Error Expansions for Multidimensional Trapezoidal Rules with Sidi Transformations*

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Abstract

In 1993, Sidi introduced a set of trigonometric transformations, $x = \psi(t)$ that improve the effectiveness of the one-dimensional trapezoidal quadrature rule for a finite interval. In this paper, we extend Sidi's approach to product multidimensional quadrature over $[0,1]^N$. We establish the Euler-Maclaurin expansion for this rule, both in the case of a regular integrand function $f(x)$ and in the cases when $f(x)$ has homogeneous singularities confined to vertices.

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1 Introduction and Outline

Elementary transformations, helpful in integrating $f(x)$ over a finite interval $[0,1]$, include some of the form $x = \psi(t)$, where

$$\psi(0) = 0 \qquad \psi(1) = 1 \qquad \psi'(t) > 0 \qquad \forall \quad t \in (0,1). \tag{1.1}$$

This transforms an integrand as follows:

$$If = \int_0^1 f(x)dx = \int_0^1 f(\psi(t))\psi'(t)dt = IF, \tag{1.2}$$

where

$$F(t) = f(\psi(t))\psi'(t) \tag{1.3}$$

is termed the transformed function. Transformations of this type are as old as integral calculus itself; traditionally, they are used when a primitive for $F(t)$ is more readily available than one for $f(x)$.

Naturally, such a transformation may be used to replace $f(x)$ by $F(t)$ when an economic way to integrate $F(t)$ numerically is available. In numerical quadrature, one useful approach is to choose $\psi(t)$ so that $F(t)$ is more amenable to integration by the trapezoidal rule than is $f(x)$. This situation occurs when $\psi(t)$ is chosen so that $\psi'(t)$ is relatively "flat" at both ends. In this context, properties (1.1) are obligatory. However, for efficiency, one would like

$$\psi^{(s)}(0) = \psi^{(s)}(1) = 0 \qquad s \in [1,p] \tag{1.4}$$

for a moderate or large value of p. For computing purposes as well as theoretical analysis, a transformation whose derivative is symmetric is often convenient; that is,

$$\psi'(1-t) = \psi'(t). \tag{1.5}$$

While individual numerical approaches of this type must be as old as computing machines themselves, the first systematic investigation appears to be due to Korobov [4] in 1963. He introduced a

set of polynomial transformation functions that satisfied (1.1) and (1.4). Independently, at about the same time, Sag and Szekeres [11] popularized the approach. Their transformation function

$$\psi(t) = \frac{1}{2}(1 + \tanh(1/(1-t) - 1/t))$$

has a symmetric derivative and satisfies (1.4) for all finite p. Since then, several authors have developed the technique. Among the better known methods are the IMT transformations [3]. For more information, one may refer to Davis and Rabinowitz [2], pp. 142 et seq.

In 1993, Sidi introduced a promising set of transformations in which ψ_p' is a trigonometric polynomial of period 2 and degree p satisfying (1.1), (1.4), and (1.5). Unlike Korobov's polynomials, Sidi's functions possess symmetry about each endpoint. Sidi derived a recursive relation for the numerical evaluation of the transformations and some error expansions, useful for extrapolation. He showed by example that these transformations were indeed efficient.

Laurie [5] discussed in 1996 polynomial transformations which, like Sidi's trigonometric transformations, are more efficient than Korobov's polynomial transformations. In the present paper we restrict to Sidi's transformations. We expect however that the results extend to Laurie's transformations, but only partially since the symmetry of Sidi's transformations about the endpoints is not shared by Laurie's polynomial transformations.

The present paper is about integration over $[0,1]^N$ using Sidi's transformation for each of the N components. We are particularly interested in quadrature error expansions of the Euler-Maclaurin type. When the integrand function is regular, the expansion (Theorem 5.2) turns out to be precisely what one might expect from the one-dimensional theory. Our principal result, Theorem 6.9, specifies the nature of the corresponding expansion when $f(\mathbf{x})$ has an algebraic singularity at a vertex.

This paper is arranged as follows. In Section 2, relevant general background material is discussed. In Sections 3 and 4, Sidi's transformations are defined and one-dimensional results relevant to the subsequent N-dimensional theory are derived. These add little to Sidi's results [10], but establish the notation, emphasize the expansions, and provide proofs that generalize in a straightforward manner. In Section 5 we treat the somewhat pedestrian case when $f(\mathbf{x})$ is regular. The principal results of the rest of this paper appear in Section 6. As in previous theory, these expansions depend on homogeneous functions (see Definition 6.2). The key Theorem 6.6 specifies an expansion of $F(\mathbf{t})$ in terms of homogeneous functions when $f(\mathbf{x})$ is itself one. Exploiting the standard N-dimensional error expansion (Theorem 6.3), we obtain Theorem 6.7. This is a weak

form of the principal theorem, as it includes, in the expansion, many terms that in fact vanish. In Section 8 we show, using analytical continuation in the complex plane, that these terms in the final expansion do indeed vanish. Two appendixes, which are technical in nature, contain our long, but straightforward, proofs of Theorems 6.6 and 6.3.

2 Background

Let If stand for the finite integral of $f(x)$ over the interval [0,1],and let $Qf = Q_x f(x)$ be its approximation using a quadrature rule Q. Throughout this paper, we treat only quadrature rules that integrate constant functions exactly. Denote by $Q^{(m)}$ the m-copy version of Q

$$Q^{(m)}f := \sum_{k=0}^{m-1} \frac{1}{m} Q_x f\left(\frac{x+k}{m}\right) = Q_x\left(\frac{1}{m}\sum_{k=0}^{m-1} f\left(\frac{x+k}{m}\right)\right). \tag{2.1}$$

Applied to an offset trapezoidal rule, the Euler-Maclaurin expansion takes the form

$$\frac{1}{m}\sum_{k=0}^{m-1} f\left(\frac{x+k}{m}\right) = \sum_{s=0}^{q}\int_0^1 f^{(s)}(t)dt\frac{\beta_s(x)}{m^s s!} + \frac{1}{m^q}\int_0^1 f^{(q)}(t)h_q(x-mt)dt, \quad (x \in [0,1]), \tag{2.2}$$

where β_s is the Bernoulli polynomial of degree s and

$$h_q(x) = \frac{\beta_q(x-[x])}{q!}.$$

Observe that the first term in this expansion is If. Applied in the context of (2.1), the Euler-Maclaurin expansion provides an asymptotic expansion for the error of a general m-copy rule applied to a regular integrand $f(x)$ as stated in the following theorem.

Theorem 2.1 *When $f(x)$ and its first q derivatives are integrable over* $[0,1]$,

$$Q^{(m)}f - If = \sum_{s=1}^{q}\frac{B_s(Q,f)}{m^s} + o(m^{-q}), \tag{2.3}$$

where

$$B_s(Q,f) = c_s(Q)\int_0^1 f^{(s)}(t)dt = c_s(Q)\left(f^{(s-1)}(1) - f^{(s-1)}(0)\right) \tag{2.4}$$

and

$$c_s(Q) = Q_x(\beta_s(x)/s!). \tag{2.5}$$

When $f(x)$ has singular behavior within the interval [0,1], expansion (2.3) is not valid. However, for the special case $f(x) = f_\alpha(x) = x^\alpha$, when $\alpha > -1$, Navot [8] has shown

$$Q^{(m)} f_\alpha - I f_\alpha = \frac{A(Q, f_\alpha)}{m^{\alpha+1}} + \sum_{s=1}^{q} \frac{B_s(Q, f_\alpha)}{m^s} + o(m^{-q}), \tag{2.6}$$

where

$$B_s(Q, f_\alpha) = c_s(Q) f_\alpha^{(s-1)}(1) \tag{2.7}$$

and

$$A(Q, f_\alpha) = Q_x(\zeta(-\alpha; x)). \tag{2.8}$$

Here $\zeta(s; x)$ is the generalized zeta function, that is the meromorphic extension w.r.t. s of the series $\sum_{k=0}^{\infty}(x+k)^{-s}$. Note that expression (2.7) coincides with (2.4) when $Re(\alpha) > s - 1$ and that it represents its analytic continuation w.r.t. α for the other values of α.

By extension, when $f(x) = x^\alpha g(x)$ and $g(x)$ is smooth so that it can be expanded in a Taylor series about the origin, we may obtain a correspondent to Theorem 2.1.

Theorem 2.2 *When $f(x) = x^\alpha g(x)$ and $g(x)$ and its first q derivatives are integrable over $[0, 1]$,*

$$Q^{(m)} f - I f = \sum_{t} \frac{A_t(Q, f)}{m^{\alpha+1+t}} + \sum_{s=1}^{q} \frac{B_s(Q, f)}{m^s} + o(m^{-q}), \tag{2.9}$$

where the index t in the first summation runs through the nonnegative integers not larger than $q - Re(\alpha) - 1$ and

$$B_s(Q, f) = c_s(Q) f^{(s-1)}(1). \tag{2.10}$$

When Q involves a function value $f(0)$ that is not defined, formulas (2.6) and (2.9) remain valid when $f(0)$ is replaced by zero. Colloquially, the singularity may be ignored.

