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Lattice rules of minimal and maximal rank with good figures of merit

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Abstract

For periodic integrands with unit period in each variable, certain error bounds for lattice rules are conveniently characterised by the figure of merit ρ, which was originally introduced in the context of number theoretic rules. The problem of finding good rules of order N (that is, having N distinct nodes) then becomes that of finding rules with large values of ρ. This paper presents efficient search methods for the discovery of rank 1 rules, and of maximal rank rules of high order, which possess good figures of merit. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

Lattice rules are quasi-Monte Carlo multidimensional quadrature rules defined on the unit hypercube $[0,1)^s$. These rules have been extensively studied in recent years, and the reader is referred to Niederreiter [19] and Sloan and Joe [23] for the basic definitions and results. This paper presents methods for finding rank 1 lattice rules and 2^s copies of rank 1 rules (which terms we define later in this section) that are optimal, in a particular sense.

It is known [24] that an s-dimensional lattice rule Q_L can be expressed in the form of a nonrepetitive sum:

$$Q_L(f) = \frac{1}{N}\sum_{j_1=0}^{n_1-1}\cdots\sum_{j_m=0}^{n_m-1} f\left(\left\{\sum_{i=1}^{m}\frac{j_i}{n_i}\boldsymbol{g}_i\right\}\right), \tag{1.1}$$

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where $m \leqslant s$, the vectors $\boldsymbol{g}_1,\dots,\boldsymbol{g}_m$ are fixed integral vectors called *generators* of the rule, $N=\prod_{i=1}^{m} n_i$ is its *order*, and $n_{i+1} \mid n_i$ for $i=1,\dots,m-1$, with $n_m > 1$. The number m is called the *rank* of the rule and $n_1,\dots,n_m,1,\dots,1$, with $s-m$ units, are its *invariants*. The braces in (1.1) indicate that addition is modulo $\mathbb{Z}^s$ which, in the case that f is 1-periodic in each variable, is clearly equivalent to using the usual addition operation in $\mathbb{R}^s$. A rank 1 rule is *simple* if it has a generator with one component that has value 1. The *integration lattice* L of the rule (1.1) is the set of linear combinations with integer coefficients of $\{\boldsymbol{g}_1/n_1,\dots,\boldsymbol{g}_m/n_m,\boldsymbol{e}_1,\dots,\boldsymbol{e}_s\}$, where $\boldsymbol{e}_1,\dots,\boldsymbol{e}_s$ are the standard Cartesian basis vectors in $\mathbb{R}^s$. Different choices of generators may yield different integration lattices and quadrature rules. Where necessary we shall denote by $L(\boldsymbol{g}_1/n_1,\dots,\boldsymbol{g}_m/n_m)$ the integration lattice with generators $\boldsymbol{g}_1/n_1,\dots,\boldsymbol{g}_m/n_m$.

Informally, two lattice rules are *geometrically equivalent* if the quadrature points of one can be transformed into those of the other by a symmetry of the cube. More formally, we may give an operational definition of the notion as follows.

Definition 1.1. Let $N > 1$. Two s-dimensional integration lattices L_1 and L_2 are *geometrically equivalent* if and only if L_2 is the image of L_1 under a finite sequence of operations on $\mathbb{R}^s$ of the form: S_1: $\mathscr{U}_i(\boldsymbol{x})=\boldsymbol{U}_i\boldsymbol{x}$, where $\boldsymbol{U}_i$ is the identity matrix with the ith diagonal element replaced by -1, or S_2: $\mathscr{V}_{ij}(\boldsymbol{x})=\boldsymbol{P}_{ij}\boldsymbol{x}$, where $\boldsymbol{P}_{ij}$ is a permutation matrix which interchanges elements i and j of $\boldsymbol{x}$ on premultiplication.

The lattice rules Q_{L_1} and Q_{L_2} are geometrically equivalent, denoted by $Q_{\mathrm{L}_L} \overset{g}{\sim} Q_{\mathrm{L}_2}$, if and only if L_1 and L_2 are geometrically equivalent.

Geometric equivalence of rules has been investigated in previous works [10,15,25]. In [10,15] it was noted that, for a given set of lattice rules, geometric equivalence is an equivalence relation. We shall refer to the corresponding equivalence classes as *geometry classes*.

The quality of a lattice rule — in particular, its suitability for use with periodic integrands having unit period in each variable — is often assessed by the values of

$$\rho(L)=\min\{r(\boldsymbol{h})\colon \boldsymbol{h}\in L^{\perp}-\{\boldsymbol{0}\}\}$$

and

$$P_\alpha = \sum_{\mathbf{h}\in L^{\perp}-\{\mathbf{0}\}} \frac{1}{r(\mathbf{h})^{\alpha}},$$

where $L^{\perp}=\{\mathbf{h}\in\mathbb{Z}^s\colon \forall\mathbf{x}\in L, \mathbf{x}\cdot\mathbf{h}\in\mathbb{Z}\}$ is the *dual* of the integration lattice L and $r(\mathbf{h})=\prod_{i=1}^{s}\max\{1,|h_i|\}$ for $\mathbf{h}\in\mathbb{Z}^s$. The series for P_α converges for $\alpha > 1$. The most commonly used values of α are even positive integers, for which a closed-form expression for P_α is available (see for example [23]). Geometrically equivalent rules have equal values of ρ and of P_α.

There have been a number of previous papers concerned with searches in dimensions exceeding 2 for lattice rules that perform well with respect to ρ and P_α. Some early numerical results were reported in [22], with later results in [2,5,9,18] being concerned with searches over sets of rank 1 simple rules only. Later results reported in [4,7,15–17,25] are from searches over other classes of rules.

