NOTES ON A SEARCH FOR OPTIMAL LATTICE RULES*

James Lyness**
Mathematics and Computer Science Division
Argonne National Laboratory, Argonne, IL 60439, U.S.A.

Ronald Cools
Department of Computer Science, Katholieke Universiteit Leuven
Celestijnenlaan 200A, B-3001 Heverlee, Belgium

In this paper some of the results of a recent computer search [CoLy99] for optimal three- and four-dimensional lattice rules of specified trigonometric degree are discussed. The theory is presented in a general frame emphasising the special nature of lattice rules among the rules of specified trigonometric degree.

1 Background Material

In this paper we discuss some of the results of a recent computer search [CoLy99] for optimal s-dimensional lattice rules of specified trigonometric degree.

An s-dimensional cubature formula (or rule) Qf for $[0,1)^s$ is a weighted sum of function values

$$Qf := \sum_{j=1}^{N(Q)} w_j f(\mathbf{x}_j), \tag{1.1}$$

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which approximates in some way the integral

$$If := \int_{[0,1)^s} f(\mathbf{x})d\mathbf{x}. \tag{1.2}$$

A cubature formula of *enhanced* trigonometric degree δ is one that integrates exactly all trigonometric polynomials (with respect to period [0,1)) of degree $\delta - 1$. An *optimal* rule Q of enhanced degree δ is one whose abscissa count $N(Q)$ is as small as or smaller than the abscissa count $N(Q')$ of any other rule Q' of the same enhanced degree δ. A lattice rule $Q(\Lambda)$ is an equal-weight cubature formula ($w_j = 1/N(Q)$) whose abscissas $\mathbf{x}_j$ lie in $\Lambda \cap [0,1)^s$, where Λ is an integration lattice. For a lattice rule $Q(\Lambda)$ to be of enhanced degree δ, the dual lattice $\Lambda^\perp$ can have no elements $\mathbf{h}$ for which $|\mathbf{h}| \in [1, \delta - 1]$. In the following subsections, the concepts mentioned above are properly connected, with the necessary theorems being referenced or proved. In what follows, we denote by $\mathbf{e}_i$ a unit vector whose components coincide with the i-th row of the $s \times s$ identity matrix I. (Note that, in common English usage, the word *rule* may be used for *cubature formula*.)

1.1 Integration Lattices

An *integration lattice* $\mathcal{L}[t, D, Z, s]$ is specified by positive integers t, $d_1, d_2, \ldots, d_t$ and the elements of a $t \times s$ integer matrix Z. Here, D is the diagonal $t \times t$ matrix $D = \text{diag}\{d_1, d_2, \ldots, d_t\}$, and we denote the i-th row of Z by $\mathbf{z}_i$.

Definition 1 *The* integration *lattice* $\mathcal{L}[t, D, Z, s]$ *comprises all points that may be expressed in the form*

$$\mathbf{p} = \sum_{i=1}^{t} j_i \mathbf{z}_i / d_i + \sum_{i=1}^{s} k_i \mathbf{e}_i \tag{1.3}$$

for some selection of integers j_i *and* k_i.

This lattice is said to be *generated* by the $t + s$ generators $\mathbf{z}_i/d_i$ $i = 1, 2, \ldots, t$ and $\mathbf{e}_i$ $i = 1, 2, \ldots, s$.

It is readily verified that this set of points satisfies the standard definition of a lattice, that is, $\mathbf{p}_1, \mathbf{p}_2 \in \Lambda \Rightarrow \mathbf{p}_1 - \mathbf{p}_2 \in \Lambda$, and, since

$\mathbf{p} \det D \in \mathbb{Z}^s$ for all $\mathbf{p}$, there are no points of accumulation. Moreover, the subset of these points, obtained by assigning $j_1 = j_2 = \cdots = j_k = 0$, constitutes the *unit lattice* Λ_0, also known as $\mathbb{Z}^s$. Thus, $\Lambda \supseteq \Lambda_0$, which is the condition that a given lattice Λ is an *integration* lattice.

