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ASYMPTOTIC EXPANSIONS OF GAUSS-LEGENDRE QUADRATURE RULES FOR INTEGRALS WITH ENDPOINT SINGULARITIES

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This paper is dedicated to the memory of Professor Philip Rabinowitz

ABSTRACT. Let $I[f] = \int_{-1}^{1} f(x) dx$, where $f \in C^{\infty}(-1, 1)$, and let $G_n[f] = \sum_{i=1}^{n} w_{ni} f(x_{ni})$ be the *n*-point Gauss–Legendre quadrature approximation to I[f]. In this paper, we derive an asymptotic expansion as $n \to \infty$ for the error $E_n[f] = I[f] - G_n[f]$ when f(x) has general algebraic-logarithmic singularities at one or both endpoints. We assume that f(x) has asymptotic expansions of the forms

$$f(x) \sim \sum_{s=0}^{\infty} U_s (\log(1-x))(1-x)^{\alpha_s} \text{ as } x \to 1-,$$

$$f(x) \sim \sum_{s=0}^{\infty} V_s (\log(1+x))(1+x)^{\beta_s} \text{ as } x \to -1+,$$

where $U_s(y)$ and $V_s(y)$ are some polynomials in y. Here, α_s and β_s are, in general, complex and $\Re \alpha_s, \Re \beta_s > -1$. An important special case is that in which $U_s(y)$ and $V_s(y)$ are constant polynomials; for this case, the asymptotic expansion of $E_n[f]$ assumes the form

$$E_n[f] \sim \sum_{\substack{s=0\\\alpha_s \notin \mathbb{Z}^+}}^\infty \sum_{i=1}^\infty a_{si} h^{\alpha_s+i} + \sum_{\substack{s=0\\\beta_s \notin \mathbb{Z}^+}}^\infty \sum_{i=1}^\infty b_{si} h^{\beta_s+i} \quad \text{as $n \to \infty$,}$$

where $h = (n + 1/2)^{-2}$, $\mathbb{Z}^+ = \{0, 1, 2, \ldots\}$, and a_{si} and b_{si} are constants independent of n.

1. INTRODUCTION

Consider the problem of approximating finite-range integrals of the form

m

(1.1)
$$I[f] = \int_{-1}^{1} f(x) \, dx$$

by the *n*-point Gauss–Legendre quadrature rule

(1.2)
$$G_n[f] = \sum_{i=1}^n w_{ni} f(x_{ni}),$$

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where x_{ni} are the abscissas [the zeros of $P_n(x)$, the *n*th Legendre polynomial] and w_{ni} are the corresponding weights. Let

$$(1.3) E_n[f] = I[f] - G_n[f]$$

denote the error in this approximation.

When $f \in C^{\infty}[-1, 1]$, the error $E_n[f]$ tends to zero as $n \to \infty$ faster than all negative powers of n, that is, $E_n[f] = o(n^{-\mu})$ as $n \to \infty$ for every $\mu > 0$. In particular, when f(z) is analytic in an open set of the z-plane that contains the interval [-1, 1] in its interior, it holds that $E_n[f] = O(e^{-\sigma n})$ as $n \to \infty$ for some $\sigma > 0$. See Davis and Rabinowitz [2, p. 312].

When f(x) has integrable singularities in (-1, 1) and/or at one or both endpoints $x = \pm 1$, $E_n[f]$ tends to zero slowly, its rate of decay depending on the strength of the singularities. For example, when $f(x) = (1 - x)^{\alpha}g(x)$, with $\Re \alpha > -1$ but $\alpha \neq 0, 1, \ldots$, and $g \in C^{\infty}[-1, 1]$, it is known that $E_n[f] = O(n^{-2\alpha-2})$ as $n \to \infty$. See [2, p. 313].

A much refined version of this result was given by Verlinden [11, Theorem 1]. For future reference, we reproduce Verlinden's result next:

Theorem 1.1. Let $f(x) = (1-x)^{\alpha}g(x)$, with $\Re \alpha > -1$ but $\alpha \neq 0, 1, \ldots$, and g(z) analytic in an open set that contains the interval [-1, 1] in its interior. Then, with $h = (n + 1/2)^{-2}$, $E_n[f]$ has the asymptotic expansion

(1.4)
$$E_n[f] \sim \sum_{k=1}^{\infty} a_k h^{\alpha+k} \quad as \ n \to \infty.$$

Here, a_k are some constants independent of n.

The proof of Verlinden's theorem is quite difficult and makes use of an important asymptotic result of Elliott [3] concerning the Jacobi polynomials and their corresponding functions of the second kind.

Interestingly, the asymptotic expansion in Theorem 1.1 resembles, in its form, the generalized Euler-Maclaurin expansion of Navot [4] for the trapezoidal rule approximation to the integral $\int_{-1}^{1} (1-x)^{\alpha} g(x) dx$. Thus, it could be viewed as an analogue of this Euler-Maclaurin expansion in the context of Gauss-Legendre quadrature. Verlinden [11] has also applied the Richardson extrapolation in conjunction with this expansion for approximating $\int_{-1}^{1} (1-x)^{\alpha} g(x) dx$ with high accuracy. For Euler-Maclaurin expansions and the Richardson extrapolation, see Atkinson [1], Ralston and Rabinowitz [7], Stoer and Bulirsch [10], and Sidi [8], for example.

In [11], Verlinden also gives an asymptotic expansion for the case in which f(x) has an algebraic-logarithmic endpoint singularity. He considers specifically $f(x) = \log(1-x)(1-x)^{\alpha}g(x)$, and shows that the asymptotic expansion of $E_n[f]$ in this case is obtained by differentiating that of Theorem 1.1 with respect to α term by term.