In all of these searches, the rules being sought are specified by generator sets, either of the integration lattice or of its dual. However, different generator sets may generate the same rule, or a geometrically equivalent rule. If the number of such unnecessary investigations can be reduced, the efficiency of the search procedure may be enhanced. The results in [14,21] describe strategies for the unique specification of certain lattice rules.

For searches which use ρ as the figure of merit it is also worth noting that the calculation of $\rho(L)$ for a given lattice L is relatively time consuming. Consequently, the efficiency of the search procedure may be enhanced by eliminating from consideration, prior to the calculation of $\rho(L)$, any rule Q_{L} such that it is known a priori that there exists a rule Q'_{L} of lower order satisfying $\rho(L) \leqslant \rho(L')$, or of equal order satisfying $\rho(L) < \rho(L')$, since in these cases Q'_{L} is superior to Q_{L} with respect to ρ.

Definition 1.2. We shall say that an s-dimensional lattice rule Q_{L} of order N is *bestρ with respect to a set S of lattice rules* if, when $Q'_{\mathrm{L}} \in S$:
(1) if order$(Q'_{\mathrm{L}}) < N$, then $\rho(L') < \rho(L)$, and
(2) if order$(Q'_{\mathrm{L}}) = N$, then $\rho(L') \leqslant \rho(L)$.

Most computer searches with respect to ρ use a variety of strategies to eliminate inferior rules prior to the calculation of ρ, as well as to reduce redundancy in the search due to the inclusion of generator sets corresponding to the same, or geometrically equivalent, rules. In this regard the work of Maissoneuve [18] appears to be fundamental, with both [9,2] following the previous author's general approach. These papers are concerned exclusively with finding rank 1 simple rules which are bestρ with respect to the set of rank 1 simple rules in three, four and five dimensions. Lyness and Sørevik [15,16] have incorporated some of the methods used by these authors in the 'rank 1 simple' phase of searches for rules which are bestρ with respect to the sets of all three-dimensional lattice rules and all four-dimensional lattice rules, respectively. The same authors, in [17], develop techniques for finding good, although not necessarily bestρ, rules of higher order by scaling rules of low order along some axes and copying the scaled rules along these axes. More recently Disney [3] has applied techniques similar to those of earlier authors in searches in dimensions three to ten for rules which are bestρ with respect to the set of 2^s copies of rank 1 simple rules.

Definition 1.3. The n^s copy $Q^{(n)}$ of a quadrature rule Q is the rule obtained by subdividing the closed unit cube $[0,1]^s$ into n^s cubes each of side n^{-1}, and applying a properly scaled version of the rule Q to each smaller cube.

It is clear (for example, see [18]) that, without loss of generality, we may restrict complete searches of rank 1 rules to considering only rules having an *ordered generator*, which term we define in Section 2. Similar restrictions may be applied when searching 2^s copies of rank 1 rules. In dimension three the tables of Maisonneuve [18] and Kedem and Zaremba [9] extend to rules of order N not exceeding 6066. In dimension four the tables of Maisonneuve [18] and Bourdeau and Pitre [2] extend to $N = 3298$. In dimension five the latter authors reach $N = 772$. Lyness and Sørevik, treating all lattice rules and not only rank 1 rules, reach $N = 3916$ in dimension three [15] and $N = 562$ in dimension four [16]. Disney [3] incorporated the techniques developed in earlier searches into searches for 2^s copies of rank 1 simple rules, producing some very good rules of orders ranging from approximately 100 000 in dimension three to approximately 300 000 in dimension ten. In this paper we investigate the extension of these techniques to the case of non-simple rank 1 rules and their 2^s copies.

In Section 2 we identify a rank 1 search set, that is, a set of generators of rank 1 rules, including non-simple rules, to be considered which contains at least one representative from each geometry class. The set to be identified is chosen to enhance the efficiency of the search procedure. In Section 3 we extend the elimination strategy of Maisonneuve [18] to dimensions exceeding four and to the case of non-simple rules, and in Section 4 to 2^s copies of rank 1 rules. Numerical results are presented in Sections 5 and 6.

Note. In parts of this paper we make use of the elementary theory of linear Diophantine equations. A useful summary of the results we require is available in [20].

2. Theoretical considerations for a full rank 1 search

Following [18] we may begin the determination of a search set by restricting g_i, for $i \in \{1,\dots,s\}$, to the set $\{1,\dots,N/2\}$ since it is clear that every rank 1 rule of order N has a generator $\boldsymbol{g}/N$ with elements in this set, or is geometrically equivalent to a rule which has such a generator. If there is an i such that $g_i = 1$ then the rule is simple. If for some i we have $\gcd(g_i, N) = 1$ then there exist integers c_1, c_2 such that $c_1 g_i + c_2 N = 1$, that is, $c_1 g_i \equiv 1 \,(\mathrm{mod}\, N)$, and the rule is again simple since $c_1\boldsymbol{g}/N \,(\mathrm{mod}\, \mathbb{Z}^s)$ also generates Q_{L} and has 1 as its ith component. Conversely, if $\gcd(g_i, N) > 1$ for every $i \in \{1,\dots,s\}$ then there are no integers i, c_1, c_2 such that $c_1 g_i + c_2 N = 1$, and the rule is not simple. Finally, we note that every simple rule is geometrically equivalent to a simple rule having a generator $\boldsymbol{g}/N$ such that $g_1 = 1$. Thus the case of simple rules may be covered by considering generators with $g_1 = 1$. For such generators it is again clear that we may restrict g_i, for $i \in \{2,\dots,s\}$, to the set $\{1,\dots,N/2\}$.

