Cubature Rules of Prescribed Merit*

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Abstract

We introduce a criterion for the evaluation of multidimensional quadrature, or cubature, rules for the hypercube: this is the *merit* of a rule, which is closely related to its trigonometric degree, and which reduces to the Zaremba figure of merit in the case of a lattice rule. We derive a family of rules Q_k^s having dimension s and merit 2^k. These rules seem to be competitive with lattice rules with respect to the merit that can be achieved with a given number of abscissas.

Key words. cubature, merit, multidimensional quadrature

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1 Introduction

Several measures of multidimensional quadrature, or cubature, rules have been conventionally used to evaluate their cost effectiveness. For integration over $[0,1]^s$ the most familiar is the algebraic polynomial degree. Another, relevant to integrands with a continuous periodic extension, is the trigonometric polynomial degree. In the corresponding evaluation of lattice rules (see Sloan and Kachoyan 1987, Lyness 1989, Niederreiter 1992, Sloan and Joe 1994), several other measures are used; one of these is the Zaremba figure of merit. This and the trigonometric degree are closely related, both being based on the ability of the rule to integrate correctly a different but similar set of low-degree trigonometric polynomials.

In this paper we introduce the *merit* of a quadrature rule. It is relevant to any quadrature rule designed for integrands with a periodic extension. In the case of a lattice rule, it reduces to the Zaremba figure of merit.

In Section 2 we provide some of the underlying theory. In Section 3 we introduce a construction that builds an s-dimensional rule of specified merit from a set of $(s-1)$-dimensional rules having the same or lower merit. This construction provides many possibilities for designing rules of moderate merit. In Section 4 and subsequently, we present

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a thorough description of one family. Each member, denoted by Q_k^s, is a well-defined s-dimensional quadrature rule of merit 2^k, which is symmetric under permutations of the s variables. The weights take $s+k$ different values, of which some may be negative or zero. If the points with zero weights are retained, then Q_{k-1}^s is embedded in Q_k^s .

We shall see that the number of function values required by the rule Q_k^s satisfies

$$\rho < N < \rho \left(\log_2 \rho + \frac{3s-4}{2}\right)^{s-1} /(s-1)!, \tag{1.1}$$

where ρ is the merit, namely, where $\rho = 2^k$. This number is satisfactory when compared with the known bounds for lattice rules: (1.1) implies

$$\rho > \frac{(s-1)!N}{\left(\log_2 \rho + \frac{3s-4}{2}\right)^{s-1}} > \frac{(s-1)!N}{\left(\log_2 N + \frac{3s-4}{2}\right)^{s-1}}, \tag{1.2}$$

whereas Zaremba (1974) shows that, for $s \geq 2$ and for every sufficiently large integer N, there exists a lattice rule with N function evaluations and with merit ρ satisfying

$$\rho > \frac{(s-1)!N}{(2\log_e \rho)^{s-1}} > \frac{(s-1)!N}{(2\log_e N)^{s-1}}. \tag{1.3}$$

The orders of the lower bounds in (1.2) and (1.3) as $N \to \infty$ are the same, namely, $O(N/(\log_e N)^{s-1})$, but the asymptotic constant in (1.2) is bigger, and hence better.

An important practical aspect of these merit rules is that a straightforward construction is available. In contrast, good lattice rules in dimensions $s > 2$ can be found only by a search.

In this paper, we exploit the rectangle rule

$$R_k f = \frac{1}{2^k} \sum_{i=0}^{2^k-1} f(i/2^k), \qquad k \geq 1,$$

to construct higher dimensional rules, all of which have abscissas in $[0,1)^s$. This results in rules Q_k^s which are not symmetric with respect to the center of the hypercube. One could equally well base the theory on the trapezoidal rule

$$T_k f = \frac{1}{2^k} \left(\frac{1}{2} f(0) + \sum_{i=1}^{2^k-1} f(i/2^k) + \frac{1}{2} f(1) \right),$$

which is symmetric. This would lead to symmetrized versions of rules Q_k^s using abscissas in $[0,1]^s$. When $f(\mathbf{x})$ is periodic, these approximations coincide. The reader should bear in mind that it is for periodic integrands that this theory is designed. When the integrand is not periodic, we suggest that a symmetrized version of Q_k^s be used.

2 Merit

In this section, we apply the definition of Zaremba's figure of merit in a wider context, in order to define (in (2.13) below) the merit $\rho(P)$ of an arbitrary linear functional of the form

$$Pf = \sum_{j=1}^{\nu} w_j f(\mathbf{x}_j), \tag{2.1}$$

where $\mathbf{x}_j \in R^s$ for $1 \le j \le s$. To this end, we denote the Fourier coefficients $\hat{f}_{\mathbf{h}}$ of the integrand function $f(\mathbf{x})$ by

$$\hat{f}_{\mathbf{h}} = \int_{[0,1]^s} f(\mathbf{x}) e^{-2\pi i \mathbf{h}.\mathbf{x}} d\mathbf{x}$$

and assume for the present that f has an absolutely convergent Fourier series

$$f(\mathbf{x}) = \sum_{\mathbf{h} \in \Lambda_0} \hat{f}_{\mathbf{h}} e^{2\pi i \mathbf{h}.\mathbf{x}}. \tag{2.2}$$

Here Λ_0 is the s-dimensional unit lattice. Thus f has a 1-periodic continuous extension with respect to each component of $\mathbf{x}$. Introducing the Fourier series representation into (2.1), we find

$$Pf = \sum_{\mathbf{h} \in \Lambda_0} d_{\mathbf{h}}(P) \hat{f}_{\mathbf{h}}, \tag{2.3}$$

where the coefficients (which we shall refer to as *error coefficients*) are given by

$$d_{\mathbf{h}}(P) = P(e^{2\pi i \mathbf{h}.\mathbf{x}}). \tag{2.4}$$

Equation (2.3) is a natural minor generalization of the classical Poisson summation formula. Almost every serious cubature rule provides an approximation to

$$If = \hat{f}_{\mathbf{0}} = \int f(\mathbf{x}) d\mathbf{x}, \tag{2.5}$$

which is exact when $f(\mathbf{x})$ is constant. To this end, we reserve the term *cubature rule* for the principal special case of (2.1) as follows.

