ERROR BOUNDS FOR THE NUMERICAL INTEGRATION OF FUNCTIONS WITH LIMITED SMOOTHNESS

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Abstract. We discuss the numerical approximation of weighted integrals by certain interpolatory quadrature formulas. Our class of integration rules includes, among others, the Gauss formula and the Clenshaw-Curtis method. The integrand functions are assumed to have an $s$th (generalized) derivative that is of bounded variation. We demonstrate that, under this assumption, the error for the $n$-point quadrature formula can be bounded by $O(n^{-s-1})$. Our class of functions is closely related to a class recently investigated by Xiang and Bornemann (SIAM J. Numer. Anal. 50 (2012), 2581–2587) that is defined in terms of the decay behaviour of the integrand function’s Chebyshev coefficients. Owing to this relation, our theorems open a possible path for a significant generalization of the results by Xiang and Bornemann and for proving a conjecture of theirs.

Key words. Numerical integration; Gauss quadrature; Clenshaw-Curtis quadrature; error bound; Peano kernel; bounded variation.

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1. Introduction. The numerical approximation of weighted integrals of the form

$$I_w[f] := \int_{-1}^{1} w(x)f(x) \, dx$$

by means of interpolatory quadrature formulas, where $w$ is a nonnegative integrable weight function and $f$ possesses certain smoothness properties, is a classical topic of research that has recently drawn some new attention. Specifically, Xiang and Bornemann [16] discussed this problem for the class of functions

$$X^s := \left\{ f \in C([-1, 1]) : f(x) = \sum_{j=0}^{\infty} a_j T_j(x), \quad |a_j| = O(j^{-s-1}) \right\}$$

for arbitrary $s > 0$. In eq. (1.2), the $a_j$ are the coefficients of the Chebyshev expansion of $f$; it is well known that they can be expressed in the form

$$a_j = \frac{2}{\pi} \int_{-1}^{1} (1 - x^2)^{-1/2} f(x) T_j(x) \, dx$$

where, as usual, $T_j$ denotes the $j$th Chebyshev polynomial of the first kind. The prime in the summation in eq. (1.2) indicates that the summand for $j = 0$ must be halved. In [16], Xiang and Bornemann approximated the integral $I_w[f]$ for $f \in X^s$ and $w \equiv 1$ by the $n$-point Clenshaw-Curtis formula $Q_n^{CC}$ and the $n$-point Gauss quadrature formula $Q_n^{G}$, respectively, and demonstrated that the resulting errors behave as

$$R_n^{CC}[f] := I_w[f] - Q_n^{CC}[f] = O(n^{-s-1}) \quad \text{for } s > 0,$$

$$R_n^{G}[f] := I_w[f] - Q_n^{G}[f] = O(n^{-s-1}) \quad \text{for } s \geq 2,$$

and they conjectured that the estimate (1.3b) is valid also for $0 < s < 2$.

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The goal of this paper is to place these results and conjectures into the context of classical quadrature theory. In particular it is our hope to open up a new path to a possible proof of the conjecture mentioned above and to showing that relations like those of eqs. (1.3a) and (1.3b) actually hold for very many types of quadrature formulas and a large class of weight functions.

Our approach is based on the observation (cf. [14] §4 or [15] Chap. 19) that, for \( s \in \mathbb{N} \), the class \( X^s \) is very closely related to the sets \( V_s \) and \( V_s^T \) defined by

\[
V_s := \{ f \in A^s[-1,1] : \text{Var } f^{(s)} < \infty \} \quad (1.4a) \\
\text{and} \quad V_s^T := \{ f \in A^s[-1,1] : \| f^{(s)} \|_T < \infty \}. \quad (1.4b)
\]

Here, \( A^s[-1,1] \) denotes the set of functions with an absolutely continuous \((s-1)\)st derivative, \( \text{Var } g \) denotes the total variation of the function \( g \) on the interval \([-1,1]\), and

\[
\| u \|_T = \int_{-1}^{1} (1-x^2)^{-1/2} \, du(x).
\]