Definition 2.1. Let N be a positive integer. We shall say that a set $\mathscr{G}_I(N)$ of integers is *exhaustive* if and only if each rank 1 rule of order N either has a generator $\boldsymbol{g}/N$ such that $g_1 \in \mathscr{G}_I(N)$, or is geometrically equivalent to such a rule. We shall say that an exhaustive set is *minimal* if there exists no exhaustive set with fewer elements.

We observe that, for $N > 1$, the set

$$\mathscr{G}_I(N) = \{1\} \cup \{m\colon 0 < m \leqslant N/2,\ \gcd(m, N) > 1\} \tag{2.1}$$

is exhaustive. However it is not, in general, minimal. For example, it is an immediate corollary of Theorem 2.5 below that, for N a prime power, the set $\mathscr{G}_I(N) = \{1\}$ is exhaustive and minimal. To identify a minimal exhaustive set for arbitrary N we generalise the notion of ‘simple’ rules. For a given rank 1 rule Q_{L}, the smallest positive integer component of any quadrature point must be a divisor of the order N. Clearly, the least such value must occur in a generator — for simple rules this value is 1, and more generally we shall call this value the *simplicity* of the rule.

Definition 2.2. Let $N > 1$ and let $\boldsymbol{g}/N$ generate the s-dimensional rule Q_{L} of order N, where $g_i \neq 0$ for $i = 1,\dots,s$. Define the *simplicity of* $\boldsymbol{g}$ *with respect to* N and the *simplicity of* Q_{L}, denoted respectively, by $\mathrm{simp}(\boldsymbol{g},N)$ and $\mathrm{simp}(Q_\mathrm{L})$, by

$$\mathrm{simp}(Q_\mathrm{L}) = \mathrm{simp}(\boldsymbol{g},N) = \min\{\gcd(g_i,N)\colon\ i=1,\dots,s\}.$$

It is shown in [10, Section 3.2] that $\mathrm{simp}(Q_\mathrm{L})$ is well defined, that is, it is independent of the choice of generator for a given rule. The values assumed by $\mathrm{simp}(Q_\mathrm{L})$, where Q_L ranges over the set of s-dimensional rank 1 rules of order N, are positive divisors of N. These values will be called the *simplicity residues* of N.

Definition 2.3. Let $N>1$. A point $\boldsymbol{g}\in\mathbb{Z}^s$ is said to be *ordered with respect to* N if $\boldsymbol{g}/N$ generates an s-dimensional rank 1 rule and

$$1\leqslant \mathrm{simp}(\boldsymbol{g},N) = \gcd(g_1,N) = g_1 \leqslant g_2 \leqslant \cdots \leqslant g_s \leqslant N/2.$$

A rule $Q_\mathrm{L}(\boldsymbol{g}/N)$ of order N is said to be *ordered* if it has a generator $\boldsymbol{g}/N$ such that $\boldsymbol{g}$ is ordered with respect to N.

Definition 2.4. Define a partial order relation on a set of s-dimensional ordered generators in which two vectors $\boldsymbol{g}_1/N_1$ and $\boldsymbol{g}_2/N_2$, where $\boldsymbol{g}_i=(g_{i,1},\dots,g_{i,s})$, are comparable if and only if $N_1=N_2=N$, say. For comparable vectors we shall say that $\boldsymbol{g}_1/N$ *precedes* $\boldsymbol{g}_2/N$, or is a *precedent* of $\boldsymbol{g}_2/N$ (denoted by $\boldsymbol{g}_1/N \prec \boldsymbol{g}_2/N$), if there is a $j\in\{1,\dots,s\}$ such that $g_{1,i}=g_{2,i}$ for $1\leqslant i<j$ and $g_{1,j}<g_{2,j}$. We shall say that $\boldsymbol{g}/N$ is *primary in its geometry class* if it has no precedents amongst the generators of rules in the geometry class of $Q_\mathrm{L}(\boldsymbol{g}/N)$.

In [10, Section 3.2] it was shown that every rank 1 rule is geometrically equivalent to an ordered rule with the same simplicity. From this it follows immediately that, for $N>1$, the simplicity residues of N form an exhaustive set. The next result identifies a minimal exhaustive set. The proof is straightforward and the interested reader is referred to Langtry [10]. We note that it may also be shown [10, Theorem 3.2.17] that we may further modify the procedure by restricting the other components of $\boldsymbol{g}$ to be multiples of the proper divisors of N which are greater than or equal to g_1.

Theorem 2.5 ([10, Theorem 3.2.18]). *Let $N>1$ and let k be the number of positive proper divisors of N. Define*

$$\mathscr{G}_I(N) = \{m_i\colon\ 1\leqslant i\leqslant k;\, m_i\,|\,N;\, m_{i+1}>m_i>0;\quad \exists \bar{m}>m_i \text{ such that } \bar{m}\,|\,N \text{ and } \gcd(m_i,\bar{m})=1)\},\tag{2.2}$$

that is, the ordered set of positive divisors of N such that, for each element of the set, there exists a larger divisor of N to which the element is relatively prime. Then $\mathscr{G}_I(N)$ is a minimal exhaustive set and is precisely the set of simplicity residues of N.