When Q is a symmetric rule, we may exploit the symmetry property of the Bernoulli polynomial β_s to establish that $c_s(Q)$ vanishes when s is odd. It follows that for both (2.4) and (2.7), we have

$$B_s(Q, f) = 0 \qquad \forall \quad s \text{ odd and symmetric } Q. \tag{2.11}$$

The expansions in either of the above theorems may, as appropriate, be used to construct an extrapolation technique for numerical quadrature. In the application of these extrapolation methods, detailed expressions for the coefficients A_t and B_s are not required. It is important,however, to know whether any coefficients vanish so that the corresponding terms may be removed from

the expansion before any extrapolation takes place, thus improving the convergence rate. A major concern in this paper is the vanishing (or otherwise) of coefficients in expansions of this general nature.

A traditional integration procedure which uses extrapolation is Romberg integration [9] (see also Bauer, Rutishauser, and Stiefel [1] . This is based on (2.3) using mesh ratios $m_i = 2^i$, $i = 0, 1, 2, \ldots$, and setting Q to be the endpoint trapezoidal rule. This quadrature formula is symmetric and, in setting up the extrapolation, (2.11) is invoked to remove the odd parity terms from this expansion.

3 Sidi Transformations ($f(x)$ Regular)

The family $\psi_p(t)$ of transformation functions introduced by Sidi [10] may be defined for all positive integer p by

$$\psi_p'(t) = \kappa_p(\sin \pi t)^p, \tag{3.1}$$

where the (normalizing) constant κ_p is chosen to validate (1.1). These satisfy (1.1), (1.5), and (1.4) for the stated value of p. We shall denote the transformed integrand by

$$F_p(t) = f(\psi_p(t))\psi_p'(t). \tag{3.2}$$

Thus, when $f(x)$ is regular, so is $F_p(x)$. In our treatment we restrict ourselves to the trapezoidal rule

$$R^{(m)}f := \frac{1}{2m}f(0) + \sum_{j=1}^{m-1} f(j/m) + \frac{1}{2m}f(1) := \frac{1}{m}\sum_{j=0}^{m}{}'' f(j/m) \tag{3.3}$$

for the integration[1]. However, as demonstrated by Sidi, the theory may be applied to the midpoint rule, and even to more sophisticated symmetric rules, with virtually no modification. Note first that

$$R^{(m)}F_p = \frac{1}{m}\sum_{j=0}^{m}{}'' F_p(j/m) = \sum_{j=0}^{m}{}'' f\left(\psi_p(j/m)\right)\psi_p'(j/m)/m. \tag{3.4}$$

Thus, $R^{(m)}F_p$ can be considered to be a symmetric quadrature rule $Q_p^{[m]}f$ having abscissas $\psi_p(j/m)$ and weights $m^{-1}\psi_p'(j/m)$. In general (i.e., except in the special case $p = 0$), no endpoint function

[1] The double prime attached to the summation symbol indicates that both the first and the last term in the summation are to be halved.

values are needed. Specializing (2.3) and (2.4) to the trapezoidal rule, we state

$$R^{(m)}F_p - If \simeq \sum_{s=1} \frac{B_s(R,F_p)}{m^s} \simeq \sum_{s=1} \frac{c_s(R)(F_p^{(s-1)}(1) - F_p^{(s-1)}(0))}{m^s}. \tag{3.5}$$

The rest of this section is devoted to the vanishing of individual terms in this expansion (3.5). To this end we examine the early coefficients in the Taylor expansion of $F_p(t)$ about $t = 0$. From expression (3.1) we see that for any positive integer r,

$$\psi_p'(t) = c_p t^p + c_{p+2} t^{p+2} + \ldots + \mathcal{O}(t^{p+2r}) \tag{3.6}$$

and that

$$\psi_p(t) = \int_0^t \psi_p'(t)dt = \mathcal{O}(t^{p+1}).$$

Thus,

$$\begin{aligned} F_p(t) &= f(\psi_p(t))\,\psi_p'(t) = (f(0) + f'(0)\psi_p(t) + \ldots)\,\psi_p'(t) \\ &= \left(f(0) + \mathcal{O}(t^{p+1})\right)\psi_p'(t) \\ &= f(0)\psi_p'(t) + \psi_p'(t)\mathcal{O}(t^{p+1}) \qquad (3.7) \\ &= f(0)(c_p t^p + c_{p+2}t^{p+2} + \ldots) + \mathcal{O}(t^{2p+1}). \qquad (3.8) \end{aligned}$$

While the second term here is of order $\mathcal{O}(t^{2p+1})$, the first involves alternate powers of t starting with t^p. Thus, we have

$$\begin{aligned} F_p^{(s)}(0) &= 0 \qquad s \in [0, p-1] \\ F_p^{(s)}(0) &= 0 \qquad (p+s) \text{ odd } s \in [1, 2p]. \end{aligned} \tag{3.9}$$

An identical argument gives corresponding results for the $t = 1$ end of the integration interval. Setting these results in (3.5), and recalling that $B_s = 0$ for all odd s (see (2.11)), we find immediately

$$B_s(R,F_p) = c_s(R)\int_0^1 \frac{\partial^s}{\partial t^s}\left(f(\psi_p(t))\psi_p'(t)\right)dt = 0 \quad p \text{ even}, s \in [2, 2p]. \tag{3.10}$$

Note that in the above expression, when $s \in [p, 2p]$, two distinct situations occur. On one hand, when p is even, either the factor $c_s(R)$ is zero or its cofactor is zero, but not in general both. On the other hand, when p is odd, either both $c_s(R)$ and its cofactor are zero or, in general, neither. Hence we have the following specialization of Theorem 2.1.

Theorem 3.1 *When p is an integer and $f(x)$ has integrable derivatives of order q over $[0,1]$, then*

$$R^{(m)}F_p - If = \sum_{\substack{s \text{ even} \\ s \in [\overline{p}+1,\, q]}} \frac{B_s(R, F_p)}{m^s} + o(m^{-q}). \tag{3.11}$$

where $\overline{p} = 2p+1$ or p depending on whether p is even or odd.

4 Sidi Transformations for $f(x) = x^\alpha g(x)$

We now look at the case when $f(x)$ has an algebraic singularity. Our first lemma is not directly concerned with quadrature. It simply specifies the nature of the singularity of $F_p(t)$ when

$$f(x) = f_\alpha(x) = x^\alpha. \tag{4.1}$$

Lemma 4.1 *When $f(x)$ is of form (4.1), the function $F_p(t)$ takes the form*

$$F_p(t) = f_\alpha(\psi_p(t))\psi_p'(t) = t^\beta g_e(t), \tag{4.2}$$

where

$$\beta = (\alpha+1)(p+1) - 1 \tag{4.3}$$

and $g_e(t)$ is an even regular function with $g_e(0) \neq 0$.

Proof. It is convenient to use $g_e(t)$ generically for an even regular function with $g_e(0) \neq 0$. Thus (3.6) may be expressed as $\psi_p'(t) = t^p g_e(t)$, from which it follows that $\psi_p(t) = t^{p+1} g_e(t)$ and

$$F_p(t) = t^{\alpha(p+1)}(g_e(t))^\alpha t^p g_e(t) = t^\beta g_e(t). \tag{4.4}$$

∎

Having established the nature of the singularity of $F_p(x)$ at the origin, we may now apply Navot's expansion (2.6), in the same way as it was applied to derive (2.9), to establish the expansion in the following theorem.

Theorem 4.2 *When p is an integer and $f(x) = x^\alpha$,*

$$R^{(m)}F_p \simeq If + \sum_{\substack{t=0 \\ t \text{ even}}} \frac{A_{\beta+1+t}(R,F_p)}{m^{\beta+1+t}} + \sum_{\substack{s \text{ even} \\ s \geq \overline{p}+1}} \frac{B_s(R,F_p)}{m^s}, \tag{4.5}$$

where $\beta = (\alpha+1)(p+1) - 1$, and $\overline{p} = 2p+1$ or p depending on whether p is even or odd.

When β is an integer, the first summation is void.

Proof. Here, the restriction of the summation index t to even values is a direct consequence of the factor $g_e(t)$ in (4.2). Straightforward substitution as indicated then gives the result, except that, without further examination, the sum over s would appear to include all positive even integers. To establish the stated restriction to $s \geq \overline{p}+1$, we note that, from (2.7), we have

$$B_s(R,F_p) = c_s(R)F_p^{(s-1)}(1),$$

and in view of (3.9) and (2.11) this vanishes for all even s in $[2, \overline{p}-1]$. (Note that the behavior of $F_p(t)$ near $t = 0$ is not relevant here.)

∎

Up to this point, the results coincide with those given by Sidi. (At most, we have given explicitly the terms in the expansion that are implicit in Sidi's work.) We have modified some proofs in order to facilitate a subsequent generalization to a multidimensional context.

5 Multidimensional Transformation (Regular)

When $f(\mathbf{x})$ is regular, the theory surrounding integration over $[0,1]^N$ using the Cartesian product of N one-dimensional Sidi transformations is straightforward. One may allow different meshes m_i in each component and different p-values, say p_i, without seriously disturbing this straightforward theory.