For later reference we also define the set

\[
V_0 := \{ f \in C[-1,1] : \text{Var } f < \infty \}. \quad (1.5)
\]

For the function classes \( V_s \) with \( s \in \mathbb{N}_0 \), classical Peano kernel theory [2] provides very accurate error estimates in a rather general setting covering a broad class of weight functions and many different quadrature formulas [3] [9]. It is well known that \( V_s \) is a proper subset of \( X^s \) for all \( s \in \mathbb{N} \) [15] Chap. 10, and we believe that the difference set \( X^s \setminus V_s \) is sufficiently small to allow us to carry over the bounds established for \( V_s \) to \( X^s \).

In the context of this paper, by a quadrature formula we will mean a linear functional \( Q \) of the form

\[
Q[f] := \sum_{j=1}^{n} a_j f(x_j)
\]

with certain nodes \(-1 \leq x_1 < x_2 < \ldots < x_n \leq 1\) and weights \( a_j \in \mathbb{R} \). Moreover, following the common terminology in numerical integration [2], we will say that such a quadrature formula is positive if \( a_j \geq 0 \) for all \( j \), and we shall say that a formula is interpolatory of \( Q[p] = I_w[p] \) for all \( p \in \mathcal{P}_{n-1} \), the set of all polynomials of degree not exceeding \( n-1 \).

The most important quadrature formulas to which our theorems below can be applied are as follows:

(i) The Gauss formula \( Q^G_n \) is the \( n \)-point quadrature formula uniquely defined by the condition that \( Q^G_n[p] = I_w[p] \) for all \( p \in \mathcal{P}_{2n-1} \) (cf. [11] [2]).

(ii) The left Radau formula \( Q^{Ra}_{n-1} \) is defined by the requirements that \( x_1 = -1 \) and that \( Q^{Ra}_{n-1}[p] = I_w[p] \) for all \( p \in \mathcal{P}_{2n-2} \). Similarly, the right Radau formula \( Q^{Ra,+1}_n \) is defined by the same exactness condition and the relation \( x_n = 1 \) (cf. [11]).

(iii) The Kronrod formula \( Q^{Kr}_{2n+1} \) is defined by requiring that \( Q^{Kr}_{2n+1}[p] = I_w[p] \) for all \( p \in \mathcal{P}_{3n+1} \) and that the set of nodes of \( Q^{Kr}_{2n+1} \) be a superset of the set of nodes of the Gauss formula \( Q^G_n \) (cf. [4] [8]).

(iv) The Pólya formula \( Q^{Po}_n \) is the interpolatory quadrature formula whose nodes are the zeros of the Chebyshev polynomial of the first kind \( T_n \) (cf. [14]).
(v) The Filippi formula $Q_{n}^{\text{Fi}}$ is the interpolatory quadrature formula whose nodes are the zeros of the Chebyshev polynomial of the second kind $U_{n}$ (cf. [4]).

(vi) For $n \geq 2$, the Clenshaw-Curtis formula $Q_{n}^{\text{CC}}$ is the interpolatory quadrature formula whose nodes are the zeros of the polynomial $(1-x^{2})U_{n-2}(x)$ (cf. [3]).

2. Estimates for functions from the set $V_{s}$. We shall first discuss error estimates for functions from the set $V_{s}$ with some $s \in \mathbb{N}_{0}$. For this set of functions, the Peano kernel theorem provides a most useful representation of the quadrature error. Here and in the following, by $(t)^{m}_{+}$ we denote the truncated power function defined by

$$(t)^{m}_{+} := (\max\{0, t\})^{m}$$

for $m > 0$ and

$$(t)^{0}_{+} := \begin{cases} 0 & \text{for } t < 0, \\ 1/2 & \text{for } t = 0, \\ 1 & \text{for } t > 0. \end{cases}$$