Example. For $N=56=2^3.7$ the divisors are 1, 2, 4, 7, 8, 14, 28 and the simplicity residues are 1, 2, 4, 7. For the 56-point three-dimensional rule $Q_\mathrm{L}(\boldsymbol{g}/N)$ with $\boldsymbol{g}=(20,35,14)$ we have $\gcd(20,56)=4$, $\gcd(35,56)=7$, $\gcd(14,56)=14$ and so $\mathrm{simp}(Q_\mathrm{L})=4$. In fact, $20\equiv 4\times 5 \pmod{56}$ and so Q_L is also generated by $5^{-1}\boldsymbol{g}/56$, where 5^{-1} denotes the multiplicative inverse of 5 modulo 56, that is, 45.

In particular, we have $45\boldsymbol{g} \equiv (4,7,14)\,(\mathrm{mod}\,56)$, which is ordered with respect to 56 and primary in its geometry class.

3. Preliminary eliminations in a full search of rank 1 rules

In her searches over rules of increasing order $N=2,3,\ldots$ for those which are best ρ with respect to the set of rank 1 simple rules in dimensions three and four, Maisonneuve [18] developed a technique for eliminating from the search, prior to the calculation of their ρ values, large numbers of rules which could be predicted to have values of ρ less than the highest value found up to that point in the search. Such rules clearly cannot be best ρ and, since the calculation of ρ is computationally intensive, this strategy significantly enhanced the efficiency of the search procedure. Lyness and Sørevik [15] have used this technique in their algorithm for determining rules that are best ρ with respect to the set of all rules in a given dimension.

This strategy can be extended in a straightforward way to searches over rank 1 rules of all simplicities in dimensions $s\geqslant 2$. For $N = 2,3,\ldots,$ and given $\rho_0 = \rho(L(\boldsymbol{g}'/N'))$ achieved for some $N' < N$, increment ρ_0 and eliminate $\boldsymbol{g}$ such that $\rho(L(\boldsymbol{g}/N)) < \rho_0$.

The elimination strategy we shall use consists of, for each value of g_1 and for $k = 2,\ldots,s$, successively identifying $(k-1)$-tuples of the form $(g_{i_2},\ldots,g_{i_k})$ such that a vector $\boldsymbol{g}$ containing such a sub-tuple must satisfy $\rho(L(\boldsymbol{g}/N)) < \rho_0$. Such sub-tuples we shall refer to as 'bad' for the given values of N and ρ_0. Clearly, any tuple $(g_{i_2},\ldots,g_{i_k})$ which contains a bad sub-tuple is itself bad, since if

$$g_1h_1 + g_{i_2}h_{i_2} + \cdots + g_{i_{k-1}}h_{i_{k-1}} = \lambda N \quad \text{and} \quad r(h_1,h_{i_2},\ldots,h_{i_{k-1}}) < \rho_0$$

then

$$g_1h_1 + g_{i_2}h_{i_2} + \cdots + g_{i_{k-1}}h_{i_{k-1}} + g_{i_k}0 = \lambda N \quad \text{and} \quad r(h_1,h_{i_2},\ldots,h_{i_{k-1}},0) < \rho_0.$$

It follows that a good tuple can contain no bad sub-tuples. In the remainder of this section we describe a procedure for constructing sets $\mathscr{G}_T(N,\rho_0,k)$ of good tuples.

Theorem 3.1. *Let N, s be integers greater than* 1 *and let ρ_0 be a positive integer. Then a set $\mathscr{G}_T(N,\rho_0,s)$ can be explicitly constructed such that*: (*a*) *$\rho(L(\boldsymbol{g}/N))\geqslant\rho_0$ for all $\boldsymbol{g}\in\mathscr{G}_T(N,\rho_0,s)$; and* (*b*) *for every s-dimensional rank* 1 *lattice rule Q_{L}' of order N such that $\rho(L')\geqslant\rho_0$, there exists a $\boldsymbol{g}\in\mathscr{G}_T(N,\rho_0,s)$ such that Q_{L}' is geometrically equivalent to the rule generated by $\boldsymbol{g}/N$.*

Proof. The proof is given in three parts.

(i) *Overall strategy*: Given N, by Theorem 2.5 we need consider only those $\boldsymbol{g}$ with values of g_1 contained in the set $\mathscr{G}_I(N)$ of simplicity residues defined in (2.2). By Definition 2.2 and [10, Theorem 3.2.17], for each value of g_1 we need consider only vectors $\boldsymbol{g}$ whose remaining components g_i are drawn from the set $\mathscr{G}_I(N,g_1) = \{km\colon m\,|\,N, g_1\leqslant m, km\leqslant N/2\}$. To construct $\mathscr{G}_T(N,\rho_0,s)$ we begin by constructing, for each g_1, a set of candidate pairs $\mathscr{G}_I(N,\rho_0,g_1) = \{g_1\}\times\mathscr{G}_I(N,g_1)$ and, by elimination from this set, a set $\mathscr{G}_T(N,\rho_0,g_1,2)\subseteq\mathscr{G}_I(N,\rho_0,g_1)$ of good pairs (g_1,g_{i_2}), that is, pairs with values of g_{i_2} such that $\rho(L((g_1,g_{i_2})/N))\geqslant\rho_0$. As we have noted, pairs with values of g_{i_2} such that $\rho(L((g_1,g_{i_2})/N)) < \rho_0$ are undesirable since if $\boldsymbol{g}$ contains such a pair then there is a nonzero

$\boldsymbol{h}=(h_1,0,\ldots,0,h_{i_2},0,\ldots,0)\in L^{\perp}(\boldsymbol{g}/N)$ such that $r(\boldsymbol{h})<\rho_0$, and thus $\rho(L(\boldsymbol{g}/N))<\rho_0$. For similar reasons, a good point $\boldsymbol{g}$ may contain no bad k-tuples for $k=2,\ldots,s$. An elimination strategy for the construction of $\mathscr{G}_T(N,\rho_0,g_1,2)$ is described in detail in (ii) below.

