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The Error Norm of Certain Gaussian Quadrature Formulae

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Abstract. We consider Gauss quadrature formulae Q_n, $n \in \mathbf{N}$, approximating the integral $I(f) := \int_{-1}^{1} w(x)f(x)\,dx$, $w = W/p_i$, $i = 1, 2$, with $W(x) = (1-x)^\alpha(1+x)^\beta$, $\alpha, \beta = \pm 1/2$ and $p_1(x) = 1 + a^2 + 2ax$, $p_2(x) = (2b+1)x^2 + b^2$, $b > 0$. In certain spaces of analytic functions the error functional $R_n := I - Q_n$ is continuous. In [1] and [2] estimates for $\|R_n\|$ are given for a wide class of weight functions. Here, for a restricted class of weight functions, we calculate the norm of R_n explicitly.

1. Introduction. Consider the integral I,

$$I(f) = \int_{-1}^{1} w(x)f(x)\,dx, \qquad w \geqslant 0,\ \|w\|_1 > 0,$$

approximated by the Gaussian quadrature formula Q_n,

$$Q_n(f) = \sum_{i=1}^{n} w_i f(x_i).$$

Let P_k, $P_k(x) = \alpha_k x^k + \beta_k x^{k-1} + \cdots$, $\alpha_k > 0$, $k \in \mathbf{N}_0$, be the orthonormal polynomials corresponding to the weight function w, i.e.,

$$\int_{-1}^{1} w(x)P_i(x)P_j(x)\,dx = \delta_{ij}.$$

The following classical representation for the error term $R_n(f) := I(f) - Q_n(f)$ can be found, e.g., in [4, p. 75],

$$\bigwedge_{f \in C^{2n}[-1,1]} \ \bigvee_{\xi \in (-1,1)} R_n(f) = \frac{1}{(2n)!\alpha_n^2} f^{(2n)}(\xi). \tag{1.1}$$

The estimate

$$|R_n(f)| \leqslant \frac{1}{(2n)!\alpha_n^2} \|f^{(2n)}\|_\infty, \tag{1.2}$$

following immediately from (1.1), is often unsatisfactory, since bounds for higher derivatives are required, and, in addition, the calculation usually has to be repeated for different values of n.

For analytic functions Hämmerlin [8] suggested the following method for obtaining derivative-free error estimates: Let $q_\kappa(x) := x^\kappa$, $\kappa \in \mathbf{N}_0$, $r > 1$ and $C_r := \{z \in \mathbf{C}: |z| < r\}$. For a function f holomorphic in C_r,

$$f(z) = \sum_{\kappa=0}^{\infty} \alpha_\kappa^f z^\kappa, \qquad z \in C_r, \tag{1.3}$$

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define

$$|f|_r := \sup\left\{|\alpha_\kappa^f| r^\kappa : \kappa \in \mathbf{N}_0 \text{ and } R_n(q_\kappa) \neq 0\right\}. \tag{1.4}$$

In the space

$$X_r := \left\{f : f \text{ holomorphic in } C_r \text{ and } |f|_r < \infty\right\}$$

$|\cdot|_r$ is a seminorm. The error functional R_n is continuous in $(X_r, |\cdot|_r)$, and for the error norm

$$\|R_n\| := \sup\left\{\frac{|R_n(f)|}{|f|_r} : f \in X_r, |f|_r \neq 0\right\}$$

the relation

$$\|R_n\| = \sum_{\kappa=0}^{\infty} \frac{|R_n(q_\kappa)|}{r^\kappa} \tag{1.5}$$

holds (see [8], [1], [2]).

For the weight functions considered here, either the condition

$$w(\cdot)/w(-\cdot) \quad \text{is nondecreasing} \tag{1.6}$$

or the condition

$$w(\cdot)/w(-\cdot) \quad \text{is nonincreasing} \tag{1.7}$$

is valid.

