JOURNAL OF APPROXIMATION THEORY **81**, 397–405 (1995)

Error Bounds for Optimal Definite Quadrature Formulae

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Communicated by Allan Pinkus

Received December 2, 1993; accepted in revised form May 4, 1994

Definite quadrature formulae are used to obtain inclusions for the integral of a function f for which $f^{(r)}$ has no sign change. In this paper, error bounds for optimal definite quadrature formulae for the classes $C^r[0, 1]$ $(r \geqslant 1)$ are considered. In the case of odd r (except for special cases), such estimates seem to be unknown. © 1995 Academic Press, Inc.

1. INTRODUCTION AND RESULTS

Let

$$Q_n[f] = \sum_{i=1}^{n} a_i f(\xi_i) \ (0 \leqslant \xi_1 < \cdots < \xi_n \leqslant 1) \tag{1.1}$$

be a quadrature formula for $I[f] = \int_0^1 f(x)\,dx$. If there exists a constant $c_{n,r} = c_{n,r}(Q_n)$ (with $r \geqslant 1$), such that

$$R_n[f] = I[f] - Q_n[f] = c_{n,r} f^{(r)}(\xi) \tag{1.2}$$

for every $f \in C^r[0, 1]$ (with some $\xi \in [0, 1]$ depending on f), then the quadrature formula Q_n is called definite of order r (positive definite, if $c_{n,r} > 0$, and negative definite, if $c_{n,r} < 0$). Definite quadrature formulae are of interest to obtain guaranteed inclusions for the integral. E.g., if $f^{(r)} \geqslant 0$,

* Supported by the European Economic Community under Grant ERB-CIPA-CT-92-2055, and by the Bulgarian Ministry of Science under Grant No. NI-1023.

0021-9045/95 $6.00

Q_n^+ is a positive definite and Q_n^- a negative definite quadrature formula, then $Q_n^+[f] \leqslant I[f] \leqslant Q_n^-[f]$.

Quadrature formulae with smallest positive or largest negative $c_{n,r}$ are called optimal definite quadrature formulae. The existence of optimal definite quadrature formulae was first proven by Schmeisser [9] for even r, and for arbitrary r and more general boundary conditions by Jetter [3] and Lange [5]. Uniqueness has been proven by Lange [5], [6]. Jetter [3] and Lange [5] have also proven some further properties and characterizations of the optimal definite quadrature formulae (see also Brass [2], ch. VII.8).

The topic of this paper are the error constants of the optimal definite quadrature formulae, i.e.,

$$c_{n,r}^+ := \inf\{c_{n,r}(Q_n) : Q_n \text{ is positive definite of order } r\},$$

$$c_{n,r}^- := \sup\{c_{n,r}(Q_n) : Q_n \text{ is negative definite of order } r\}$$

(by definition, $c_{n,r}^+ \geqslant 0$ and $c_{n,r}^- \leqslant 0$). For even r, Lange [5] has shown that

$$c_{n,r}^+ = -\frac{B_r(j/2)}{n^r}\left(1 + O\left(\frac{1}{n}\right)\right) \quad \text{if} \quad r = 4m + 2j, \tag{1.3}$$

$$c_{n,r}^- = -\frac{B_r(j/2)}{n^r}\left(1 + O\left(\frac{1}{n}\right)\right) \quad \text{if} \quad r = 4m + 2 - 2j \tag{1.4}$$

for $j = 0$, 1, where B_r is the Bernoulli polynomial of order r with leading coefficient $1/r!$. (Schmeisser [9] has proven this for optimal definite quadrature formulae with equidistant nodes.)

The following theorem gives explicit bounds for $c_{n,r}^+$ and $c_{n,r}^-$.

