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The Euler-Maclaurin Expansion for the Simplex*

By J. N. Lyness and K. K. Puri**

Abstract. A natural extension of the one-dimensional trapezoidal rule to the simplex $0 \leqq x_i \leqq 1$, $\sum x_i \leqq 1$, is a rule Rf which uses as abscissas all those points on a hyper-rectangular lattice of spacing $h = 1/m$ which lie within the simplex, assigning an equal weight to each interior point. In this paper, rules of this type are defined and some of their properties are derived. In particular, it is shown that the error functional satisfies an Euler-Maclaurin expansion of the type

$$Rf - If \sim A_1 h + A_2 h^2 + \cdots + A_p h^p + O(h^{p+1})$$

so long as $f(\mathbf{x})$ and its partial derivatives of order up to p are continuous. Conditions under which this asymptotic series terminates are given, together with the condition for odd terms to drop out leaving an even expansion. The application to Romberg integration is discussed.

1. Introduction. In the theory of Romberg integration, the Euler-Maclaurin expansion

$$R^{[m,\alpha]}f - If = \sum_{q=1}^{p-1} a_q/m^q + E_p^{[m,\alpha]}f \tag{1.1}$$

plays a fundamental role. Here, $R^{[m,\alpha]}f$ stands for an m-panel (offset) trapezoidal rule approximation (see (2.1) below) to

$$If = \int_0^1 f(x)\,dx, \tag{1.2}$$

the quantities a_q are independent of m, and the remainder term satisfies the order relation

$$E_p^{[m,\alpha]}f \sim O(m^{-p}). \tag{1.3}$$

In addition, when $f(x)$ is a polynomial of degree d or less

$$a_q = 0, \qquad q > d, \tag{1.4}$$

and

$$E_p^{[m,\alpha]}f = 0, \qquad p > d. \tag{1.5}$$

Also, in the case where $R^{[m,\alpha]}f$ is a symmetric rule, i.e., the midpoint ($\alpha = 0$) or the endpoint ($\alpha = 1$) trapezoidal rule, it can be shown that

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(1.6) $$a_q = 0, \qquad q \text{ odd}.$$

The results given above are very well known and occur implicitly or explicitly in many papers about Romberg integration such as [3] or [4]. An exhaustive list of such papers is given in a recent survey article by Joyce [5].

It is a straightforward matter to generalize these results to apply to integration over an s-dimensional hypercube. With certain self-evident modification of notation, the difference between product trapezoidal type rule approximations and the integral over the hypercube is also described by an expansion of type (1.1). The statements embodying Eqs. (1.3) to (1.6) are also valid in this wider context. In the case of (1.6), the symmetry required is in each one-dimensional trapezoidal rule which is used to form the product. The theory for the hypercube is given in Baker and Hodgson [2]. In this paper, we are concerned with obtaining analogous results for the simplex. To this end, we introduce the simplex weighted product trapezoidal rule. In the case of the right-angled triangle

$$\Delta_2; \quad x \geqq 0; \quad y \geqq 0; \quad x + y \leqq 1$$

this rule is of the form

$$Rf = \frac{1}{m^2} \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \theta_{j,k} f\left(\frac{j + t_{\alpha_1}}{m}, \frac{k + t_{\alpha_2}}{m}\right),$$

the $\theta_{j,k}$ taking the value 1 if the abscissa is strictly within the triangle and zero if the abscissa is strictly outside the triangle. The specification of $\theta_{j,k}$ if the abscissa lies on an edge of the triangle is discussed in detail below.

We assume that $f(\mathbf{x})$ has a sufficient number of continuous derivatives and derive analogues of the various results mentioned above. The principal results are derived in Sections 4 and 5 and are embodied in Theorems 4.29, 5.10 and 5.15. In Section 6, we discuss the polynomial degree of these rules and we discuss some of the simpler two- and three-dimensional rules in Section 7. Like the one-dimensional trapezoidal rule, individually, these rules are not particularly useful in practice. However, they are powerful when used as the basis of Romberg integration. This is discussed in Section 8.

2. One-Dimensional Notation and Results. This section is devoted to establishing a basic notation and to restating certain known results which will be employed later on. We define a one-dimensional trapezoidal rule operator for an arbitrary interval $[a, b]$ as follows:

(2.1) $$R_x^{[m,\alpha]}[a, b]f(x) = \frac{1}{m} \sum_{j=-\infty}^{\infty} \theta_j f(x_j)$$

where

(2.2) $$x_j = (j - 1 + t_\alpha)/m$$

and

(2.3) $$t_\alpha = (1 + \alpha)/2, \qquad |\alpha| \leqq 1.$$

Essentially, $\theta_j = 1$ when $a < x_j < b$ and $\theta_j = 0$ when x_j lies outside the interval. To take care of the cases when x_j lies at a or at b and the special case when $b = a$

(and even the case when $b < a$ which is not used subsequently), we define θ_i as follows:

$$\begin{aligned} \operatorname{sgn}(x) &= x/|x|, \qquad x \neq 0, \\ &= 0, \qquad x = 0, \\ \theta_i &= \tfrac{1}{2}(\operatorname{sgn}(x_i - a) - \operatorname{sgn}(x_i - b)). \end{aligned} \tag{2.4}$$

In the cases which arise in this paper ($a \leqq b$), we find

$$\begin{aligned} \theta_i &= 1, \qquad a < x_i < b, \\ \theta_i &= \tfrac{1}{2}, \qquad x_i = a < b \text{ or } a < b = x_i, \\ \theta_i &= 0, \qquad a = b, \\ \theta_i &= 0, \qquad \text{otherwise}. \end{aligned} \tag{2.5}$$

We shall write

$$R^{[m,\alpha]}[a, b]f = R_x^{[m,\alpha]}[a, b]f(x) \tag{2.6}$$

and

$$R^{[m,\alpha]}f = R^{[m,\alpha]}[0, 1]f \tag{2.7}$$

in cases where no confusion is likely to arise. This notation is entirely consistent with the notation used in previous papers [6]. However, the superscript m has geometrical significance only as an inverse step length

$$m = 1/h \tag{2.8}$$

and corresponds to the number of panels only in the case that the interval $[a, b]$ happens to be of unit length.

In a corresponding manner, we define

$$I_x[a, b]f(x) = I[a, b]f = \int_a^b f(x)\, dx. \tag{2.9}$$

In the sequel, we require the generalization of the Euler-Maclaurin summation formula given in (2.10) below. This is proved in Lyness [6, p. 62]. (Note that this is not simply a scaled version of the conventional Euler-Maclaurin expansion. In this generalization, the length of the integration interval $[a, b]$ is not an integer multiple of the spacing $1/m$ between function values.) This is

$$\begin{aligned} &R^{[m,\alpha]}[a, b]f - I[a, b]f \\ &= \sum_{q=1}^{p-1} \frac{1}{m^q} \left\{ \frac{\bar{B}_q(t_\alpha - mb)}{q!} f^{(q-1)}(b) - \frac{\bar{B}_q(t_\alpha - ma)}{q!} f^{(q-1)}(a) \right\} + E_p^{[m,\alpha]}[a, b]f \end{aligned} \tag{2.10}$$

where

$$\begin{aligned} E_p^{[m,\alpha]}[a, b]f = \frac{1}{m^p} \Bigg\{ &\frac{\bar{B}_p(t_\alpha - mb)}{p!} f^{(p-1)}(b) - \frac{\bar{B}_p(t_\alpha - ma)}{p!} f^{(p-1)}(a) \\ &- \int_a^b f^{(p)}(x) \frac{\bar{B}_p(t_\alpha - mx)}{p!}\, dx \Bigg\}. \end{aligned} \tag{2.11}$$

Here, the functions $\bar{B}_q(t)$ are periodic Bernoulli functions, which have unit period. $\bar{B}_q(t)$ coincides with the Bernoulli polynomial $B_q(t)$ in the interval $0 < t < 1$, and takes the value $\frac{1}{2}(B_q(1) + B_q(0))$ when t is an integer. We follow the notation used in Abramowitz and Stegun [1, p. 803 et seq.].