In this work, we consider functions f(x) that have arbitrary algebraic-logarithmic endpoint singularities at one or both endpoints ± 1 . The class of functions we consider is more general than that considered in [11], and contains the latter as a subclass. We derive asymptotic expansions of $E_n[f]$ as $n \to \infty$ for these functions. In the next section, we state our main results on these asymptotic expansions when $f \in C^{\infty}(-1, 1)$ and mention some important special cases. In Section 3, we present the proofs of these results. In Section 4, we extend the results of Section 2 to the case in which f(x) is only in $C^r(-1, 1)$ for some nonnegative integer r.

2. Statement of main results

Throughout this section, we assume that the function f(x) in (1.1)–(1.3) has the following properties:

1. $f \in C^{\infty}(-1, 1)$ and has the asymptotic expansions

(2.1)
$$f(x) \sim \sum_{s=0}^{\infty} U_s (\log(1-x))(1-x)^{\alpha_s} \text{ as } x \to 1-,$$
$$f(x) \sim \sum_{s=0}^{\infty} V_s (\log(1+x))(1+x)^{\beta_s} \text{ as } x \to -1+,$$

where $U_s(y)$ and $V_s(y)$ are some polynomials in y, and α_s and β_s are, in general, complex and satisfy

(2.2)
$$\begin{array}{l} -1 < \Re \alpha_0 \leq \Re \alpha_1 \leq \Re \alpha_2 \leq \cdots; \quad \lim_{s \to \infty} \Re \alpha_s = +\infty, \\ -1 < \Re \beta_0 \leq \Re \beta_1 \leq \Re \beta_2 \leq \cdots; \quad \lim_{s \to \infty} \Re \beta_s = +\infty. \end{array}$$

Here, $\Re z$ stands for the real part of z.

2. If we let $u_s = \deg(U_s)$ and $v_s = \deg(V_s)$, then the α_s and β_s are ordered such that

(2.3)
$$u_s \ge u_{s+1}$$
 if $\Re \alpha_{s+1} = \Re \alpha_s; \quad v_s \ge v_{s+1}$ if $\Re \beta_{s+1} = \Re \beta_s.$

3. By (2.1), we mean that, for each r = 1, 2, ...,

(2.4)

$$f(x) - \sum_{s=0}^{r-1} U_s (\log(1-x))(1-x)^{\alpha_s}$$

$$= O(U_r (\log(1-x))(1-x)^{\alpha_r}) \quad \text{as } x \to 1-,$$

$$f(x) - \sum_{s=0}^{r-1} V_s (\log(1+x))(1+x)^{\beta_s}$$

$$= O(V_r (\log(1+x))(1+x)^{\beta_r}) \quad \text{as } x \to -1+.$$

4. For each k = 1, 2, ..., the kth derivative of f(x) also has asymptotic expansions as $x \to \pm 1$ that are obtained by differentiating those in (2.1) term by term.

The following are consequences of (2.2) and (2.3):

- (i) There are only a finite number of α_s that have the same real parts. Similarly, there are only a finite number of β_s that have the same real parts. Consequently, $\Re \alpha_s < \Re \alpha_{s+1}$ and $\Re \beta_{s'} < \Re \beta_{s'+1}$ for infinitely many values of the indices s and s'.
- (ii) The sequences $\{U_s(\log(1-x))(1-x)^{\alpha_s}\}_{s=0}^{\infty}$ and $\{V_s(\log(1+x))(1+x)^{\beta_s}\}_{s=0}^{\infty}$ are asymptotic scales. For a discussion of asymptotic scales, see Olver [5, p. 25], for example. Thus, also by (2.4), the expansions in (2.1) are genuine asymptotic expansions.

A key result that we will use to state and prove our main theorems is essentially given in [11, Section 6]; it is also a corollary of Theorem 1.1 corresponding to the case $g(x) \equiv 1$ there. We state it below as Theorem 2.1. To that effect, let us define

(2.5)
$$f_{\omega}^{\pm}(x) = (1 \pm x)^{\omega}.$$

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Then

(2.6)
$$I[f_{\omega}^{+}] = I[f_{\omega}^{-}] = \frac{2^{\omega+1}}{\omega+1}, \quad \Re \omega > -1.$$

By the symmetry of the Gauss-Legendre quadrature formulas, namely, by the fact that $x_{n,n-i+1} = -x_{ni}$ and $w_{n,n-i+1} = w_{ni}$ for all *i* in (1.2), we also have

$$(2.7) G_n[f_{\omega}^+] = G_n[f_{\omega}^-],$$

so that

(2.8)
$$E_n[f_{\omega}^+] = E_n[f_{\omega}^-]$$

Theorem 2.1. Let $f_{\omega}^{\pm}(x)$ be as in (2.5), with $\Re \omega > -1$ but $\omega \notin \mathbb{Z}^+$, where $\mathbb{Z}^+ = \{0, 1, 2, \ldots\}$. Then, with $h = (n + 1/2)^{-2}$, $E_n[f_{\omega}^{\pm}]$ has the asymptotic expansion

(2.9)
$$E_n[f_{\omega}^{\pm}] \sim \sum_{k=1}^{\infty} c_k(\omega) h^{\omega+k} \quad as \ n \to \infty,$$

that is valid uniformly in every strip $-1 < d_1 \leq \Re \omega \leq d_2 < \infty$ of the ω -plane. The $c_k(\omega)$ are analytic functions of ω for $\Re \omega > -1$ (same functions for f_{ω}^+ and for f_{ω}^-). When $\omega \in \mathbb{Z}^+$, for each $k = 0, 1, \ldots$, it holds that $c_k(\omega) = 0$; in this case, we also have $E_n[f_{\omega}^{\pm}] = 0$ for all $n \geq (\omega + 1)/2$.