In two dimensions, the Euler-Maclaurin expansion of a double sum may be simply obtained. One sets

$$\frac{1}{m^2}\sum_{k_1=0}^{m-1}\sum_{k_2=0}^{m-1} f\left(\frac{x_1+k_1}{m}, \frac{x_2+k_2}{m}\right) = \frac{1}{m}\sum_{k=0}^{m-1} s(\frac{x_1+k}{m}, x_2), \tag{5.1}$$

where

$$s(x_1, x_2) = \frac{1}{m} \sum_{k=0}^{m-1} f\left(x_1, \frac{x_2 + k}{m}\right), \tag{5.2}$$

and applies the one-dimensional Euler-Maclaurin expansion (2.2) to the sum (5.2), treating x_1 as an incidental parameter. One then substitutes this expansion into the right of (5.1) and applies the Euler-Maclaurin expansion to sum each element of this expansion in the x_1-direction.

In N dimensions, an iterated procedure of this sort gives

$$\begin{aligned} \frac{1}{m^N} \sum_{\mathbf{k} \in \{0,1,\ldots,m-1\}^N} f\left(\frac{\mathbf{x}+\mathbf{k}}{m}\right) &= \sum_{|\mathbf{s}| \le q} \frac{1}{m^{|\mathbf{s}|}} \int_{[0,1]^N} f^{(\mathbf{s})}(\mathbf{t}) d^N\mathbf{t} \prod_{i=1}^N \frac{\beta_{s_i}(x_i)}{s_i!} \\ &\quad + \frac{1}{m^q} \sum_{|\mathbf{s}|=q} \int_{[0,1]^N} f^{(\mathbf{s})}(\mathbf{t}) h_{\mathbf{s}}(\mathbf{x}; m\mathbf{t}) d^N\mathbf{t}. \end{aligned} \tag{5.3}$$

Here $|\mathbf{s}| = |(s_1, \ldots, s_N)| := s_1 + \cdots + s_N$ and

$$f^{(\mathbf{s})}(\mathbf{t}) := \frac{\partial^{s_1 + \cdots + s_N} f}{\partial t_1^{s_1} \cdots \partial t_N^{s_N}}(t_1, \ldots, t_N).$$

The representation of the kernels $h_{\mathbf{s}}(\mathbf{x}; \mathbf{t})$ was studied in [6]. We need only recall that these kernels are bounded and periodic with period 1 in each t_i and that

$$\int_{[0,1]^N} h_{\mathbf{s}}(\mathbf{x}; \mathbf{t}) d^N\mathbf{t} = 0.$$

Equation (5.3) readily provides an N-dimensional version of Theorem 2.1, but limited to m-copies of one-point rules $Q(f) = f(\mathbf{x})$. However, one may expand a general quadrature rule Q in terms of one-point rules, and so obtain the following general theorem.

Theorem 5.1 *When $f(\mathbf{x})$ together with all partial derivatives of total order q or less are integrable over $[0,1]^N$, then*

$$Q^{(m)} f - If = \sum_{s=1}^{q} \frac{B_s(Q, f)}{m^s} + o(m^{-q}), \tag{5.4}$$

where

$$B_s(Q, f) = \sum_{|\mathbf{s}|=s} B_{\mathbf{s}}(Q, f) = \sum_{|\mathbf{s}|=s} c_{\mathbf{s}}(Q) \int_{[0,1]^N} f^{(\mathbf{s})}(\mathbf{x}) d^N\mathbf{x} \tag{5.5}$$

and

$$c_{(s_1,\ldots,s_N)}(Q) = Q_{(x_1,\ldots,x_N)} \left(\prod_{i=1}^N \frac{\beta_{s_i}(x_i)}{s_i!} \right). \tag{5.6}$$

We now apply this theorem to the N-dimensional product R of the m-copy one-dimensional trapezoidal rules to the function

$$F_p(\mathbf{t}) = f(\psi_p(t_1), \psi_p(t_2), \ldots, \psi_p(t_N)) \prod_{i=1}^{N} \psi_p'(t_i). \tag{5.7}$$

We find quite generally that, when $f(\mathbf{x})$ and all derivatives of total order q are integrable,

$$R^{(m)}F_p - IF_p = \sum_{s=1}^{q} \frac{B_s(R, F_p)}{m^s} + o(m^{-q}), \tag{5.8}$$

where

$$B_s(R, F_p) = \sum_{\Sigma s_i = s} B_{s_1, s_2, \ldots, s_N}(R, F_p) \tag{5.9}$$

and

$$\begin{aligned} B_{s_1, s_2, \ldots, s_N}(R, F_p) &= \prod_{i=1}^{N} c_{s_i}(R) \\ &\times \int_0^1 \ldots \int_0^1 \frac{\partial^s}{\partial t_1^{s_1} \partial t_2^{s_2} \ldots \partial t_N^{s_N}} (f(\psi_p(t_1), \psi_p(t_2) \ldots \psi_p(t_N)) \prod_{i=1}^{N} \psi_p'(t_i)) d^N \mathbf{t}. \end{aligned} \tag{5.10}$$

Examination of the integral in (5.10) shows that each one-dimensional integration is independent of the others and coincides in form with the one in (3.10) when one treats the other $(N-1)$ variables t_i as independent parameters. One may then apply the result (3.10) to each component in turn to find

$$B_{s_1, s_2 \ldots s_N}(R, F_p) = 0 \qquad \text{when any } s_i \in [1, 2p+1], \tag{5.11}$$

giving

$$B_s(R, F_p) = 0 \qquad\qquad s \in [1, 2p+1], \tag{5.12}$$

which provides an N-dimensional version of Theorem 3.1 s follows.

Theorem 5.2 *When p is an integer and $f(\mathbf{x})$ has integrable derivatives of order q over $[0,1]^N$ and F_p is given by (5.7)*

$$R^{(m)}F_p - If = \sum_{\substack{s \text{ even} \\ s \in [\overline{p}+1, q]}} \frac{B_s(R, F_p)}{m^s} + o(m^{-q}), \tag{5.13}$$

where $\overline{p} = 2p+1$ or p depending on whether p is even or odd.

6 Singular Multidimensional Integrand

In this section we are interested in multidimensional integrands that are smooth except at the origin. First we consider homogeneous functions and subsequently functions that can be expanded in homogeneous functions. Finally we study the effect of such singularities at the origin when Sidi's transformation is applied.

Definition 6.1 *Let $R \subset \mathbb{R}^N$ be open. Then we say that a function f on R is* **smooth** *if its partial derivatives $f^{(\mathbf{k})}$ of all orders $\mathbf{k} \in \mathbb{N}^N$ exist and are continuous on R.*
If R is not open but is contained in the closure of its interior, then we say that a function f on R is **smooth** *if it is smooth on the interior of R and if the partial derivatives of f of all orders extend to a continuous function on R.*

We shall use the following region of $[0,\infty)^N$:

$$L^N[a,b] := \{(x_1,\ldots,x_N) \mid \forall i : x_i \geq 0 \text{ and } a \leq \max_j x_j \leq b\} \tag{6.1}$$

and its limit cases

$$L^N(0,b] := \bigcup_{a>0} L^N[a,b] \quad L^N[a,\infty) := \bigcup_{b>0} L^N[a,b] \quad L^N(0,\infty) := \bigcup_{b>a>0} L^N[a,b]. \tag{6.2}$$

These are known as L-shaped regions because, in two dimensions, they resemble the letter L.

Several coefficients given below have integral representations in terms of these L-shaped regions. Of these, some require integrals on $U^N = L^N[1,1]$, which may be expressed as a sum of $(N-1)$-dimensional integrals as follows:

$$\int_{U^N} f(\mathbf{x}) d^{N-1}\mathbf{x} := \sum_{j=1}^{N} \int_0^1 \cdots \int_0^1 f(x_1,\ldots,x_{j-1},1,x_{j+1},\ldots,x_N) dx_1 \cdots dx_{j-1} dx_{j+1} \cdots dx_N. \tag{6.3}$$

Definition 6.2 *Let $R \subset \mathbb{R}^N$ be a cone, that is, for all $\mathbf{x} \in R$ and for all $\lambda > 0$,*

$$\lambda \mathbf{x} \in R.$$

A function $f(\mathbf{x})$ on R is **homogeneous** *of degree α when, for all $\mathbf{x} \in R$ and for all $\lambda > 0$,*

$$f(\lambda \mathbf{x}) = \lambda^\alpha f(\mathbf{x}).$$

Two-dimensional examples include

$$x^{\frac{1}{2}},\ (x^2+y^2)^{\beta/2},\ (x+2y)^{\gamma}$$

which are homogeneous of degrees $\frac{1}{2}$, β, and γ, respectively. In this paper we are only interested in homogeneous functions that are smooth on $L^N(0,+\infty)$, i.e. singular only at the origin. The last 2 functions satisfy this condition, the first function $x^{\frac{1}{2}}$ not, because this function is singular along the whole line $x=0$.

In [7] Lyness gives a set of results relating to integrands having homogeneous and logarithmic singularities at vertices. Some of these are generalizations of Navot's one-dimensional expansion (2.6). A fundamental result is the following theorem.