One property of the Bernoulli functions, which is fundamental to the work in Section 4, is that

$$\bar{B}_q(x) \in C^{q-2}(-\infty, \infty) \tag{2.12}$$

but that, for $q \geqq 1$, the $(q - 1)$th derivative of $\bar{B}_q(x)$ is discontinuous at integer values of x.

As it is written, the expansion in (2.10) is not in general an expansion in inverse powers of m because the coefficients such as $\bar{B}_q(t_\alpha - mb)$ themselves depend on m. Because of the complicated character of this dependence, involving derivative discontinuities, an asymptotic expansion in inverse powers of m cannot be constructed and so Romberg integration based on $R^{[m,\alpha]}[a, b]f$ cannot be justified. In the special case in which $a = 0, b = 1$, since mb and ma are integers, this dependence on m drops out. Expansion (2.10) then reduces to the conventional Euler-Maclaurin expansion which is an asymptotic expansion in inverse powers of m, and is the basis of Romberg integration.

3. Product Trapezoidal Rules for the Simplex. We treat an s-dimensional simplex Δ_s defined by

$$\Delta_s : x_i \geqq 0, \qquad i = 1, 2, \cdots, s, \qquad \sum_{i=1}^{s} x_i \leqq 1. \tag{3.1}$$

In two dimensions, this is the right-angled triangle having vertices (1, 0), (0, 0), (0, 1). If the coordinates of a point satisfy

$$x_i > 0, \qquad i = 1, 2, \cdots, s, \qquad \sum_{i=1}^{s} x_i < 1, \tag{3.1a}$$

we term the point an *interior point*. If the coordinates satisfy (3.1) but not (3.1a), we term the point a *boundary point*. We denote the integral of $f(\mathbf{x})$ over the simplex by

$$I_{\Delta_s} f = \int_{\Delta_s} f(x_1, x_2, \cdots, x_s)\, dx_1\, dx_2 \cdots dx_s. \tag{3.2}$$

This integral may be expressed in terms of the one-dimensional operators of Section 2 in various ways depending on the coordinate system used and the order of integration. If one uses the coordinate system (3.1), one finds $s!$ different orders of integration are available. For example, in two dimensions one may write

$$I_{\Delta_2} f = I_x[0, 1] I_y[0, 1 - x] f(x, y) \tag{3.3}$$

or

$$I_{\Delta_2} f = I_y[0, 1] I_x[0, 1 - y] f(x, y). \tag{3.4}$$

We are interested in quadrature rules which are natural extensions of the one-dimensional trapezoidal rule. Relations (3.3) and (3.4) suggest quadrature rules of the form

$$R_{12}f = R_x^{[m_1,\alpha_1]}[0, 1]R_y^{[m_2,\alpha_2]}[0, 1 - x]f(x, y), \tag{3.5}$$

or

$$R_{21}f = R_y^{[m_2,\alpha_2]}[0, 1]R_x^{[m_1,\alpha_1]}[0, 1 - y]f(x, y). \tag{3.6}$$

Both of these rules are referred to subsequently as "basic simplex weighted product trapezoidal rules." This term is defined below in Definition 3.13.

Applying definition (2.1) we find that

$$R_{12}f = \frac{1}{m_1 m_2} \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \theta_{i,j} f\left(\frac{i - 1 + t_{\alpha_1}}{m_1}, \frac{j - 1 + t_{\alpha_2}}{m_2}\right), \tag{3.7}$$

where $\theta_{i,j}$ has to be determined from (2.1). The form of $\theta_{i,j}$ is

$$\theta_{i,j} = \theta_i \theta_j(i) \tag{3.8}$$

where

$$\theta_i = 0, \tfrac{1}{2}, 1, \tag{3.9}$$

depending on the position of $(i - 1 + t_{\alpha_1})/m_1$ with respect to the interval [0, 1] and

$$\theta_j(i) = 0, \tfrac{1}{2}, 1, \tag{3.10}$$

depending on the position of $(j - 1 + t_{\alpha_2})/m_2$ with respect to the interval $[0, 1 - (i - 1 + t_{\alpha_1})/m_1]$.

Clearly, for interior points $\theta_{i,j} = 1$ and for exterior points $\theta_{i,j} = 0$. However, for points on the boundary, one can obtain some unexpected values of $\theta_{i,j}$. This is discussed in more detail in Section 7. For the moment, we remark that in the case

$$m_1 = m_2 = m, \qquad t_{\alpha_1} = t_{\alpha_2} = 0, \tag{3.11}$$

the rules $R_{12}f$ and $R_{21}f$ are actually different from each other. The respective weighting factors $\theta_{i,j}$ are listed in Table 7.6. However, this inconvenience does not always occur, even if boundary points are involved. If in place of (3.11), we assign

$$m_1 = m_2 = m, \qquad t_{\alpha_1} = t_{\alpha_2} = \tfrac{1}{2}, \tag{3.12}$$

then $R_{12}f$ and $R_{21}f$ given by (3.5) and (3.6) are identical. This rule has points having weighting factor $\frac{1}{2}$ on the boundary $x + y = 1$.

Definition 3.13. A *basic* simplex weighted product trapezoidal rule for the s-dimensional simplex Δ_s is a sum of function values of the form

$$\begin{aligned} &R_{x_1}^{[m_1,\alpha_1]}[0, 1]R_{x_2}^{[m_2,\alpha_2]}[0, 1 - x_1]R_{x_3}^{[m_3,\alpha_3]}[0, 1 - x_1 - x_2] \\ &\qquad \cdots R_{x_s}^{[m_s,\alpha_s]}\left[0, 1 - \sum_{j=1}^{s-1} x_j\right] f(x_1, x_2, \cdots, x_s) \end{aligned} \tag{3.13}$$

or a similar sum in which the variables $x_1, x_2, \cdots, x_s$ are permuted in the rule operators (but not in the function arguments). Here, Δ_s is defined by (3.1) above and the constituent one-dimensional trapezoidal rule operators are defined by (2.1) above. The basic simplex weighted product trapezoidal rule Rf enjoys the following properties:

(1) All abscissas lie on a rectangular grid which includes points of the form

$$(t_{\alpha_1} + k_1)/m_1, (t_{\alpha_2} + k_2)/m_2, \cdots, \quad (t_{\alpha_s} + k_s)/m_s,$$

where k_i are positive or negative integers or zero. (The values of $t_{\alpha_i} = (\alpha_i + 1)/2$ and m_i are specified in (3.13).)

(2) The weight attached to each abscissa is

$$\theta_k/(m_1 m_2 \cdots m_s)$$

where $\theta_k = 1$ if the point is strictly inside Δ_s and $\theta_k = 0$ if the point is strictly outside Δ_s.

(3) The value of θ_k when the point is on the boundary of Δ_s is determined from (3.13) and (2.1) and (2.4). However, it may take only one of the $s + 2$ values

$$\theta = 1, 1/2, 1/4, \cdots, 1/2^s \quad \text{or} \quad 0. \tag{3.14}$$

Some examples of basic simplex weighted product trapezoidal rules in two and three dimensions are given in Section 7. It appears that they are not usually symmetric and that there are other more natural rules which satisfy properties (1) and (2) but not property (3). We refer to these simply as follows.

Definition 3.15. A simplex weighted product trapezoidal rule Rf is a sum of function values satisfying properties (1) and (2) above. An example is the symmetric sum

$$R_S f = \tfrac{1}{2}(R_{12}f + R_{21}f) \tag{3.16}$$

defined by (3.5) and (3.6) above with $m_1 = m_2 = m$; $t_{\alpha_1} = t_{\alpha_2} = 0$ as in (3.11). This rule is not basic as it does not satisfy property (3) and cannot be expressed in form (3.13). However, it does satisfy properties (1) and (2) and is in addition symmetric in the interchange of the x and y coordinates.