We now state the main results of this work. We start with the following special case of pure algebraic (nonlogarithmic) endpoint singularities that is important and of interest in itself:

Theorem 2.2. Let f(x) be exactly as described in the first paragraph of this section with the same notation, $U_s(y) = A_s \neq 0$ and $V_s(y) = B_s \neq 0$ being constant polynomials for all s. Then, with $h = (n + 1/2)^{-2}$ and $\mathbb{Z}^+ = \{0, 1, 2, ...\}$, it holds that

$$(2.10) \quad E_n[f] \sim \sum_{\substack{s=0\\\alpha_s \notin \mathbb{Z}^+}}^{\infty} A_s \sum_{k=1}^{\infty} c_k(\alpha_s) h^{\alpha_s+k} + \sum_{\substack{s=0\\\beta_s \notin \mathbb{Z}^+}}^{\infty} B_s \sum_{k=1}^{\infty} c_k(\beta_s) h^{\beta_s+k} \quad as \ n \to \infty.$$

Here, $c_k(\omega)$ are precisely as given in Theorem 2.1.

Remarks.

- 1. By (2.2), the sequences $\{h^{\alpha_s+k}\}_{s=0}^{\infty}$ and $\{h^{\beta_s+k}\}_{s=0}^{\infty}$ are asymptotic scales as $n \to \infty$, and the expansion in (2.10) is a genuine asymptotic expansion when its terms are reordered according to their size.
- 2. Note that, when $U_s(y)$ and $V_s(y)$ are constants, the nonnegative integer powers $(1-x)^s$ and $(1+x)^s$, if present in the asymptotic expansions of (2.1), do not contribute to the expansion of $E_n[f]$ as $n \to \infty$.
- 3. In case α_s, β_s are all nonnegative integers in Theorem 2.2, of course, $f \in C^{\infty}[-1, 1]$, and the asymptotic expansion in (2.10) is empty (zero). This does not necessarily mean that $E_n[f] = 0$, however. It only means that $E_n[f]$ tends to zero as $n \to \infty$ faster than all negative powers of n, which is consistent with the known result we mentioned in Section 1. Of course, when f(x) is a polynomial, $E_n[f] = 0$ for all large n.
- 4. If $\alpha_s = \alpha + s$ and $\beta_s = s$ for all s = 0, 1, ..., in Theorem 2.2, then f(x) is of the form $f(x) = (1-x)^{\alpha}g(x)$ with $g \in C^{\infty}[-1,1]$, and $A_s = (-1)^s g^{(s)}(1)/s!$,

 $s = 0, 1, \ldots$ In this case, the second double sum in (2.10) disappears and the first double sum can be rearranged so that

(2.11)
$$E_n[f] \sim \sum_{k=1}^{\infty} a_k h^{\alpha+k} \text{ as } n \to \infty,$$

where a_k are functions of α given by

(2.12)
$$a_k = \left[\sum_{s=0}^{k-1} A_s c_{k-s}(\alpha+k)\right], \quad k = 1, 2, \dots,$$

and are analytic in every strip $-1 < d_1 \leq \Re \alpha \leq d_2 < \infty$ of the α -plane. Thus, Theorem 2.2 reduces to the result of Verlinden given in Theorem 1.1; however, it is more general since the function g(z) now is not assumed to be analytic in an open set in the z-plane containing the interval [-1, 1] but is assumed to be in $C^{\infty}[-1, 1]$ only.

5. If $\alpha_s = \alpha + s$ and $\beta_s = \beta + s$ for all s = 0, 1, ..., in Theorem 2.2, then f(x) is of the form $f(x) = (1-x)^{\alpha}(1+x)^{\beta}g(x)$ with $g \in C^{\infty}[-1, 1]$, and A_s and B_s are given by

(2.13)
$$A_{s} = \frac{(-1)^{s}}{s!} \frac{d^{s}}{dx^{s}} \left[(1+x)^{\beta} g(x) \right] \Big|_{x=1} = (-1)^{s} \sum_{i=0}^{s} \binom{\beta}{i} \frac{g^{(s-i)}(1)}{(s-i)!} 2^{\beta-i},$$
$$B_{s} = \frac{1}{s!} \frac{d^{s}}{dx^{s}} \left[(1-x)^{\alpha} g(x) \right] \Big|_{x=-1} = \sum_{i=0}^{s} (-1)^{i} \binom{\alpha}{i} \frac{g^{(s-i)}(-1)}{(s-i)!} 2^{\alpha-i}.$$

Note that A_s are entire functions of β only, while B_s are entire functions of α only. In this case, by rearranging both of the double sums in (2.10), we have the following generalization of Theorem 1.1 for algebraic singularities at both endpoints:

(2.14)
$$E_n[f] \sim \sum_{k=1}^{\infty} a_k h^{\alpha+k} + \sum_{k=1}^{\infty} b_k h^{\beta+k} \quad \text{as } n \to \infty.$$

Here, a_k and b_k are functions of both α and β given by

(2.15)
$$a_k = \sum_{s=0}^{k-1} A_s c_{k-s}(\alpha+k), \quad b_k = \sum_{s=0}^{k-1} B_s c_{k-s}(\beta+k), \quad k = 1, 2, \dots,$$

and are analytic when α and β are such that $-1 < d_1 \leq \Re \alpha \leq d_2 < \infty$ and $-1 < d'_1 \leq \Re \beta \leq d'_2 < \infty$, respectively.