Theorem 6.3 *Let $f(\mathbf{x})$ be homogeneous of degree α and smooth on $L^N(0,\infty)$. Then, if $\alpha+N \notin \mathbb{N}$ and $q > Re(\alpha)+N$,*

$$Q^{(m)}f = \frac{A(Q,f)}{m^{\alpha+N}} + \sum_{s=0}^{q} \frac{B_s(Q,f)}{m^s} + \frac{R_q(Q,m,f)}{m^q}, \tag{6.4}$$

where

$$B_s(Q,f) = \frac{1}{\alpha+N-s} \sum_{|\mathbf{s}|=s} c_{\mathbf{s}}(Q) \int_{U^N} f^{(\mathbf{s})}(\mathbf{x}) d^{N-1}\mathbf{x} \tag{6.5}$$

$$A(Q,f) = Qf - \sum_{s=0}^{q} B_s(Q,f) + \sum_{|\mathbf{s}|=q} \int_{L^N[1,\infty)} Q_{\mathbf{x}} h_{\mathbf{s}}(\mathbf{x},\mathbf{t}) f^{(\mathbf{s})}(\mathbf{t}) d^N\mathbf{t} \tag{6.6}$$

$$R_q(Q,m,f) = -m^{q-\alpha-N} \sum_{|\mathbf{s}|=q} \int_{L^N[m,\infty)} Q_{\mathbf{x}} h_{\mathbf{s}}(\mathbf{x},\mathbf{t}) f^{(\mathbf{s})}(\mathbf{t}) d^N\mathbf{t} = O(1). \tag{6.7}$$

When Q is symmetric w.r.t. the center of the cube $[0,1]^N$, then $B_s(Q,f)=0$ for s odd.

This was proved first by Lyness [7]. A separate proof is given in Appendix A which provides naturally this form of coefficient and is valid in the wider context of complex α and $Re(\alpha) < -N$.

We shall now apply this theorem in a context in which the integrand is not homogeneous but admits an expansion in homogeneous functions.

Definition 6.4 *Let f be a smooth function on $R \subset \mathbb{R}^N$. Let $(f_j)_{j=0}^{\infty}$ be a sequence of smooth homogeneous functions on a cone containing R, and let δ_j denote the degree of f_j. Then we say that f can be expanded in the f_j, and we write*

$$f \sim \sum_{j=0}^{\infty} f_j$$

if, for each $q \in \mathbb{R}$, the set

$$J_q = \{j \in I\!N : Re(\delta_j) \leq q\}$$

is finite and if the remainder $r_q(\mathbf{x})$, defined by

$$f = \sum_{j \in J_q} f_j + r_q \tag{6.8}$$

satisfies the following condition. For each $\mathbf{k} \in I\!N^N$ there exists an $M_{\mathbf{k}} > 0$ such that

$$\forall \mathbf{x} \in R : |r_q^{(\mathbf{k})}(\mathbf{x})| \leq M_k \|\mathbf{x}\|^{q-|\mathbf{k}|}. \tag{6.9}$$

Please note that, in this definition and in the sequel, the index q may take any real number and is not (as it has been) restricted to integer values.

Remarks:

- If f is smooth in a neighborhood of $\mathbf{0}$, then the Taylor expansion of f about $\mathbf{0}$ is an expansion of f in homogeneous functions of degree $(j)_{j=0}^{\infty}$.
- r_q has continuous partial derivatives up to order $\lceil \delta_q \rceil - 1$ at the origin provided the origin belongs to the closure of R.
- If f and g both admit expansions in homogeneous functions, then so do $f + g$ and fg, and these expansions are obtained by formal addition and multiplication.
- When $f(\mathbf{x}) = h(\mathbf{x})g(\mathbf{x})$, where $h(\mathbf{x})$ is a smooth homogenous function of degree α on $L^N(0, \infty)$ and $g(\mathbf{x})$ is smooth on $[0, 1]^N$, then $f(\mathbf{x})$ admits an expansion in homogeneous functions of degree $(\delta_j)_{j=0}^{\infty}$ with $\delta_j = \alpha + j$.

Theorem 6.5 *When $f(\mathbf{x})$ on $L^N(0, 1]$ admits an expansion in smooth homogeneous functions of degree $(\delta_j)_{j=0}^{\infty}$ (see Definition 6.4), whereby $\delta_j + N \notin I\!N$, $j = 0, 1, \ldots$, then*

$$Q^{(m)} f \simeq \sum_{j=0} \frac{A_j(Q, f)}{m^{\delta_j + N}} + \sum_{s=0} \frac{B_s(Q, f)}{m^s}. \tag{6.10}$$

Proof. This is a straightforward consequence of applying $Q^{(m)}$ to each term in (6.8) above and then using (6.4) for $Q^{(m)} f_j$ and (5.4) for $Q^{(m)} r_q$.

∎

Note that

$$B_s(Q, f) = \sum_{j \in J_q} B_s(Q, f_j) + B_s(Q, r_q). \tag{6.11}$$

In the one-dimensional case we showed that when $f(x) = x^\alpha$ (a homogeneous function of degree α), the transformed function $F_p(t) = f_\alpha(\psi_p(t))\psi_p'(t)$ has an expansion in terms of homogeneous functions of degrees $\beta, \beta+2, \beta+4, ...,$ where $\beta = (\alpha+1)(p+1)-1$. That straightforward theorem was easy to prove. The next theorem states the N-dimensional analogue. This theorem is independent of quadrature. It is valid for all values of α including, for example, large negative integers. Our somewhat lengthy proof may be found in Appendix B.

Theorem 6.6 *Let $f(\mathbf{x})$ be a smooth homogeneous function of degree α on $L^N(0, \infty)$. Then,*

$$F_p(t_1, t_2, , \ldots, t_N) = f(\psi_p(t_1), \psi_p(t_2), \ldots, \psi_p(t_N))\psi_p'(t_1)\psi_p'(t_2)\cdots\psi_p'(t_N) \tag{6.12}$$

has an expansion in homogeneous functions of degree $(\beta + 2j)_{j=0}^\infty$, where

$$\beta = (\alpha + N)(p + 1) - N.$$

We now arrive at the principal results of this paper. These are the appropriate error expansions when Sidi's transformation is applied in an N-dimensional context to functions having certain vertex algebraic singularities.

Our first, and basic, result is Theorem 6.7, which covers the case in which the integrand $f(\mathbf{x})$ is homogeneous. This is an N-dimensional version of Theorem 4.2.

Theorem 6.7 *Let $f(\mathbf{x})$ be a smooth homogeneous function of degree α on $L^N(0, \infty)$, and let $F_p(\mathbf{t})$ be given by (6.12); then, when $\beta + N \notin \mathbb{Z}$,*

$$R^{(m)}F_p \simeq \sum_{\substack{t=0 \\ t \text{ even}}} \frac{A_t(R, F_p)}{m^{\beta+N+t}} + \sum_{s=0} \frac{B_s(R, F_p)}{m^s}, \tag{6.13}$$

where $\beta = (\alpha + N)(p + 1) - N$ and where, as is conventional, $\mathbb{Z}$ stands for the set of all integers.

Proof. The hypotheses of this theorem coincide with those of Theorem 6.6. It follows directly from that theorem that $F_p(\mathbf{t})$ has an expansion in homogeneous functions of degrees $(\beta + 2j)_{j=0}^\infty$. This implies, in turn, that the function $F_p(\mathbf{t})$ satisfies the conditions required of $f(\mathbf{x})$ in Theorem

6.5 with $\delta_j = \beta + 2j$. Setting $Q = R$ in that theorem, we find the result (6.10) reduces to the required result (6.13) above.

∎

It will come as no surprise to the reader to learn that, as in the case of a regular integrand, many terms $B_s(R, F_p)$ in the expansion (6.13) vanish identically.

Theorem 6.8 *Under the hypotheses of Theorem 6.7 we have*

$$B_s(R, F_p) = 0, \qquad s \text{ is odd or } s \in [1, \overline{p}].$$

where, as before, $\overline{p}$ denotes either $2p+1$ or p depending on whether p is even or odd.

In Section 8, we shall treat families of homogeneous functions depending analytically on a parameter. For example, when $f(\mathbf{x})$ satisfies the hypotheses of Theorems 6.6 and 6.7, the function $f_z(\mathbf{x}) = \|\mathbf{x}\|^z f(\mathbf{x})$ is a smooth homogeneous function of degree $\alpha_z = \alpha + z$. By Theorem 6.6, the transformed function $F_{z,p}$ of f_z then admits an expansion in homogeneous functions of degrees $(\beta_z + 2j)_{j=0}^{\infty}$, with $\beta_z = \beta + (p+1)z$. The proof of Theorem 6.8 relies on Theorem 8.5 and Theorem 8.4 below. These theorems justify the extremely plausible suggestion that the expansion coefficients $B_s(R, F_{z,p})$ depend analytically on the parameter z (in the region of definition $\beta_z + N \notin \mathbb{Z}$).