Finally, we remark that our present interest in basic rules derives solely from the circumstance that we can prove our results directly and generally for these rules. Once this is done, it is sometimes possible to use these results to derive the corresponding results for the more general rules which do not satisfy property (3). This approach is employed in Section 7.

4. An Euler-Maclaurin Expansion for Δ_s. We are concerned here with deriving the Euler-Maclaurin expansion for the basic simplex weighted product trapezoidal rule over an s-dimensional simplex. We carry out the derivation for the case $s = 3$ only. The method generalizes in an obvious way. We therefore investigate the difference between the rule sum

$$Rf = R_x^{[m_1,\alpha_1]}[0, 1]R_y^{[m_2,\alpha_2]}[0, 1 - x]R_z^{[m_3,\alpha_3]}[0, 1 - x - y]f(x, y, z) \tag{4.1}$$

and the integral

$$I_{\Delta_3}f = I_x[0, 1]I_y[0, 1 - x]I_z[0, 1 - x - y]f(x, y, z) \tag{4.2}$$

which the rule sum (4.1) is supposed to approximate.

In this paper, we shall assume that $f(\mathbf{x})$ and all its partial derivatives of total order p or less are continuous in all variables within and on the boundary of the simplex Δ_s. We are interested principally in the case in which the spacing $h = 1/m$ is the same in each direction, that is

$$m_1 = m_2 = m_3 = m.$$

However, the derivation is marginally more general and allows an assignment of the form $m_3 = k_{32}m_2$; $m_2 = k_{21}m_1$, where k_{32}, k_{21} are integers. The quantity $k_{31} = k_{32}k_{21} = m_3/m_1$ also occurs in the result.

The statement that a term is $O(m^{-p})$ is taken to mean that it is $O(m_i^{-p})$ where i may be 1, 2 or 3. A situation is implied in which the values of m_i become infinite in a manner in which k_{32} and k_{21} remain constant. We commence by applying (2.10) to form an expansion for

$$\varphi(x, y) = R_z^{[m_3, \alpha_3]}[0, 1 - x - y]f(x, y, z). \tag{4.3}$$

This gives

$$\varphi(x, y) = \sum_{q_3=0}^{p-1} c_{q_3}(x, y)/m_3^{q_3} + C_p(x, y)/m_3^p, \tag{4.4}$$

where

$$c_0(x, y) = \int_0^{1-x-y} f(x, y, z)\, dz,$$

$$c_{q_3}(x, y) = \frac{\bar{B}_{q_3}(t_{\alpha_3} - m_3(1 - x - y))}{q_3!} \frac{\partial^{q_3-1}}{\partial z^{q_3-1}} f(x, y, z)\bigg|_{z=1-x-y} - \frac{\bar{B}_{q_3}(t_{\alpha_3})}{q_3!} \frac{\partial^{q_3-1}}{\partial z^{q_3-1}} f(x, y, z)\bigg|_{z=0}, \qquad q_3 \geqq 1, \tag{4.5}$$

and

$$|C_p(x, y)| < K. \tag{4.6}$$

The next stage would be to apply the same expansion (2.10) to

$$R_y^{[m_2, \alpha_2]}[0, 1 - x]\varphi(x, y).$$

Unfortunately, this is not possible because the function $\varphi(x, y)$ is not continuous in the variable y. This is obvious from its definition (4.3). As y is increased, the rule sum in (4.3) abruptly requires an additional function value. This is reflected in the coefficients $c_q(x, y)$ as these involve Bernoulli functions $\bar{B}_q(t)$ which have discontinuities in the $(q - 1)$th derivative at $t = 0, 1, \cdots$. In order to overcome this difficulty, we synthesize each function $c_{q_3}(x, y)$ as follows

$$c_{q_3}(x, y) = a_{q_3}(x, y) + b_{q_3}(x, y), \tag{4.7}$$

where

$$a_0(x, y) = c_0(x, y); \qquad b_0(x, y) = 0,$$

$$a_{q_3}(x, y) = \frac{\bar{B}_{q_3}(t_{\alpha_3} + m_3 t_{\alpha_2}/m_2 + m_3 t_{\alpha_1}/m_1)}{q_3!} \frac{\partial^{q_3-1}}{\partial z^{q_3-1}} f(x, y, z)\bigg|_{z=1-x-y} - \frac{\bar{B}_{q_3}(t_{\alpha_3})}{q_3!} \frac{\partial^{q_3-1}}{\partial z^{q_3-1}} f(x, y, z)\bigg|_{z=0}, \qquad q_3 \geqq 1, \tag{4.8}$$

and

$$b_{q_3}(x, y) = \left\{\frac{\bar{B}_{q_3}(t_{\alpha_3} - m_3(1 - x - y))}{q_3!} - \frac{\bar{B}_{q_3}(t_{\alpha_3} + m_3 t_{\alpha_2}/m_2 + m_3 t_{\alpha_1}/m_1)}{q_3!}\right\}$$

(4.9)
$$\times \frac{\partial^{q_3-1}}{\partial z^{q_3-1}} f(x, y, z)\Big|_{z=1-x-y}, \qquad q_3 \geqq 1.$$

This synthesis depends on α_1 and α_2. The functions $a_{q_3}(x, y)$ have continuous derivatives of order up to $p - q_3 + 1$ and the functions $b_{q_3}(x, y)$ contain the inconvenient discontinuities in the derivatives. In the subsequent part of the summation, each point (x_i, y_j) for function evaluation has the form

(4.10)
$$(x_i, y_j) = \left(\frac{i - 1 + t_{\alpha_1}}{m_1}, \frac{j - 1 + t_{\alpha_2}}{m_2}\right).$$

For these points, the Bernoulli functions in (4.9) are identical and so

(4.11)
$$b_{q_3}(x_i, y_j) = 0.$$

Consequently,

(4.12)
$$R^{[m_1,\alpha_1]}[0, 1]R^{[m_2,\alpha_2]}[0, 1 - x]b_{q_3}(x, y) = 0.$$

We may then replace $c_{q_3}(x, y)$ in (4.4) by its synthesis in (4.7) and, using (4.12), we find at once that

(4.13)
$$Rf = \sum_{q_3=0}^{p-1} \frac{1}{m_3^{q_3}} R^{[m_1,\alpha_1]}[0, 1]R^{[m_2,\alpha_2]}[0, 1 - x]a_{q_3}(x, y) + \frac{1}{m_3^p} R^{[m_1,\alpha_1]}[0, 1]R^{[m_2,\alpha_2]}[0, 1 - x]C_p(x, y).$$

The final term is of order m^{-p} and forms part of the ultimate remainder term. The functions $a_{q_3}(x, y)$ have continuous derivatives up to order $p - q_3 - 1$. We are now ready to carry out the second stage of the calculation which consists of using (2.10) to expand

(4.14)
$$R^{[m_2,\alpha_2]}[0, 1 - x]a_{q_3}(x, y).$$

Proceeding in an identical manner, we find

(4.15)
$$R_y^{[m_2,\alpha_2]}[0, 1 - x]a_{q_3}(x, y) = \sum_{q_2=0}^{p-q_3-1} \frac{c_{q_2,q_3}(x)}{m_2^{q_2}} + \frac{C_{p-q_3,q_3}(x)}{m_2^{p-q_3}}, \qquad q_3 = 0, 1, \cdots, p - 1.$$

Here, $C_{p-q_3,q_3}(x)$ is bounded and the other coefficients may be expressed in the form