The next theorem deals with the general case, in which algebraic-logarithmic singularities may occur at the endpoints.

Theorem 2.3. Let f(x) be exactly as described in the first paragraph of this section with the same notation, and let $U_s(y) = \sum_{i=0}^{u_s} \sigma_{si} y^i$ and $V_s(y) = \sum_{i=0}^{v_s} \tau_{si} y^i$. Denote $\frac{d}{d\omega}$ by D_{ω} . For an arbitrary polynomial $W(y) = \sum_{i=0}^{k} \epsilon_i y^i$ and an arbitrary function g that depends on ω , define also

$$W(D_{\omega})g := \sum_{i=0}^{k} \epsilon_i \left[D_{\omega}^i g \right] = \sum_{i=0}^{k} \epsilon_i \frac{d^i g}{d\omega^i}.$$

Then, with $h = (n + 1/2)^{-2}$, it holds that

(2.16)
$$E_n[f] \sim \sum_{s=0}^{\infty} \sum_{k=1}^{\infty} U_s(D_{\alpha_s}) [c_k(\alpha_s) h^{\alpha_s+k}] + \sum_{s=0}^{\infty} \sum_{k=1}^{\infty} V_s(D_{\beta_s}) [c_k(\beta_s) h^{\beta_s+k}] \quad as \ n \to \infty$$

Here, $c_k(\omega)$ are precisely as given in Theorem 2.1.

Remarks.

1. To see the explicit form of the expansion in Theorem 2.3, we also need

$$D^{i}_{\omega} \left[c_k(\omega) h^{\omega+k} \right] = h^{\omega+k} \sum_{j=0}^{i} \binom{i}{j} c_k^{(i-j)}(\omega) (\log h)^j,$$

where $c_k^{(r)}(\omega)$ stands for the *r*th derivative of $c_k(\omega)$. Using this, it can be seen, for example, that

$$U_s(D_{\alpha_s})[c_k(\alpha_s)h^{\alpha_s+k}] = h^{\alpha_s+k}\sum_{j=0}^{u_s} e_{sj}(\log h)^j,$$

where

$$e_{sj} = \sum_{i=j}^{u_s} {i \choose j} \sigma_{si} c_k^{(i-j)}(\alpha_s), \quad j = 0, 1, \dots, u_s.$$

Note that $e_{su_s} = \sigma_{su_s} c_k(\alpha_s)$. By Theorem 2.1, this implies that $e_{su_s} = 0$ when $\alpha_s \in \mathbb{Z}^+$.

Thus, (2.16) assumes the following explicit form:

$$(2.17) \quad E_n[f] \sim \sum_{s=0}^{\infty} \sum_{k=1}^{\infty} \widehat{U}_{sk}(\log h) h^{\alpha_s + k} + \sum_{s=0}^{\infty} \sum_{k=1}^{\infty} \widehat{V}_{sk}(\log h) h^{\beta_s + k} \quad \text{as } n \to \infty,$$

where $\widehat{U}_{sk}(y)$ and $\widehat{V}_{sk}(y)$ are polynomials in y with $\deg(\widehat{U}_{sk}) \leq u_s$ and $\deg(V_s) \leq v_s$. If $\alpha_s \in \mathbb{Z}^+$, then $\deg(\widehat{U}_{sk}) \leq u_s - 1$; otherwise, $\deg(\widehat{U}_{sk}) = u_s$. Similarly, if $\beta_s \in \mathbb{Z}^+$, then $\deg(\widehat{V}_{sk}) \leq v_s - 1$; otherwise, $\deg(\widehat{V}_{sk}) = v_s$. 2. Invoking now (2.2) and (2.3), we conclude that the sequences

$$\{U_s(D_{\alpha_s})[c_k(\alpha_s)h^{\alpha_s+k}]\}_{s=0}^{\infty}$$
 and $\{V_s(D_{\beta_s})[c_k(\beta_s)h^{\beta_s+k}]\}_{s=0}^{\infty}$

are asymptotic scales as $n \to \infty$, and that the expansion in (2.16) is a genuine asymptotic expansion.

3. When $\alpha_s = \alpha + s$ and $\beta_s = \beta + s$, for all $s = 0, 1, \ldots$, and $u_0 = u_1 = \cdots = p$ and $v_0 = v_1 = \cdots = q$, we can rearrange the double sums in (2.17), and obtain

(2.18)
$$E_n[f] \sim \sum_{k=1}^{\infty} \check{U}_k(\log h) h^{\alpha+k} + \sum_{k=1}^{\infty} \check{V}_k(\log h) h^{\beta+k} \quad \text{as } n \to \infty,$$

where $\check{U}_k(y) = \sum_{s=0}^{k-1} \widehat{U}_{s,k-s}(y)$ and $\check{V}_k(y) = \sum_{s=0}^{k-1} \widehat{V}_{s,k-s}(y)$ are polynomials in y of degree at most p and q, respectively. If $\alpha \in \mathbb{Z}^+$, then $\deg(\check{U}_k) \leq p-1$. Similarly, if $\beta \in \mathbb{Z}^+$, then $\deg(\check{V}_k) \leq q-1$.