It is well known that one can express any s-dimensional lattice Λ in terms of only s distinct generators. Thus, there exists an $s \times s$ matrix A whose rows $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_s$ may be used to generate Λ and (1.3) may be replaced by

$$\mathbf{p} = \sum_{i=1}^{s} \lambda_i \mathbf{a}_i = \lambda A, \tag{1.4}$$

where λ_i are integers, that is, $\lambda \in \Lambda_0$.

The reader will note that a generator matrix is not unique. When A is a generator matrix of Λ, this same lattice is generated by UA, where U is any unimodular integer matrix ($|\det U| = 1$).

1.2 Dual Lattices

Corresponding to every s-dimensional lattice Λ is its dual (or polar or reciprocal) lattice $\Lambda^\perp$. This may be defined in terms of generator matrices as follows. When the generator matrix of Λ is A, then $\Lambda^\perp$ is the lattice whose generator matrix is $B = (A^T)^{-1}$. This is a somewhat trite definition. For a more informative introduction, see [Lyn89]. It is readily shown that, when Λ is an integration lattice, that is, $\Lambda \supseteq \Lambda_0$, then $\Lambda^\perp$ is an integer lattice that is, $\Lambda^\perp \subseteq \Lambda_0$. Since all components of a point in Λ_0 are integers, the same is true for $\Lambda^\perp$, and so its generator matrix B has only integer elements. Again, UB is also a generator matrix of $\Lambda^\perp$, and it is possible to choose U so that $H = UB$ is in upper triangular lattice form (*utlf*). That is, $H_{cc} > 0$; $H_{rc} \in [0, H_{cc})$, when $r < c$ and $H_{rc} = 0$ when $r > c$. The *utlf* generator matrix H is in 1–1 correspondence with the integer lattice $\Lambda^\perp$. (This is helpful for counting the number of different lattices and for organizing a search for optimal lattices. See [LySø89].)

1.3 Lattice Rules

The *lattice rule* $Q(\Lambda)$ is a cubature formula whose abscissas lie on the intersection of an integration lattice $\Lambda = \mathcal{L}[t, D, Z, s]$ and $[0,1)^s$. It is denoted by $Q[t, D, Z, s]$ and may be defined by

$$Q[t, D, Z, s]f = \frac{1}{d_1 d_2 \ldots d_t} \sum_{j_1=1}^{d_1} \sum_{j_2=1}^{d_2} \cdots \sum_{j_t=1}^{d_t} f(\{\sum j_i \mathbf{z}_i / d_i\}), \tag{1.5}$$

where, as is conventional, $\mathbf{y} = \{\mathbf{x}\}$ is defined as the vector obtained from the fractional parts of each component of $\mathbf{x}$.

The same rule $Q(\Lambda)$ may have many different representations of this form, using different values of t and other parameters. A rule is of *rank* r if it can be expressed in this form with $t = r$, but cannot be so expressed with $t < r$. See, for example, [SlLy89]. An example of a rank-2 rule is given in Section 4. The m-copy rule defined in Section 3 when $m > 1$ is of rank s.

The number of function values $N(Q)$ used by $Q(\Lambda)$ is the number of points in $\Lambda \cap [0,1)^s$; this coincides with the density of lattice points and can be shown to be

$$N = |\det A|^{-1} = |\det B| = H_{11} H_{22} \ldots H_{ss}. \tag{1.6}$$

Unfortunately, this value is not immediately clear from (1.5). In point of fact, $N = (\det D)/k$, where k is a positive integer and, of course, $\det D = d_1 d_2 \ldots d_t$. When $k > 1$, the form (1.5) is termed *repetitive.*

The reader will note that $(s!)^{-1} |\det B|$ is the s-volume of a simplex having vertices at the s generators of $\Lambda^\perp$ and at the origin. This simplex is known as a basic simplex of the lattice $\Lambda^\perp$. In fact, any simplex constructed from $(s+1)$ distinct elements of this lattice has s-volume $k(s!)^{-1} |\det B|$, where k is a nonnegative integer.