(4.16)
$$c_{q_2,q_3}(x) = a_{q_2,q_3}(x) + b_{q_2,q_3}(x)$$

with

$$a_{0,q_3}(x) = \int_0^{1-x} a_{q_3}(x, y)\, dy; \qquad b_{0,q_3}(x) = 0,$$

$$(4.17) \qquad a_{q_2,q_3}(x) = \frac{\bar{B}_{q_2}(t_{\alpha_2} + m_2 t_{\alpha_1}/m_1)}{q_2!} \frac{\partial^{q_2-1}}{\partial y^{q_2-1}} a_{q_3}(x, y)\bigg|_{y=1-x} - \frac{\bar{B}_{q_2}(t_{\alpha_2})}{q_2!} \frac{\partial^{q_2-1}}{\partial y^{q_2-1}} a_{q_3}(x, y)\bigg|_{y=0}, \qquad q_2 \geqq 1,$$

and

$$(4.18) \qquad b_{q_2,q_3}(x) = \frac{\bar{B}_{q_2}(t_{\alpha_2} - m_2(1-x)) - \bar{B}_{q_2}(t_{\alpha_2} + m_2 t_{\alpha_1}/m_1)}{q_2!} \times \frac{\partial^{q_2-1}}{\partial y^{q_2-1}} a_{q_3}(x, y)\bigg|_{y=1-x}, \qquad q_2 \geqq 1.$$

The function $a_{q_2,q_3}(x)$ has continuous derivatives of order up to $p - q_2 - q_3 + 2$, while

$$(4.19) \qquad R_x^{[m_1,\alpha_1]}[0, 1] b_{q_2,q_3}(x) = 0.$$

Substituting these expressions into (4.13) gives

$$(4.20) \qquad \begin{aligned} Rf = {} & \sum_{q_3=0}^{p-1} \sum_{q_2=0}^{p-q_3-1} \frac{1}{m_2^{q_2} m_3^{q_3}} R_x^{[m_1,\alpha_1]}[0, 1] a_{q_2,q_3}(x) \\ & + \sum_{q_3=0}^{p-1} \frac{1}{m_3^{q_3}} \frac{1}{m_2^{p-q_3}} R_x^{[m_1,\alpha_1]}[0, 1] C_{p-q_3,q_3}(x) \\ & + \frac{1}{m_3^p} R_x^{[m_1,\alpha_1]}[0, 1] R_y^{[m_2,\alpha_2]}[0, 1-x] C_p(x, y). \end{aligned}$$

The final $p + 1$ terms here are remainder terms of order m^{-p}. The final stage, that of evaluating $R_x^{[m_1,\alpha_1]} a_{q_2,q_3}(x)$, is straightforward since there are no complications arising from a variable interval length. We use (2.10) again to obtain

$$(4.21) \qquad R_x^{[m_1,\alpha_1]}[0, 1] a_{q_2,q_3}(x) = \sum_{q_1=0}^{p-q_2-q_3-1} \frac{a_{q_1,q_2,q_3}}{m_1^{q_1}} + \frac{C_{p-q_2-q_3,q_2,q_3}}{m_1^{p-q_2-q_3}},$$

$$q_2 = 0, 1, \cdots, p - q_2 - 1, \quad q_3 = 0, 1, \cdots, p - 1,$$

where $C_{p-q_2-q_3 q_2,q_3}$ is bounded and

$$(4.22) \qquad a_{q_1,q_2,q_3} = \frac{B_{q_1}(t_{\alpha_1})}{q_1!} \left\{ \frac{\partial^{q_1-1}}{\partial x^{q_1-1}} a_{q_2,q_3}(x) \bigg|_{x=1} - \frac{\partial^{q_1-1}}{\partial x^{q_1-1}} a_{q_2,q_3}(x) \bigg|_{x=0} \right\}.$$

Substituting (4.21) into (4.20), we find

$$(4.23) \qquad Rf = \sum_{q_3=0}^{p-1} \sum_{q_2=0}^{p-q_3-1} \sum_{q_1=0}^{p-q_3-q_2-1} a_{q_1,q_2,q_3} / m_1^{q_1} m_2^{q_2} m_3^{q_3} + Ef,$$

where

$$Ef = \sum_{q_3=0}^{p-1} \sum_{q_2=0}^{p-q_3-1} \frac{C_{p-q_2-q_3,q_2,q_3}}{m_1^{p-q_2-q_3} m_2^{q_2} m_3^{q_3}} + \sum_{q_3=0}^{p-1} \frac{1}{m_3^{q_3} m_2^{p-q_3}} R_x^{[m_1,\alpha_1]}[0, 1]C_{p-q_3,q_3}(x) \tag{4.24}$$
$$+ \frac{1}{m_3^p} R_x^{[m_1,\alpha_1]}[0, 1]R_y^{[m_3,\alpha_3]}[0, 1 - x]C_p(x, y).$$

Since the functions and operators occurring here are bounded, we may write

$$|Ef| < km^{-p}. \tag{4.25}$$

To avoid unnecessary complication, we state the theorem for the case

$$m_1 = m_2 = m_3 = m. \tag{4.26}$$

We note from the definitions which lead to the constants a_{q_1,q_2,q_3}, namely (4.22), (4.17) and (4.8), that

$$a_{0,0,0} = I_{\Delta_3}f \tag{4.27}$$

and that

$$a_{q_1,q_2,q_3}, \qquad q_1 + q_2 + q_3 < p, \tag{4.28}$$

are independent of m. We also note that the remainder term Ef given by (4.24) consists of the sum of a finite number of terms, each of which is of the form C/m^p where C is bounded. This leads to the theorem.

THEOREM 4.29.

$$Rf - I_{\Delta_3}f = \sum_{q=1}^{p-1} A_q/m^q + Ef, \tag{4.29}$$

where Rf and $I_{\Delta_3}f$ are given by (4.1) *with* $m_1 = m_2 = m_3 = m$ *and* (4.2) *respectively, the quantities A_q, $q = 1, 2, \cdots, p - 1$, are independent of m and*

$$|Ef| < km^{-p}. \tag{4.30}$$

Here

$$A_q = \sum_{q_1=0}^{q} \sum_{q_2=0}^{q-q_1} a_{q_1,q_2,q-q_1-q_2}. \tag{4.31}$$

5. The Coefficients A_q. In this section, we look in some detail at the structure and properties of the coefficients A_q which occur in the Euler-Maclaurin expansion (4.29). These are functions of the rule parameters $\alpha_1, \alpha_2, \cdots, \alpha_s$ and depend also on the function $f(\mathbf{x})$. In view of the possible application of this expansion in Romberg integration, we are particularly interested in the circumstances under which certain coefficients vanish.

The principal results of this section are given in Theorems 5.10 and 5.15 below. These state that the expansion terminates if $f(\mathbf{x})$ is a polynomial and that the odd coefficients are zero if all the constituent one-dimensional trapezoidal rules are symmetric.