Condition (1.6) implies

$$R_n(q_\kappa) \geqslant 0, \qquad \kappa \in \mathbf{N}_0 \tag{1.8}$$

(see [5]). Thus, from (1.5) there follows

$$\|R_n\| = \sum_{\kappa=0}^{\infty} \frac{R_n(q_\kappa)}{r^\kappa} = R_n\left(\sum_{\kappa=0}^{\infty} \frac{q_\kappa}{r^\kappa}\right),$$

i.e.,

$$\|R_n\| = rR_n(\varphi) \quad \text{with } \varphi(x) := 1/(r-x). \tag{1.9}$$

Let the polynomial π_{n-1} of degree less than n interpolate the function φ at the abscissae $x_1, \ldots, x_n$ of Q_n. Since Q_n integrates π_{n-1} exactly, $R_n(\varphi) = R_n(\varphi - \pi_{n-1})$ holds. Setting $\Pi_n(x) := (x - x_1) \cdots (x - x_n)$, we obtain

$$\varphi(x) - \pi_{n-1}(x) = \gamma_n \Pi_n(x)/(r - x),$$

where γ_n is a constant, because the function on the left-hand side vanishes at $x_1, \ldots, x_n$. Multiplying by $r - x$ and taking the limit as $x \to r$ we obtain $\gamma_n = 1/\Pi_n(r)$ (see [3, pp. 71–72]). Thus, from (1.9) we get the representation

$$\|R_n\| = \frac{r}{\Pi_n(r)} \int_{-1}^{1} w(x) \frac{\Pi_n(x)}{r-x} dx \quad \text{with } \Pi_n(x) = \prod_{i=1}^{n} (x - x_i), \tag{1.10}$$

for weight functions satisfying (1.6).

If w satisfies (1.7),

$$(-1)^\kappa R_n(q_\kappa) \geqslant 0 \tag{1.11}$$

holds (see [5]), and we obtain similarly

$$\|R_n\| = rR_n(\psi), \qquad \psi(x) := 1/(r+x), \tag{1.12}$$

and

$$(1.13)\quad \|R_n\| = \frac{r}{\Pi_n(-r)} \int_{-1}^{1} w(x) \frac{\Pi_n(x)}{r+x} dx \quad \text{with } \Pi_n(x) = \prod_{i=1}^{n} (x - x_i).$$

In [1] and [2], estimates for $\|R_n\|$ were derived for weight functions satisfying (1.6) or (1.7), and $\|R_n\|$ was given for $w = W$. Starting from (1.10) or (1.13) respectively, in the next section we calculate the norm of R_n for weight functions w with

$$\begin{aligned} &w = W/p_i, \qquad i = 1, 2,\\ &W(x) = (1-x)^\alpha (1+x)^\beta, \qquad \alpha,\beta = \pm 1/2,\\ &p_1(x) = 1 + a^2 + 2ax,\\ &p_2(x) = (2b+1)x^2 + b^2, \qquad b > 0. \end{aligned}$$

Two numerical examples conclude the paper.

Remark. For even weight functions, (1.4) can be written as $|f|_r = \sup_{\kappa \geq n}\{|\alpha_{2\kappa}^f| r^{2\kappa}\}$ (cf. [1]). If $w(\cdot)/w(-\cdot)$ is strictly monotonic, then $R_n(q_\kappa) \neq 0$ for $\kappa \geq 2n$ (see [5]), and $|\cdot|_r$ can be equivalently defined by $|f|_r := \sup_{\kappa \geq 2n}\{|\alpha_\kappa^f| r^\kappa\}$.

2. The Norm of the Error Functional.

a. $p_1(x) = 1 + a^2 + 2ax$. The case $a = 0, \pm 1$ is treated in [1], [2] if w remains integrable. For $|a| < 1$, $a \neq 0$, put $d := 1/a$ to obtain $p_1(x) = a^2(1 + d^2 + 2dx)$, $|d| > 1$. Therefore we only consider the case $|a| > 1$.

We first summarize some results of Kumar [9] which are important for the subsequent development.

LEMMA 1. *Let $p_1(x) = 1 + a^2 + 2ax$, $|a| > 1$, $W(x) = (1-x)^\alpha(1+x)^\beta$ and $w = W/p_1$. Let T_i and U_i be the Chebyshev polynomials of the first and second kind, respectively. Then the abscissae $x_1, \ldots, x_n$ of the Gauss quadrature formula Q_n corresponding to w are the zeros of*

(i) $aT_n + T_{n-1}$ *if* $\alpha = \beta = -1/2$,

(ii) $aU_n + U_{n-1}$ *if* $\alpha = \beta = 1/2$,

(iii) $aU_n + (1+a)U_{n-1} + U_{n-2}$ *if* $\alpha = -\beta = 1/2$ *and* $n > 1$.

Remark. For $\alpha = \beta = \pm 1/2$ the condition (1.6) is satisfied if $a < -1$, the condition (1.7) if $a > 1$. For $\alpha = -\beta = -1/2$, (1.6) holds, for $\alpha = -\beta = 1/2$ we have (1.7).