Proof of Theorem 6.8. Fix an s that is odd or that does not exceed $\overline{p}$. Let f_z and $F_{z,p}$ be as in the discussion above. Then, for sufficiently large $Re(z)$, the partial derivatives of $F_{z,p}(\mathbf{x})$ of order s are continuous on $[0,1]^N$. We can then rely on Theorem 5.2 to state that $B_s(R, F_{z,p})$ vanishes for sufficiently large $Re(z)$. But, as $B_s(R, F_{z,p})$ depends analytically on z in the region $\beta_z + N \notin \mathbb{Z}$, it must vanish for all these z and in particular for $z = 0$.

∎

When a smooth function f on $L^N(0,1]$ is not homogeneous but admits an expansion in smooth homogeneous functions, then the transformed function F_p is the sum of the transformed functions on the right-hand side of (6.8). The expansion of $R^{(m)}F_p$ is then obtained by applying Theorems 6.7 and 6.8 to the f_j and (5.8) to the remainder r_q.

We now state the results of carrying out this procedure in a standard case, where $f(\mathbf{x}) = f_\alpha(\mathbf{x})g(\mathbf{x})$ and, as before, $f_\alpha(\mathbf{x})$ is a smooth homogeneous function of degree α and $g(\mathbf{x})$ is $C^\infty[0,1]^N$.

Using a multivariate Maclaurin expansion, we may expand $g(\mathbf{x})$ in a sequence of smooth homogeneous functions of nonnegative integer degree, providing an expansion for $f(\mathbf{x})$ comprising terms of homogeneous degree $\delta(j) = \alpha + j$. Each of these terms gives rise to a different function F_p, having an individual value of β and a corresponding expansion. Since successive values of α differ by one unit, the corresponding values of β differ by $p+1$ units. Applying Theorems 6.7 and 6.8 to each of these functions in turn, one finds the following.

Theorem 6.9 *When $f(\mathbf{x}) = f_\alpha(\mathbf{x})g(\mathbf{x})$ and $f_\alpha(\mathbf{x})$ is a smooth homogeneous function of degree α on $L^N(0,\infty)$ and $g(\mathbf{x})$ is $C^\infty[0,1]^N$, then*

$$R^{(m)}F_p \simeq If + \sum_{t\in\mathcal{T}} \frac{A_t(R,F_p)}{m^{\beta+N+t}} + \sum_{s\in\mathcal{S}} \frac{B_s(R,F_p)}{m^s}, \tag{6.14}$$

where $\beta = (\alpha+N)(p+1) - N$ and the integer sets $\mathcal{S}$ and $\mathcal{T}$ are

$$p \text{ odd}, \ : \mathcal{S} = \{ \text{ all even } s \geq p+1\} : \mathcal{T} = \{ \text{ all even } t \geq 0\}$$

$$p \text{ even}, \ : \mathcal{S} = \{ \text{ all even } s \geq 2p+2\} : \mathcal{T} = \{ \text{ all } t \geq 0 \text{ except odd } t \in [1, p-1]\}.$$

If $g(\mathbf{x})$ is even, i.e., if its Taylor expansion about the origin involves only monomials of even degree, then we have for even p the stronger result

$$\mathcal{S} = \{ \text{ all even } s \geq 2p+2\} : \mathcal{T} = \{ \text{ all even } t \geq 0\}.$$

The reader will notice that the nature of these expansions is unaffected when a general even function g is replaced by $g(\mathbf{x}) = 1$. In these cases, the expansion with p even requires fewer terms than with p odd. However, with general $g(\mathbf{x})$, this preference may be reversed. Ultimately, with p odd, two even sequences appear, while with p even, there is one even and one full sequence.

7 Examples

The results of theorems 6.3, 6.7 and 6.8 are illustrated for the homogeneous function $h(x,y) = (x+y)^{-3/4}$ and the result of theorem 6.9 for the function $f(x,y) = h(x,y)g(x,y)$ where

$$g(x,y) = \exp\left(\left(\frac{x+y}{2}\right)^2\right).$$

Note that $g(x, y)$ is even.

We present in Tables 1 and 2 below the Romberg (extrapolation) tables containing quadrature errors for respectively Sidi's $p = 0, 2$ and 4 transformations applied to h and f. The number of panels, m, used in the computations is 8, 16, 32, 64 and 128. The early powers of $1/m$ in the asymptotic error expansion are as follows:

- for $p = 0$ and the integrand h: 1.25, 2, 4, 6 and 8;
- for $p = 0$ and the integrand f: 1.25, 2, 3.25, 4 and 5.25;
- for $p = 2$ and both integrands : 3.75, 5.75, 6, 7.75 and 8;
- for $p = 4$ and both integrands : 6.25, 8.25, 10, 10.25 and 12.

The integrals of $h(x, y)$ and $f(x, y)$ over $[0, 1]^2$ are respectively

$$\begin{aligned} Ih &= (32/5)(2^{1/4} - 1) = 1.210925536017414827, \\ If &= 1.528421461141788355. \end{aligned}$$

8 Integrands depending Analytically on a Parameter

Many simple homogeneous functions $f(\mathbf{x})$ are naturally embedded in a family of homogeneous functions that depend analytically on the degree z. Examples include

$$\|\mathbf{x}\|^z, \qquad |\lambda x_1 + \mu x_2|^z.$$

Obviously, it is always possible to embed a homogeneous $f(\mathbf{x})$ in such a family artificially. For example, when $f(\mathbf{x})$ is of homogeneous degree α, one such family comprises the functions $f(\mathbf{x})\|\mathbf{x}\|^z$. The degree of a member of this family is $\alpha(z) = \alpha + z$.

In this section we study the analytic dependence on the parameter z of the terms appearing in the asymptotic expansion of copy rules. This study is useful for two reasons. First, the previously derived asymptotic expansions were valid only when the degrees of the homogeneous functions were not exceptional, that is not integer. Knowing the analytic behavior of the terms of the error expansion about the exceptional degrees, we may be able to obtain the error expansion for the exceptional degrees as a limit case. Second, it turns out that explicit expressions of the terms of the expansion may be simple for certain values of the parameter and complicated otherwise. Instead of working with these complicated expressions, it is often easier to interpret them as the analytic continuation of the simple expressions. The usefulness of this interpretation has appeared in Theorem 5.1, where the vanishing of some terms in the expansion was established without relying on the complicated explicit expressions of these terms.

We need a rigorous definition of analytic families of smooth functions.

Definition 8.1 *Let Ω be an open subset of $\mathbb{C}$, and let $f_z(\mathbf{x})$ be a family of smooth functions on $R \subset \mathbb{R}^n$ parametrized by $z \in \Omega$. Then we say that $f_z(\mathbf{x})$ is an* **analytic family of smooth functions** *on R if all its partial derivatives w.r.t. $\mathbf{x}$ of all orders $f_z^{(\mathbf{k})}(\mathbf{x})$ are continuous on $\Omega \times R$ and if for each fixed $\mathbf{x} \in R$, $f_z^{(\mathbf{k})}(\mathbf{x})$ is an analytic function of z on Ω.*

The key result of this section is the following somewhat trivial application of this definition to the results of Theorem 6.3.

Theorem 8.2 *Let $f_z(\mathbf{x})$ ($z \in \Omega$) be an analytic family of smooth functions on $L^N(0,\infty)$, each member of which is homogeneous of degree $\alpha(z)$, where $\alpha(z)$ depends analytically on z. Let s be*

a positive integer. Then there exists an analytic function $F_s(z)$ on Ω such that the coefficient $B_s(Q, f_z)$ in (6.5) satisfies

$$B_s(Q, f_z) = \frac{F_s(z)}{\alpha(z) + N - s} \tag{8.1}$$

when $\alpha(z) + N \notin I\!N$.

Proof. For all functions satisfying the hypothesis of the theorem, each term in the summation in (6.5) is analytic in z for all $z \in \Omega$.

∎

The use of analytic families also provides an N-dimensional analogue of formula (2.8) for the coefficient $A(Q, f)$ in Theorem 6.3. Let f be a homogeneous function of degree α, let $f_z(\mathbf{x}) = \|\mathbf{x}\|^z f(\mathbf{x})$, and, for simplicity, let Q be a one-point rule, say, $Qf = f(\mathbf{t})$. Then, when $Re(\alpha+z)+N < 0$, we have by (6.4) that

$$\begin{aligned} A(Q, f_z) &= \lim_{m\to\infty} m^{\alpha+z+N} Q^{(m)}(f_z) \\ &= \lim_{m\to\infty} \sum_{\mathbf{k}\in\{0,1,\ldots,m-1\}^N} f_z(\mathbf{t}+\mathbf{k}) \\ &= \sum_{\mathbf{k}\in I\!N^N} f_z(\mathbf{t}+\mathbf{k}). \end{aligned} \tag{8.2}$$

By (6.6), the sum (8.2) admits a meromorphic extension in z with possible simple poles at $z = -\alpha - N + s$, $s \in I\!N$. For a general Q, $A(Q, f)$ is thus equal to Q applied to the meromorphic extension of (8.2) at $z = 0$. This result was first derived in [12, 13], together with corresponding results for more general singularities.