It is difficult to write down a closed expression for A_q in conventional notation which is not unduly cumbersome. We content ourselves with a recursive definition embodied in Eqs. (5.1) to (5.5) below. For notational convenience, we define

$$\mu_j = 1 - \sum_{i=1}^{j-1} x_i; \qquad \lambda_j^1 = \sum_{l=1}^{j} k_{jl} t_{\alpha l}; \qquad \lambda_j^0 = t_{\alpha j} \tag{5.1}$$

where, as before, $k_{jl} = m_j/m_l$. Then, following through the definitions of Section 4 in an s-dimensional rather than a 3-dimensional context, we find the following recursive definition of $a_{q_1, q_2, \cdots, q_s}$:

$$a(x_1, x_2, \cdots, x_s) = f(x_1, x_2, \cdots, x_s), \tag{5.2}$$

$$\begin{aligned} &a_{q_t, q_{t+1}, \cdots, q_s}(x_1, x_2, \cdots, x_{t-1}) \\ &\quad = \frac{\bar{B}_{q_t}(\lambda_t^1)}{q_t!} \frac{\partial^{q_t - 1}}{\partial x_t^{q_t - 1}} a_{q_{t+1}, q_{t+2}, \cdots, q_s}(x_1, x_2, \cdots, x_t)\Big|_{x_t = \mu_t} \\ &\quad - \frac{\bar{B}_{q_t}(\lambda_t^0)}{q_t!} \frac{\partial^{q_t - 1}}{\partial x_t^{q_t - 1}} a_{q_{t+1}, q_{t+2}, \cdots, q_s}(x_1, x_2, \cdots, x_t)\Big|_{x_t = 0}. \end{aligned} \tag{5.3a}$$

When $q_t = 0$, this is interpreted as an integral, i.e.,

$$a_{0, q_{t+1}, \cdots, q_s}(x_1, x_2, \cdots, x_{t-1}) = \int_0^{\mu_t} a_{q_{t+1}, \cdots, q_s}(x_1, x_2, \cdots, x_t)\, dx_t. \tag{5.3b}$$

Since $\lambda_1^1 = \lambda_1^0 = t_{\alpha_1}$, the final stage, that having $t = 1$, may also be simplified. Thus,

$$a_{q_1, q_2, \cdots, q_s} = \frac{\bar{B}_{q_1}(t_{\alpha_1})}{q_1!} \int_0^1 \frac{\partial^{q_1}}{\partial x^{q_1}} a_{q_2, q_3, \cdots, q_s}(x_1)\, dx_1. \tag{5.4}$$

Finally,

$$A_q = \sum_{\Sigma q_i = q} a_{q_1, q_2, \cdots, q_s}, \tag{5.5}$$

the sum being taken over all distinct sets of nonnegative integers q_i whose sum is q.

LEMMA 5.6. *If $f(\mathbf{x})$ is a polynomial of degree d, then*

$$a_{q_1, q_2, \cdots, q_s} = 0 \quad \textit{when} \sum_{t=1}^{s} q_t > d + s - 1.$$

Proof. In this proof, the statement that a function is a polynomial of degree d' assumes its usual meaning when $d' \geqq 0$ and assumes the meaning that it is identically zero when $d' < 0$.

Let us suppose that the function $a_{q_{t+1}, \cdots, q_s}(x_1, \cdots, x_t)$ is a polynomial of degree d_t. One term in the subsequent function in (5.3a) is obtained by differentiating $q_t - 1$ times and replacing one of the variables x_t by a linear sum μ_t of the other variables. The other term is obtained in the same way, except that μ_t is replaced by zero. Thus, the subsequent function is a polynomial of degree d_{t-1} satisfying

$$d_{t-1} \leqq d_t - q_t + 1. \tag{5.7}$$

In the case in which $q_t = 0$, examination of (5.3b) yields the same result (5.7).

Thus, if $f(\mathbf{x})$ in (5.2) is of degree d applying (5.7) $(s - 1)$ times shows that the degree d_1 of $a_{q_2, q_3, \cdots, q_s}(x_1)$ satisfies

$$d_1 \leqq d - \sum_{t=2}^{s} q_t + (s - 1). \tag{5.8}$$

However, the integrand in (5.4) is zero if

$$d_1 < q_1. \tag{5.9}$$

The simple consequence of (5.8) and (5.9) is the statement of Lemma 5.6 above. Finally, since A_q is a sum of these coefficients having $\sum q_t = q$, there follows

THEOREM 5.10. *When $f(\mathbf{x})$ is a polynomial of degree d,*

$$A_q = 0, \qquad q > d + s - 1, \tag{5.10}$$

Theorem 5.10 represents a major difference between the theory as applied to the simplex given here and the corresponding much simpler theory for the hypercube. In the expansion for the hypercube, (5.10) is replaced by

$$A_q = 0, \qquad q > d \text{ (hypercube)}. \tag{5.11}$$

The difference arises at the point where the variable limits μ_i are introduced (definition (5.1)). For the hypercube, one would replace $\mu_i(x_1, x_2, \cdots, x_{i-1})$ by $\mu_i = 1$. This has the effect that (5.3a) could be replaced by an integral analogous to (5.4). Then (5.7) would be replaced by

$$d_{t-1} \leqq d_t - q_t \qquad \text{(hypercube)}. \tag{5.12}$$

This adjustment, being necessary only $(s - 1)$ times, accounts precisely for the discrepancy between (5.10) and (5.11). Incidentally, the formalism given here is quite unnecessary to derive similar results for the hypercube.

The effect of the constituent trapezoidal rules being symmetric is much easier to gauge. First, we recall that the odd Bernoulli functions satisfy

$$\bar{B}_q(n) = \bar{B}_q(n + \tfrac{1}{2}) = 0, \qquad q \text{ odd}, n \text{ integer}. \tag{5.13}$$

In (5.3a) if it happens that $\bar{B}_{q_t}(\lambda_t^1) = \bar{B}_{q_t}(\lambda_t^0) = 0$, then the function defined by (5.3a) is zero and so subsequently is $a_{q_1,q_2,\cdots,q_s}$. One of the many possible cases in which this happens is covered in the following lemma:

LEMMA 5.14. *If $2t_{\alpha_i}$ is an integer for $i = 1, 2, \cdots, s$, and q_t is odd, then*

$$a_{q_1,q_2,\cdots,q_s} = 0.$$

In expression (5.5) for A_q, we see that if q is odd, then each term in the sum on the right must contain at least one odd subscript. Thus

THEOREM 5.15. *If each constituent rule $R^{[m_i,\alpha_i]}$ in a basic simplex weighted product trapezoidal rule is either a midpoint rule ($\alpha_i = 0$) or an endpoint rule ($\alpha_i = 1$), then*

$$A_q = 0, \qquad q \text{ odd}.$$

6. The Polynomial Degree of $R^{(m)}f$. A natural question to ask about a quadrature rule is whether or not it is exact for $f(\mathbf{x}) =$ constant, i.e., is it of polynomial degree zero? In this section, we show that the basic simplex weighted product trapezoidal rules for the simplex are in general not of degree zero, though there are some exceptions to this statement.

In this section, we restrict ourselves to cases in which $m = m_1 = m_2 = \cdots = m_s$. We denote by $R^{(m)}f$ an s-dimensional basic simplex weighted product trapezoidal rule of type (3.13). We note that Theorem 5.10 warns us that we might expect a situation of this type. This states that when $f(\mathbf{x}) = 1$, i.e., is a polynomial of degree zero, then $A_q = 0$ for $q > s - 1$. Thus,

$$R^{(m)}f - If = \frac{A_1}{m} + \frac{A_2}{m^2} + \cdots + \frac{A_{s-1}}{m^{s-1}}. \tag{6.1}$$

In the 'symmetric cases' covered by Theorem 5.15, the terms A_q/m^q with q odd drop out. But there is no other reason to believe that, in this rather special case with $f(\mathbf{x}) = 1$, any of the terms in (6.1) should be zero. And if they are not zero, then $R^{(m)}f$ differs from $I_{\Delta_s}f$ and is not of degree zero.

The results of this section are Theorems 6.4 and 6.6 below. We treat the case $s \geqq 3$ first. The result in Theorem 6.4 below is proved by means of two lemmas.

LEMMA 6.2. *For $s \geqq 3$, $R^{(m)}f$, $m = 1, 2$, is not of degree zero.*

Proof. Using properties (2) and (3) of Section 3 and Eq. (3.14), we have

$$R^{(m)}f = \frac{1}{m^s} \sum_{k=1} \theta_k f(\mathbf{x}_k),$$

where

$$\theta_k = \lambda_k/2^s, \qquad \lambda_k = \text{integer}.$$

Thus, when $f(\mathbf{x}) = 1$, it follows

$$I_{\Delta_s}f = 1/s!; \qquad R^{(m)}f = \lambda/(2m)^s, \quad \lambda = \text{integer}.$$

If $I_{\Delta_s}f$ is to equal $R^{(m)}f$, then

$$\lambda = (2m)^s/s!$$

must be an integer. If $s \geqq 3$ and $m = 1$ or 2, this is clearly impossible. This establishes Lemma 6.2.