We now establish the first of our results.

THEOREM 1. *Consider $p_1(x) = 1 + a^2 + 2ax$, $|a| > 1$, $W(x) = (1-x)^\alpha(1+x)^\beta$, $w = W/p_1$. Let $\tau := r - \sqrt{r^2 - 1}$. For the norm of the error functional R_n the following is true*:

$$(2.1)\qquad \|R_n\| = \frac{2\pi r \tau^{2n}}{(\tau + a)[\tau(1 + \tau^{2n-2}) + a(1 + \tau^{2n})]\sqrt{r^2 - 1}}$$

for $\alpha = \beta = -1/2$ *and* $a < -1$,

$$(2.2)\qquad \|R_n\| = \frac{2\pi r \tau^{2n+2}\sqrt{r^2-1}}{(\tau + a)[\tau(1 - \tau^{2n}) + a(1 - \tau^{2n+2})]}$$

for $\alpha = \beta = 1/2$ *and* $a < -1$,

$$\|R_n\| = \frac{2\pi r \tau^{2n+1}}{(\tau - a)[\tau(1 + \tau^{2n-1}) - a(1 + \tau^{2n+1})]}\left(\frac{r+1}{r-1}\right)^{1/2} \tag{2.3}$$

for $\alpha = -\beta = 1/2$ *and* $n > 1$.

Proof. First, let us verify the identity (2.1). The weight function w satisfies condition (1.6) for $\alpha = \beta = -1/2$ and $a < -1$. Thus, by Lemma 1 (i) and (1.10),

$$\|R_n\| = \frac{r}{aT_n(r) + T_{n-1}(r)} \int_{-1}^{1} (1 - x^2)^{-1/2} \frac{aT_n(x) + T_{n-1}(x)}{(r - x)(1 + a^2 + 2ax)} dx \tag{2.4}$$

holds. Let the integral on the right-hand side of (2.4) be denoted by $I_n(a, r)$. Substituting $x = \cos y$ we obtain

$$I_n(a, r) = \int_0^{\pi} \frac{a\cos(ny) + \cos[(n-1)y]}{(r - \cos y)(1 + a^2 + 2a\cos y)} dy.$$

Set

$$C_n(a) := 2a\int_0^{\pi} \frac{a\cos(ny) + \cos[(n-1)y]}{1 + a^2 + 2a\cos y} dy$$

to obtain

$$I_n(a, r) = \frac{1}{1 + a^2 + 2ar}\left\{\int_0^{\pi} \frac{a\cos(ny) + \cos[(n-1)y]}{r - \cos y} dy + C_n(a)\right\}.$$

Since

$$\int_0^{\pi} \frac{\cos(my)}{r - \cos y} dy = \frac{\pi\tau^m}{\sqrt{r^2 - 1}}$$

(cf., e.g., [7, p. 112]), we have

$$I_n(a, r) = \frac{1}{1 + a^2 + 2ar}\left\{\frac{\pi\tau^{n-1}(a\tau + 1)}{\sqrt{r^2 - 1}} + C_n(a)\right\}.$$

By (1.5), $\|R_n\| = O(r^{-2n})$ holds for $r \to \infty$, and (2.4) yields $I_n(a, r) = O(r^{-n-1})$ for $r \to \infty$. Therefore $C_n(a) = 0$, which can also be established by straightforward calculation. Thus,

$$I_n(a, r) = \frac{\pi\tau^n}{(\tau + a)\sqrt{r^2 - 1}}.$$

Combining this with $T_m(r) = [(r - \sqrt{r^2 - 1})^m + (r + \sqrt{r^2 - 1})^m]/2$ (see [11, p. 5]), the relation (2.1) follows from (2.4).

(2.2) can be proved in a similar way. To prove (2.3), use the relation

$$(1 - x)[U_m(x) + U_{m-1}(x)] = T_m(x) - T_{m+1}(x),$$

which immediately follows from well-known identities for Chebyshev polynomials (cf., e.g., [11, p. 9]).

Remark. $I_n(a, r)$ is also calculated by Kumar [9] by means of the generating function for the polynomials $aT_n + T_{n-1}$.