4. The case in the preceding remark arises, for example, when

$$f(x) = (1-x)^{\alpha} (1+x)^{\beta} [\log(1-x)]^p [\log(1+x)]^q g(x)$$

with $g \in C^{\infty}[-1, 1]$. In this case, the asymptotic expansion of $E_n[f]$ can be obtained by differentiating the asymptotic expansion of $E_n[\tilde{f}]$, where $\tilde{f}(x) = (1-x)^{\alpha}(1+x)^{\beta}g(x)$, p times with respect to α and q times with respect to β . Note that $\tilde{f}(x)$ here is precisely the function f(x) given in Remark 5 following Theorem 2.2, and the asymptotic expansion of $E_n[\tilde{f}]$ is as given in (2.14) and (2.15). Recall that the a_k and b_k there are analytic functions of both α and β . Thus, applying $\partial^{p+q}/\partial \alpha^p \partial \beta^q$ to (2.14), we obtain the expansion in (2.18).

A simpler special case is one in which $\beta = 0$ and q = 0. For this case, we have $f(x) = (1 - x)^{\alpha} [\log(1 - x)]^p g(x)$ with p a positive integer and $g \in C^{\infty}[-1, 1]$. The asymptotic expansion of $E_n[f]$ is now of the form

(2.19)
$$E_n[f] \sim \sum_{k=1}^{\infty} \check{U}_k(\log h) h^{\alpha+k} \quad \text{as } n \to \infty,$$

where $U_k(y)$, as before, are polynomials in y of degree at most p, and this can be obtained by differentiating the asymptotic expansion of $E_n[\tilde{f}]$, where $\tilde{f}(x) = (1-x)^{\alpha}g(x)$, p times with respect to α . The asymptotic expansion of $E_n[\tilde{f}]$ is that given in (2.11). The case p = 1 has been given in [11, Section 6].

Just as the expansion of $E_n[f]$ (for Gauss-Legendre quadrature) in Theorem 1.1 is an analogue of Navot's generalized Euler-Maclaurin expansion (for the trapezoidal rule), those in Theorems 2.2 and 2.3 (for Gauss-Legendre quadrature) are analogues of the author's [9] recent generalizations of the Euler-Maclaurin expansion (for the trapezoidal rule) under precisely the same conditions.

3. Proofs of main results

3.1. **Proof of Theorem 2.2.** With $U_s(y) = A_s$ and $V_s(y) = B_s$, and an arbitrary positive integer m, let

$$(3.1) \ p(x) = \sum_{s=0}^{m-1} A_s (1-x)^{\alpha_s} + \sum_{s=0}^{m-1} B_s (1+x)^{\beta_s} = \sum_{s=0}^{m-1} A_s f_{\alpha_s}^-(x) + \sum_{s=0}^{m-1} B_s f_{\beta_s}^+(x).$$

Here, $f_{\omega}^{\pm}(x)$ are as defined in (2.5). Then,

(3.2)
$$f(x) = p(x) + \phi(x); \quad \phi(x) := f(x) - p(x).$$

Thus,

(3.3)
$$E_n[f] = E_n[p] + E_n[\phi].$$

By Theorem 2.1,

(3.4)
$$E_n[p] = \sum_{s=0}^{m-1} A_s E_n[f_{\alpha_s}^-] + \sum_{s=0}^{m-1} B_s E_n[f_{\beta_s}^+] \\ \sim \sum_{s=0}^{m-1} A_s \sum_{k=1}^{\infty} c_k(\alpha_s) h^{\alpha_s+k} + \sum_{s=0}^{m-1} B_s \sum_{k=1}^{\infty} c_k(\beta_s) h^{\beta_s+k} \quad \text{as } n \to \infty.$$

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We now have to analyze $E_n[\phi]$. For this, we need to know the differentiability properties of $\phi(x)$ on [-1,1]. First, $\phi \in C^{\infty}(-1,1)$. At $x = \pm 1$, $\phi(x)$ has the asymptotic expansions

(3.5)

$$\phi(x) \sim w_m^+(x) + \sum_{s=m}^{\infty} A_s (1-x)^{\alpha_s} \quad \text{as } x \to 1-; \quad w_m^+(x) = -\sum_{s=0}^{m-1} B_s (1+x)^{\beta_s},$$

$$\phi(x) \sim w_m^-(x) + \sum_{s=m}^{\infty} B_s (1+x)^{\beta_s} \quad \text{as } x \to -1+; \quad w_m^-(x) = -\sum_{s=0}^{m-1} A_s (1-x)^{\alpha_s}.$$

Note that $w_m^+(x)$ is infinitely differentiable at x = 1 while $w_m^-(x)$ is infinitely differentiable at x = -1. Thus, what determines the differentiability properties on [-1, 1] of $\phi(x)$ are the infinite sums in (3.5). By the fourth of the properties of f(x)mentioned in the beginning of Section 2, the asymptotic expansions of $\phi(x)$ in (3.5) can be differentiated termwise as many times as we wish. Then, for every positive integer j, it holds that

(3.6)

$$\frac{d^{j}}{dx^{j}}\phi(x) \sim \frac{d^{j}}{dx^{j}}w_{m}^{+}(x) + \sum_{s=m}^{\infty}A_{s}\alpha_{s}(\alpha_{s}-1)\cdots(\alpha_{s}-j+1)(1-x)^{\alpha_{s}-j} \quad \text{as } x \to 1-,$$

$$\frac{d^{j}}{dx^{j}}\phi(x) \sim \frac{d^{j}}{dx^{j}}w_{m}^{-}(x) + \sum_{s=m}^{\infty}B_{s}\beta_{s}(\beta_{s}-1)\cdots(\beta_{s}-j+1)(1+x)^{\beta_{s}-j} \quad \text{as } x \to -1+.$$

Clearly,

(3.7)
$$\lim_{x \to 1-} \frac{d^{j}}{dx^{j}} \phi(x) = -\frac{d^{j} w_{m}^{+}}{dx^{j}} \Big|_{x=1}, \quad j = 0, 1, \dots, \lceil \Re \alpha_{m} - 1 \rceil, \\\lim_{x \to -1+} \frac{d^{j}}{dx^{j}} \phi(x) = -\frac{d^{j} w_{m}^{-}}{dx^{j}} \Big|_{x=-1}, \quad j = 0, 1, \dots, \lceil \Re \beta_{m} - 1 \rceil,$$

which also means that $\phi(x)$ has $\lceil \Re \alpha_m - 1 \rceil$ continuous derivatives at x = 1 and $\lceil \Re \beta_m - 1 \rceil$ continuous derivatives at x = -1, in addition to being in $C^{\infty}(-1, 1)$. Consequently, $\phi \in C^{\kappa_m}[-1, 1]$, where $\kappa_m = \min\{\lceil \Re \alpha_m - 1 \rceil, \lceil \Re \beta_m - 1 \rceil\}$.