Definition 2.1 *The finite sum*

$$Qf = \sum w_j f(\mathbf{x}_j)$$

is termed a cubature rule *when*

$$\sum w_j = d_{\mathbf{0}}(Q) = 1. \tag{2.6}$$

In this case (2.3) may be re-expressed as

$$Qf - If = \sum_{\substack{\mathbf{h} \in \Lambda_0 \\ \mathbf{h} \neq \mathbf{0}}} d_{\mathbf{h}}(Q) \hat{f}_{\mathbf{h}}. \tag{2.7}$$

This expression for the error functional is basic to our development of rule construction criteria. In particular, it may be used to define both the trigonometric degree and the merit of a quadrature rule.

Definition 2.2 *For a linear functional P of the form (2.1), $\Delta(P)$ is the subset of Λ_0 for which*

$$d_{\mathbf{h}}(P) \neq 0. \tag{2.8}$$

Obviously (2.7) may be replaced by

$$Qf - If = \sum_{\substack{\mathbf{h} \in \Delta(Q) \\ \mathbf{h} \neq \mathbf{0}}} d_{\mathbf{h}}(Q) \hat{f}_{\mathbf{h}}. \tag{2.9}$$

When Q is a lattice rule, $\Delta(Q)$ is the dual lattice of the one defining Q. (See Sloan and Kachoyan (1987).) Because of this we refer to $\Delta(Q)$ as the $pseudo - duallattice$ associated with Q.

In general, the points of $\Delta(Q)$ do not form a lattice. For many excellent rules (for instance, product Gaussian rules), $\Delta(Q) = \Lambda_0$.

To define the trigonometric degree and the merit, respectively, we need the following. With $\mathbf{h} = (h_1, h_2, \ldots, h_s) \in \Lambda_0$, we define

$$s(\mathbf{h}) = |h_1| + |h_2| + \ldots + |h_s|, \tag{2.10}$$

$$r(\mathbf{h}) = \bar{h}_1 \bar{h}_2 \ldots \bar{h}_s, \qquad \bar{h}_i = \max(1, |h_i|). \tag{2.11}$$

Both depend only on the absolute values of the nonzero components of $\mathbf{h}$, $s(\mathbf{h})$ being their sum, and $r(\mathbf{h})$ their product. Then we have the following definitions.

Definition 2.3 *The* trigonometric degree $D(Q)$ *of a cubature rule* Q *is*

$$D(Q) = -1 + \min_{\substack{\mathbf{h} \in \Delta(Q) \\ \mathbf{h} \neq \mathbf{0}}} s(\mathbf{h}). \tag{2.12}$$

Definition 2.4 *The* merit $\rho(Q)$ *of a cubature rule* Q *is*

$$\rho(Q) = \min_{\substack{\mathbf{h} \in \Delta(Q) \\ \mathbf{h} \neq \mathbf{0}}} r(\mathbf{h}). \tag{2.13}$$

These definitions have the immediate implication

$$d_{\mathbf{0}}(Q) = 1; \quad d_{\mathbf{h}}(Q) = 0 \quad \text{when } \mathbf{h} \neq \mathbf{0} \text{ and } 0 < s(\mathbf{h}) < D(Q) + 1, \tag{2.14}$$

and

$$d_{\mathbf{0}}(Q) = 1; \quad d_{\mathbf{h}}(Q) = 0 \quad \text{when } \mathbf{h} \neq \mathbf{0} \text{ and } r(\mathbf{h}) < \rho(Q). \tag{2.15}$$

Much of the theory of merit rules depends on properties of the error coefficients $d_{\mathbf{h}}(Q)$. We note that

(1)

$$d_{\mathbf{h}}(Q_1 + Q_2) = d_{\mathbf{h}}(Q_1) + d_{\mathbf{h}}(Q_2), \tag{2.16}$$

where Q_1 and Q_2 are operators of the form (2.1).

(2) If Q is symmetric about $(\frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2})$ for periodic integrands, (i.e., if Q is unchanged when the transformation $\mathbf{x} \to (1, 1, ..., 1) - \mathbf{x}$ is applied to a periodic integrand), then

$$d_{\mathbf{h}}(Q) = d_{-\mathbf{h}}(Q). \tag{2.17}$$

(3) If $Q^{(m)}$ is the m^s-copy of Q (see, e.g., Sloan and Lyness (1989)), then

$$\begin{aligned} d_{\mathbf{h}}(Q^{(m)}) &= d_{\mathbf{h}/m}(Q) \text{ when } \mathbf{h}/m \in \Lambda_0, \\ &= 0 \text{ otherwise.} \end{aligned} \tag{2.18}$$

(4) Let $\mathbf{h} = (h_1, h_2, \ldots, h_s) = (t_1, t_2, \ldots, t_{s-1}, j) = (\mathbf{t}, j)$, and let $Q = TJ$ be the s-dimensional Cartesian product of an $s-1$ dimensional rule T with respect to the first $s-1$ components, and a one-dimensional rule J with respect to the s-th component. Then

$$d_{\mathbf{h}}(Q) = d_{\mathbf{t}}(T) d_j(J). \tag{2.19}$$

(5) Finally, if Q is a "grid" rule, that is, if all points of its abscissa set lie on a scaled unit lattice Λ_0/m, where m is an integer, then $d_{\mathbf{h}}(Q)$ is periodic in $\mathbf{h}$ with period m. That is,

$$d_{\mathbf{h}+m\mathbf{z}}(Q) = d_{\mathbf{h}}(Q), \qquad \forall \ \mathbf{z} \in \Lambda_0. \tag{2.20}$$

It appears that many rules of high trigonometric degree are grid rules.

It follows from the property (3) that

$$\Delta(Q^{(m)}) = m\Delta(Q), \tag{2.21}$$

so that the merit of an m^s-copy rule is at least m. The merit of an m^s copy of a product Gaussian rule is exactly m, since, for these rules, $\Delta(Q) = \Lambda_0$. Gaussian rules are designed for a different class of function. In the context of sets of Gaussian rules, the effect of using more points in Q is to reduce in an overall manner the values of $|d_{\mathbf{h}}(Q)|$ rather than to eliminate any.