1.4 Fourier Series and Trigonometric Polynomials

We treat the s-dimensional hypercube $[0,1)^s$. For many functions, the Fourier series

$$\bar{f}(\mathbf{x}) = \sum_{\mathbf{h} \in \mathbb{Z}^s} \hat{f}_{\mathbf{h}} e^{2\pi i \mathbf{h}.\mathbf{x}} \tag{1.7}$$

converges and coincides with $f(\mathbf{x})$ in $(0,1)^s$. Here

$$\hat{f}_{\mathbf{h}} = \int_{[0,1)^s} f(\mathbf{x}) \mathrm{e}^{-2\pi i \mathbf{h}.\mathbf{x}} d\mathbf{x} \tag{1.8}$$

is a Fourier coefficient of $f(\mathbf{x})$. A trigonometric polynomial is simply a function $f(\mathbf{x})$, having only a finite number of nonvanishing Fourier coefficients. To quantify this, we define a subset $\Omega(x,\delta)$ of the s-dimensional unit lattice

$$\Omega(s,\delta) = \{\mathbf{h} \text{ such that } |\mathbf{h}| := |h_1| + |h_2| + \cdots + |h_s| < \delta\}. \tag{1.9}$$

Definition 2 $f(\mathbf{x})$ *is an s-dimensional trigonometric polynomial of degree d (or enhanced degree $\delta = d+1$) when its only nonzero Fourier coefficients $\hat{f}_{\mathbf{h}}$ are those for which $\mathbf{h} \in \Omega(s,\delta)$.*

1.5 Lattice Rules of Specified Trigonometric Degree

The discretization error of any cubature formula may be expressed in terms of the Fourier coefficients of the integrand function. To this end, we apply the operator Q to the Fourier series (1.7) above to obtain

$$Qf = \sum_{\mathbf{h} \in \mathbb{Z}^s} \hat{f}_{\mathbf{h}} d_{\mathbf{h}}(Q), \tag{1.10}$$

where we have defined

$$d_{\mathbf{h}}(Q) := Q(\mathrm{e}^{2\pi i \mathbf{h}.\mathbf{x}}) = \sum_{j=1}^{N(Q)} w_j \mathrm{e}^{2\pi i \mathbf{h}.\mathbf{x}_j}. \tag{1.11}$$

Equation (1.10) above may be considered a generalization of the Poisson summation formula, which in one dimension connects a sum of equally spaced function values with a sum of equally spaced Fourier transforms. When Q is a lattice rule, many coefficients $d_{\mathbf{h}}(Q)$ in (1.11) vanish.

Theorem 1 *When $Q = Q(\Lambda)$ is a lattice rule,*

$$d_{\mathbf{h}}(Q) = \begin{cases} 1 & \text{for all } \mathbf{h} \in \Lambda^{\perp} \\ 0 & \text{otherwise.} \end{cases}$$

There are several straightforward ways of proving this. See, for example, [Lyn89].

Applying this result to (1.10) in the case that Q is a lattice rule gives

$$Q(\Lambda)f = \sum_{\mathbf{h}\in\Lambda^{\perp}} \hat{f}_{\mathbf{h}}. \tag{1.12}$$

We are now in a position to derive a criterion for the enhanced degree of a lattice rule. Recalling that $\hat{f}_{\mathbf{0}} = If$, we rewrite this equation in the form

$$Ef := Q(\Lambda)f - If = \sum_{\substack{\mathbf{h}\in\Lambda^{\perp} \\ 0<|\mathbf{h}|<\delta}} \hat{f}_{\mathbf{h}} + \sum_{\substack{\mathbf{h}\in\Lambda^{\perp} \\ |\mathbf{h}|\geq\delta}} \hat{f}_{\mathbf{h}}. \tag{1.13}$$

When $f(\mathbf{x})$ is a trigonometric polynomial of enhanced degree δ, in view of Definition 2 above, every term in the final summation is zero. Because of this, the condition for Ef to be zero must be that the first summation is also zero; this implies that $\Lambda^{\perp}$ contains no elements $\mathbf{h}$ for which $0 < |\mathbf{h}| < \delta$.