Next, it is known that

(3.8)
$$|E_n[\phi]| \le 4 \min_{q \in \Pi_{2n-1}} ||\phi - q||,$$

where Π_k is the set of all polynomials of degree at most k and

$$||F|| = \max_{x \in [-1,1]} |F(x)|,$$

and that

(3.9)
$$\min_{q \in \Pi_N} \|F - q\| = O(N^{-k}) \text{ as } N \to \infty, \text{ when } F \in C^k[-1,1],$$

by one of Jackson's theorems. For (3.8), see [2, Section 4.8, pp. 332–333], and for Jackson's theorem leading to (3.9), see Powell [6, Section 16.3, pp. 194–198], for

example. Thus,

(3.10)
$$\min_{q \in \Pi_{2n-1}} \|\phi - q\| = O(n^{-\kappa_m}) = O(h^{\kappa_m/2}) \quad \text{as } n \to \infty$$

From (3.8) and (3.10), it therefore follows that

(3.11)
$$E_n[\phi] = O(h^{\kappa_m/2}) \quad \text{as } n \to \infty.$$

Combining (3.4) and (3.11) in (3.3), and considering only those terms with $\Re \alpha_s + k < \Re \alpha_m$ and $\Re \beta_s + k < \Re \beta_m$ in, respectively, the first and second double summations in (3.4), we have

$$(3.12) E_n[f] = \sum_{\substack{0 \le s \le m-1\\1 \le k < \Re(\alpha_m - \alpha_s)}} A_s c_k(\alpha_s) h^{\alpha_s + k} + O(h^{\alpha_m}) + \sum_{\substack{0 \le s \le m-1\\1 \le k < \Re(\beta_m - \beta_s)}}^{m-1} B_s c_k(\beta_s) h^{\beta_s + k} + O(h^{\beta_m}) + O(h^{\kappa_m/2}) \quad \text{as } n \to \infty.$$

Now, $\lim_{m\to\infty} \kappa_m = \infty$ and $\lim_{m\to\infty} \Re \alpha_m = \infty$ and $\lim_{m\to\infty} \Re \beta_m = \infty$ simultaneously, by (2.2). From this and from (3.12), we conclude that $E_n[f]$ has the true asymptotic expansion

$$(3.13) \qquad E_n[f] \sim \sum_{s=0}^{\infty} A_s \sum_{k=1}^{\infty} c_k(\alpha_s) h^{\alpha_s+k} + \sum_{s=0}^{\infty} B_s \sum_{k=1}^{\infty} c_k(\beta_s) h^{\beta_s+k} \quad \text{as } n \to \infty.$$

Finally, the result in (2.10) follows by invoking the fact that $c_k(\omega) = 0$ when $\omega \in \mathbb{Z}^+$.

3.2. **Proof of Theorem 2.3.** We first observe that, with $f_{\omega}^{\pm}(x)$ as defined in (2.5),

(3.14)
$$f_{\omega,i}^{\pm}(x) := [\log(1\pm x)]^i (1\pm x)^{\omega} = \frac{d^i}{d\omega^i} f_{\omega}^{\pm}(x).$$

Consequently, we also have

(3.15)
$$I[f_{\omega,i}^{\pm}] = \frac{d^i}{d\omega^i} I[f_{\omega}^{\pm}] = \frac{d^i}{d\omega^i} \frac{2^{\omega+1}}{\omega+1}$$

and

(3.16)
$$G_n[f_{\omega,i}^{\pm}] = \frac{d^i}{d\omega^i} G_n[f_{\omega}^{\pm}],$$

and hence

(3.17)
$$E_n[f_{\omega,i}^{\pm}] = \frac{d^i}{d\omega^i} E_n[f_{\omega}^{\pm}]$$

The following theorem, which we employ in our proof, essentially follows from [11, Section 6].

Theorem 3.1. Let $\Re \omega > -1$. Then, with $h = (n + 1/2)^{-2}$, for each $i = 1, 2, ..., E_n[f_{\omega,i}^{\pm}]$ has the asymptotic expansion

(3.18)
$$E_n[f_{\omega,i}^{\pm}] \sim \sum_{k=1}^{\infty} \frac{d^i}{d\omega^i} [c_k(\omega)h^{\omega+k}] \quad as \ n \to \infty,$$

that is valid uniformly in every strip $-1 < d_1 \leq \Re \omega \leq d_2 < \infty$ of the ω -plane.

Remark. In other words, the asymptotic expansion of $E_n[f_{\omega,i}^{\pm}]$ is obtained by differentiating that of $E_n[f_{\omega}^{\pm}]$ *i* times term by term. Note, however, that even though $c_k(\omega)$ vanish when $\omega \in \mathbb{Z}^+$, $c_k^{(i)}(\omega)$ do not have to.

