_{2n+1}^{GK}[T_{3n+2+\kappa}]|\int_{-1}^{1}\left|\frac{2}{\pi}\frac{(3n+2+\kappa)!2^{3n+2+\kappa}}{(6n+4+2\kappa)!}(1-x^2)^{3n+2+\kappa-1/2}\right|dx \\ &\qquad+ \frac{1}{(3n+2+\kappa)!2^{3n+1+\kappa}}\left\{\frac{2(6n+4+2\kappa)!}{(6n+6+2\kappa)!}\frac{6n+6+2\kappa}{6n+3+2\kappa}\right\}^{1/2} \\ &\qquad\cdot \sup_{\mu\ge 2}|R_{2n+1}^{GK}[T_{3n+2+\kappa+\mu}]|. \end{aligned}$$

Since

$$\int_{-1}^{1} |(1-x^2)^{3n+2+\kappa-1/2}|\,dx = \frac{\Gamma(\frac{1}{2})\Gamma(3n+2+\kappa+\frac{1}{2})}{\Gamma(3n+3+\kappa)}$$

and $\sup_{\mu\geq 2} |R_{2n+1}^{GK}[T_{3n+2+\mu}]| \leq 4$, we find

$$c_{3n+2+\kappa}(R_{2n+1}^{GK}) \leq \frac{1}{(3n+2+\kappa)!2^{3n+1+\kappa}} \cdot \left(|R_{2n+1}^{GK}[T_{3n+2+\kappa}]| + \frac{4\sqrt{2}}{\sqrt{(6n+3+2\kappa)(6n+5+2\kappa)}} \right).$$

Using (6), (7), (8), (9), and (10), we conclude the result after some simplifying calculation. □

Proof of Lemma 1. The recursion formula (2) for α_ν and $\alpha_{\nu-1}$, respectively, is

$$\alpha_\nu = -f_\nu - \sum_{\mu=1}^{\nu-1} \alpha_\mu f_{\nu-\mu}, \qquad 0 = -f_{\nu-1} - \sum_{\mu=1}^{\nu-1} \alpha_\mu f_{\nu-1-\mu}.$$

Multiplication of the first by $f_{\nu-1}$ and the second by $-f_\nu$, and summation, yields

$$f_{\nu-1}\alpha_\nu = \sum_{\mu=1}^{\nu-1} \alpha_\mu [f_{\nu-1-\mu} f_\nu - f_{\nu-\mu} f_{\nu-1}] = \sum_{\mu=1}^{\nu-1} \alpha_\mu f_{\nu-1} f_{\nu-1-\mu} (\sigma_\nu - \sigma_{\nu-\mu})$$
$$= f_{\nu-1} \sum_{\mu=1}^{\nu-1} \alpha_\mu f_{\nu-1-\mu} (\sigma_\nu - \sigma_{\nu-\mu}),$$

leading to the first assertion (see also [6] for this method). Using $f_\nu > 0$ and $\sigma_\nu - \sigma_{\nu-\mu} > 0$ for $\mu = 1, \dots, \nu-1$, we find that all terms in the right-hand sum have the same sign, and we conclude the second assertion, using the monotonicity of (σ_ν). Since $(-\alpha_{\nu+1})$ is completely monotonic, the last two inequalities of Lemma 1 follow readily. □

Proof of the Corollary. Theorem 4 of [2] states that

$$c_{3n+2+\kappa}(R_{2n+1}^{G}) \leq \overline{c}_{3n+2+\kappa}(R_{2n+1}^{G}),$$

where

$$\overline{c}_{3n+2+\kappa}(R_{2n+1}^{G}) := \frac{\pi}{(3n+2+\kappa)!2^{3n+2+\kappa}} \cdot \left\{ \frac{(n-\kappa)!(6n+4+2\kappa)!}{(7n+4+\kappa)!} \frac{7n+4+\kappa}{8n+4} \cdot \left(1 + \frac{5}{3} \frac{(n+1-\kappa)(n+2-\kappa)}{(6n+3+2\kappa)(7n+5+\kappa)} \right) \right\}^{1/2}.$$