Theorem 2 *$Q(\Lambda)$ is of enhanced degree δ if and only if $\Lambda^{\perp}$ contains no elements, other than the origin within $\Omega(s,\delta)$.*

This result could equally well be established using (1.11) by constructing moment equations. A set of moment equations is

$$d_{\mathbf{0}}(Q) = 1 \qquad d_{\mathbf{h}}(Q) = 0 \quad \forall\ 0 < \mathbf{h} < \delta,$$

whether or not Q is a lattice rule. Theorem 2 may be expressed in other ways. For example,

$$\delta = \min_{\substack{\mathbf{h}\neq 0 \\ \mathbf{h}\in\Lambda^{\perp}}} |\mathbf{h}|. \tag{1.14}$$

In classical lattice theory, the term *admissible* is used for this concept. A lattice Λ is termed Ω-admissible if it contains no elements other than the origin within Ω. Thus, δ is the largest integer for which $\Lambda^{\perp}$ is $\Omega(s,\delta)$-admissible.

2 The Search for Optimal Rules

Every cubature formula Q has an abscissa set. We denote by $N(Q)$ the number of abscissas in this set. All these may be taken to be in $[0,1)^s$. We define $N_{\min}(s,\delta)$ to be the minimal number $N(Q)$ of abscissas needed by any cubature formula Q of enhanced trigonometric degree δ. Any formula Q of this enhanced degree δ for which $N(Q) = N_{\min}(s,\delta)$ is termed an *optimal* rule. Our searches have all been limited to lattice rules, and the more expensive searches to subsets of lattice rules. We have been particularly careful to specify the subset of lattice rules with respect to which each individual result is optimal.

The final paragraph of the preceding section indicates that many properties of interest of $Q(\Lambda)$ are geometric properties of $\Lambda^\perp$; these may be conveniently obtained from its generator matrix, B or H. For example, the abscissa count $N(Q)$ is simply $s!V$, V being the s-volume of the basic simplex of $\Lambda^\perp$. In terms of the generator matrix, this is simply $|\det B|$ or $\det H = H_{11}H_{22}\dots H_{ss}$. The enhanced degree of Q is simply the shortest L_1 distance of any element of $\Lambda^\perp$ from the origin, as specified by (1.14) above. Moreover, there is a 1–1 correspondence between an integer lattice and its generator matrix in utlf.

This all suggests a somewhat indirect class of search procedure, one based on searching sets of integer lattices, $\Lambda^\perp$. Finally, when the search is complete and the "best" lattices found, then and only then need Λ and $Q(\Lambda)$ be constructed.

The search population comprises sets of integer lattices. Each lattice is represented by a generator matrix. Several searches for rules having optimal Zaremba indices are described in [LySø91]. In these, $\Lambda^\perp$ is represented by its utlf generator H. In the current search, a different generator, described below, is used.

Besides indicating a method for an exhaustive search, the theory of the preceding section, in particular the final theorem, suggests some obvious characteristics we might expect to find in the dual lattice of an optimal rule. Indeed, our recent major search [CoLy99] was confined to areas where promising lattices seemed likely to occur. The next paragraph is adapted from [CoLy99], where a complete description of this search may be found.

A dynamic approach to the problem of finding an optimal rule might start with a lattice that is comfortably of enhanced degree δ and has a high abscissa count. We perturb this given $\Omega(s,\delta)$-admissible lattice $\Lambda^\perp$, with a view to reducing the s-volume of its unit cell but keeping it $\Omega(s,\delta)$-admissible, that is, not allowing any lattice point to enter the fixed region $\Omega(s,\delta)$. It is reasonable to believe that the process of making this unit cell small, that is, making the lattice $\Lambda^\perp$ denser and reducing its order, would, in general, move lattice points towards the origin. This process would be seriously inhibited by the boundary of $\Omega(s,\delta)$. Ultimately (as the wiggle room disappears), one would expect progress to come to a complete stop (grind to a halt) at a stage where many points of $\Lambda^\perp$ were (jammed) on this boundary. Thus, it is plausible to believe that the lattice Λ of an *optimal* lattice rule $Q(\Lambda)$ of enhanced degree δ will have a dual lattice $\Lambda^\perp$ with many elements on this boundary. The underlying feature of our search is that it is limited to dual lattices having this property.