The behavior of the coefficients $B_s(Q, f)$ and $A(Q, f)$ in Theorem 6.3 near the poles is not without interest. Suppose $\alpha(z_0) + N = s \in I\!N$ but $\alpha(z) + N \neq s$ for $z \neq z_0$ but close to z_0. Then the only terms in (6.4) that are not analytic at z_0 are the A-term and the B_s-term, but it is readily verified that their sum has a limit as $z \to z_0$. Results given in [7] and [12, 13] show that this limit is of the form

$$\lim_{z\to z_0} \frac{A(Q, f_z)}{m^{\alpha(z)+N}} + \frac{B_s(Q, f_z)}{m^s} = \frac{C(Q, f_{z_0}) \log m + D(Q, f_{z_0})}{m^s}.$$

The expansion in the exceptional case $\alpha + N \in I\!N$ is simply the limit of the expansion in the regular case $\alpha + N \notin I\!N$.

The remainder of this section is devoted to establishing the analyticity of the coefficients B_s in a wider context. This comprises a somewhat pedestrian extension of definitions and results. The next definition extends Definition 6.4 to analytic families of functions.

Definition 8.3 *Let f_z be an analytic family of smooth functions on $R \subset \mathbb{R}^N$ where z runs through Ω. Let $(f_{j,z})_{j=0}^{\infty}$ be a sequence of analytic families of smooth homogeneous functions on a cone containing R, and let $\delta_j(z)$ denote the degree of $f_{j,z}$. Then we say that f_z can be expanded in the $f_{j,z}$ analytically in z, and we write*

$$f_z \sim \sum_{j=0}^{\infty} f_{j,z}$$

if, for each $q \in \mathbb{R}$ and each compact subset K of Ω, the set

$$J_{q,K} = \{j \in I\!N : Re(\delta_j(z)) \leq q \text{ for some } z \in K\}$$

is finite and if the remainder $r_{q,K,z}(\mathbf{x})$, defined by

$$f_z = \sum_{j \in J_{q,K}} f_{j,z} + r_{q,K,z} \tag{8.3}$$

satisfies the following condition. For each $\mathbf{k} \in I\!N^N$ there exists an $M_{\mathbf{k}} > 0$ such that

$$\forall \mathbf{x} \in R, \forall z \in K : |r_{q,K,z}^{(\mathbf{k})}(\mathbf{x})| \leq M_{\mathbf{k}} \|\mathbf{x}\|^{q-|\mathbf{k}|}. \tag{8.4}$$

Theorem 8.4 *Let $f_z(\mathbf{x})$ $(z \in \Omega)$ be an analytic family of smooth functions on $L^N(0,1]$ that can be expanded in homogeneous functions of degrees $(\delta_j(z))_{j=0}^{\infty}$ as in Definition 8.3. Let s be a positive integer. Then there exists a sequence of analytic functions $(F_{j,s}(z))_{j=0}^{\infty}$ on Ω such that for all $q > s$ and all compact subsets K of Ω, the coefficient $B_s(Q, f_z)$ in (6.10) admits the expansion*

$$B_s(Q, f_z) = \sum_{j \in J_{q,K}} \frac{F_{j,s}(z)}{\delta_j(z) + N - s} + R_{q,K,s}(z), \tag{8.5}$$

when $\delta_j(z) + N \notin I\!N$ for all $j \in J_{q,K}$. Here $R_{q,K,s}(z)$ is a continuous function on K that is analytic in the interior of K.

Proof. Applying (6.11) to f_z given in (8.3), we find

$$B_s(Q, f_z) = \sum_{j \in J_{q,K}} B_s(Q, f_{j,z}) + B_s(Q, r_{q,K,z}). \tag{8.6}$$

By (6.5), or better, by Theorem 8.2 there exist analytic functions $F_{j,s}(z)$ on Ω such that

$$B_s(Q, f_{j,z}) = \frac{F_{j,s}(z)}{\delta_j(z) + N - s}, \tag{8.7}$$

when $\delta_j(z) + N \notin I\!N$. By (5.5), $R_{q,K,s}(z) = B_s(Q, r_{q,K,z})$ $(z \in K)$ can be expressed as a linear combination of the integrals on the cube $[0,1]^N$ of the partial derivatives of order s of $r_{q,K,z}(\mathbf{x})$. We now consider an approximation to $R_{q,K,s}(z)$. This is $R_{\epsilon,q,K,s}(z)$ $(\epsilon > 0)$, an expression obtained from (5.5) by replacing these integrals on the cube by integrals on the region $L^N[\epsilon, 1]$. Since the partial derivatives of $r_{q,K,z}(\mathbf{x})$ depend analytically on z when $\mathbf{x}$ is restricted to $L^N[\epsilon, 1]$, we have that $R_{\epsilon,q,K,s}(z)$ is an analytic function on Ω. By (8.4), as $\epsilon \to 0^+$, $R_{\epsilon,q,K,s}(z)$ converges to $R_{q,K,s}(z)$, uniformly for $z \in K$. Hence, since $R_{q,K,s}(z)$ is the uniform limit of continuous functions on K, it is itself continuous on K, and, since it is the uniform limit of analytic functions on the interior of K, it is itself analytic on the interior of K.

∎

Note that the exceptional case, $\delta_j + N \in I\!N$ for some $j \in I\!N$, not considered in Theorem 6.5, can be treated as a limit case of that theorem.

Theorem 6.6 can also be extended to the context of analytic families.

Theorem 8.5 *If in Theorem 6.6 $f(\mathbf{x})$ depends analytically on a parameter, then the expansion of (6.12) also depends analytically on that parameter.*

The proof of this theorem is given in Appendix B as a supplement to the proof of Theorem 6.6.

A Proof of Theorem 6.3 and An Associated Lemma

Theorem 6.3 specifies the quadrature error expansion for a homogeneous integrand function with a vertex singularity. The coefficients are in terms of integrals over L-shaped regions defined in (6.1) and over U^N defined in (6.3).

The proof of Theorem 6.3 relies on the following lemma.

Lemma A.1 *Let $f(\mathbf{x})$ be a homogeneous function of degree $\alpha \in \mathbb{C}$ that is continuous on $L^N(0, \infty)$. Then, if $\alpha + N \neq 0$ and $0 < a < b$,*

$$\int_{L^N[a,b]} f(\mathbf{x}) d^N\mathbf{x} = \frac{b^{\alpha+N} - a^{\alpha+N}}{\alpha + N} \int_{U^N} f(\mathbf{x}) d^{N-1}\mathbf{x}.$$

Proof. We subdivide $L^N[a,b]$ in N parts

$$L^N[a,b] = \bigcup_{j=1}^{N} L_j^N[a,b],$$

where

$$\begin{aligned} L_j^N[a,b] &= \{(x_1,\ldots,x_N) \in L^N[a,b] : x_j = \max\{x_1,\ldots,x_N\}\} \\ &= \{t(u_1,\ldots,u_{j-1},1,u_{j+1},\ldots,u_N) : t \in [a,b], u_1,\ldots,u_{j-1},u_{j+1},\ldots,u_N \in [0,1]\}. \end{aligned}$$

Then we have

$$\int_{L^N[a,b]} f(\mathbf{x}) d^N\mathbf{x} = \sum_{j=1}^{N} \int_{L_j^N[a,b]} f(\mathbf{x}) d^N\mathbf{x}.$$

The j th integral in this sum is computed by the change of variable $x_j = t$ and $x_k = tu_k$ $(k \neq j)$.

$$\begin{aligned} &\int_{L_j^N[a,b]} f(\mathbf{x}) d^N\mathbf{x} \\ &= \int_a^b \int_0^1 \cdots \int_0^1 f(tu_1,\ldots,tu_{j-1},t,tu_{j+1},\ldots,tu_N) t^{N-1} dt du_1 \cdots du_{j-1} du_{j+1} \cdots du_N \\ &= \int_a^b t^{\alpha+N-1} dt \int_0^1 \cdots \int_0^1 f(u_1,\ldots,u_{j-1},1,u_{j+1},\ldots,u_N) du_1 \cdots du_{j-1} du_{j+1} \cdots du_N \\ &= \frac{b^{\alpha+N} - a^{\alpha+N}}{\alpha+N} \int_0^1 \cdots \int_0^1 f(u_1,\ldots,u_{j-1},1,u_{j+1},\ldots,u_N) du_1 \cdots du_{j-1} du_{j+1} \cdots du_N. \end{aligned}$$

Summation over j completes the proof.