**Theorem 2.1** (Peano kernel theorem). Let $w$ be a nonnegative integrable weight function on $[-1, 1]$ and let $Q$ be a quadrature formula with associated remainder term $R := I_{w} - Q$. Assume that $R[p] = 0$ whenever $p \in \mathbb{P}_{m}$ for some $m \in \mathbb{N}_{0}$. Then, for all $f \in V_{m}$, the remainder $R[f]$ can be expressed as a Stieltjes integral

$$R[f] = \int_{-1}^{1} K_{m+1}(R; x) d f^{(m)}(x)$$

(2.1)

where

$$K_{m+1}(R; x) := \frac{1}{m!} R[(\cdot - x)^{m}]_{+}$$

is the $(m+1)$st Peano kernel of $R$. Hence we have the error estimate

$$|R[f]| \leq \|K_{m+1}(R; \cdot)\|_{\infty} \cdot \text{Var } f^{(m)}. \quad (2.2)$$

A proof for this result may be found in [7] (where $K_{m+1}$ is called an influence function) or [11 Thm. 17]; see also [2, §§4.2 and 4.4]. The more general case where $R$ is an arbitrary continuous linear functional on $C[-1, 1]$ requires a slightly more tedious proof in the case $m = 0$ because the truncated power function of order 0 is discontinuous; we refer to the classical books of Sard [13] or Riesz and Sz.-Nagy [12] for details.

We note an immediate nonclassical consequence of eq. (2.1) that may prove useful in the context of the seminorm $\| \cdot \|_{T}$:

**Corollary 2.2.** Under the assumptions of the Peano kernel theorem, we have that

$$|R[f]| \leq \sup_{-1 \leq x \leq 1} (1 - x^{2})^{1/2} |K_{m+1}(x)| \cdot \|f^{(m)}\|_{T}. \quad (2.3)$$

**Proof.** The statement follows directly from the definition of $\| \cdot \|_{T}$ and eq. (2.1).
It is evident from eqs. (2.2) and (2.3) that upper bounds for the (weighted) supremum norm of the Peano kernel of the quadrature error will immediately yield error bounds for the function sets \( V_m \) and \( V_m^T \). Fortunately, such bounds are readily available for various important classes of quadrature formulas.

**Theorem 2.3.** Let \( w : (-1, 1) \to \mathbb{R} \) be a nonnegative and integrable weight function and assume that there exists some \( M > 0 \) such that \( w(x) \leq M(1-x^2)^{-1/2} \) for all \( x \in (-1, 1) \). For \( n = 1, 2, 3, \ldots \), let \( Q_n \) be a positive interpolatory quadrature formula with \( n \) nodes and let \( R_n := I_w - Q_n \) be the associated remainder term. Then, for all \( m = 0, 1, 2, \ldots \), we have

\[
\|K_{m+1}(R_n; \cdot)\|_\infty = O(n^{-m-1}) \quad (n \to \infty).
\]

**Proof.** This result follows from a classical statement of Freud [5]; see also [9] for additional details including a discussion of the constants implied in the \( O \)-term. \( \square \)

**Remark 2.1.** It is well known that the class of quadrature formulas covered by Theorem 2.3 contains, in particular,

(i) the Gauss and Radau formulas for all weight functions admissible under the conditions of the theorem [1],

(ii) the formulas of Clenshaw-Curtis, Filippi and Polya, at least for the standard weight function \( w \equiv 1 \),

(iii) the Gauss-Kronrod formulas for the ultraspherical weight functions \( w_\lambda(x) = (1-x^2)^{\lambda-1/2} \) where \( \lambda \in [0, 1] \cup \{3\} \), cf. [10] where it is also conjectured that all \( \lambda \in [0, 3] \) are admissible.