THEOREM 1.1. (a) *For even r with $2 \leqslant r \leqslant 2n$, there holds*

$$c_{n,r}^+ \leqslant -\frac{B_r(j/2)}{(n+1-r/2)^r} \quad \textit{if} \quad r = 4m + 2j,\ j = 0, 1.$$

(b) *For even r with $2 \leqslant r \leqslant 2n-2$, there holds*

$$c_{n,r}^- \geqslant -\frac{B_r(j/2)}{(n-r/2)^r} \quad \textit{if} \quad r = 4m + 2 - 2j,\ j = 0, 1.$$

(c) *For odd r with $1 \leqslant r \leqslant 2n-1$, there holds*

$$c_{n,r}^+ \leqslant \frac{\|B_r\|}{(n-(r-1)/2)^r} \quad \textit{and} \quad c_{n,r}^- \geqslant -\frac{\|B_r\|}{(n-(r-1)/2)^r},$$

where $\|\cdot\|$ denotes the supremum norm on $[0, 1]$.

For even r, the bounds given above were also obtained by Strauss [8] (though not in relation to optimal definite quadrature formulae), but the comparison theorem that Strauss uses cannot be applied to yield the result for odd r. A comparison of (a) and (b) with (1.3) and (1.4) shows that these bounds are asymptotically sharp for even r. For odd r, we could not find any result on the size of $c_{n,r}^{+}$ or $c_{n,r}^{-}$ in the literature (except for special cases). Therefore, the bounds given above for odd r seem to be the first available. They are essentially of the same form as for even r (see (2.10), (2.11)), and we conjecture that they are also asymptotically sharp. For $r=1$, 2, there holds equality in Theorem 1.1 (see also the remark below). For $r=3$, 4, Lange [5] has computed $c_{n,3}^{+}(=-c_{n,3}^{-})$ and $c_{n,4}^{+}$ numerically for $n=3, ..., 30$. Using this results, one obtains

$$\frac{\|B_r\|}{n^r} < c_{n,r}^{+} < \frac{\|B_r\|}{(n-1)^r} \qquad \text{for} \quad r=3,\ 4 \text{ and } n=3, ..., 30,$$

where $\|B_3\| = \sqrt{3}/216$ and $\|B_4\| = -B_4(0) = 1/720$. This indicates that the estimates of Theorem 1.1 are quite good.

Jetter [3] and Lange [5] have shown that optimal definite formulae are of Gauss type for certain spaces S of splines with double knots, i.e., they are formulae with minimal number of nodes and the property that $R_n[f]=0$ for all $f \in S$. More precisely, for even r, the optimal positive definite formulae are Gauss formulae, and the optimal negative definite formulae are Lobatto formulae. For odd r, the optimal positive definite formulae are left, and the optimal negative definite formulae are right Radau formulae. Except for special cases, neither the knots of the splines nor the nodes ξ_i of the quadrature formulae are known. As an immediate consequence of this fact that optimal definite formulae are of Gauss type, and of Theorem 1.1, we obtain the following corollary.

COROLLARY 1.1. *Let Q_n be an optimal definite n-point quadrature formula of order r with λ nodes at* 0 *or* 1 *(i.e.,* $\lambda \in \{0, 1, 2\}$*). Then*

$$|c_{n,r}(Q_n)| \leqslant \frac{\|B_r\|}{(n+1-(r+\lambda)/2)^r}.$$

Remark. For fixed n, the highest possible value for r is $r=2n$. In this case, the Gauss-Legendre formula is the optimal positive definite quadrature formula of order $2n$ (a negative definite quadrature formula of order $2n$ does not exist). The optimal definite formulae for $r=1$ are the compound left and right rectangular rule, and for $r=2$ the compound midpoint and the compound trapezoidal rule.

2. The Proof

In the proof of Theorem 1.1, Gauss type formulae for spaces of splines with double and equidistant knots are considered. Error bounds for these formulae are obtained by comparison with shifted Bernoulli monosplines, using the Budan-Fourier Theorem for splines. (More precisely, this means that we obtain pointwise estimates of the highest Peano kernels of the Gaussian formulae by modified Bernoulli monosplines defined in (2.2) and (2.7) below. These pointwise estimates, which may be of interest by themselves, are given in (2.5) for the Gauss formulae, in (2.6) for the Lobatto formulae, and in (2.8) and (2.9) for the Radau formulae). The error bounds obtained in this way are also error bounds for the optimal definite formulae, and are stated in Theorem 1.1. Because of the result of Lange, this means that, for even r, Gauss type formulae for spaces of splines with double, equidistant knots are asymptotically optimal definite formulae of order r.