In three dimensions, our population comprised all integer lattices generated by $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$, where these lay on different faces of the octahedron $\Omega(3,\delta)$. None have enhanced degree exceeding δ. In our search, we check the abscissa count first. If this is the smallest yet encountered, we carry out the longer task of calculating the enhanced degree. If this turns out to be δ, we retain this lattice $\Lambda^\perp$ as a candidate for an optimal lattice.

These remarks are intended only to give the underlying idea of the search. A proper description even in three dimensions is far longer. In higher dimensions there are many complications that we do not discuss here.

The cost in computer time of this search is enormous. The complexity is high but not more than δ^{s^2-1}. However, after code development and calculations lasting over one year, we have found what are probably the optimal lattice rules for $s=3$, $\delta<54$, and for $s=4$, $\delta<23$. Unfortunately, we cannot affirm that these are optimal in a general sense. In [CoLy99] we have introduced definitions (K-optimal) which specify the precise sense in which these rules are optimal.

3 The rho-index $\rho(Q)$

In this section, we simply state some examples of the results we found. The reader interested in a complete set of results should refer to [CoLy99]. There we give seventy-six lattice rules, all optimal in some sense, each specified in terms of its utlf matrix H. These are presented in three pages of tabular material, which we do not reproduce here. However, we do reproduce below two figures in which a rule may be represented by a single point. In these two figures we have included a majority of the rules discovered by our search, as well as some other rules.

Definition 3 *Let an s-dimensional cubature rule Q have abscissa count N and strict enhanced trigonometric degree δ. Then its ρ-*index *$\rho(Q)$ is*

$$\rho(Q) := \delta^s/(s!N). \tag{3.1}$$

In earlier papers, the concept of an efficiency indicator was used. We believe that the efficiency indicator has now outlived its usefulness; we recommend using the ρ-index instead. Naturally, this suggestion has no effect on the depth and nature of research about optimal rules. It simply provides a way of illustrating results. The reader might compare Figures 1 and 2 below with corresponding figures that use the efficiency indicator as ordinate. Figures 1 and 2 are reasonably compact (in a nontechnical sense). The following theoretical results show why.

Definition 4 *The m-copy (or m^s-copy) of an s-dimensional cubature formula (1.1) is*

$$Q^{(m)}f = \sum_{k_1=0}^{m-1}\sum_{k_2=0}^{m-1}\cdots\sum_{k_s=0}^{m-1}\sum_{j=1}^{N}\frac{w_j}{m^s}f\left(\frac{\mathbf{x}_j+(k_1,k_2,\ldots,k_s)}{m}\right). \tag{3.2}$$