We end this section by noticing that the norms of the Peano kernels of a type of quadrature formulas based on completely different construction principles also show the same decay behaviour. To this end, we restrict our attention to the weight function \( w \equiv 1 \) and let \( Q \) be an arbitrary quadrature formula given by

\[
Q[f] = \sum_{j=1}^{\ell} a_j f(x_j)
\]

that satisfies the condition \( R[p] := I_w[p] - Q[p] = 0 \) for all \( p \in \mathcal{P}_m \). We can then subdivide the basic interval \([-1, 1]\) into \( n \) subintervals of length \( 2/\ell \), affinely transform \( Q \) to each of these subintervals and add up the resulting formulas, thus obtaining the \( n \)-fold compound quadrature formula with respect to the elementary formula \( Q \), denoted and defined by

\[
Q^{(n)}[f] := \frac{1}{n} \sum_{\nu=1}^{n} \sum_{j=1}^{\ell} a_j f \left( -1 + \frac{1}{n} (x_j + 2\nu - 1) \right).
\]

As usual we will denote the associated error term by \( R^{(n)} := I_w - Q^{(n)} \). In view of the considerations above, it is then clear that the Peano kernels \( K_{m+1}(R; \cdot) \) and \( K_{m+1}(R^{(n)}; \cdot) \) exist for all \( n = 1, 2, \ldots \). In fact, the kernels \( K_{m+1}(R^{(n)}; \cdot) \) can be obtained by a simple affine mapping from the kernel \( K_{m+1}(R; \cdot) \), and this yields an immediate bound on their supremum norms:

**Theorem 2.4.** Under the assumptions above, we have

\[
\|K_{m+1}(R^{(n)}; \cdot)\|_\infty = 2^{m+1} \|K_{m+1}(R; \cdot)\|_\infty \cdot n^{-m-1}.
\]

**Proof.** This is a direct consequence of [11, Thm. 93]. \( \square \)
It should be noted that, asymptotically, the number of nodes of $Q^{(n)}$ is a constant multiple of $n$. Precisely speaking, $Q^{(n)}$ has $\ell n$ nodes if and only if at most one of the points $\pm 1$ is a node of the underlying elementary formula $Q$: if both these points are nodes of $Q$ then $Q^{(n)}$ has $(\ell - 1)n + 1$ nodes. Thus, the computational cost of evaluating $Q^{(n)}$ is $O(n)$ operations.

We hence conclude that the errors of compound quadrature formulas have the same asymptotic decay rate, but the implied constants may differ from those of the interpolatory rules discussed in Theorem 2.3. The more important difference is, though, that bounds of the form

$$|R[f]| \leq cn^{-s-1} \text{Var } f^{(s)}$$

follow for the interpolatory rules of Theorems 2.3 for arbitrary $s \in \mathbb{N}_0$ whereas they are valid for the compound rules of Theorem 2.4 only for $s = 0, 1, \ldots, \hat{s}$ where

$$\hat{s} := \sup\{\sigma \in \mathbb{N}_0 : R[p] = 0 \text{ for all } p \in \mathcal{P}_\sigma\}.$$

In summary, we have thus shown:

**Theorem 2.5.**

(i) Let $Q_n$ be a positive $n$-point interpolatory quadrature formula for a weight function that satisfies the assumptions of Theorem 2.3. Then, for all $s \in \mathbb{N}_0$ there exists a constant $c_s$ such that for all $f \in V_s$ we have the error bound

$$|R_n[f]| \leq c_s n^{-s-1} \text{Var } f^{(s)} = O(n^{-s-1}).$$

(ii) For every $n \in \mathbb{N}$, let $Q^{(n)}$ be a compound quadrature formula with the same elementary quadrature formula $Q$, and let

$$\hat{s} := \sup\{\sigma \in \mathbb{N}_0 : R[p] = 0 \text{ for all } p \in \mathcal{P}_\sigma\}.$$

Then, for all $s \in \{0, 1, \ldots, \hat{s}\}$ there exists a constant $c_s$ such that for all $f \in V_s$ we have the error bound

$$|R^{(n)}[f]| \leq c_s n^{-s-1} \text{Var } f^{(s)} = O(n^{-s-1}).$$

**3. Future work and further comments.** In view of Theorem 2.5 and the above mentioned close relation between the sets $V_s$ and $X^*$, the error bounds provided by Xiang and Bornemann appear to be rather natural and not unexpected. In particular the yit very nicely into the classical theory.