For an arbitrary positive integer m, let

(3.19)
$$p(x) = \sum_{s=0}^{m-1} U_s (\log(1-x))(1-x)^{\alpha_s} + \sum_{s=0}^{m-1} V_s (\log(1+x))(1+x)^{\beta_s}$$
$$= \sum_{s=0}^{m-1} \sum_{i=0}^{u_s} \sigma_{si} f_{\alpha_{s,i}}^-(x) + \sum_{s=0}^{m-1} \sum_{i=0}^{v_s} \tau_{si} f_{\beta_s,i}^+(x),$$

and write, as before,

(3.20)
$$f(x) = p(x) + \phi(x); \quad \phi(x) := f(x) - p(x),$$

and

(3.21)
$$E_n[f] = E_n[p] + E_n[\phi],$$

However, this time,

(3.22)
$$E_n[p] = \sum_{s=0}^{m-1} \sum_{i=0}^{u_s} \sigma_{si} E_n[f_{\alpha_s,i}^-] + \sum_{s=0}^{m-1} \sum_{i=0}^{v_s} \tau_{si} E_n[f_{\beta_s,i}^+].$$

By Theorem 3.1, this gives

(3.23)
$$E_n[p] \sim \sum_{s=0}^{m-1} \sum_{k=1}^{\infty} U_s(D_{\alpha_s}) [c_k(\alpha_s) h^{\alpha_s+k}] + \sum_{s=0}^{m-1} \sum_{k=1}^{\infty} V_s(D_{\beta_s}) [c_k(\beta_s) h^{\beta_s+k}] \quad \text{as } n \to \infty.$$

To analyze $E_n[\phi]$, we again need to study the differentiability properties of $\phi(x)$ on [-1, 1]. Clearly, $\phi \in C^{\infty}(-1, 1)$. At $x = \pm 1$, $\phi(x)$ has the asymptotic expansions

(3.24)

$$\phi(x) \sim w_m^+(x) + \sum_{s=m}^{\infty} \sum_{i=0}^{u_s} \sigma_{si} [\log(1-x)]^i (1-x)^{\alpha_s} \quad \text{as } x \to 1-,$$

$$\phi(x) \sim w_m^-(x) + \sum_{s=m}^{\infty} \sum_{i=0}^{v_s} \tau_{si} [\log(1+x)]^i (1+x)^{\beta_s} \quad \text{as } x \to -1+$$

with

(3.25)
$$w_m^+(x) = -\sum_{s=0}^{m-1} V_s (\log(1+x))(1+x)^{\beta_s},$$
$$w_m^-(x) = -\sum_{s=0}^{m-1} U_s (\log(1-x))(1-x)^{\alpha_s}.$$

As was the case in the proof of Theorem 2.2, again $w_m^+(x)$ is infinitely differentiable at x = 1 while $w_m^-(x)$ is infinitely differentiable at x = -1. By the fourth of the properties of f(x) mentioned in the beginning of Section 2, the asymptotic expansions of $\phi(x)$ in (3.24) can be differentiated termwise as many times as we wish. Then, for every positive integer j, it holds that

(3.26)
$$\frac{d^{j}}{dx^{j}}\phi(x) \sim \frac{d^{j}}{dx^{j}}w_{m}^{+}(x) + \sum_{s=m}^{\infty} \widetilde{U}_{s}(\log(1-x))(1-x)^{\alpha_{s}-j} \quad \text{as } x \to 1-,$$
$$\frac{d^{j}}{dx^{j}}\phi(x) \sim \frac{d^{j}}{dx^{j}}w_{m}^{-}(x) + \sum_{s=m}^{\infty} \widetilde{V}_{s}(\log(1+x))(1+x)^{\beta_{s}-j} \quad \text{as } x \to -1+,$$

where $\widetilde{U}_s(y)$ and $\widetilde{V}_s(y)$ are polynomials in y of degree u_s and v_s , respectively. It is easy to see that, in this case too, we have

(3.27)
$$\lim_{x \to 1-} \frac{d^j}{dx^j} \phi(x) = -\frac{d^j w_m^+}{dx^j} \Big|_{x=1}, \quad j = 0, 1, \dots, \lceil \Re \alpha_m - 1 \rceil,$$
$$\lim_{x \to -1+} \frac{d^j}{dx^j} \phi(x) = -\frac{d^j w_m^-}{dx^j} \Big|_{x=-1}, \quad j = 0, 1, \dots, \lceil \Re \beta_m - 1 \rceil,$$

which also means that $\phi(x)$ has $\lceil \Re \alpha_m - 1 \rceil$ continuous derivatives at x = 1 and $\lceil \Re \beta_m - 1 \rceil$ continuous derivatives at x = -1, in addition to being in $C^{\infty}(-1, 1)$. Consequently, $\phi \in C^{\kappa_m}[-1, 1]$, where $\kappa_m = \min\{\lceil \Re \alpha_m - 1 \rceil, \lceil \Re \beta_m - 1 \rceil\}$.

The proof of Theorem 2.3 can now be completed as that of Theorem 2.2. We leave the details to the reader.

4. Extensions

In the preceding sections, we assumed that the function f(x) is infinitely differentiable on (-1, 1). However, the proofs of Theorems 2.2 and 2.3 suggest that these theorems can be extended to the case in which the function f(x) is not necessarily in $C^{\infty}(-1, 1)$.