LEMMA 6.3. *If $R^{(m)}f$ is of degree zero for $s - 1$ distinct values of m, then it is of degree zero for all m.*

Proof. Let $A_1, A_2, \cdots, A_{s-1}$ stand for the values of the coefficients in the case that $f(\mathbf{x}) = 1$. Then, if the $s - 1$ distinct values are $m_1, m_2, \cdots, m_{s-1}$, we have

$$0 = R^{(m_i)}f - I_{\Delta_s}f = \sum_{j=1}^{s-1} A_j/m_i^j, \qquad i = 1, 2, \cdots, s-1.$$

This is a set of $s - 1$ linear homogeneous equations in $s - 1$ unknowns A_j with a nonsingular coefficient matrix. This has the unique solution $A_1 = A_2 = \cdots = A_{s-1} = 0$. Consequently,

$$R^{(m)}f - I_{\Delta_s}f = \sum_{j=1}^{s-1} A_j/m^j = 0 \quad \text{all } m.$$

The immediate consequence of Lemmas 6.2 and 6.3 is

THEOREM 6.4. *For $s \geqq 3$, the basic simplex weighted product trapezoidal rule $R^{(m)}f$ is of degree zero for at most $s - 2$ special values of m.*

The two-dimensional case requires special treatment. Theorem 5.10 gives, for $f(\mathbf{x}) = 1$,

$$R^{(m)}f - If = A_1/m$$

and Theorem 5.15 shows

(6.5) $$A_1 = 0, \quad t_{\alpha_1} = 0, \tfrac{1}{2} \quad \textit{and} \quad t_{\alpha_2} = 0, \tfrac{1}{2}.$$

However, a direct evaluation of A_1 when $f(\mathbf{x}) = 1$ leads to some other cases in which A_1 is zero. We find

$$A_1 = \bar{B}_1(t_{\alpha_2} + t_{\alpha_1}) - \bar{B}_1(t_{\alpha_1}) - \bar{B}_1(t_{\alpha_2}) \qquad (f(\mathbf{x}) = 1; s = 2),$$

where

$$\bar{B}_1(x) = x - \tfrac{1}{2}, \qquad 0 < x < 1,$$
$$\bar{B}_1(x + 1) = \bar{B}_1(x), \qquad \text{all } x,$$
$$\bar{B}_1(0) = \bar{B}_1(1) = 0.$$

This leads to

$$A_1 = 0, \qquad t_{\alpha_1} = 0, \quad \text{any } t_{\alpha_2},$$
$$A_1 = 0, \qquad t_{\alpha_2} = 0, \quad \text{any } t_{\alpha_1},$$
$$A_1 = 0, \qquad t_{\alpha_1} + t_{\alpha_2} = 1.$$

These include (6.5) above. In fact, these are precisely the cases in which the rule $R^{(1)}f$ includes a boundary point, thus making it possible for $R^{(1)}f = \frac{1}{2} = If$.

THEOREM 6.6. *When* $s = 2$, $R^{(m)}f$ *is of degree zero if and only if either* $t_{\alpha_1} = 0$ *or* $t_{\alpha_2} = 0$ *or* $t_{\alpha_1} + t_{\alpha_2} = 1$.

7. Examples of Two- and Three-Dimensional Rules. Up to this point, we have considered only families of basic rules defined by product one-dimensional operators of form (3.13). This restriction arose simply because only in these cases is any reasonably general method for establishing the Euler-Maclaurin expansion known to us. In this section, we consider, in certain very special cases, the rules obtained using a different, intuitive approach. This discussion is limited to 'centre' rules and 'vertex' rules and is also limited to two- and three-dimensional simplexes.

Definition 7.1. A two-dimensional vertex rule is one of the form

(7.1) $$R^{(m)}f = \frac{1}{m^2} \sum_{i=0}^{m} \sum_{j=0}^{m-i} \theta_{i,j} f(i/m, j/m)$$

where

(7.2) $$\theta_{i,j} = 1, \qquad (i/m, j/m) \text{ is an interior point.}$$

The main interest centres on the definition of $\theta_{i,j}$ when $(i/m, j/m)$ is a boundary point.

Two examples of two-dimensional vertex rules have been considered in the previous sections. These are

(7.3) $$R_{12}^{(m)}f = R_x^{[m,1]}[0, 1]R_y^{[m,1]}[0, 1 - x]f(x, y),$$

(7.4) $$R_{21}^{(m)}f = R_y^{[m,1]}[0, 1]R_x^{[m,1]}[0, 1 - y]f(x, y).$$

As mentioned in Section 3, these are different from each other. A 'natural' rule may be obtained using various intuitive approaches. The grid lines divide the simplex into squares and right angled triangles. If we assign to each square the weight $\frac{1}{4}m^2$ at each corner and to each triangle the weights $\frac{1}{4}m^2$, $\frac{1}{8}m^2$, $\frac{1}{8}m^2$ at the right angle vertex and the other two vertices, we obtain a natural rule $R_s^{(m)}f$. It appears that

$$R_s^{(m)}f = \tfrac{1}{2}(R_{12}^{(m)}f + R_{21}^{(m)}f). \tag{7.5}$$

The weight factors $\theta_{i,j}$ are listed in Table 7.6.

TABLE 7.6

	$R_{21}^{(m)}$	$R_{12}^{(m)}$	$R_s^{(m)}$
interior	1	1	1
edge but not vertex	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
vertex (0, 0)	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
vertex (1, 0)	$\frac{1}{4}$	0	$\frac{1}{8}$
vertex (0, 1)	0	$\frac{1}{4}$	$\frac{1}{8}$

We make the following remarks:

1. All three rules are of polynomial degree zero. None is of polynomial degree 1.
2. All three have an even error expansion of the form

$$R^{(m)}f - I_{\Delta_2}f = A_2/m^2 + A_4/m^4 + \cdots . \tag{7.7}$$

3. Since

$$\begin{aligned} R_s^{(m)}f &= R_{12}f + \frac{1}{8m^2}(f(0, 1) - f(1, 0)) \\ &= R_{21}f - \frac{1}{8m^2}(f(0, 1) - f(1, 0)), \end{aligned} \tag{7.8}$$

the coefficients $A_4, A_6, \cdots$ in (7.7) are the same for all three rules. The coefficient A_2 differs from one rule to another according to (7.8).

Definition 7.9. A three-dimensional vertex rule is one of the form

$$R^{(m)}f = \frac{1}{m^3}\sum_{i=0}^{m}\sum_{j=0}^{m-i}\sum_{k=0}^{m-i-j}{}' \theta_{i,j}f\left(\frac{i}{m}, \frac{j}{m}, \frac{k}{m}\right), \tag{7.9}$$

where

$$\theta_{i,j,k} = 1, \qquad (i/m, j/m, k/m) \text{ is an interior point.} \tag{7.10}$$