We introduce here two one-dimensional functionals which are useful subsequently. These are the 2^k-panel rectangle rule

$$R_k f = \frac{1}{2^k} \sum_{i=0}^{2^k-1} f(i/2^k), \qquad k \geq 1, \tag{2.22}$$

and the 2^{k+1}-point alternating null rule

$$\begin{aligned} W_k f &= R_{k+1} f - R_k f \\ &= \frac{1}{2^{k+1}} \sum_{i=0}^{2^{k+1}-1} (-1)^{i+1} f(i/2^{k+1}), \qquad k \geq 1. \end{aligned} \tag{2.23}$$

It is easy to verify that, when $k \geq 1$,

$$d_j(R_k) = 1 \qquad \text{when} \qquad j/2^k = \text{integer}, \tag{2.24}$$

$$d_j(W_k) = -1 \qquad \text{when} \qquad j/2^k = \text{odd integer}, \tag{2.25}$$

and all other error coefficients of R_k and W_k are zero. It follows that R_k and W_k have merit 2^k. For later convenience, we collect together some useful special cases.

Lemma 2.5 *For $k \geq 1$, the following results are valid:*

$$d_0(R_1) = 1, \qquad d_0(W_k) = 0, \tag{2.26}$$

$$d_j(R_1) = d_j(W_k) = 0 \qquad \forall odd\ j. \tag{2.27}$$

When j is even, and so representable uniquely in the form $j = 2^m(2l+1)$ with l, m integer and $m \geq 1$,

$$\begin{array}{l} d_j(W_m) = -1 \\ d_j(W_k) = 0 \quad when \qquad k \neq m \\ d_j(R_1) = 1. \end{array} \tag{2.28}$$

3 A Recursive Construction of Rules with Prescribed Merit

In this section we establish the following theorem.

Theorem 3.1 *For positive integer k, let Q_k be an s-dimensional cubature rule, defined by*

$$Q_k = T_k R_1 + T_{k-1} W_1 + T_{k-2} W_2 + \ldots + T_1 W_{k-1}, \tag{3.1}$$

where T_i $(i = 1, 2, \ldots)$ is an $(s-1)$-dimensional cubature rule, R_i is the one-dimensional 2^i-panel rectangle rule, and $W_i = R_{i+1} - R_i$. Assume that for all i = 1,2,...,k the merit of T_i is 2^i or greater. Then the merit of Q_k is 2^k or greater.

To prove the theorem, we first establish a relation between the error coefficients $d_{\mathbf{h}}(Q_k) = d_{\mathbf{t},j}(Q_k)$ and $d_{\mathbf{t}}(T_i)$, $i = 1, 2, \ldots, k$. This is based only on (3.1) and the results in Lemma 2.5 of the preceding section.

Lemma 3.2 *Let Q_k be given by (3.1), and let $k \geq 1$. If j is odd, then*

$$d_{\mathbf{t},j}(Q_k) = 0. \tag{3.2}$$

If $j = 2^m(2l+1)$ with $m \in [1, k-1]$ then,

$$d_{\mathbf{t},j}(Q_k) = d_{\mathbf{t}}(T_k) - d_{\mathbf{t}}(T_{k-m}). \tag{3.3}$$

If $j = 0$, or if $j = 2^m(2l+1)$ with $m \geq k$, then

$$d_{\mathbf{t},j}(Q_k) = d_{\mathbf{t}}(T_k). \tag{3.4}$$

Proof. In view of (2.16) and (2.19), it follows from (3.1) that

$$d_{\mathbf{t},j}(Q_k) = d_{\mathbf{t}}(T_k) d_j(R_1) + \sum_{i=1}^{k-1} d_{\mathbf{t}}(T_{k-i}) d_j(W_i). \tag{3.5}$$

We simply apply the results of Lemma 2.5 to remove the dependence on R_1 and W_i. When $j = 0$ or j is odd, the result follows from (2.26) and (2.27). When j is even, we find from (2.28) that at most one term in the sum over i contributes, this term having $i = m$ when

m is defined by $j = 2^m(2l+1)$. Naturally, this term appears only if this value of j occurs in the summation, that is, only if $m \in [1, k-1]$. In this case we recover (3.3). Otherwise we find (3.4). ∎

As a special case of (3.4), note that $d_{\mathbf{0},0}(Q_k) = d_{\mathbf{0}}(T_k)$, so that Q_k is indeed a quadrature rule in the sense of Definition 2.1.

We now proceed to the proof of Theorem 3.1.

Proof. By assumption, for all $i \in [1, k]$, the merit of T_i is 2^i or greater; that is to say,

$$d_{\mathbf{t}}(T_i) = 0 \quad \text{if} \quad \mathbf{t} \neq \mathbf{0} \quad \text{and} \quad \bar{t}_1 \ldots \bar{t}_{s-1} < 2^i. \tag{3.6}$$

To establish the theorem, we have to show that

$$d_{\mathbf{h}}(Q_k) = d_{\mathbf{t},j}(Q_k) = 0 \tag{3.7}$$

whenever

$$\bar{t}_1 \ldots \bar{t}_{s-1}\bar{j} < 2^k \quad \text{and} \quad (\mathbf{t}, j) \neq (\mathbf{0}, 0). \tag{3.8}$$

When $\mathbf{t} = \mathbf{0}$, we see from (3.5), (2.6), and (2.16) that

$$\begin{aligned} d_{\mathbf{0},j}(Q_k) &= d_j(R_1 + W_1 + W_2 + \ldots + W_{k-1}) \\ &= d_j(R_k), \end{aligned}$$

which by (2.24) vanishes for $0 < |j| < 2^k$. Now consider $\mathbf{t} \neq \mathbf{0}$. When $j = 0$, the result follows from (3.4) by applying (3.6) with $i = k$. When j is odd, the result is given immediately by (3.2). When $j = 2^m(2l+1)$, we have $\bar{j} \geq 2^m$; thus for $m \geq k$ there is nothing to prove, while for $m \in [1, k-1]$ it suffices to show that (3.7) holds whenever

$$\bar{t}_1 \ldots \bar{t}_{s-1} < 2^{k-m}.$$

This follows from (3.3) on applying (3.6) once with $i = k - m$ and again with $i = k$. ∎

4 A Specific Family: The Meritorious Rules

Theorem 3.1 may be used to define a set of s-dimensional rules Q_k^s having merit 2^k for $s \geq 1$ and $k \geq 1$ recursively, so long as the recursion is anchored by defining Q_k^1, $k \geq 1$. This may be done in many ways. The rest of this paper is about a particular set of rules defined as follows.