More generally, for $k=3,\ldots,s$, we construct by elimination successive sets $\mathscr{G}_T(N,\rho_0,g_1,k)$ of good ordered k-tuples, that is, tuples $(g_1,g_{i_2},\ldots,g_{i_k})$ such that $\rho(L((g_1,g_{i_2}\ldots,g_{i_k})/N))\geqslant\rho_0$. The construction proceeds as follows: since no good tuple may contain a bad sub-tuple we must have $(g_1,g_{i_2},\ldots,g_{i_{k-1}})$, a good $(k-1)$-tuple. Thus we may form, for each good $(k-1)$-tuple $(g_1,g_{i_2},\ldots,g_{i_{k-1}})$, a set

$$\mathscr{G}_I(N,\rho_0,g_1,g_{i_2},\ldots,g_{i_{k-1}})=\{(g_1,g_{i_2},\ldots,g_{i_{k-1}},g_{i_k}):\ g_{i_k}\in\mathscr{G}_I(N,g_1),g_{i_k}\geqslant g_{i_{k-1}}\}\tag{3.1}$$

of candidate k-tuples. From this set we eliminate all elements which have a bad $(k-1)$-tuple, yielding a reduced set $\hat{\mathscr{G}}_I(N,\rho_0,g_1,g_{i_2},\ldots,g_{i_{k-1}})$ of candidate k-tuples having no bad sub-tuples. This step requires the storage of all good (or alternatively, all bad) $(k-1)$-tuples, that is, the set $\mathscr{G}_T(N,\rho_0,g_1,k-1)$. Then we eliminate from the set $\hat{\mathscr{G}}_I(N,\rho_0,g_1,g_{i_2},\ldots,g_{i_{k-1}})$ all bad k-tuples, yielding a set $\hat{\mathscr{G}}_T(N,\rho_0,g_1,g_{i_2},\ldots,g_{i_{k-1}})$ of good k-tuples derived from $(g_1,g_{i_2},\ldots,g_{i_{k-1}})$. The elimination scheme itself is described in (iii) below. The set

$$\mathscr{G}_T(N,\rho_0,g_1,k)=\bigcup_{(g_1,g_{i_2},\ldots,g_{i_{k-1}})\in\mathscr{G}_T(N,\rho_o,g_1,k-1)}\hat{\mathscr{G}}_T(N,\rho_0,g_1,g_{i_2},\ldots,g_{i_{k-1}})$$

is then the set of good k-tuples. By induction it follows that $\mathscr{G}_T(N,\rho_0,g_1,s)$ is precisely the set of points $\boldsymbol{g}$, with first component g_1, that are ordered with respect to N and satisfy $\rho(L(\boldsymbol{g}/N))\geqslant\rho_0$. The required set is then given by

$$\mathscr{G}_T(N,\rho_0,s)=\bigcup_{g_1\in\mathscr{G}_I(N)}\mathscr{G}_T(N,\rho_0,g_1,s).$$

(ii) *Construction of* $\mathscr{G}_T(N,\rho_0,g_1,2)$: From the set

$$\mathscr{G}_I(N,\rho_0,g_1)=\{g_1\}\times\mathscr{G}_I(N,g_1)\tag{3.2}$$

we wish to eliminate 2-tuples (g_1,g_{i_2}) with values of g_{i_2} such that $\rho(L(\boldsymbol{g}/N))<\rho_0$, in particular, values for which there exist integers h_1,h_{i_2}, not both zero, and λ satisfying both

$$g_1h_1+g_{i_2}h_{i_2}=\lambda N\tag{3.3}$$

and

$$r(h_1,h_{i_2})=\bar{h}_1\bar{h}_{i_2}<\rho_0,\tag{3.4}$$

where $\bar{h}_i=\max(1,|h_i|)$.

Since $\boldsymbol{h}\in L^{\perp}$ if and only if $-\boldsymbol{h}\in L^{\perp}$ and $r(\boldsymbol{h})=r(-\boldsymbol{h})$, it follows that we may arbitrarily fix the sign of one component of $\boldsymbol{h}$. We shall require $h_{i_2}\geqslant 0$. In this case it is clear that if relations (3.3) and (3.4) are satisfied for a particular g_{i_2}, then $0<\bar{h}_{i_2}<\rho_0$ and hence

$$0\leqslant|h_1|<\frac{\rho_0}{\bar{h}_{i_2}}.\tag{3.5}$$

Combining (3.3) and (3.5) yields

$$|g_1h_1|=|\lambda N-g_{i_2}h_{i_2}|<\frac{g_1\rho_0}{\bar{h}_{i_2}}.\tag{3.6}$$

The values of g_{i_2} which satisfy both this bound and Eq. (3.3) for suitable λ and h_{i_2} are bad for the given g_1 and may be found by enumeration over h_{i_2} and λ. However, bounds on λ that are independent of g_{i_2} are required for the enumeration. Solving the inequality in (3.6) for λ we obtain

$$\frac{1}{N}\left(g_{i_2}h_{i_2} - \frac{g_1\rho_0}{\bar{h}_{i_2}}\right) < \lambda < \frac{1}{N}\left(g_{i_2}h_{i_2} + \frac{g_1\rho_0}{\bar{h}_{i_2}}\right).$$