The previous sections provide six examples. These are 'basic' rules of form (3.13), namely

$$R_{i,j,k}^{(m)}f = R_{x_i}^{[m,1]}[0, 1]R_{x_j}^{[m,1]}[0, 1 - x_i]R_{x_k}^{[m,1]}[0, 1 - x_i - x_j]f(x_1, x_2, x_3) \tag{7.11}$$

where $\{i, j, k\}$ is a permutation of $\{1, 2, 3\}$. It turns out that these rules are identical in pairs; thus,

$$R_{i,j,k}^{(m)}f = R_{j,i,k}^{(m)}f. \tag{7.12}$$

The weighting factors $\theta_{i,j,k}$ corresponding to these rules and to another rule $R_N^{(m)}$ are listed in Table 7.13. Here, we have used the following abbreviation:

$$\text{Face}^* = \text{Face but not edge,}$$

$$\text{Edge}^* = \text{Edge but not vertex,}$$

$$\sigma = x_1 + x_2 + x_3 - 1.$$

TABLE 7.13

	$R_{231}^{(m)}$ or $R_{321}^{(m)}$	$R_{312}^{(m)}$ or $R_{132}^{(m)}$	$R_{123}^{(m)}$ or $R_{213}^{(m)}$	$R_N^{(m)}$
interior	1	1	1	1
Face* $x_i = 0$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
Face* $\sigma = 0$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
Edge* $x_i = x_j = 0$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
Edge* $\sigma = x_1 = 0$	0	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{5}{36}$
$\sigma = x_2 = 0$	$\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{5}{36}$
$\sigma = x_3 = 0$	$\frac{1}{4}$	$\frac{1}{4}$	0	$\frac{5}{36}$
Vertex (0, 0, 0)	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
(1, 0, 0)	$\frac{1}{8}$	0	0	$\frac{1}{72}$
(0, 1, 0)	0	$\frac{1}{8}$	0	$\frac{1}{72}$
(0, 0, 1)	0	0	$\frac{1}{8}$	$\frac{1}{72}$

The three product rules have an even expansion

$$R^{(m)}f - I_{\Delta_3}f = A_2/m^2 + A_4/m^4 + \cdots . \tag{7.14}$$

However, they are not of degree zero. In fact,

$$R_{i,j,k}^{(m)}f - I_{\Delta_3}f = \frac{1/12}{m^2}, \qquad f(\mathbf{x}) = 1. \tag{7.15}$$

Since this relation is satisfied by all three rules, it is also satisfied by their symmetrized sum

$$R_s^{(m)}f = \tfrac{1}{3}(R_{231}^{(m)}f + R_{312}^{(m)}f + R_{123}^{(m)}f). \tag{7.16}$$

The weighting factors for $R_s^{(m)}$ are not given in Table 7.13 explicitly.

Because the rule $R_s^{(m)}f$ does not integrate the constant function correctly, a rule $R_N^{(m)}f$ which does integrate the constant function was constructed. The weight factors for this rule appear in Table 7.13. The specifications for this rule are as follows:

(1) It should be of form (7.9).

(2) It should be symmetric under permutations of the variables x, y, z.

(3) Points which do not lie on the plane $x + y + z = 1$ should have the natural weighting factors 1, $\frac{1}{2}$, $\frac{1}{4}$, $\frac{1}{8}$ according as they are interior, face, edge or vertex points.

(4) Three other weighting factors θ_F, θ_E, θ_V are assigned for points on the plane $x + y + z = 1$ according as they are face, edge or vertex points.

(5) The rule should be of degree zero.

This led unambiguously to the weights listed under R_Nf in Table 7.13. Note that conditions (1) through (4) are satisfied by a three-parameter set of rules including, for example, the symmetric rule $R_s^{(m)}f$. The single condition (5)

(7.17) $$R_N^{(m)}f = I_{\Delta_3}f, \qquad f(\mathbf{x}) = 1 \quad \text{all integer } m,$$

gives three linear equations in the three unknown weighting factors θ_F, θ_E, θ_V. There are other ways of setting up specifications which lead to the same rule. This rule is clearly not a linear combination of basic simplex weighted product trapeziodal rules as defined in (3.15). Thus, it is of interest to investigate its properties to see whether it has an Euler-Maclaurin expansion and, if it does, whether the coefficients satisfy Theorems 5.10 and 5.15.

Direct examination of Table 7.13 gives

(7.18) $$R_N^{(m)}f - R_{123}^{(m)}f = \lambda_1 m^{-2}R^{[m,1]}\varphi_1 + \lambda_2 m^{-2}R^{[m,1]}\varphi_2 + \lambda_3 m^{-2}R^{[m,3]}\varphi_3,$$

where

(7.19) $$\lambda_1 = \lambda_2 = \tfrac{5}{36} - \tfrac{1}{4}, \qquad \lambda_3 = \tfrac{5}{36},$$

and $\varphi_i(t)$ are one-dimensional functions defined by

(7.20) $$\varphi_1(t) = f(0, t, 1-t); \quad \varphi_2(t) = f(1-t, 0, t); \quad \varphi_3(t) = f(t, 1-t, 0).$$

Since both $R_{123}^{(m)}f$ and $R^{[m,1]}\varphi$ have even expansions in powers of $1/m$, so has $R_N^{(m)}f$. This establishes that Theorems 4.29 and 5.15 are satisfied also by $R_N^{(m)}f$.

To proceed, we invoke the Euler-Maclaurin expansion for $R^{[m,1]}\varphi_i$. Thus,

(7.21) $$R^{[m,1]}\varphi_i = \sum_{q=0}^{p-3} \alpha_q^{(i)}/m^q + E_{p-2}^{[m,1]}\varphi_i,$$

where

(7.22) $$\alpha_q^{(i)} = \frac{\bar{B}_q(1)}{q!}\int_0^1 \varphi_i^{(q)}(t)\,dt.$$

In view of Eq. (1.6),

(7.23) $$\alpha_q^{(i)} = 0, \qquad q \text{ odd}.$$

Also, if $f(\mathbf{x})$ is a polynomial of degree d or less, so is $\varphi_i(x)$ and so

(7.24) $$\alpha_q^{(i)} = 0, \qquad q > d.$$

Collecting these results, we find

(7.25) $$R_N^{(m)}f - I_{\Delta_3}f = A_2^{(N)}/m^2 + A_4^{(N)}/m^4 + \cdots,$$

where

(7.26) $$A_q^{(N)} = A_q + \sum_{i=1}^{3} \lambda_i \alpha_{q-2}^{(i)}$$

and A_q are the coefficients corresponding to $R_{123}^{(m)}f$. In view of Theorem 5.10 and (7.24) above,

(7.27) $$A_q^{(N)} = 0, \qquad q > d + 2.$$

This establishes that the coefficients corresponding to the rule $R_N^{(m)}f$ also satisfy Theorem 5.10.

The two- and three-dimensional 'centre' rules are not nearly so complicated. In two dimensions, the two rules

$$R_{ij}^{(m)}f = R_{x_i}^{[m,0]}[0, 1]R_{x_j}^{[m,0]}[0, 1 - x_i]f(x_1, x_2), \tag{7.28}$$

with $\{i, j\} = \{1, 2\}$ or $\{2, 1\}$, coincide. They assign weighting factors 1 to interior points and $\frac{1}{2}$ to points on the edge $x + y = 1$. There are no points on the other edges or at the vertices. This rule is of degree zero.

In three dimensions, all six rules

$$R_{ijk}^{(m)}f = R_{x_i}^{[m,0]}[0, 1]R_{x_j}^{[m,0]}[0, 1 - x_i]R_{x_k}^{[m,0]}[0, 1 - x_i - x_j]f(x_1, x_2, x_3) \tag{7.29}$$

coincide. There are no boundary points. This rule is not of degree zero, and there is no obvious 'natural' rule of this type. In fact,

$$R_{123}^{(m)}f - I_{\Delta_3}f = \frac{-1/6}{m^2}, \qquad f(\mathbf{x}) = 1. \tag{7.30}$$

An interesting point to notice is that, when $m = 1$, none of the points lie within the simplex and so

$$R_{123}^{(1)}f = 0. \tag{7.31}$$

8. Romberg Integration. The natural application of these expansions is to Romberg integration for a simplex. In general, one chooses a set of mesh ratios $m_0, m_1, m_2, \cdots$ and constructs a Romberg T-table of the following form:

$$\begin{array}{cccc} T_0^0 & & & \\ T_0^1 & T_1^0 & & \\ T_0^2 & T_1^1 & T_2^0 & \\ T_0^3 & T_1^2 & T_2^1 & T_3^0 \end{array} \tag{8.1}$$