Definition 4.1 *For $k \geq 1$, the* meritorious *rules Q_k^s are defined by*

$$\begin{array}{ll} Q_k^1 = R_k, & k \geq 1, \\ Q_k^s = Q_k^{s-1} R_1 + \sum_{j=1}^{k-1} Q_{k-j}^{s-1} W_j, & s > 1,\ k \geq 1. \end{array} \tag{4.1}$$

It follows immediately from Theorem 3.1 that Q_k^s is an s-dimensional cubature rule for which $\rho(Q_k^s) = 2^k$.

Equations (4.1) may be re-expressed in various forms. It is convenient to extend the rule definitions in the following way:

$$R_0 f = 0; \quad W_0 f = R_1 f; \quad Q_j^s = 0 \qquad \forall j \leq 0. \tag{4.2}$$

(Note that the first member of (4.2) is not a natural extension of (2.22). However, once this has been enforced, the second and third members follow naturally.) With this convention we find, using $W_j = R_{j+1} - R_j$,

$$Q_k^s = \sum_{i=0}^{k-1} (Q_{i+1}^{s-1} - Q_i^{s-1}) R_{k-i}. \tag{4.3}$$

Also we may write (4.1) in the form

$$Q_k^1 = \sum_{j=0}^{k-1} W_j, \tag{4.4}$$

$$Q_k^s = \sum_{j=0}^{k-1} Q_{k-j}^{s-1} W_j \qquad \text{for} \quad \text{s} > 1.$$

Using this, we easily obtain by induction the following theorem.

Theorem 4.2 *For $k \geq 1$ we have*

$$Q_k^s = \sum_{j_1 + \ldots + j_s \leq k-1} W_{j_1} W_{j_2} \ldots W_{j_s}.$$

In this form it is apparent that the construction is a special case of a construction used by Smoljak (1963), sometimes known as the method of hyperbolic cross points. It follows that Q_k^s is symmetric under permutations of the components of $\mathbf{x}$, and under reflections of the form $x_i \to 1 - x_i$ when the rule is applied to periodic functions.

Corollary 4.3 *The rule Q_k^s is invariant under all permutations and reflections of the components of* $\mathbf{x}$.

It is instructive to examine briefly some of the properties of the two-dimensional rules. Direct substitution of the first member of (4.1) into the second gives

$$\begin{aligned} Q_k^2 &= R_k R_1 + \sum_{j=1}^{k-1} R_{k-j} W_j \\ &= \sum_{j=0}^{k-1} R_{k-j} R_{j+1} - \sum_{j=1}^{k-1} R_{k-j} R_j \\ &= S_k^2 - S_{k-1}^2 \qquad k \geq 1, \end{aligned}$$

where S_k^2 is defined by

$$S_k^2 = 0 \qquad \text{when} \qquad k \leq 0$$

and

$$S_k^2 = R_k R_1 + R_{k-1} R_2 + \ldots + R_1 R_k \qquad \text{when} \qquad k \geq 1.$$

In this form it is apparent that Q_k^2 is the "blending rectangle rule" proposed by Delvos (1990). A figure showing the abscissas of a 2-dimensional rule is presented in Section 5.

We shall now generalize this theory to s-dimensions.

Definition 4.4 *For $k \geq 1$, the symmetric functionals S_k^s are defined by*

$$\begin{aligned} S_k^1 &= R_k, \\ S_k^s &= \sum_{\substack{\Sigma j_i = k+s-1 \\ j_i \geq 1}} R_{j_1} R_{j_2} \ldots R_{j_s} \qquad \textit{for} \qquad s > 1. \end{aligned} \tag{4.5}$$

This sum in (4.5) is over all s-partitions of $k + s - 1$ whose elements are positive. A trivial consequence, which could also be used as a definition, is

$$\begin{aligned} S_k^1 &= R_k, \\ S_k^s &= \sum_{i=1}^{k} S_{k+1-i}^{s-1} R_i \qquad \text{for} \qquad s > 1. \end{aligned} \tag{4.6}$$

Theorem 4.5 *For $k \geq 1$ and $s \geq 1$,*

$$Q_k^s = \sum_j (-1)^j \binom{s-1}{j} S_{k-j}^s. \tag{4.7}$$

The limits on this sum over j are 0 and $\min(k, s) - 1$. However, the conventions

$$\binom{a}{b} = 0 \text{ when } b < 0 \text{ or } b > a, \qquad \binom{0}{0} = 1, \qquad \text{and} \qquad S_j^s = 0 \text{ when } j \leq 0 \tag{4.8}$$

allow us to suppress these limits.

Proof. We use induction on s, noting that the result is certainly true when $s = 1$. For $s \geq 2$, assume that (4.7) is valid with s replaced by $s - 1$. Then for $i \geq 0$

$$\begin{aligned} Q_{i+1}^{s-1} - Q_i^{s-1} &= \sum_j (-1)^j \binom{s-2}{j} S_{i+1-j}^{s-1} - \sum_j (-1)^j \binom{s-2}{j} S_{i-j}^{s-1} \\ &= \sum_j (-1)^j \binom{s-2}{j} S_{i+1-j}^{s-1} + \sum_j (-1)^j \binom{s-2}{j-1} S_{i-j+1}^{s-1} \\ &= \sum_j (-1)^j S_{i-j+1}^{s-1} \binom{s-1}{j}, \end{aligned} \tag{4.9}$$

where, in the last step, we have used the Pascal triangle binomial coefficient identity. Then (4.3) gives

$$Q_k^s = \sum_{i=0}^{k-1} \sum_j (-1)^j S_{i-j+1}^{s-1} \binom{s-1}{j} R_{k-i}$$

$$
\begin{aligned}
&= \sum_j (-1)^j \begin{pmatrix} s-1 \\ j \end{pmatrix} \sum_{i=1}^{k} S^{s-1}_{k-j+1-i} R_i \\
&= \sum_j (-1)^j \begin{pmatrix} s-1 \\ j \end{pmatrix} S^s_{k-j}, \qquad (4.10)
\end{aligned}
$$