∎

Proof of Theorem 6.3. As f is homogeneous of degree α, we have

$$\frac{1}{m^N} \sum_{\mathbf{k} \in \{0,1,\ldots,m-1\}^N} f\left(\frac{\mathbf{x}+\mathbf{k}}{m}\right) = \frac{1}{m^{\alpha+N}} f(\mathbf{x}) + \frac{1}{m^{\alpha+N}} \sum_{\mathbf{0} \neq \mathbf{k} \in \{0,1,\ldots,m-1\}^N} f_{\mathbf{k}}(\mathbf{x}), \tag{A.1}$$

where $f_{\mathbf{k}}(\mathbf{x}) = f(\mathbf{k}+\mathbf{x})$. As $f_{\mathbf{k}}$ is smooth on $[0,1]^N$, it can be replaced by its Euler-Maclaurin expansion (5.3) (with $m = 1$)

$$f_{\mathbf{k}}(\mathbf{x}) = \sum_{|\mathbf{s}| \leq q} \int_{[0,1]^N} f^{(\mathbf{s})}(\mathbf{t}+\mathbf{k}) d^N\mathbf{t} \prod_{i=1}^{N} \frac{\beta_{s_i}(x_i)}{s_i!} + \sum_{|\mathbf{s}|=q} \int_{[0,1]^N} f^{(\mathbf{s})}(\mathbf{t}+\mathbf{k}) h_{\mathbf{s}}(\mathbf{x};\mathbf{t}+\mathbf{k}) d^N\mathbf{t}.$$

Here we have used the periodicity of the kernel $h_{\mathbf{s}}$. $L^N[1,m]$ may be subdivided into m^N identical unit cubes, aligned with the axes. We denote the cube $[k_1,k_1+1] \times [k_2,k_2+1] \times \cdots \times [k_N,k_N+1]$

by $\mathbf{k}+[0,1]^N$; summation over $\mathbf{k}$ yields

$$\sum_{\mathbf{0}\neq\mathbf{k}\in\{0,1,\ldots,m-1\}^N} f_{\mathbf{k}}(\mathbf{x}) = \sum_{|\mathbf{s}|\leq q}\int_{L^N[1,m]} f^{(\mathbf{s})}(\mathbf{t})d^N\mathbf{t}\prod_{i=1}^N \frac{\beta_{s_i}(x_i)}{s_i!} \tag{A.2}$$

$$+\sum_{|\mathbf{s}|=q}\int_{L^N[1,m]} f^{(\mathbf{s})}(\mathbf{t})h_{\mathbf{s}}(\mathbf{x};\mathbf{t})d^N\mathbf{t}. \tag{A.3}$$

The integrand $f^{(\mathbf{s})}$ in (A.2) is homogeneous of degree $\alpha-|\mathbf{s}|$. Therefore, by Lemma A.1, we can write

$$\int_{L^N[1,m]} f^{(\mathbf{s})}(\mathbf{t})d^N\mathbf{t} = \frac{m^{\alpha-|\mathbf{s}|+N}-1}{\alpha-|\mathbf{s}|+N}\int_{U^N} f^{(\mathbf{s})}(\mathbf{t})d^N\mathbf{t}. \tag{A.4}$$

Each integral over $L^N[1,m]$ in (A.3) may be expressed as the difference of the integral over $L^N[1,\infty)$ and the integral over $L^N[m,\infty)$. Separating the terms with different asymptotic behavior w.r.t. m, and applying Q to the sum (A.1), gives the relation (6.4).

To bound $|R_q(Q,m,f)|$, we use the fact that $|Q_{\mathbf{x}}h_{\mathbf{s}}(\mathbf{x},\mathbf{t})|$ is bounded in $\mathbf{t}$, say by M_q, and that $|f^{(\mathbf{s})}|$ is homogeneous of degree $Re(\alpha)-q$. This gives

$$\begin{aligned}|R_q(Q,m,f)| &\leq m^{q-Re(\alpha)-N}\sum_{|\mathbf{s}|=q} M_q\int_{L^N[m,\infty)}|f^{(\mathbf{s})}(\mathbf{t})|d^N\mathbf{t}\\ &= \frac{M_q}{q-Re(\alpha)-N}\sum_{|\mathbf{s}|=q}\int_{U^N}|f^{(\mathbf{s})}(\mathbf{t})|d^{N-1}\mathbf{t}.\end{aligned}$$

∎

B Proof of Theorem 6.6 and Theorem 8.5

These concern the expansion of $F_p(\mathbf{t})$ when $f(\mathbf{x})$ is homogeneous of degree α. We define

$$g(x_1,\ldots,x_N) = f(x_1^{p+1},\ldots,x_N^{p+1}). \tag{B.1}$$

Then g is a smooth homogeneous function of degree $\gamma=(p+1)\alpha$ on $[0,\infty)^N\setminus\{\mathbf{0}\}$. Obviously, we have

$$f(\psi_p(t_1),\ldots,\psi_p(t_N)) = g(\phi(t_1),\ldots,\phi(t_N)), \tag{B.2}$$

where

$$\phi(t) = (\psi_p(t))^{\frac{1}{p+1}}. \tag{B.3}$$

This function $\phi : [0,1] \to [0,1]$ is smooth, and there exist constants $b > a > 0$ such that

$$at \leq \phi(t) \leq bt. \tag{B.4}$$

We can decompose $\phi(t)$ as

$$\phi(t) = ct + t^3 h(t), \tag{B.5}$$

where $a \leq c \leq b$ and $h(t)$ is a smooth function with an expansion in even powers of t.

We will now show that $g(\phi(t_1), \ldots, \phi(t_N))$ admits an expansion in homogeneous functions of degrees $(\gamma + 2j)_{j=0}^{\infty}$.

Fix an arbitrary real number q, and choose $p \in I\!N$ sufficiently large so that

$$Re(\gamma) + 2p > q. \tag{B.6}$$

We have the Taylor expansion

$$g(\mathbf{x} + \mathbf{y}) = \sum_{k=0}^{p-1} H_k(g; \mathbf{x}, \mathbf{y}) + R_p(g; \mathbf{x}, \mathbf{y}). \tag{B.7}$$

Here

$$H_k(g; \mathbf{x}, \mathbf{y}) = \sum_{|\mathbf{k}|=k} g^{(\mathbf{k})}(\mathbf{x}) \frac{y_1^{k_1} \cdots y_N^{k_N}}{k_1! \cdots k_N!} \tag{B.8}$$

and

$$R_p(g; \mathbf{x}, \mathbf{y}) = \sum_{|\mathbf{k}|=p} g^{(\mathbf{k})}(\mathbf{x} + \theta \mathbf{y}) \frac{y_1^{k_1} \cdots y_N^{k_N}}{k_1! \cdots k_N!} \tag{B.9}$$

for some $\theta \in (0,1)$. In this Taylor expansion, we substitute

$$x_j = ct_j, \qquad y_j = t_j^3 h(t_j). \tag{B.10}$$

This gives, from (B.5),

$$g(\phi(t_1), \ldots, \phi(t_N)) = \sum_{k=0}^{p-1} H_k(g; c\mathbf{t}, (t_1^3 h(t_1), \ldots, t_N^3 h(t_N))) + R_p(g; c\mathbf{t}, (t_1^3 h(t_1), \ldots, t_N^3 h(t_N))). \tag{B.11}$$

Here

$$H_k(g; c\mathbf{t}, (t_1^3 h(t_1), \ldots, t_N^3 h(t_N))) = \sum_{|\mathbf{k}|=k} g^{(\mathbf{k})}(c\mathbf{t}) t_1^{3k_1} \cdots t_N^{3k_N} \frac{h(t_1)^{k_1} \cdots h(t_N)^{k_N}}{k_1! \cdots k_N!}. \tag{B.12}$$

Each term in this sum is a homogeneous function of degree $\gamma - k + 3k$ multiplied with a smooth function that admits a Taylor expansion in homogeneous polynomials of even degree. Hence, (B.12) admits an expansion in smooth homogeneous functions of degrees $(\gamma + 2k + 2j)_{j=0}^{\infty}$. We now search a bound for the remainder

$$R_p(g; c\mathbf{t}, (t_1^3 h(t_1), \ldots, t_N^3 h(t_N))) = \sum_{|\mathbf{k}|=p} g^{(\mathbf{k})}(ct_1 + \theta t_1^3 h(t_1), \ldots, ct_N + \theta t_N^3 h(t_N)) t_1^{3k_1} \cdots t_N^{3k_N} \frac{h(t_1)^{k_1} \cdots h(t_N)^{k_N}}{k_1! \cdots k_N!}. \quad \text{(B.13)}$$

Let G_p be sufficiently large so that for all $\mathbf{x} \in [0, \infty)^N$ with $\|\mathbf{x}\| = 1$ and all $\mathbf{k} \in I\!N^N$ with $|\mathbf{k}| \leq p$, we have

$$|g^{(\mathbf{k})}(\mathbf{x})| \leq G_p. \quad \text{(B.14)}$$

Then we have for $|\mathbf{k}| = p$ that

$$|g^{(\mathbf{k})}(ct_1 + \theta t_1^3 h(t_1), \ldots, ct_N + \theta t_N^3 h(t_N))| \leq G_p \|(ct_1 + \theta t_1^3 h(t_1), \ldots, ct_N + \theta t_N^3 h(t_N))\|^{Re(\gamma)-p}. \quad \text{(B.15)}$$

By (B.4), we have that

$$at \leq ct + \theta t^3 h(t) = (1-\theta)ct + \theta\phi(t) \leq bt,$$

whence

$$|g^{(\mathbf{k})}(ct_1 + \theta t_1^3 h(t_1), \ldots, ct_N + \theta t_N^3 h(t_N))| \leq G_p \|\mathbf{t}\|^{Re(\gamma)-p} \max\{a^{Re(\gamma)-p}, b^{Re(\gamma)-p}\}. \quad \text{(B.16)}$$