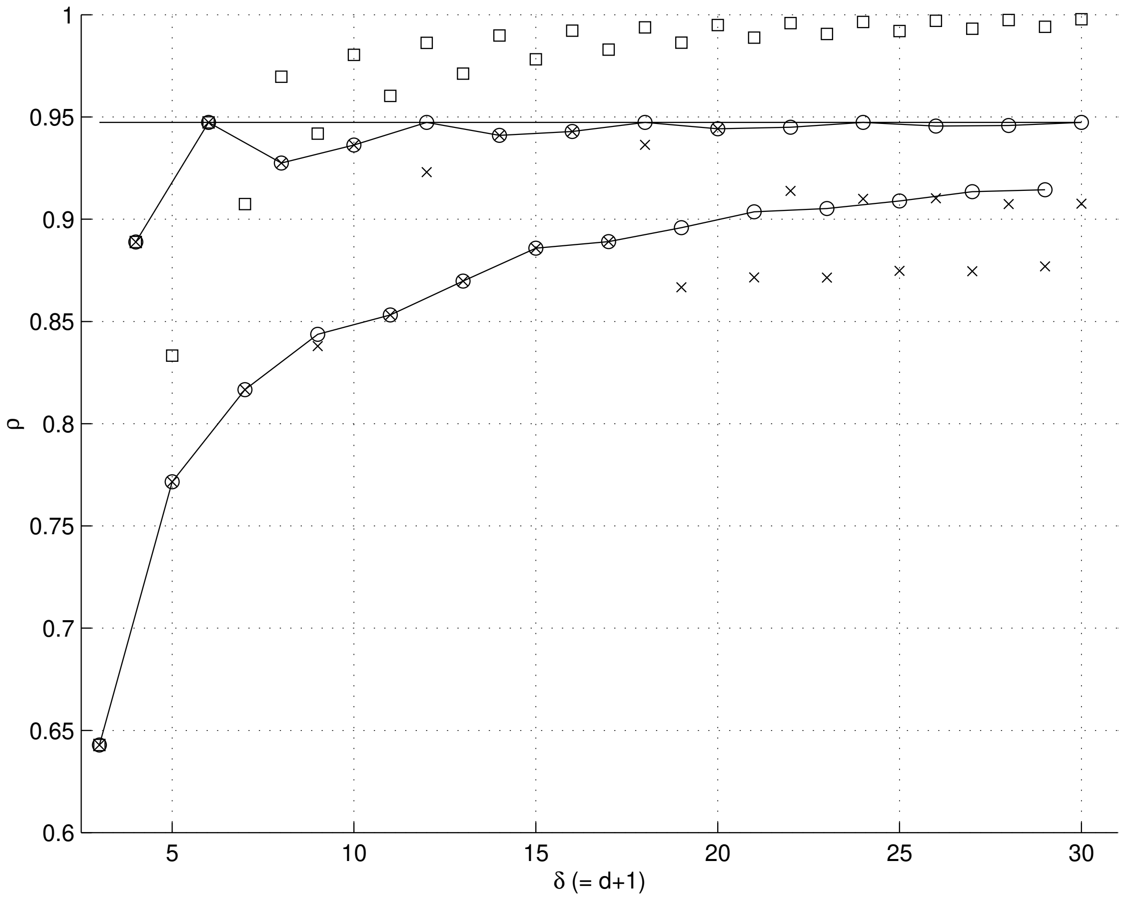

Figure 1: ρ as a function of δ for three-dimensional rules

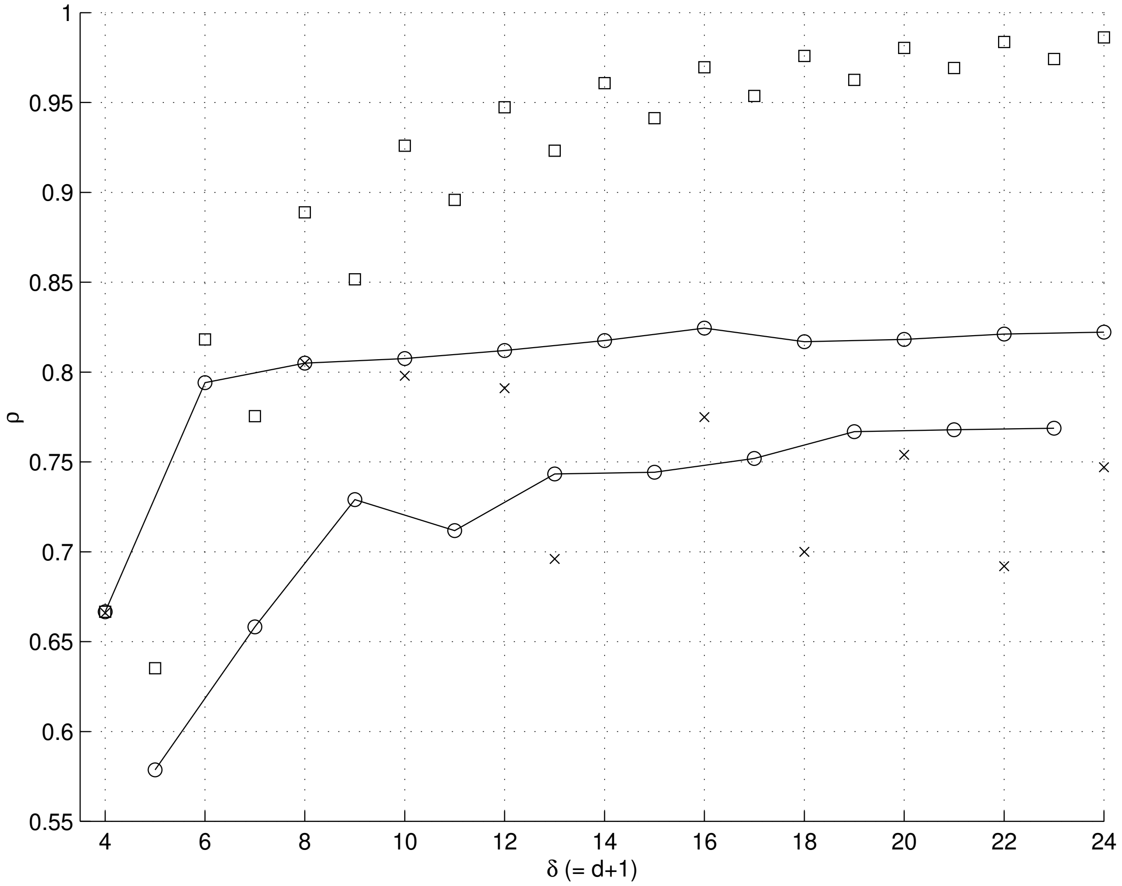

Figure 2: ρ as a function of δ for four-dimensional rules

$\times$ Rules appearing in recent papers

$\circ$ Rules appearing in [CoLy99]

$\square$ The Möller Bound N_{ME}

This is, of course, the rule obtained by partitioning $[0,1]^s$ in a natural way into m^s identical squares and applying a properly scaled version of Q to each. It is almost self-evident that the m-copy of a lattice rule is also a lattice rule.

Theorem 3 *When Q is a cubature formula of enhanced degree δ having abscissa count N, then $Q^{(m)}$ is a cubature formula of enhanced degree $s\delta$ and abscissa count $\delta^s N$.*

A proof restricted to lattice rules is almost self-evident, since the effect of taking an m-copy is to replace Λ by $(1/m)\Lambda$ and $\Lambda^\perp$ by $m\Lambda^\perp$. However, the general proof is also straightforward.

Corollary 1 *The ρ-indices of a cubature formula Q and any of its m-copies $Q^{(m)}$ are identical. That is,*

$$\rho(Q^{(m)}) = \rho(Q). \tag{3.3}$$

This follows immediately from (3.1).

The second relevant result concerns $N_{ME}(s,\delta)$, the well-known lower bound on the abscissa count of any s-dimensional rule of enhanced trigonometric degree δ. This bound is sometimes called Möller's lower bound, although Möller considered only the algebraic degree [Möl79]. All results known to us on lower bounds are contained in [Coo97]; see in particular subsections 7.1 and 8.3. For odd values of δ the bound is classical. For even values of δ it is mentioned in [Nos85] and derived in [Mys87], extending Möller's result. Using this result, one can easily show that $\rho(\tilde{Q}) \leq 1$ for a hypothetical rule $\tilde{Q}$ of degree δ and abscissa count N_{ME}. Since no actual rule of this degree can have a lower abscissa count, we find

$$\rho(Q) \leq \rho(\tilde{Q}) \leq 1. \tag{3.4}$$

In Figures 1 and 2, every point entry represents a cubature formula. In view of (3.4) above, there can be no entries above $\rho = 1$. The square entries are the hypothetical rules $\tilde{Q}$ mentioned above. Because of Möller's bound, there can be no entries above these.