where, in the last step, we have used (4.6). This establishes the theorem. ∎

We close this section by noting some elementary embedding properties of the abscissa sets of S^s_k and Q^s_k. Using (4.6), we note that

$$S^s_{k+1} = \sum_{i=1}^{k+1} S^{s-1}_{k+2-i} R_i = \sum_{i=0}^{k} S^{s-1}_{k+1-i} R_{i+1},$$

while

$$S^s_k = \sum_{i=1}^{k} S^{s-1}_{k+1-i} R_i.$$

Since every point of R_i is contained in R_{i+1} it follows that

$$\mathcal{A}(S^s_k) \subseteq \mathcal{A}(S^s_{k+1}), \qquad (4.11)$$

where$\mathcal{A}(Q)$ is the abscissa set of the functional Q; thus the abscissa sets for each term on the right of (4.7) are all contained in the abscissa set of S^s_k, and so

$$\mathcal{A}(Q^s_k) \subseteq \mathcal{A}(S^s_k). \qquad (4.12)$$

In Section 6 we shall give a bound on the number of points $N^s_k = \nu(S^s_k)$ required by S^s_k. This is then also a bound on $\nu(Q^s_k)$. The next lemma follows from (4.5) and (4.7).

Lemma. *All points of S^s_k and of Q^s_k lie on $2^{-k}\Lambda_0$.*

That is, all points are of the form $\mathbf{z}/2^k$, where $\mathbf{z} \in \Lambda_0$. A detailed analysis of the location and nature of these points will appear in the next section.

5 The Structure of the Rules Q^s_k

In the preceding sections, we defined these rules recursively, defining an s-dimensional rule in terms of combinations of products of lower-dimensional rules. This approach turned out to be useful for establishing the existence of rules of specified merit. However, it is highly inconvenient for practical use. In this section we re-express these rules in terms of abscissas and weights. In so doing, we find a remarkable structure.

We note, once more, that all abscissas required by either S^s_k or by Q^s_k lie in $[0,1)^s$ on a grid of mesh $1/2^k$. That is, every abscissa is of the form

$$(j_1, j_2, \ldots, j_s)/2^k, \qquad j_i \in [0, 2^k).$$

Thus, each of these points may be expressed in the form

$$\mathbf{x} = \left(\frac{i_1}{2^{\lambda_1}}, \frac{i_2}{2^{\lambda_2}}, \ldots, \frac{i_s}{2^{\lambda_s}} \right), \tag{5.1}$$

where either i_j is an odd integer and $\lambda_j \in [1,k]$ or $i_j = 0$ and $\lambda_j = 1$. Note that λ_j is the number of binary digits after the "point" in the binary representation of the j-th component, except that, if this component is zero, then λ_j is set to 1 (and not, as might have been expected, to zero).

Definition 5.1 *The* length $l(\mathbf{x})$ *of a point* $\mathbf{x}$ *expressed in the form (5.1), with* i_j *an odd integer and* $\lambda_j \in [1,k]$ *or* $i_j = 0$ *and* $\lambda_j = 1$*, is*

$$l(\mathbf{x}) = \lambda_1 + \lambda_2 + \ldots + \lambda_s.$$

We refer to points that can be expressed in this form as *finite length points.* In this section, we shall establish that all points used by Q_k^s are finite length points, of length $s \le l \le s + k - 1$.

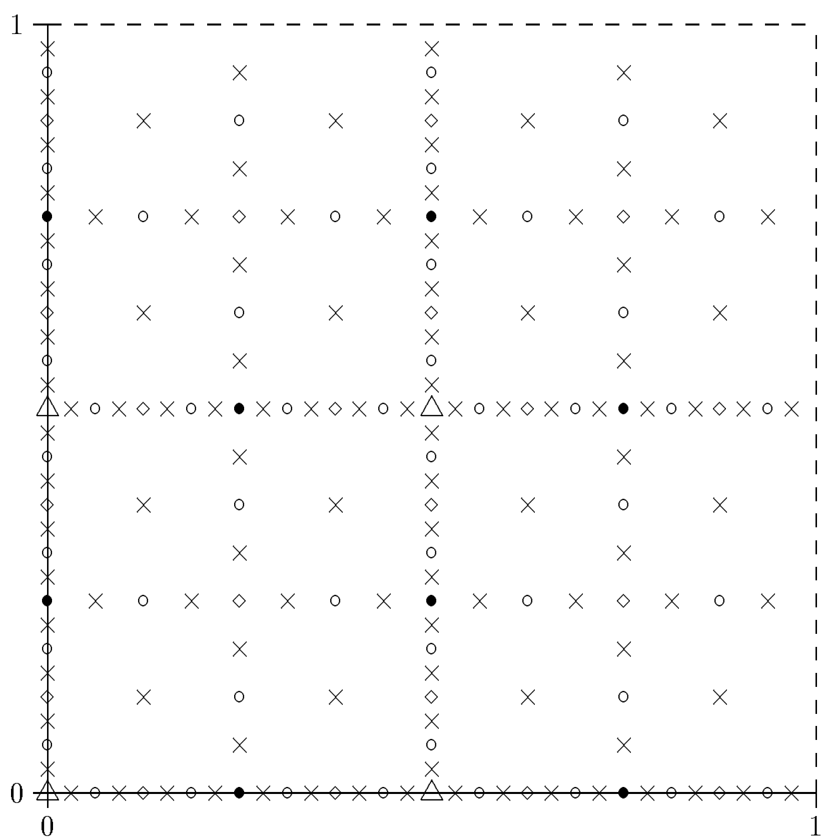

Figure 1. Abscissas for S_k^2, and hence also for the 2-dimensional rules Q_k^2, for $k = 5$. Abscissas of length 2, 3, 4, 5, and 6 are denoted by $\triangle$, $\bullet$, $\diamond$, $\circ$, and $\times$, respectively.