The method of proof is essentially the same as in our previous paper [4]. We will use the Budan-Fourrier Theorem in the form stated in [4], which is a slight modification of the version of de Boor and Schoenberg [1] (for convenience, we restate it below). For $\bar{a} = (a_1, ..., a_n) \in \mathbb{R}^n$, denote by $S^-(\bar{a})$ the number of strong sign changes in the sequence $a_1, a_2, ..., a_n$, and by $S^+(\bar{a})$ the number of weak sign changes in this sequence. For a spline function f of degree n with simple knots, $Z_{f^{(n)}}(a, b)$ denotes the number of strong sign changes of $f^{(n)}$ in (a, b), and $Z_f(a, b)$ denotes the total number of zeros of f in (a, b).

Theorem 2.1 (Budan-Fourier Theorem for Splines). *If f is a polynomial spline of exact degree n on (a, b) (i.e., of degree n with $f^{(n)}(t) \neq 0$ for some $t \in (a, b)$) with finitely many (active) knots in (a, b), all simple, then*

$$\begin{aligned} Z_f(a, b) \leqslant Z_{f^{(n)}}(a, b) &+ S^-(f(a), f'(a), ..., f^{(n-1)}(a), f^{(n)}(\sigma+)) \\ &- S^+(f(b), f'(b), ..., f^{(n-1)}(b), f^{(n)}(\tau-)), \end{aligned}$$

where $[\sigma, \tau] \subset [a, b]$ is the largest interval such that $f^{(n)}(\sigma+) \neq 0$ and $f^{(n)}(\tau-) \neq 0$.

Proof of Theorem 1.1. Since the cases $r = 1, 2$ are explicitly known, we can assume that $r \geqslant 3$. For $N \geqslant 1$, let $\tau_i = i/N$ and

$$S_{N,r} = \{f \in C^{r-3}[0, 1] : f_{|(\tau_{i-1}, \tau_i)} \in \pi_{r-1} \text{ for } i = 1, ..., N\}, \tag{2.1}$$

where π_{r-1} denotes the space of polynomials of degree strictly less than r ($\dim S_{N,r} = r + 2(N-1)$). We consider Gauss type formulae related to $S_{N,r}$, i.e., quadrature formulae which are exact for $S_{N,r}$, and which have a minimal number of nodes. Since $\pi_{r-1} \subset S_{N,r}$, these quadrature formulae are also exact for π_{r-1}, so that their Peano kernels of order r exist. These Peano kernels have a maximal number of zeros, and the zeros of the Peano kernels in $(0, 1)$ are the knots of the corresponding spline space. Since $S_{N,r}$ has only double knots $\tau_1, ..., \tau_{N-1}$, the Peano kernels have only double zeros in $(0, 1)$ and therefore no sign change, i.e., they are definite. Of importance for the proof is also the fact that the weights a_i of Gauss type formulae are always positive.

In the following, $N = n - m + 1$, where either $r = 2m$ or $r = 2m + 1$.

(a) Let $r = 2m$, and let $Q_n^G[f] = \sum_{i=1}^n a_i^G f(\xi_i^G)$ with $0 < \xi_1^G < \cdots < \xi_n^G < 1$ be the Gauss formula related to $S_{N,r}$. Let $K_{n,r}^G \geqslant 0$ be the Peano kernel of order r of Q_n^G. We will compare $K_{n,r}^G$ with the following monosplines (B_r^* is the Bernoulli monospline of order r, i.e., the 1-periodic extension of $B_{r\,|\,[0,1)}$):

$$K_j(x) = \frac{1}{N^r}\left(B_r^*\left(Nx + \frac{j}{2}\right) - B_r\left(\frac{j}{2}\right)\right) \qquad \text{for} \quad j = 0, 1. \tag{2.2}$$