COROLLARY 1. *Let* $p_1(x) = 1 + a^2 + 2ax$, $|a| > 1$, $W(x) = (1-x)^\alpha(1+x)^\beta$ *and* $w = W/p_1$. *Then the norm of* R_n *can be expressed as*

$$\|R_n\| = \frac{2\pi r \tau^{2n}}{(\tau - a)\left[\tau(1+\tau^{2n-2}) - a(1+\tau^{2n})\right]\sqrt{r^2-1}} \tag{2.5}$$

if $\alpha = \beta = -1/2$ *and* $a > 1$, *and as*

$$\|R_n\| = \frac{2\pi r \tau^{2n+2}\sqrt{r^2-1}}{(\tau - a)\left[\tau(1-\tau^{2n}) - a(1-\tau^{2n+2})\right]} \tag{2.6}$$

if $\alpha = \beta = 1/2$ *and* $a > 1$, *and as*

$$\|R_n\| = \frac{2\pi r \tau^{2n+1}}{(\tau + a)\left[\tau(1+\tau^{2n-1}) + a(1+\tau^{2n+1})\right]}\left(\frac{r+1}{r-1}\right)^{1/2} \tag{2.7}$$

if $\alpha = -\beta = -1/2$ *and* $n > 1$.

Proof. Let R_n and R_n^* be the error functionals corresponding to the weight functions w and $w(-\cdot)$, respectively. Then obviously $R_n(q_\kappa) = (-1)^\kappa R_n^*(q_\kappa)$ holds, and thus $\|R_n\| = \|R_n^*\|$. Hence, the corollary immediately follows from Theorem 1.

b. $p_2(x) = (2b+1)x^2 + b^2$, $b > 0$. We first summarize some results of Kumar [10] which are needed in the sequel.

LEMMA 2. *Let* $p_2(x) = (2b+1)x^2 + b^2$, $b > 0$, $W(x) = (1-x)^\alpha(1+x)^\beta$ *and* $w = W/p_2$. *The abscissae* $x_1, \ldots, x_n$ *of the Gauss quadrature formula* Q_n *corresponding to* w *are the zeros of*

(i) $(2b+1)T_n + T_{n-2}$ *if* $\alpha = \beta = -1/2$ *and* $n > 1$,
(ii) $(2b+1)U_n + U_{n-2}$ *if* $\alpha = \beta = 1/2$ *and* $n > 1$,
(iii) $(2b+1)(U_n + U_{n-1}) + U_{n-2} + U_{n-3}$ *if* $\alpha = -\beta = 1/2$ *and* $n > 2$.

Our second result is presented in the following theorem.

THEOREM 2. *Let* $p_2(x) = (2b+1)x^2 + b^2$, $b > 0$, $W(x) = (1-x)^\alpha(1+x)^\beta$ *and* $w = W/p_2$. *For the norm of the error functional we have*:

$$\|R_n\| = \frac{4\pi r \tau^{2n}}{(b + r\tau)\left[(2b+1)(1+\tau^{2n}) + \tau^2(1+\tau^{2n-4})\right]\sqrt{r^2-1}} \tag{2.8}$$

for $\alpha = \beta = -1/2$, $n > 1$,

$$\|R_n\| = \frac{4\pi r \tau^{2n+2}\sqrt{r^2-1}}{(b + r\tau)\left[(2b+1)(1-\tau^{2n+2}) + \tau^2(1-\tau^{2n-2})\right]} \tag{2.9}$$

for $\alpha = \beta = 1/2$, $n > 1$, *and*

$$\|R_n\| = \frac{4\pi r \tau^{2n+1}}{(b + r\tau)\left[(2b+1)(1+\tau^{2n+1}) + \tau^2(1+\tau^{2n-1})\right]}\left(\frac{r+1}{r-1}\right)^{1/2} \tag{2.10}$$

for $\alpha = -\beta = 1/2$, $n > 2$.

Proof. In this case (1.7) holds, and the results follow from (1.13) using Lemma 2. Symmetry arguments yield the following corollary.

COROLLARY 2. *Let* $w(x) = ((1+x)/(1-x))^{1/2}/[(2b+1)x^2 + b^2]$, $b > 0$. *The norm of the error functional corresponding to* w *is then given by* (2.10) *also*.

Remark. Let $K_n(z) := R_n(\varphi_z)$, $\varphi_z(x) := 1/(z-x)$, $|z| = r$. If f is holomorphic in a region B including C_r the representation

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

holds. Gautschi and Varga [6] showed that for weight functions satisfying either (1.6) or (1.7)

$$\max_{|z|=r} |K_n(z)| = \max\{K_n(r), |K_n(-r)|\} = \sum_{\kappa=0}^{\infty} \frac{|R_n(q_\kappa)|}{r^{\kappa+1}}$$

holds. Therefore, we have $\max_{|z|=r}|K_n(z)| = \|R_n\|/r$, and for the weight functions considered here $\max_{|z|=r}|K_n(z)|$ has also been determined.