Definition 5.2 *The set* $\mathcal{S}^s(l)$ *comprises all points in* $[0,1)^s$ *of length* l*.*

We denote a sum of function values over this set by

$$S^s(l)f = \sum_{\mathbf{x}\in\mathcal{S}^s(l)} f(\mathbf{x}). \tag{5.2}$$

Note that this sum is defined quite independently of any quadrature rule. It is evident that

$$S^s(l) = \sum_{\lambda+\mu=l} S^{s-1}(\lambda)S^1(\mu). \tag{5.3}$$

Theorem 5.3 *For* $k \geq 1$,

$$S_k^s f = 2^{-(s+k-1)} \sum_{l=s}^{s+k-1} a_{s,s+k-l} S^s(l)f, \tag{5.4}$$

where

$$a_{s,r} = \left(\begin{array}{c} s+r-2 \\ s-1 \end{array} \right) = \left(\begin{array}{c} s+r-2 \\ r-1 \end{array} \right), \qquad r \geq 1. \tag{5.5}$$

The reader should note that this structure is unexpectedly simple. First, the abscissas of $S_k^s f$ comprise only points of lengths s through $s+k-1$ and comprise all these points. Second, all abscissas of the same length carry the same weight. Third, while the weight of a point of length l in S_k^s depends on s, k, and l, each weight may be readily expressed as $2^{-(s+k-1)}$ multiplied by a function of two parameters only, namely, s and $k-l$. Moreover, in a sequential calculation, to evaluate $S_{k+1}^s f$ after $S_k^s f$, one need treat only one further set of points, namely, $\mathcal{S}^s(k+s)$, and one more weight, $a_{s,k+1}$; for one simply reassigns the previous weights (remembering to include an additional 2^{-1} factor). In Figure 1 we show the abscissas of S_k^2, and hence of Q_k^2, for $k=5$, with abscissas of different length shown by different symbols.

Proof. We shall prove Theorem 5.3 by induction on s. This is anchored by the following lemma.

Lemma 5.4 *For* $k \geq 1$*,*

$$Q_k^1 f = S_k^1 f = 2^{-k} \sum_{l=1}^{k} S^1(l)f. \tag{5.6}$$

Proof. In view of the definitions of the preceding section, this rule is simply the 2^k panel rectangle rule. Applying Definitions 5.1 and 5.2 in one dimension, we find

$$\begin{aligned} \mathcal{S}^1(1) &= \left\{0, \tfrac{1}{2}\right\}, \\ \mathcal{S}^1(2) &= \left\{\tfrac{1}{4}, \tfrac{3}{4}\right\}, \\ \mathcal{S}^1(3) &= \left\{\tfrac{1}{8}, \tfrac{3}{8}, \tfrac{5}{8}, \tfrac{7}{8}\right\}, \end{aligned}$$

and so forth. It is obvious that the expression on the right of (5.6) is precisely the rectangle rule, establishing the lemma. ∎

The lemma is seen to coincide with Theorem 5.3 in the case that $s = 1$, since in this case the coefficients $a_{s,r}$ required in (5.4) have the value 1.

Now we provide the induction step for Theorem 5.3. Suppose the equation (5.4) is valid for all k with s replaced by $s-1$; that is, suppose

$$S_k^{s-1} f = 2^{-(s+k-2)} \sum_{l=s-1}^{s+k-2} \binom{2s+k-l-4}{s-2} S^{s-1}(l) f, \qquad k \geq 1. \tag{5.7}$$

Now from (4.6) we have

$$S_r^s = \sum_{k=1}^{r} S_k^{s-1} R_{r+1-k}, \qquad r \geq 1. \tag{5.8}$$

Since S_k^{s-1} contains only points of lengths $s-1$ to $s+k-2$, and R_i contains only points of lengths 1 to i, it follows that the term $S_k^{s-1} R_{r+1-k}$ contains only points of lengths s to $s+r-1$. Now consider a particular point $\mathbf{x} = (\mathbf{y}, z)$, where $\mathbf{y}$ is a point of S_r^{s-1} of length λ, and z is a point of R_r of length μ, with $s \leq \lambda + \mu \leq s+r-1$. The k-th term of (5.8) involves this point if and only if $s-1 \leq \lambda \leq s+k-2$ and $1 \leq \mu \leq r+1-k$, which together imply

$$\lambda - s + 2 \leq k \leq -\mu + r + 1.$$

For k in this range, the weight associated with the point $\mathbf{y}$ in S_k^{s-1} is, from (5.7),

$$2^{-(s+k-2)} \binom{2s+k-\lambda-4}{s-2},$$

while the weight associated with the point z in R_{r+1-k} is 2^{-r-1+k}. Thus, the total weight associated with the point $(\mathbf{y}, z)$ in the sum (5.8) is

$$\begin{aligned} \sum_{k=\lambda-s+2}^{-\mu+r+1} 2^{-(s+r-1)} \binom{2s+k-\lambda-4}{s-2} &= 2^{-(s+r-1)} \sum_{m=1}^{s+r-\lambda-\mu} \binom{s+m-3}{s-2} \\ &= 2^{-(s+r-1)} \binom{2s+r-\lambda-\mu-2}{s-1}, \end{aligned}$$

where in the last step we used the well-known identity

$$\binom{a}{a} + \binom{a+1}{a} + \ldots + \binom{b}{a} = \binom{b+1}{a+1},$$

easily proved by induction. Since the length of the point $(\mathbf{y}, z)$ is $l = \lambda + \mu$, we may use (5.3) and recover (5.4). ∎

To obtain an analogous formula for the rule Q_k^s, we simply apply Theorem 4.5. This gives the following corollary to Theorem 5.3.

Corollary 5.5

$$Q_k^s f = 2^{-(s+k-1)} \sum_{l=s}^{s+k-1} w_{s,s+k-l} S^s(l) f, \qquad k \geq 1, \tag{5.9}$$

where

$$w_{s,r} = \sum_{j=0}^{\min(r,s)-1} (-1)^j \binom{s-1}{j} 2^j a_{s,r-j}, \qquad r \geq 1. \tag{5.10}$$

Note that Q_k^s uses the weights $w_{s,1}, ..., w_{s,k}$; the weight $w_{s,k}$ is associated with the abscissas of shortest length s, the weight $w_{s,1}$ with the abscissas of greatest length $s+k-1$. There are simple generating functions for these weights.