Together with the observation that $g_{i_2} \in \mathscr{G}_I(N, g_1)$, this yields

$$\frac{1}{N}\left(h_{i_2}\min(\mathscr{G}_I(N,g_1)) - \frac{g_1\rho_0}{\bar{h}_{i_2}}\right) < \lambda < \frac{1}{N}\left(h_{i_2}\max(\mathscr{G}_I(N,g_1)) + \frac{g_1\rho_0}{\bar{h}_{i_2}}\right). \tag{3.7}$$

If the set $\mathscr{G}_I(N, g_1)$ is held in storage then the minimum and maximum values which appear in this relation are easily determined and (3.7) gives the bounds on λ required for the enumeration. For each value of h_{i_2} and λ, then, the values of g_{i_2} to be eliminated are those for which there exists an $h_1 \in \mathbb{Z}$ satisfying (3.3). Now, if $h_{i_2} = 0$ then (3.3) reduces to $g_1h_1 = \lambda N$, yielding no information about g_{i_2} and hence no eliminations from $\mathscr{G}_I(N, \rho_0, g_1)$. If on the other hand $h_{i_2} \neq 0$, let $d = \gcd(g_1, h_{i_2})$. Then there exists a value of h_1 which satisfies (3.3) if and only if $d|\lambda N$. In this case we observe from (3.3) that we can find $x_0 \in \{0,\dots,h_{i_2}-1\}$ such that $g_1x_0 \equiv \lambda N \pmod{h_{i_2}}$. Let $y_0 = (\lambda N - g_1x_0)/h_{i_2}$, then values of h_1 and g_{i_2} which satisfy (3.3) are of the form

$$h_1 = x_0 + \frac{h_{i_2}}{d}t, \qquad g_{i_2} = y_0 - \frac{g_1}{d}t$$

for $t \in \mathbb{Z}$. Enumerating over those values of t such that $|h_1| < \rho_0/\bar{h}_{i_2}$, that is, since $h_{i_2} > 0$,

$$-\frac{d}{h_{i_2}}\left(x_0 + \frac{\rho_0}{h_{i_2}}\right) < t < \frac{d}{h_{i_2}}\left(-x_0 + \frac{\rho_0}{h_{i_2}}\right),$$

now yields precisely the pairs (g_1, g_{i_2}) to be eliminated from $\mathscr{G}_I(N, \rho_0, g_1)$ in order to obtain $\mathscr{G}_T(N, \rho_0, g_1, 2)$.

(iii) *The general case. Construction of* $\hat{\mathscr{G}}_T(N, \rho_0, g_1, g_{i_2}, \dots, g_{i_{k-1}})$, for $k \geqslant 3$. Given $\mathscr{G}_I(N, \rho_0, g_1, g_{i_2}, \dots, g_{i_{k-1}})$ as defined in (3.1), with $g_1, g_{i_2}, \dots, g_{i_{k-1}}$ known, we first eliminate k-tuples containing known bad $(k-1)$-tuples to obtain the set $\hat{\mathscr{G}}_I(N, \rho_0, g_1, g_{i_2}, \dots, g_{i_{k-1}})$. We then seek to eliminate k-tuples $(g_1, g_{i_2}, \dots, g_{i_k})$ such that there exist integers $\lambda, h_1, h_{i_2}, \dots, h_{i_k}$, all nonzero except possibly for λ and h_1, satisfying both

$$g_1h_1 + g_{i_2}h_{i_2} + \cdots + g_{i_k}h_{i_k} = \lambda N \tag{3.8}$$

and

$$\bar{h}_1\bar{h}_{i_2}\cdots\bar{h}_{i_k} < \rho_0. \tag{3.9}$$

The assumption that h_{i_j} is nonzero, for $j \in \{2,\dots,k\}$, is justified by the observation that tuples which would be eliminated were this was not the case would already have been eliminated during an iteration with a smaller value of k (in the case that this value is 2, by using the procedure described in (ii) above). The value of h_1 may, however, be zero. Again we may arbitrarily fix the sign of one component of $\boldsymbol{h}$, and in particular, we shall require that $h_{i_k} > 0$. From (3.8) we have

$$|g_1h_1| = |\lambda N - (g_{i_2}h_{i_2} + \cdots + g_{i_k}h_{i_k})| \tag{3.10}$$

and from (3.9) it follows that we may require

$$\begin{aligned} 0 &< \quad h_{i_k} \quad < \rho_0, \\ 0 &< |h_{i_{k-1}}| < \frac{\rho_0}{h_{i_k}}, \\ &\quad\vdots \\ 0 &< \quad |h_{i_2}| \quad < \frac{\rho_0}{|h_{i_3}\cdots h_{i_k}|} \\ &\quad |h_1| \quad < \frac{\rho_0}{|h_{i_2}\cdots h_{i_k}|}. \end{aligned} \tag{3.11}$$

Combining (3.10) and the final inequality of (3.11) yields

$$|g_1h_1| = |\lambda N - (g_{i_2}h_{i_2} + \cdots + g_{i_k}h_{i_k})| < \frac{g_1\rho_0}{|h_{i_2}\cdots h_{i_k}|}. \tag{3.12}$$