Theorems 4.1 and 4.2 below are extensions of Theorems 2.2 and 2.3, respectively, precisely to this case. In these theorems, we assume that f(x) is exactly as in the first paragraph of Section 2, except that it ceases to be infinitely differentiable at a finite number of points in (-1, 1), and that it is in $C^r(-1, 1)$ for some nonnegative integer r. Of course, f(x) continues to be infinitely differentiable in the open intervals $(-1, -1 + \eta)$ and $(1 - \eta, 1)$, where η is sufficiently small and, in addition, as $x \to \pm 1$, f(x) has the asymptotic expansions given in (2.1), with (2.2)-(2.4). Below, we adopt the notation of Sections 2 and 3.

Theorem 4.1. Let f(x) be as in the second paragraph of this section with the same notation, $U_s(y) = A_s \neq 0$ and $V_s(y) = B_s \neq 0$ being constant polynomials for all s. Let m_- and m_+ be the smallest integers for which

(4.1)
$$r < \Re \alpha_{m_{-}} \quad and \quad r < \Re \beta_{m_{+}}.$$

Then, with $h = (n + 1/2)^{-2}$ and $\mathbb{Z}^+ = \{0, 1, 2, ...\}$, it holds that

$$(4.2) \quad E_n[f] = \sum_{\substack{s=0\\\alpha_s \notin \mathbb{Z}^+}}^{m_- - 1} \sum_{k=1}^{\lceil r/2 - \Re \alpha_s - 1 \rceil} A_s c_k(\alpha_s) h^{\alpha_s + k} + \sum_{\substack{s=0\\\beta_s \notin \mathbb{Z}^+}}^{m_+ - 1} \sum_{k=1}^{\lceil r/2 - \Re \beta_s - 1 \rceil} B_s c_k(\beta_s) h^{\beta_s + k} + O\left(h^{r/2}\right) \quad as \ n \to \infty.$$

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Theorem 4.2. Let f(x) be as in the second paragraph of this section with the same notation, $U_s(y)$ and $V_s(y)$ being polynomials in y of degree u_s and v_s , respectively. Let m_- and m_+ be the smallest integers for which

(4.3) $r < \Re \alpha_{m_-} \quad and \quad r < \Re \beta_{m_+}.$

Then, with $h = (n + 1/2)^{-2}$, it holds that

(4.4)
$$E_{n}[f] = \sum_{s=0}^{m_{-}-1} \sum_{k=1}^{\lceil r/2 - \Re \alpha_{s} - 1 \rceil} U_{s}(D_{\alpha_{s}}) [c_{k}(\alpha_{s})h^{\alpha_{s}+k}] + \sum_{s=0}^{m_{+}-1} \sum_{k=1}^{\lceil r/2 - \Re \beta_{s} - 1 \rceil} V_{s}(D_{\beta_{s}}) [c_{k}(\beta_{s})h^{\beta_{s}+k}] + O(h^{r/2}) \quad as \ n \to \infty.$$

The proof of Theorem 4.1 is achieved precisely as that of Theorem 2.2 by modifying p(x) in (3.1) as in

(4.5)
$$p(x) = \sum_{s=0}^{m_{-}-1} A_s (1-x)^{\alpha_s} + \sum_{s=0}^{m_{+}-1} B_s (1+x)^{\beta_s}.$$

Similarly, the proof of Theorem 4.2 is achieved precisely as that of Theorem 2.3 by modifying p(x) in (3.19) as in

(4.6)
$$p(x) = \sum_{s=0}^{m_{-}-1} U_s (\log(1-x))(1-x)^{\alpha_s} + \sum_{s=0}^{m_{+}-1} V_s (\log(1+x))(1+x)^{\beta_s}.$$

In both cases, the functions $\phi(x) := f(x) - p(x)$ are in $C^r[-1, 1]$ so that $E_n[\phi] = O(h^{r/2})$ as $n \to \infty$. We leave the details to the reader.

Note that the summations over the α_s (the β_s) in (4.2) and (4.4) are empty in case $\Re \alpha_0 \ge r/2 - 1$ ($\Re \beta_0 \ge r/2 - 1$).

References

- K.E. Atkinson. An Introduction to Numerical Analysis. Wiley, New York, 1978. MR504339 (80a:65001)
- P.J. Davis and P. Rabinowitz. Methods of Numerical Integration. Academic Press, New York, second edition, 1984. MR760629 (86d:65004)
- [3] D. Elliott. Uniform asymptotic expansions of the Jacobi polynomials and an associated function. Math. Comp., 25:309–315, 1971. MR0294737 (45:3805)
- [4] I. Navot. An extension of the Euler-Maclaurin summation formula to functions with a branch singularity. J. Math. and Phys., 40:271–276, 1961. MR0140876 (25:4290)
- [5] F.W.J. Olver. Asymptotics and Special Functions. Academic Press, New York, 1974. MR0435697 (55:8655)
- M.J.D. Powell. Approximation Theory and Methods. Cambridge University Press, Cambridge, 1981. MR604014 (82f:41001)
- [7] A. Ralston and P. Rabinowitz. A First Course in Numerical Analysis. McGraw-Hill, New York, second edition, 1978. MR0494814 (58:13599)
- [8] A. Sidi. Practical Extrapolation Methods: Theory and Applications. Number 10 in Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, Cambridge, 2003. MR1994507 (2004e:65005)
- [9] A. Sidi. Euler-Maclaurin expansions for integrals with endpoint singularities: a new perspective. Numer. Math., 98:371–387, 2004. MR2092747 (2005g:65012)
- [10] J. Stoer and R. Bulirsch. Introduction to Numerical Analysis. Springer-Verlag, New York, third edition, 2002. MR1923481 (2003d:65001)
- [11] P. Verlinden. Acceleration of Gauss-Legendre quadrature for an integrand with an endpoint singularity. J. Comp. Appl. Math., 77:277–287, 1997. MR1440013 (98f:65029)

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