Theorem 5.6 *The weights $a_{s,r}$ and $w_{s,r}$ of (5.5) and (5.10) are generated by*

$$A(x,y) := xy(1-x-y)^{-1} = \sum_{r=1}^{\infty}\sum_{s=1}^{\infty} a_{s,r} x^r y^s \tag{5.11}$$

and

$$W(x,y) := xy(1-x-y+2xy)^{-1} = \sum_{r=1}^{\infty}\sum_{s=1}^{\infty} w_{s,r} x^r y^s. \tag{5.12}$$

Proof. Using the binomial expansion and the elementary relation

$$(-1)^j \binom{-s}{j} = \binom{s+j-1}{s-1},$$

we find

$$x(1-x)^{-s} = \sum_{j=0}^{\infty} \binom{s+j-1}{s-1} x^{j+1}. \tag{5.13}$$

Setting $j = r-1$ in this and inserting expression (5.5) for $a_{s,r}$ gives

$$x(1-x)^{-s} = \sum_{r=1}^{\infty} a_{s,r} x^r. \tag{5.14}$$

After multiplying by y^s and summing over s, we find a geometric series on the left-hand side. Simplifying this yields (5.11), establishing the first part of this theorem.

It follows directly from (5.10) that

$$\sum_{r=1}^{\infty} w_{s,r} x^r = \sum_{r=1}^{\infty} x^r \sum_{j=0}^{\min(r,s)-1} (-1)^j \binom{s-1}{j} 2^j a_{s,r-j}. \tag{5.15}$$

Inverting the summation order, we find after a minor rearrangement that the right-hand side is

$$\sum_{j=0}^{s-1} x^j (-1)^j \binom{s-1}{j} 2^j \sum_{r=j+1}^{\infty} a_{s,r-j} x^{r-j}. \tag{5.16}$$

The reader will recognize the sum over r as the one in (5.14), after which the sum over j gives $(1-2x)^{s-1}$, establishing

$$\sum_{r=1}^{\infty} w_{s,r} x^r = x(1-x)^{-s}(1-2x)^{s-1}. \tag{5.17}$$

When treated in the same way as we treated (5.14) above, this yields (5.12). ∎

All of the weights $a_{s,r}$, being binomial coefficients, are positive. Some of the weights $w_{s,r}$ are negative and some zero. Note that (5.17) is also a generating function, which may in some cases be more convenient than the more elegant (5.12).

Corollary 5.7 *$a_{s,r} = a_{r,s}$ and $w_{s,r} = w_{r,s}$, and for even s, $w_{s,s}$ is zero.*

Proof. The symmetry of the coefficients is an immediate consequence of the symmetry of the generating functions (5.11), (5.12). (The symmetry of $a_{s,r}$ is also apparent in (5.5).) The final part follows from elementary manipulation of the generating function (5.12). First, we establish that

$$W(x,y) = \sum_{r=1}^{\infty}\sum_{s=1}^{\infty} w_{s,r}x^s y^r = \sum_{t=1}^{\infty}(-1)^{t-1}[xy/(1-x)(1-y)]^t. \tag{5.18}$$

Then, applying the binomial theorem to each individual element $(1-x)^{-t}$ and $(1-y)^{-t}$ in this sum and extraction of the coefficient of $(xy)^s$ gives

$$w_{s,s} = \sum_{t=1}^{s}(-1)^{t-1}\begin{pmatrix} s-1 \\ t-1 \end{pmatrix}^2.$$

The right-hand side is identical to the coefficient of z^{s-1} in the expansion of $(1+z)^{s-1}(1-z)^{s-1}$. Since this is an even function of z, when s is even the coefficient of z^{s-1} is zero, implying $w_{s,s} = 0$. ∎

The authors have encountered no other cases of zero $w_{s,r}$. For s and $r \leq 8$, the weights $w_{s,r}$ are tabulated in the Appendix.

6 The Number of Abscissas

This section is concerned with the number of points required by the meritorious rule Q_k^s. We shall generally denote by $\nu(P)$ the number of points required by an operator P. Further, we abbreviate

$$N_k^s = \nu(S_k^s),$$
$$\nu(S^s(l)) = \nu^s(l).$$

As in preceding sections, we deal first with the symmetric operator S_k^s. This may be generated by the use of (4.6), which states

$$S_k^s = \sum_{i=1}^{k} S_{k+1-i}^{s-1} R_i. \tag{6.1}$$

Here R_i is the 2^i panel rectangle rule, which as in Lemma 5.4 may be expressed as

$$R_i f = \frac{1}{2^i}\sum_{j=1}^{i} S^1(j)f, \qquad i \geq 1, \tag{6.2}$$

where $S^1(j)$ is the set of one-dimensional points of length j. Substitution of (6.2) into (6.1) and a rearrangement of the order of summation give

$$S_k^s = \sum_{j=1}^{k} \sum_{i=j}^{k} \frac{1}{2^i} S_{k+1-i}^{s-1} S^1(j). \tag{6.3}$$

In this sum the terms with different index j represent distinct points, as the x_s-components of points with different values of j have different lengths, and so are distinct. Associated with each index j is a sum of symmetric operators S_{k+1-i}^{s-1}. These form embedded sets: all points of S_{k+1-i}^{s-1} with $i > j$ are included in S_{k+1-j}^{s-1}. Consequently, in determining the number of *distinct* points, we need consider only those elements in this sum having $i = j$. This gives

$$\nu(S_k^s) = \sum_{j=1}^{k} \nu(S_{k+1-j}^{s-1}) \nu(S^1(j)), \tag{6.4}$$

where $\nu(S^1(j)) = \nu^1(j) = \delta_{j,1} + 2^{j-1}$ is the number of one-dimensional points of length j.