Taking the modulus of (B.13) and substituting (B.16) in it, we have

$$\begin{aligned} &|R_p(g; c\mathbf{t}, (t_1^3 h(t_1), \ldots, t_N^3 h(t_N)))| \\ &\leq G_p \|\mathbf{t}\|^{Re(\gamma)-p} \max\{a^{Re(\gamma)-p}, b^{Re(\gamma)-p}\} \|\mathbf{t}\|^{3p} \frac{(|h_1(t_1)| + \cdots + |h_N(t_N)|)^p}{p!} \quad \text{(B.17)} \\ &\leq M\|\mathbf{t}\|^q \quad \text{(B.18)} \end{aligned}$$

for some $M > 0$. To obtain similar bounds for the partial derivatives of the remainder (B.13), we observe that we have the following rules of differentiation:

$$\begin{aligned} \frac{\partial}{\partial x_j} H_k(g; \mathbf{x}, \mathbf{y}) &= H_k(\frac{\partial g}{\partial x_j}; \mathbf{x}, \mathbf{y}) \\ \frac{\partial}{\partial y_j} H_k(g; \mathbf{x}, \mathbf{y}) &= H_{k-1}(\frac{\partial g}{\partial x_j}; \mathbf{x}, \mathbf{y}) \quad (k > 0), \end{aligned}$$

whence, using (B.7), also

$$\begin{aligned}\frac{\partial}{\partial x_j}R_p(g;\mathbf{x},\mathbf{y}) &= R_p(\frac{\partial g}{\partial x_j};\mathbf{x},\mathbf{y})\\ \frac{\partial}{\partial y_j}R_p(g;\mathbf{x},\mathbf{y}) &= R_{p-1}(\frac{\partial g}{\partial x_j};\mathbf{x},\mathbf{y}) \quad (p>0).\end{aligned}$$

By induction on s, we now show that each partial derivative of order s of (B.13) can be written as a finite sum of terms of the form

$$R_{p-l}(\tilde{g};c\mathbf{t},(t_1^3h(t_1),\ldots,t_N^3h(t_N)))\pi(\mathbf{t})\sigma(\mathbf{t}), \tag{B.19}$$

where $\tilde{g}$ is a partial derivative of g of order $k+l$, $\pi(\mathbf{t})$ is a homogeneous polynomial of degree $2l-m$, and $\sigma(\mathbf{t})$ is smooth. k, l, and m are nonnegative, and

$$k+l+m \leq s. \tag{B.20}$$

For $s=0$ this obviously holds. It remains to check that differentiating (B.19) w.r.t. t_j gives a finite sum of terms of the same type as (B.19) but with s incremented with 1. Differentiating the first factor of (B.19) w.r.t. t_j gives by the chain rule 2 terms to which the above rules of differentiation can be applied. The derivative of (B.19) w.r.t. t_j consists of the sum of the following four terms, the first two of which are are produced by differentiating the first factor of (B.19):

$$R_{p-l}(\frac{\partial\tilde{g}}{\partial x_j};c\mathbf{t},(t_1^3h(t_1),\ldots,t_N^3h(t_N)))c\pi(\mathbf{t})\sigma(\mathbf{t}),$$

which is of the same type as (B.19) but with k and s incremented with 1,

$$R_{p-l-1}(\frac{\partial\tilde{g}}{\partial x_j};c\mathbf{t},(t_1^3h(t_1),\ldots,t_N^3h(t_N)))\left(t_j^2\pi(\mathbf{t})\right)\left((3h(t_j)+t_1h'(t_j))\sigma(\mathbf{t})\right),$$

which is of the same type as (B.19) but with l and s incremented with 1,

$$R_{p-l}(\tilde{g};c\mathbf{t},(t_1^3h(t_1),\ldots,t_N^3h(t_N)))\frac{\partial\pi}{\partial t_j}(\mathbf{t})\sigma(\mathbf{t}),$$

which is of the same type as (B.19) but with m and s incremented with 1, and finally

$$R_{p-l}(\tilde{g};c\mathbf{t},(t_1^3h(t_1),\ldots,t_N^3h(t_N)))\pi(\mathbf{t})\frac{\partial\sigma}{\partial t_j}(\mathbf{t}),$$

which is of the same type as (B.19) with s incremented with 1.

Using (B.17), we can bound the modulus of (B.19) by

$$\|\mathbf{t}\|^{(Re(\gamma)-(k+l))+2(p-l)}\|\mathbf{t}\|^{2l-m} = \|\mathbf{t}\|^{Re(\gamma)+2p-k-l-m}$$

multiplied by a constant factor, and this can be further bounded by $M_s\|\mathbf{t}\|^{q-s}$ for some $M_s > 0$. We thus have shown that the remainder (B.13) and its partial derivatives are suitably bounded. We conclude that $f(\psi_p(t_1), \ldots, \psi_p(t_N)) = g(\phi(t_1), \ldots, \phi(t_N))$ admits an expansion in smooth homogeneous functions of degrees $(\gamma + 2j)_{j=0}^{\infty}$. The desired expansion for $F_p(t_1, \ldots, t_N)$ is established by multiplying this expansion with the expansion of the $\psi_p'(t_j)$. This completes the proof of Theorem 6.6.

Now consider the case when f depends analytically on a parameter $z \in \Omega$. Then clearly g also depends analytically on that parameter, and both α and γ are analytic functions of z. It is immediate that the expansion of (B.12) then analytically depends on z. Let K be an arbitrary compact subset of Ω. Then we can choose p sufficiently large so that (B.6) holds for all $z \in K$, and we can also choose G_p and M sufficiently large so that (B.14) and (B.18) hold for all $z \in K$. Observe that in (B.19), the functions $\pi(\mathbf{t})$ and $\sigma(\mathbf{t})$ are independent of z. Therefore, it is readily verified that the constant M_s can be chosen so that the bound $M_s\|\mathbf{t}\|^{q-s}$ for the modulus of (B.19) holds for all $z \in K$. This shows that the expansion of $g(\phi(t_1), \ldots, \phi(t_N))$ depends analytically on z and thus also the expansion of $F_p(t_1, \ldots, t_N)$. This completes the proof of Theorem 8.5

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Table 1: Errors in extrapolation table for the integrand h

$p = 0$	$m = 8$	-0.2748e-01				
			0.1078e-02			
	$m = 16$	-0.1093e-01		-0.3781e-06		
			0.2692e-03		-0.1792e-09	
	$m = 32$	-0.4439e-02		-0.2380e-07		-0.3220e-13
			0.6728e-04		-0.2833e-11	
	$m = 64$	-0.1827e-02		-0.1490e-08		
			0.1682e-04			
	$m = 128$	-0.7586e-03				
$p = 2$	$m = 8$	-0.3624e-03				
			0.3229e-05			
	$m = 16$	-0.2395e-04		0.8779e-10		
			0.6009e-07		-0.1061e-10	
	$m = 32$	-0.1724e-05		-0.9076e-11		-0.2465e-13
			0.1108e-08		-0.7394e-13	
	$m = 64$	-0.1271e-06		-0.2145e-12		
			0.2037e-10			
	$m = 128$	-0.9430e-08				
$p = 4$	$m = 8$	0.3522e-03				
			0.2017e-05			
	$m = 16$	0.6619e-05		0.5179e-08		
			0.1179e-07		0.3499e-11	
	$m = 32$	0.9859e-07		0.8553e-11		0.1332e-14
			0.4725e-10		0.4441e-14	
	$m = 64$	0.1342e-08		0.1266De13		
			0.1679e-12			
	$m = 128$	0.1780e-10				

Table 2: Errors in extrapolation table for the integrand f.

$p = 0$	$m = 8$	-0.2630e-01				
			0.7290e-03			
	$m = 16$	-0.1063e-01		-0.7695e-07		
			0.1822e-03		0.1187e-07	
	$m = 32$	-0.4365e-02		0.2537e-08		0.1536e-10
			0.4555e-04		0.7565e-09	
	$m = 64$	-0.1809e-02		0.9436e-09		
			0.1139e-04			
	$m = 128$	-0.7540e-03				
$p = 2$	$m = 8$	-0.3605e-03				
			0.3103e-05			
	$m = 16$	-0.2392e-04		0.6257e-09		
			0.5827e-07		-0.1302e-10	
	$m = 32$	-0.1724e-05		-0.3044e-11		-0.2354e-13
			0.1080e-08		-0.8371e-13	
	$m = 64$	-0.1271e-06		-0.1301e-12		
			0.1994e-10			
	$m = 128$	-0.9430e-08				
$p = 4$	$m = 8$	0.3527e-03				
			0.2011e-05			
	$m = 16$	0.6619e-05		0.5197e-08		
			0.1179e-07		0.3486e-11	
	$m = 32$	0.9859e-07		0.8558e-11		-0.8882e-15
			0.4725e-10		0.1998e-14	
	$m = 64$	0.1342e-08		0.1021e-13		
			0.1654e-12			
	$m = 128$	0.1780e-10				