However, in view of (3.3), every point on this figure gives rise to an infinite sequence of other points; specifically, a point at (δ, ρ) implies there is a sequence of points at $(m\delta, \rho)$ for all positive integer m. In general, these points are not shown.

It is apparent, then, that rules of particular interest have entries in the part of this figure lying in a strip bounded above by $\rho = 1$ and below by one of the previous entries. The reasoning here extends to s-dimensions.

4 Some Specific Results for $s = 4$, $\delta = 16$

The four-dimensional rule with the highest ρ-index known to us is one with $\delta = 16$. In this section we first give several examples of rules having enhanced degree $\delta = 16$. We then make some general points in terms of these examples.

In 1991, Noskov published [Nos91] two rank-1 simple rules having $\delta = 16$. These were of the form

$$Qf = \frac{1}{N} \sum_{j=1}^{N} f\left(\{j\mathbf{z}/N\}\right). \tag{4.1}$$

One is a member of a family of rules specified for all $\delta = 4k, k = 1, 2, \ldots$; the member with $\delta = 16$ has

$$N = 3544;\ \mathbf{z} = (1, 17, 129, 985);\ \mu = 192. \tag{4.2}$$

(See Section 5 for the multiplicity μ.) Another, found by experiment, has

$$N = 3522;\ \mathbf{z} = (1, 17, 195, 949);\ \mu = 192. \tag{4.3}$$

Almost ten years later, in the course of the exhaustive search described above, we came across the rank-1 simple rule with

$$N = 3376;\ \mathbf{z} = (1, 169, 1091, 1387);\ \mu = 192. \tag{4.4}$$

This may or may not be an optimal rank-1 rule; however it is not an optimal lattice rule of this degree. In [CoLy99], a rank-2 rule is listed. Since it has rank 2, it cannot be written in rank-1 form (4.1) above. One $D - Z$ representation is

$$Qf = \frac{1}{3312} \sum_{j=1}^{1656} \sum_{k=1}^{2} f\left(\left\{\frac{j\mathbf{z}_2}{1656} + \frac{k\mathbf{e}_1}{2}\right\}\right), \tag{4.5}$$

with

$$N = 3312;\ \mathbf{z}_2 = (1431, 919, 495, 1);\ \mathbf{e}_1 = (1, 0, 0, 0);\ \mu = 96.$$

It has *not* been shown that this is a generally optimal rule. It is K-optimal with respect to a reduced family. Thus, there could possibly be: (i) a K-optimal rule; (ii) a lattice rule; (iii) a general rule; having successively higher values of ρ.

5 Symmetric Equivalence

In the context of lattice searches, the concept of symmetric equivalent sets of lattices was first extensively developed in [LySø91]. The first paragraph of Section 3 of [CoLy99] also provides a good introduction to these ideas.

Briefly, a lattice Λ is symmetrically equivalent to another lattice Λ' if one can obtain Λ from Λ' by elementary rotations or inversions of the coordinate axis system. For example, in four dimensions ($s = 4$), any particular lattice is one of a set of μ lattices, each of which is a symmetric copy of any other. In general, μ can be as high as $2^{s-1}s! = 192$. In fact, many lattices Λ' have built in additional symmetry, and the multiplicity of the symmetric equivalent set to which Λ' belongs may be any integer of the form $192/k$, where k is a positive integer.

It is intuitively obvious that many characteristics of each lattice, including its abscissa count and its trigonometric degree, are shared by each lattice in a set of symmetric equivalents. Thus, considerable effort in a search could be saved if only one member of each set were treated. Specifically, whether the search is taking place on a personal computer or on a state-of-the-art supercomputer, avoiding such duplication of effort might reduce the computer time required in a four-dimensional search from N hours to N minutes. However, our own experience in several comparable searches is that it is extremely difficult to exploit the symmetry effectively.

Further information with detailed proofs about lattice rules in general may be obtained from [SlJo94]. Much of the background for our search may be found in [CoSl96].

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It is *not* intended that this statement be published with the paper.