In a similar fashion to the derivation of (3.7) we then obtain the following bounds on λ:

$$\begin{aligned} &\frac{1}{N}\left(g_{i_2}h_{i_2} + \cdots + g_{\min_k}h_{i_k} - \frac{g_1\rho_0}{|h_{i_2}\cdots h_{i_k}|}\right) < \lambda \\ &\quad < \frac{1}{N}\left(g_{i_2}h_{i_2} + \cdots + g_{\max_k}h_{i_k} + \frac{g_1\rho_0}{|h_{i_2}\ldots h_{i_k}|}\right), \end{aligned} \tag{3.13}$$

where $g_{\min_k}$ and $g_{\max_k}$ are, respectively, the minimum and maximum of the set

$$\{g_{i_k}\colon (g_1, g_{i_2}, \ldots, g_{i_k}) \in \mathscr{G}_I(N, \rho_0, g_1, g_{i_2}, \ldots, g_{i_{k-1}})\}.$$

Enumeration over values of $h_{i_2}, \ldots, h_{i_k}$ and λ satisfying (3.11) and (3.13) respectively yields the tuples to be eliminated from $\hat{\mathscr{G}}_I(N, \rho_0, g_1, g_{i_2}, \ldots, g_{i_{k-1}})$. These are the tuples for which, for given $h_{i_2}, \ldots, h_{i_k}$ and λ, there exists $h_1 \in \mathbb{Z}$ satisfying (3.8). Let

$$g_1h_1 + g_{i_k}h_{i_k} = \lambda N - g_{i_2}h_{i_2} - \cdots - g_{i_{k-1}}h_{i_{k-1}} = M, \tag{3.14}$$

say, and let $d = \gcd(g_1, h_{i_k})$. Then $d > 0$ and as in (ii) above, provided that $d \mid M$, we may find $x_0 \in \{0, \ldots, h_{i_k} - 1\}$ such that $g_1x_0 \equiv M \pmod{h_{i_k}}$. Let $y_0 = (M - g_1x_0)/h_{i_k}$. The solutions h_1 and g_{i_k} to (3.14) yield the tuples $(g_1, g_{i_2}, \ldots, g_{i_k})$ to be eliminated from $\hat{\mathscr{G}}_I(N, \rho_0, g_1, g_{i_2}, \ldots, g_{ik-1})$. These solutions are of the form

$$h_1 = x_0 + \frac{h_{i_k}}{d}t, \qquad g_{i_k} = y_0 - \frac{g_1}{d}t,$$

where $t \in \mathbb{Z}$. Enumeration over the values of t such that $|h_1| < \rho_0/|h_{i_2}\cdots h_{i_k}|$, that is, since $d, h_{i_k} > 0$,

$$-\frac{d}{h_{i_k}}\left(x_0 + \frac{\rho_0}{|h_{i_2}\cdots h_{i_k}|}\right) < t < \frac{d}{h_{i_k}}\left(-x_0 + \frac{\rho_0}{|h_{i_2}\cdots h_{i_k}|}\right),$$

gives precisely the tuples to be eliminated from $\hat{\mathscr{G}}_I(N, \rho_0, g_1, g_{i_2}, \ldots, g_{i_{k-1}})$ to yield $\hat{\mathscr{G}}_T(N, \rho_0, g_1, \ldots, g_{i_{k-1}})$.

As a final remark on the elimination scheme we note that, at the conclusion of the preliminary eliminations, any vector $\boldsymbol{g}$ such that $\gcd(g_1, \ldots, g_s, N) > 1$ should be eliminated since the corresponding rules are clearly of order $N/\gcd(g_1, \ldots, g_s, N) < N$. □

In practice, during a search ρ_0 usually exceeds by 1 the highest value of ρ achieved for a lower value of N. If, for a given N, the set $\mathscr{G}_T(N,\rho_0,s)$ is empty then we may immediately increment N and repeat the search procedure with the current value of ρ_0. Otherwise, the set contains at least one vector which is best ρ with respect to the search set. In practice, the set is usually empty, or contains only a small number of elements, in which case the best ρ elements may be identified by direct evaluation of ρ as described, for example, in [18]. The values of N and ρ_0 are then updated and the search procedure repeated with the new value of ρ_0.

4. Searches for 2^s copies of rank 1 rules

In a number of previous searches the class of rules to be considered has been restricted in various ways, thereby allowing higher orders of rules to be reached in the search. These searches include those of Korobov-type rank 1 rules reported by Maisonneuve [18], the sample rank 1 and rank 2 searches of Sloan and Walsh [25], the sample searches of 2^s copies of rank 1 simple rules reported by Disney and Sloan [4], and of intermediate rank rules reported by Joe and Disney [7], and the searches of rules formed by component scaling reported by Lyness and Sørevik [17]. A comparison of the numerical results obtained in these searches suggests that certain sets of higher rank rules contain rules which are at least competitive with the best known rank 1 rules of similar orders (see, for example, the tables of best ρ rules in [15,16] and the comparison of the results of Sloan and Walsh [25] with those of Disney and Sloan presented in [4]). This suggestion is in fact due to Disney and Sloan [4], and is in accord with the theoretical results concerning copy rules and intermediate rank rules presented in [4,7]. These authors point out that, in practice, information about certain higher rank rules of relatively large orders can be ascertained more efficiently by examining related rank 1 rules of smaller orders, and in particular that searches of sets of these higher rank rules can be carried out by searching for rank 1 rules of relatively low order that perform well with respect to slightly modified figures of merit. Disney and Sloan [4] note that if a rule Q has lattice L then $Q^{(n)}$ — that is, the n^s copy of Q — has lattice $(1/n)L$ and dual lattice $nL^{\perp}$. Hence they show that

$$P_\alpha(Q^{(n)}) = P_{\alpha,n}(Q) = Q(f_{\alpha,n}) - 1,$$

where

$$f_{\alpha,n}(\boldsymbol{x}) = \sum_{\boldsymbol{h}\in\mathbb{Z}^s} \frac{1}{r(n\boldsymbol{h})^\alpha} \mathrm{e}^{\mathrm{i}2\pi\boldsymbol{h}\cdot\boldsymbol{x}}.$$

They point out that, for α an even positive integer, an explicit expression can be obtained for the function $f_{\alpha,n}$ in terms of the Bernoulli polynomials. In fact, these expressions are given by Joe and Sloan [8, Eqs. (5.6)–(5.8)] and the recurrence relation for the Bernoulli polynomials $B_n(x)$, $n = 1,2,\ldots$, is given in [28, p. 60, 6, Lemma 6.6]. Maisonneuve [18, p. 124] gives explicit expressions for B_2 and B_4.