K_j has the knots $x_{k,j} = (k - j/2)/N$ for $k = 1, ..., N + j - 1$, and double zeros at τ_i for $i = 1, ..., N - 1$. The functions $g_j := K_j - K_{n,r}^G$ are spline functions of degree $r - 1$ with simple knots $\{x_{k,j}\}_{k=1}^{N+j-1} \cup \{\xi_k^G\}_{k=1}^n$, and with double zeros at $\tau_1, ..., \tau_{N-1}$. Using the sign properties of the Bernoulli polynomials, we obtain, with the abbreviation

$$\bar{v}_j := 0, 0, (-1)^{m-2+j}, 0, ..., (-1)^{1+j}, 0, (-1)^{0+j}$$

that

$$S^-(g_j(0), ..., g_j^{(r-1)}(\sigma+)) = S^-(\bar{v}_j, *) \leqslant m - j,$$
$$S^+(g_j(1), ..., g_j^{(r-1)}(\tau-)) = S^+(\bar{v}_j, *) \geqslant m + 1 - j$$

for $j = 0, 1$, where the last entries marked by $*$ are in part unknown. In any case their exact value is of no importance here. The Budan-Fourier Theorem yields

$$2N - 2 \leqslant Z_{g_j}(0, 1) \leqslant Z_{g_j^{(r-1)}}(0, 1) - 1. \tag{2.3}$$

For $x \in (0, 1)$, $g_j^{(r-1)}$ is explicitly given by

$$g_j^{(r-1)}(x) = -\frac{1-j}{2N} - \frac{1}{N}\sum_{k=1}^{N+j-1}(x - x_{k,j})_+^0 + \sum_{k=1}^n a_k^G (x - \xi_k^G)_+^0,$$

and, since $a_k^G > 0$ for all k, it is easy to count the maximal number of sign changes of $g_j^{(r-1)}$, which yields

$$Z_{g_j^{(r-1)}}(0, 1) \leqslant 2N-1. \tag{2.4}$$

In view of (2.3), we conclude that g_j has no other zeros in (0, 1) except the double zeros at the τ_i. But a double zero in the sense of de Boor and Schoenberg [1] cannot be a sign change, and therefore g_j does not change sign in (0, 1). We obtain

$$0 \leqslant K_{n,r}^G \leqslant K_0 \text{ for even } m, \text{ and } 0 \leqslant K_{n,r}^G \leqslant K_1 \text{ for odd } m. \tag{2.5}$$

Therefore,

$$c_{n,r}^+ \leqslant c_{n,r}(Q_n^G) = I[K_{n,r}^G] \leqslant I[K_j],$$

where $j=0$ for even m and $j=1$ for odd m. Then the explicit calculation of $I[K_j]$ completes the proof of part (a).

(b) Let $r=2m$, and let $K_{n+1,r}^L \leqslant 0$ be the Peano kernel of order r of the $(n+1)$-point Lobatto formula related to $S_{N,r}$, $Q_{n+1}^L[f] = \sum_{i=0}^n a_i^L f(\xi_i^L)$ with $0 = \xi_0^L < \cdots < \xi_n^L = 1$. We compare $K_{n+1,r}^L$ with the same monosplines K_j as in (a). Therefore, we now define the functions g_j by $g_j = K_j - K_{n+1,r}^L$. We obtain the same estimates for S^- and S^+ as in (a), so that (2.3) holds, and from

$$g_j^{(r-1)}(x) = a_0^L - \frac{1-j}{2N} - \frac{1}{N} \sum_{k=1}^{N+j-1} (x - x_{k,j})_+^0 + \sum_{k=1}^{n-1} a_k^L (x - \xi_k^L)_+^0$$

for $x \in (0, 1)$, we obtain that also (2.4) holds. Finally,

$$0 \geqslant K_{n+1,r}^L \geqslant K_0 \text{ for odd } m, \text{ and } 0 \geqslant K_{n+1,r}^L \geqslant K_1 \text{ for even } m, \tag{2.6}$$

which, in the same way as in (a), yields lower bounds for $c_{n+1,r}^-$ and proves part (b).