The elements of the first column are obtained from

$$T_0^i = R^{(m_i)}f \tag{8.2}$$

and elements of subsequent columns using

$$T_p^k = T_{p-1}^{k+1} + \mu_{k,p}(T_{p-1}^{k+1} - T_{p-1}^k). \tag{8.3}$$

If, as is usually the case, $R^{(m)}f - If$ has an even expansion, then

$$\mu_{k,p} = m_k^2/(m_{k+p}^2 - m_k^2). \tag{8.4}$$

If one had chosen a rule for which the expansion is not known to be even, a situation which is avoided in practice, then

$$\mu_{k,p} = m_k/(m_{k+p} - m_k). \tag{8.5}$$

In the one-dimensional case in which a standard choice of the symmetric rule $R^{[m,1]}f$ in (8.2) is made, each element T_p^k in the table represents an approximation to If of polynomial degree $2p + 1$. This follows quite simply from (1.4) and (1.6) namely,

$$a_q = 0, \qquad q > d, \tag{8.6}$$

$$a_q = 0, \qquad q \text{ odd}. \tag{8.7}$$

In the case of integration over a hypercube using product symmetric trapezoidal rules, the same result holds. See for example Baker and Hodgson [2].

However, in the case of the s-dimensional simplex, (8.6) and (8.7) have to be replaced by

$$A_q = 0, \qquad q > d + s - 1, \tag{8.8}$$

$$A_q = 0, \qquad q \text{ odd}. \tag{8.9}$$

This leads to the following theorem:

THEOREM 8.10. *If* $R^{(m)}f$ *is an s-dimensional basic simplex weighted product trapezoidal rule of type* (3.13) *having an even expansion* ($\alpha_i = 0$ *or* 1), *the elements* T_p^k *of the T-table* (8.1) *defined by* (8.2), (8.3), (8.4) *are of polynomial degree*

$$D = 2p + 2 - s.$$

The only significance of a negative value of D is that the result is not exact when $f(\mathbf{x})$ = constant. A corresponding theorem of little present practical interest applies to the case where the Euler-Maclaurin expansion is not an even expansion. This is

THEOREM 8.11. *If* $R^{(m)}f$ *is an s-dimensional basic simplex weighted product trapezoidal rule of type* (3.13), *the elements* T_p^k *of the T-table* (8.1) *defined by* (8.2), (8.3), (8.5) *are of polynomial degree*

$$D = p + 1 - s.$$

These theorems depend only on the results embodied in Theorems 4.29, 5.10 and 5.15. Since the two-dimensional rule $R_s^{(m)}f$ given by (7.5) and the three-dimensional rule $R_N^{(m)}f$ given in Table 7.13 have Euler-Maclaurin expansions whose coefficients have the properties described by these theorems, these rules may be also used as a basis for Romberg integration and the elements of the T-table have the same degree as that given in Theorem 8.10. If Romberg integration is to be used, it appears that the use of $R_N^{(m)}f$ rather than $R_{123}^{(m)}f$ requires marginally more function values. The only gain seems to be that the first column is exact in the special case in which $f(\mathbf{x})$ = constant. There is no obvious reason for believing any other elements of the T-table are more or less accurate in any general case.

So far as comparing $R_s^{(m)}f$ and $R_{12}^{(m)}f$ is concerned, the situation, though rather trivial, does have one point of interest. All elements in the T-table other than the first column are identical. A moment's reflection indicates that these elements are actually independent of the values of $f(1, 0)$ and $f(0, 1)$ and $f(0, 0)$ since these occur in every rule sum with coefficient k/m^2 and are automatically eliminated at the first eliminating stage. So if Romberg integration is to be used, and elements of the first column are not going to be taken seriously, then the rule

$$R^{(m)}f = R_{12}^{(m)}f - \frac{1}{4m^2}(f(0, 0) + f(1, 0)) \tag{8.12}$$

gives identical results to $R_{12}^{(m)}f$, but requires two fewer function values. Using a criterion based on error per number of function values, a rule which does not integrate $f(\mathbf{x}) = 1$ exactly shows up to advantage over one which does. There are other very special cases in which a rule which is not symmetric but which has an even expansion may be useful. Suppose, in three dimensions,

$$f(x, y, z) = \varphi(x, y, z)/(x + y - 1), \tag{8.13}$$

where $\varphi(x, y, z)$ is easily evaluated and is zero on the plane $x + y - 1 = 0$. The rule $R_{123}^{(m)}f$ does not require function values at points for which $x + y = 1$ and so the inconvenience of special coding for this case would be avoided.

There is another rather interesting phenomenon which occurs when Romberg integration is used for the three-dimensional simplex using the centre rule (7.29). If the mesh sequence $m_0, m_1, m_2, \cdots$ includes

$$m_0 = 1, \tag{8.14}$$

we find

$$T_0^0 = R_{123}^{(1)}f = 0, \tag{8.15}$$

an approximation obtained at the cost of no function values at all. A natural immediate reaction would be to ignore this and to choose a different mesh sequence. However, if one considers T_0^0 as an intermediate quantity which will be combined with T_0^1 to form T_1^0, it appears that there is no reason to disregard it at all. In particular, if

$$m_1 = 2, \tag{8.16}$$

we find

$$T_0^1 = R_{123}^{(2)}f = \tfrac{1}{4}f(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}) \tag{8.17}$$

and

$$T_1^0 = T_0^1 - \tfrac{1}{3}(T_0^1 - T_0^0) = \tfrac{1}{6}f(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}). \tag{8.18}$$

Since the point $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ is the centroid of the tetrahedron Δ_3, this is an approximation of degree 1 in accordance with Theorem 8.10 and, clearly, a more appropriate approximation than T_0^1, although the same number of function values is involved. The effect of the approximation $T_0^0 = 0$ in the Romberg table is only to adjust the ratios in which the other approximations T_0^i are combined by the procedure in such a way as to ensure the proper polynomial degree of the other elements.

9. Concluding Remarks. The principal results given in this paper are very simple in structure. Essentially they are embodied in only three theorems (4.29, 5.10 and 5.15). These state broadly:

(i) A basic simplex weighted trapezoidal product rule does have an Euler-Maclaurin expansion.

(ii) This is an even expansion if the constituent rules are symmetric.

(iii) The expansion terminates at a specified point if $f(\mathbf{x})$ is a polynomial of particular degree.

Only the third result is different in detail from the corresponding result for the hypercube.

The theory as presented here suffers from several defects. First of all, the basic elements which are the basic simplex weighted product trapezoidal rules are not symmetric. Secondly, the proof of these various properties involves an excessive amount of manipulation of an elementary nature. Thirdly, naturally arising rules such as $R_N^{(m)}f$ are not covered directly by the theory and subsidiary calculations are necessary to produce precisely corresponding results.

There are, of course, other branches of numerical analysis where the derivation of aesthetically satisfying results involves a mass of unpalatable algebra. One branch is high-order Runge-Kutta integration. Another branch is the one-dimensional Euler-Maclaurin expansion in the case in which $f(x)$ includes an algebraic or logarithmic singularity. In that branch, the initial publication by Navot [8] of results whose proof was most unaesthetic in 1960–1962 led ultimately to simpler proofs by Lyness and Ninham [7] and to more general results over a course of ten years. It is the authors' hope that the same sort of phenomenon may occur here.

However, any easier approach must lead to the same curiosities in the results. The same exceptions to the general remarks about the degree of a two-dimensional rule as described in Section 6 must occur. Also, the fact that basic rules which are not of degree zero may be used in Romberg integration to form approximations of high polynomial degree must also form part of the theory. In the authors' view, the situation described at the end of Section 8 in which the element $T_0^0 = 0$ is included in theRomberg T-table epitomizes the difference between s-dimensional quadrature over the simplex and over the hypercube.

Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Department of Mathematics and Astronomy
University of Maine at Orono
Orono, Maine 04473

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