For $N_k^s = \nu(S_k^s)$, we find the recursion relation

$$N_k^s = N_k^{s-1} + \sum_{j=1}^{k} N_{k+1-j}^{s-1} 2^{j-1}, \qquad k \geq 1, s \geq 2. \tag{6.5}$$

(Note that the $j = 1$ term occurs twice.) This is anchored by

$$N_k^1 = 2^k, \qquad k \geq 1. \tag{6.6}$$

The values N_k^s for $s \leq 4$ and $k \leq 8$ are listed in the Appendix. Expressions for the rules of dimension up to four are

$$\begin{aligned} N_k^1 &= 2^k, \\ N_k^2 &= 2^k(k+1), \\ N_k^3 &= 2^k(k^2+5k+2)/2, \\ N_k^4 &= 2^k(k^3+12k^2+29k+6)/6. \end{aligned}$$

To obtain a convenient bound, we proceed as follows. We set

$$N_k^s = 2^k p_{s-1}(k), \qquad k \geq 1. \tag{6.7}$$

Then substitution into (6.5) and (6.6) gives

$$\begin{aligned} p_s(k) &= p_{s-1}(k) + \sum_{j=1}^{k} p_{s-1}(j), \qquad k \geq 1, \quad s \geq 1, \\ p_0(k) &= 1. \end{aligned}$$

This, in fact, defines a set of polynomials, p_s, of degree indicated by the subscript. Since $p_{s-1}(k)$ is a positive integer, it is clear from (6.7) that $N_k^s \geq 2^k = \rho$, with equality only if $s = 1$. Computation of the values of $p_{s-1}(k)$ is most easily effected by means of the identity

$$p_s(k) = p_s(k-1) + 2p_{s-1}(k) - p_{s-1}(k-1), \qquad k \geq 1, \quad s \geq 1, \quad \text{with} \quad p_s(0) = 1, \quad s \geq 1. \tag{6.8}$$

One may obtain a simple upper bound on N_k^s by showing first by induction that

$$p_s(k) \leq (k+2s-1)(k+2s-2)\dots(k+s)/s!, \tag{6.9}$$

and then applying the arithmetic mean, geometric mean inequality to obtain

$$p_s(k) < (k + \tfrac{3}{2}s - \tfrac{1}{2})^s/s!. \tag{6.10}$$

Substituting this in (6.7) gives

$$N_k^s < 2^k \left(k + \frac{3s-4}{2}\right)^{s-1} /(s-1)!\,. \tag{6.11}$$

As remarked earlier, it is known that $w_{s,s} = 0$ when s is even. On recalling (4.12), this leads to the bounds

$$\begin{aligned} \nu(Q_k^s) &\leq N_k^s, && s \text{ odd, or } s \text{ even and } k < s, \\ \nu(Q_k^s) &\leq N_k^s - \nu^s(k), && s \text{ even and } k \geq s. \end{aligned}$$

A numerical investigation confirms that for $s < 8$ all coefficients $w_{s,r}$ other than $w_{s,s}$ for even s are nonzero. Thus the inequalities may be replaced by equalities for all $s < 8$; we conjecture they may always be replaced by equalities.

Note that the bound (1.1) follows from (6.11), since the merit is $\rho = 2^k$.

A procedure similar to the one described above may be used to construct formulas analogous to (6.5) to (6.8) for $\nu^s(l)$, the number of $s-$dimensional points of length l. Alternatively, an immediate corollary of Theorem 5.3 is that

$$N_k^s = \nu^s(s) + \nu^s(s+1) + \dots + \nu^s(s+k-1), \qquad s, k \geq 1, \tag{6.12}$$

giving immediately

$$\nu^s(s) = N_1^s = 2^s; \qquad \nu^s(l) = N_{l-s+1}^s - N_{l-s}^s, \qquad l > s \geq 1. \tag{6.13}$$

Invoking (6.7), we find, after some manipulation, that

$$\nu^s(l) = 2^{l-s} q_{s-1}(l) + \delta_{l,s}, \qquad l \geq s \geq 1, \tag{6.14}$$

where

$$q_{s-1}(l) = 2p_{s-1}(l-s+1) - p_{s-1}(l-s), \qquad l \geq s \geq 1. \tag{6.15}$$

These polynomials satisfy recursion relations similar in form to those satisfied by $p_s(k)$.

Acknowledgment

We are indebted to Dr. Michael D. Hirschhorn of the University of New South Wales for Theorem 5.6 and Corollary 5.7.

APPENDIX

Weights and Abscissas

The cubature rule Q_k^s of Section 4 is an s-dimensional quadrature rule for $[0,1)^s$ having merit $\rho = 2^k$. It has the form

$$Q_k^s f = 2^{-(s+k-1)} \sum_{l=s}^{s+k-1} w_{s,s+k-l} S^s(l) f.$$

Here $S^s(l)f$ is the sum of function values over all distinct s-dimensional points of length l, as defined in Definition 5.1, and the weights are given by (5.10). Some numerical values are given in the following tables.

Table 1. Weight coefficients $w_{s,r}$

	$r=1$	$r=2$	$r=3$	$r=4$	$r=5$	$r=6$	$r=7$	$r=8$
$s=1$	1	1	1	1	1	1	1	1
$s=2$	1	0	-1	-2	-3	-4	-5	-6
$s=3$	1	-1	-2	-2	-1	1	4	8
$s=4$	1	-2	-2	0	3	6	8	8
$s=5$	1	-3	-1	3	6	6	2	-6
$s=6$	1	-4	1	6	6	0	-10	-20
$s=7$	1	-5	4	8	2	-10	-20	-20
$s=8$	1	-6	8	8	-6	-20	-20	0

Table 2. The number $\nu^s(l)$ of points of length l

	$l=s$	$l=s+1$	$l=s+2$	$l=s+3$	$l=s+4$	$l=s+5$	$l=s+6$	$l=s+7$
$s=1$	2	2	4	8	16	32	64	128
$s=2$	4	8	20	48	112	256	576	1280
$s=3$	8	24	72	200	528	1344	3328	8064
$s=4$	16	64	224	704	2064	5760	15488	40448
$s=5$	32	160	640	2240	7200	21792	63040	176000
$s=6$	64	384	1728	6656	23232	75648	233792	693504
$s=7$	128	896	4480	18816	70784	246400	809088	2537600
$s=8$	256	2048	11264	51200	206336	763904	2653184	8763392

Table 3. The number N_k^s of abscissas required by S_k^s

	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$	$k=6$	$k=7$	$k=8$
$s=1$	2	4	8	16	32	64	128	256
$s=2$	4	12	32	80	192	448	1024	2304
$s=3$	8	32	104	304	832	2176	5504	13568
$s=4$	16	80	304	1008	3072	8832	24320	64768
$s=5$	32	192	832	3072	10272	32064	95104	271104
$s=6$	64	448	2176	8832	32064	107712	341504	1035108
$s=7$	128	1024	5504	24320	95104	341504	1150592	3688192
$s=8$	256	2304	13568	64768	271104	1035108	3688192	12451584

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