(c) Let $r = 2m+1$. In this case, the left and right Radau quadrature formulae related to $S_{N,r}$ will be considered, $Q_{n+1}^{Ri}[f] = \sum_{i=0}^{n+1} a_i^{Ri} f(\xi_i^{Ri})$ with $0 = \xi_0^{Ri} < \cdots < \xi_{n+1}^{Ri} = 1$, where $i=0$ and $a_{n+1}^{R0} = 0$ for the left Radau formula, and $i=1$ and $a_0^{R1} = 0$ for the right Radau formula (the Radau formulae have a node only at one endpoint, but to unify the presentation, we have added a node with corresponding weight equal to zero at the other endpoint). Let $K_{n+1,r}^{R0} \geqslant 0$ and $K_{n+1,r}^{R1} \leqslant 0$ denote the Peano kernels of order r of the left and right Radau formula, respectively. These Peano kernels again have double zeros at $\tau_1, ..., \tau_{N-1}$. Let $\Theta_0 = \Theta_{0,m} < \Theta_1 = \Theta_{1,m}$ denote the zeros of B_{2m} in (0, 1), and define monosplines L_j by

$$L_j(x) = -\frac{1}{N^r} (B_r^*(Nx + \Theta_j) - B_r(\Theta_j)) \qquad \text{for} \quad j = 0, 1, \tag{2.7}$$

and spline functions $g_{i,j}$ by $g_{i,j} = L_j - K^{Ri}_{n+1,r}$ for $i, j \in \{0, 1\}$. In $(0, 1)$, L_j has N simple knots $x_{k,j} = (k - \Theta_j)/N$ for $k = 1, ..., N$. Moreover, L_j and therefore also $g_{i,j}$ have double zeros at τ_k, $k = 1, ..., N-1$. The calculation of the number of sign changes of the derivatives of $g_{i,j}$ at 0 and 1 makes use of the fact that the sequence $\{\Theta_{0,k}\}_{k=1}^{\infty}$ is monotone increasing, and that the sequence $\{\Theta_{1,k}\}_{k=1}^{\infty}$ is monotone decreasing (Ostrowski [7]). There holds

$$g^{(r-1)}_{i,j}(0+) = \frac{1-2\Theta_j}{2N} - a^{Ri}_0 \text{ and } g^{(r-1)}_{i,j}(1-) = \frac{1-2\Theta_j}{2N} + a^{Ri}_{n+1}.$$

In some cases, this derivatives may be equal to zero, and it is then necessary to choose $\sigma > 0$ or $\tau < 1$, resp., in the Budan-Fourier Theorem. For this reason, we assign the following values to σ and $\vartheta_{i,0}$, depending on the sign of $g^{(r-1)}_{i,0}(0+)$, and to τ and $\vartheta_{i,1}$, depending on the sign of $g^{(r-1)}_{i,1}(1-)$:

$g^{(r-1)}_{i,0}(0+)$	σ	$\vartheta_{i,0}$	$g^{(r-1)}_{i,1}(1-)$	τ	$\vartheta_{i,1}$
>0	$=0$	$=0$	>0	$=1$	$=1$
$=0$	>0	$=1$	$=0$	<1	$=1$
<0	$=0$	$=1$	<0	$=1$	$=0$

(there holds $\vartheta_{1,1} = \vartheta_{0,0}$, and $\vartheta_{0,1} = \vartheta_{1,0} = 0$, because of $\Theta_0 = 1 - \Theta_1$ and $a^{R1}_{n+1} = a^{R0}_0$). In the other cases of interest, the sign of $g^{(r-1)}_{i,j}$ is explicitly known, namely, $g^{(r-1)}_{i,j}(0+) < 0$ and $g^{(r-1)}_{i,j}(1-) > 0$ for $i = 0, 1$. With the abbreviation

$$\bar{v}_0 := 0, 0, (-1)^{m-1}, (-1)^{m-2}, (-1)^{m-2}, ..., (-1)^1, (-1)^1, (-1)^0$$

$$\bar{v}_1 := 0, 0, (-1)^{m-2}, (-1)^{m-2}, (-1)^{m-3}, ..., (-1)^1, (-1)^0, (-1)^0$$