Using the lower bounds (1) for $c_{3n+2+\kappa}(R_{2n+1}^{GK})$, the following inequality can be proved for $n \geq 4$ after some (elementary) calculation involving Stirling's formula:

$$\frac{c_{3n+2+\kappa}(R_{2n+1}^{G})}{c_{3n+2+\kappa}(R_{2n+1}^{GK})} < c \cdot n^{23/4} \left(\sqrt{\frac{6^6}{7^7}} \right)^n, \tag{11}$$

with $c = 0.62$. Inequality (11) yields $c_{3n+2+\kappa}(R_{2n+1}^{G}) \le c_{3n+2+\kappa}(R_{2n+1}^{GK})$ for $n \ge 10$ and $c_{3n+2+\kappa}(R_{2n+1}^{G})/c_{3n+2+\kappa}(R_{2n+1}^{GK}) \le 3^{-n+1}$ for $n \ge 68$, where for $1 \le n \le 9$ and $15 \le n \le 68$, respectively, the results can be proved numerically (cf. [4]). In [2, Theorem 4] it is stated that the upper bound $\overline{c}_{3n+2+\kappa}(R_{2n+1}^{G})$ can only be improved by $O(n^{3/4})$. Using this result and the remark in §1 to obtain also a lower bound for the ratio in (11), the corollary follows. □

3. Further remarks

1. Using similar methods as described above, respective results can be obtained in the more general case of an ultraspherical weight function (cf. [4]). For $w(x) = (1-x^2)^{\lambda-1/2}$, $\lambda \in (0, 1)$, $n \ge 4$, $\kappa = \lfloor \frac{n+1}{2} \rfloor - \lfloor \frac{n}{2} \rfloor$ there holds $c_{3n+2+\kappa}(R_{2n+1}^{GK}) \le \overline{c}_{3n+2+\kappa}(R_{2n+1}^{GK})$, where

$$\begin{aligned}\overline{c}_{3n+2+\kappa}&(R_{2n+1}^{GK})\\ &:= \frac{1}{(3n+2+\kappa)!2^{3n+1+\kappa}}\left(\frac{\pi\lambda}{2^{2\lambda-1}\Gamma(1-\lambda)}\frac{9n+4\lambda}{9n-3\kappa+4\lambda}\right.\\ &\qquad\cdot\left\{\frac{6(2n+2+\lambda)}{(n+\lambda-1+\kappa)(9n+4\lambda)}\right\}^{\lambda}\\ &\qquad\left.+\frac{2\sqrt{\pi}(\lambda+(1+\kappa)/4)^{\lambda-1}}{\sqrt{(6n+3+2\kappa)(6n+5+2\kappa)}}\right).\end{aligned}$$

Lower bounds for $c_{3n+2+\kappa}(R_{2n+1}^{GK})$ can be found in [4], which for the quality of the upper bounds yield

$$\frac{\overline{c}_{3n+2+\kappa}(R_{2n+1}^{GK})}{c_{3n+2+\kappa}(R_{2n+1}^{GK})} = O(n^{3+1/\lambda}).$$

The corresponding error constants of Q_{2n+1}^{G} are again significantly smaller (cf. [4]).

2. Using the methods derived in the proof of the theorem in §1, we can also prove bounds for the error constants $c_{3n+2+\kappa-s}(R_{2n+1}^{GK})$ of nonmaximum order (cf. [4] for details). In the case of constant $s \in \mathbb{N}$, these bounds are again better than the hitherto best-known bounds. For their quality we can prove

$$\frac{\overline{c}_{3n+2+\kappa-s}(R_{2n+1}^{GK})}{c_{3n+2+\kappa-s}(R_{2n+1}^{GK})} = O(n^{5+(s/2)}).$$

In the case $s = s(n) \in \mathbb{N}$, $\lim_{n\to\infty} \frac{3n+2+\kappa-s}{n} = A > 0$, the new bounds are of quality

$$\lim_{n\to\infty} \sqrt[n]{\frac{\overline{c}_{3n+2+\kappa-s}(R_{2n+1}^{GK})}{c_{3n+2+\kappa-s}(R_{2n+1}^{GK})}} = \frac{A^A(3-A)^{(3-A)/2}(3+A)^{(3+A)/2}}{3^3(2A)^A}.$$

The corresponding error constants of Q_{2n+1}^{G} can be proved to be significantly smaller for $2 < A \le 3$.

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