A close inspection shows that Theorem 2.5 covers certain cases not yet handled by Xiang and Bornemann. In particular,

- it is valid for $s = 0$ for the Clenshaw-Curtis formula and for $s \in \{0, 1\}$ for the Gauss formula,
- it also holds (for all $s \in \mathbb{N}_0$) for a large class of other interpolatory quadrature formulas,
- it allows to treat the problem for weight functions other than the Legendre weight $w \equiv 1$,
- and it can be applied to compound quadrature rules for sufficiently small $s$.

On the other hand, it is not directly applicable for $s \notin \mathbb{N}_0$, and it does not yet cover the full function class $X^*$. Nevertheless we hope that a combination of our approach with other methods will be able to provide the missing elements that first extend our results to the sets $X^*$, $s \in \mathbb{N}_0$, by a more detailed investigation of the relations

$$|R[f]| \leq cn^{-s-1} \text{Var } f^{(s)}$$
between the sets $V_s$ and $X_s$, thus showing that the asymptotic decay behaviour that we have proven to hold in $V_s$ for our large classes of weight functions and quadrature formulas are also valid in $X_s$. This should hopefully then be augmented by suitable techniques permitting to prove the results also to $X_s$ with $s \notin \mathbb{N}$.

We end our paper with some comments regarding certain statements on questions relevant in this context that were given in the recent literature. To be precise, the corresponding chapter of Trefethen’s recent book [15, Chap. 19] appears to contain two mistakes. Trefethen’s opinion (private communication) is that these are typographical errors.

Specifically, Trefethen [15, eq. (19.10)] writes that, for every $\nu \in \mathbb{N}$, there exists a constant $c_\nu$ such that the Gaussian quadrature formula satisfies

$$|R_n^{G}| \leq c_\nu n^{-2\nu - 1} \text{Var} f^{(\nu)}$$  \hspace{1cm} (3.1)

for all sufficiently large $n$ if $f^{(\nu)}$ is of bounded variation. If this were true, then it would follow, since the bound from eq. (2.2) is clearly unimprovable, that

$$|K_{\nu + 1}(R_n^{G}; x)| \leq c_\nu n^{-2\nu - 1}$$  \hspace{1cm} (3.2)

for all $x \in [-1, 1]$ and all $\nu \in \mathbb{N}$ if $n$ is sufficiently large. In view of the well known relation $K_{\nu + 1}(R_n^{G}; x) = -\int_{-1}^{x} K_m(R_n^{G}; x) \, dx$ (cf. [1, Thm. 16]) for sufficiently large $n$, this would imply

$$\|K_{\nu + 2}(R_n^{G}; \cdot)\|_1 \leq 2 \|K_{\nu + 2}(R_n^{G}; \cdot)\|_\infty \leq 2 \sup_{x \in [-1, 1]} \left| \int_{-1}^{x} K_{\nu + 1}(R_n^{G}; t) \, dt \right|$$

$$\leq 4 \sup_{x \in [-1, 1]} |K_{\nu + 1}(R_n^{G}; x)| \leq 4 c_\nu n^{-2\nu - 1}.$$  

For $\nu > 1$ this, however, contradicts the well known result [9] that

$$\|K_{\nu + 2}(R_n^{G}; \cdot)\|_1 = C_\nu n^{-\nu-2}(1 + o(1))$$

with a certain constant $C_\nu$ that is also discussed in detail in [9]. We thus conclude that [15, eq. (19.10)] is incorrect for $\nu > 1$.

In the same way we can see that the corresponding statement claimed for the Clenshaw-Curtis formula [15, eq. (19.12)] is not true either. A comparison with the original source [14] reveals the correct form.

Clearly the even stronger statement [15, p. 151] that the bounds [15 eqs. (19.10) and (19.12)] can be improved by a factor of $1/n$ is not valid either when applied to the inequalities in the misprinted form given in [15]; the true interpretation of these statements needs to be based on the appropriately corrected form of [15 eqs. (19.10) and (19.12)].

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