we obtain, for $i = 0, 1$,

$$S^-(g_{i,0}(0), ..., g^{(r-1)}_{i,0}(\sigma+)) = S^-(\bar{v}_0, g^{(r-1)}_{i,0}(\sigma+)) \leqslant m - 1 + \vartheta_{i,0},$$

$$S^+(g_{i,0}(1), ..., g^{(r-1)}_{i,0}(1-)) = S^+(\bar{v}_0, g^{(r-1)}_{i,0}(1-)) = m + 1,$$

$$S^-(g_{i,1}(0), ..., g^{(r-1)}_{i,1}(0+)) = S^-(\bar{v}_1, g^{(r-1)}_{i,1}(0+)) = m - 1,$$

$$S^+(g_{i,1}(1), ..., g^{(r-1)}_{i,1}(\tau-)) = S^+(\bar{v}_1, g^{(r-1)}_{i,1}(\tau-)) \geqslant m + 1 - \vartheta_{i,1}.$$

Application of the Budan-Fourier Theorem now yields

$$2N - 2 \leqslant Z_{g_{i,j}}(0, 1) \leqslant Z_{g^{(r-1)}_{i,j}}(0, 1) - 2 + \vartheta_{i,j}$$

for $i, j \in \{0, 1\}$. The $(r-1)$-st derivatives of the $g_{i,j}$ are explicitly given by

$$g_{i,j}^{(r-1)}(x) = \frac{1-2\Theta_j}{2N} - a_0^{Ri} + \frac{1}{N} \sum_{k=1}^{N} (x - x_{k,j})_+^0 - \sum_{k=1}^{n} a_k^{Ri}(x - \xi_k^{Ri})_+^0.$$

Again, $a_k^{Ri} > 0$ (with the exception of $a_0^{R1} = a_{n+1}^{R0} = 0$), which can be used to obtain upper bounds for the number of sign changes of $g_{i,j}^{(r-1)}$ (where one has also to take into consideration that the sum of the positive jumps is 1, but the sum of the negative jumps is $-\sum_{k=1}^{n} a_k^{Ri} = -1 + a_0^{Ri} + a_{n+1}^{Ri}$, so that the sum of all jumps is $a_0^{Ri} + a_{n+1}^{Ri}$). We obtain

$$Z_{g_{i,j}^{(r-1)}}(0, 1) \leqslant 2N - \vartheta_{i,j},$$

and therefore we conclude that the $g_{i,j}$ have no other zeros in $(0, 1)$ except the double zeros $\tau_1, \ldots, \tau_{N-1}$, which yields that

$$0 \geqslant K_{n+1,r}^{R1} \geqslant L_0 \text{ if } m \text{ is even, } 0 \geqslant K_{n+1,r}^{R1} \geqslant L_1 \text{ if } m \text{ is odd,} \tag{2.8}$$

$$0 \leqslant K_{n+1,r}^{R0} \leqslant L_0 \text{ if } m \text{ is odd, } 0 \leqslant K_{n+1,r}^{R0} \leqslant L_1 \text{ if } m \text{ is even.} \tag{2.9}$$

From this, we obtain the estimates

$$c_{n+1,r}^{+} \leqslant I[K_{n+1,r}^{R1}] \leqslant \frac{1}{(n+1-(r-1)/2)^r} \times \begin{cases} B_r(\Theta_0) & \text{for } r = 4m+3, \\ B_r(\Theta_1) & \text{for } r = 4m+1, \end{cases} \tag{2.10}$$

$$c_{n+1,r}^{-} \geqslant I[K_{n+1,r}^{R0}] \geqslant \frac{1}{(n+1-(r-1)/2)^r} \times \begin{cases} B_r(\Theta_0) & \text{for } r = 4m+1, \\ B_r(\Theta_1) & \text{for } r = 4m+3, \end{cases} \tag{2.11}$$

which proves part (c) (note that $|B_r(\Theta_0)| = |B_r(\Theta_1)| = \|B_r\|$). ∎

ACKNOWLEDGMENTS

The authors than Professor H. Brass for having brought to their attention the paper of A. Ostrowski. The research in this paper was conducted during a stay of the second author at the Technical University of Braunschweig, which was supported by the European Economic Community.

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