3. Numerical Results. For $f \in X_\rho$, $|R_n(f)|$ is bounded by $\|R_n\|\,|f|_r$, $r \in (1, \rho]$. Therefore,

$$|R_n(f)| \leqslant \inf_{1<r\leqslant\rho} \left(\|R_n\|\,|f|_r\right) \tag{3.1}$$

holds. (Although not explicitly noted, $\|R_n\|$ is obviously a function of r.) Estimating $|f|_r$ by $\|f\|_{2,r}$,

$$\|f\|_{2,r} := \frac{1}{\sqrt{2\pi r}}\left(\int_{|z|=r} |f(z)|^2 |dz|\right)^{1/2},$$

or by $\max_{|z|=r}|f(z)|$, which exist at least for $r < \rho$, we obtain

$$|R_n(f)| \leqslant \inf_{1<r<\rho} \left(\|R_n\|\,\|f\|_{2,r}\right) \tag{3.2}$$

and

$$|R_n(f)| \leqslant \inf_{1<r<\rho} \left(\|R_n\| \max_{|z|=r}|f(z)|\right), \tag{3.3}$$

respectively (see [8]). The sharpness of these estimates is demonstrated by two numerical examples.

Example 1. Let $f(z) := \exp(z)$, $f \in X_r$, $r > 1$ ($\rho = \infty$). Approximate the integral

$$\int_{-1}^{1} \frac{1}{(3+2\sqrt{2})(1+x^2)\sqrt{1-x^2}} f(x)\, dx$$

by the Gaussian quadrature formula Q_2 corresponding to

$$w(x) = \frac{1}{(3+2\sqrt{2})(1+x^2)\sqrt{1-x^2}}.$$

The abscissae and the weights of Q_2 are given in [10]. The remainder term is $R_2(f) = 2.016 \cdot 10^{-3}$. Setting $b = 1+\sqrt{2}$ and $n = 2$ in (2.8), we obtain the norm of the error functional R_2. With $|f|_r = r^4/24$ for $1 < r \leqslant \sqrt{30}$, $|f|_r = r^6/720$ for $\sqrt{30} < r \leqslant \sqrt{56}$, and so on, and $\max_{|z|=r}|f(z)| = \exp(r)$, (3.1) and (3.3) yield for $|R_2(f)|$ the bounds $2.019 \cdot 10^{-3}$ ($r = 5.45$) and $1.073 \cdot 10^{-2}$ ($r = 4.15$), respectively.

Example 2. Let

$$f(z) = \sum_{\kappa=4}^{\infty} \left(\frac{z}{2}\right)^{\kappa} = \frac{1}{8}\frac{z^4}{2 - z}, \qquad f \in X_r \text{ for } r \in (1,2] \ (\rho = 2).$$

The remainder term $R_2(f)$ for the approximation of

$$\int_{-1}^{1} \frac{1}{(5 + 4x)\sqrt{1 - x^2}} f(x)\, dx$$

by the Gaussian quadrature formula Q_2 corresponding to

$$w(x) = \frac{1}{(5 + 4x)\sqrt{1 - x^2}}$$

is $7.18 \cdot 10^{-3}$. The abscissae of Q_2 are the zeros of $2T_2 + T_1$ (Lemma 1(i), $a = 2$). We have

$$|f|_r = \frac{r^4}{16}, \qquad \|f\|_{2,r} = \left[\sum_{\kappa=4}^{\infty} \left(\frac{r}{2}\right)^{2\kappa}\right]^{1/2} = \frac{r^4}{8\sqrt{4 - r^2}}$$

(cf. [8]) and $\max_{|z|=r}|f(z)| = r^4/(16 - 8r)$. Setting $a = 2$ and $n = 2$ in (2.5), we obtain the norm of R_2. Now, from (3.1), (3.2) and (3.3), we get for $|R_2(f)|$ the bounds $1.25 \cdot 10^{-2}$ ($r = 2$), $3.06 \cdot 10^{-2}$ ($r = 1.65$) and $8.75 \cdot 10^{-2}$ ($r = 1.50$), respectively.

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