In later work Disney [3] has extended the work of Maisonneuve [18] and Lyness and Sorevik [15] to produce an efficient search algorithm for rules that are best ρ with respect to the set of 2^s copies of rank 1 simple rules. The 2^s copy $Q^{(2)}$ of a rank 1 rule with generator $\boldsymbol{g}/\tilde{N}$ has $N = 2^s\tilde{N}$

points and is given by

$$\frac{1}{2^s\tilde{N}}\sum_{j_1=0}^{1}\cdots\sum_{j_s=0}^{1}\sum_{i=0}^{\tilde{N}-1} f\left(\left\{\frac{i}{2\tilde{N}}\boldsymbol{g}+\frac{(j_1,\ldots,j_s)}{2}\right\}\right).$$

The search procedure in [3] also relies on the preliminary elimination, from a set of candidate generators $\boldsymbol{g}/\tilde{N}$ of rank 1 rules, of those generators for which there exists an $\boldsymbol{h}\in L^{\perp}(\boldsymbol{g}/\tilde{N})$ and an integer λ such that, for some $k\leqslant s$,

(i) $h_{i_2},\ldots,h_{i_k}$ are non zero,

(ii) $2h_1+g_{i_2}2h_{i_2}+\cdots+g_{i_k}2h_{i_k}=\lambda 2^s\tilde{N}$, and

(iii) $2\bar{h}_1\cdots 2\bar{h}_{i_k}<\rho_0$, where ρ_0 is the current target value for ρ.

Clearly, the method of preliminary eliminations for exhaustive rank 1 searches described in Section 3, which is based directly on the method of Maisonneuve [18], may be similarly extended to searches for best ρ 2^s copies of rank 1 rules of all simplicities.

Theorem 4.1. *Let $n>1$ and $Q_{\mathrm{L}_L}^{(n)}$ and $Q_{\mathrm{L}_2}^{(n)}$ be the n^s copies of Q_{L_L} and Q_{L_2}, respectively. Then Q_{L_L} is geometrically equivalent to Q_{L_2} if and only if $Q_{\mathrm{L}_L}^{(n)}$ is geometrically equivalent to $Q_{\mathrm{L}_2}^{(n)}$.*

Proof. Assume that $Q_{\mathrm{L}_L}\overset{g}{\sim}Q_{\mathrm{L}_2}$. Then clearly these rules are of equal order say $\tilde{N}$, and there exists a finite composition $\mathscr{T}=\mathscr{T}_t\circ\cdots\circ\mathscr{T}_1$ of operations, of the forms $\mathscr{U}_i,\mathscr{V}_{ij}$ described in Definition 1.1, such that $L_2=\mathscr{T}(L_1)$. Let $L_1^{(n)}$ and $L_2^{(n)}$ be the integration lattices corresponding to $Q_{\mathrm{L}_L}^{(n)}$ and $Q_{\mathrm{L}_2}^{(n)}$, respectively. Clearly, if $L_3=\mathscr{U}_i(L_1)$ then

$$L_3^{(n)}=n^{-1}L_3=n^{-1}\mathscr{U}_i(L_1)=\mathscr{U}_i(n^{-1}L_1)=\mathscr{U}_i(L_1^{(n)}).$$

Similarly, if $L_3=\mathscr{V}_{ij}(L_1)$ then $L_3^{(n)}=\mathscr{V}_{ij}(L_1^{(n)})$ and it follows that $L_2^{(n)}$ is geometrically equivalent to $L_1^{(n)}$. The converse is established by a similar argument. □

Together with [10, Theorem 3.2.17] and the observation that every geometry class of rank 1 rules of order $\tilde{N}>1$ has a unique primary ordered rule, Theorem 4.1 yields the following corollaries.

Corollary 4.2. *The n^s copy of a rank 1 rule of order $\tilde{N}>1$ is geometrically equivalent to the n^s copy of a unique primary ordered rank 1 rule.*

Corollary 4.3. *The n^s copy of a rank 1 rule of order $\tilde{N}>1$ is geometrically equivalent to the n^s copy of a rank 1 ordered rule with generator $\boldsymbol{g}/\tilde{N}$ such that $\boldsymbol{g}$ is ordered with respect to $\tilde{N}$, and the components of $\boldsymbol{g}$ are multiples of proper divisors of $\tilde{N}$ and satisfy* $\mathrm{simp}(\boldsymbol{g},\tilde{N})\leqslant g_j\leqslant\tilde{N}/2$.

The next result now justifies the adaptation of the construction of Theorem 3.1 to searches over n^s-copies of rank 1 rules.

Theorem 4.4. *Let $\tilde{N}$, n, s be integers greater than 1 and let ρ_0 be a positive integer. Denote by $L^{(n)}$ the integration lattice corresponding to the n^s copy of the rank 1 lattice rule with integration lattice L. Then a set $\mathscr{G}_T^{(n)}(\tilde{N},\rho_0,s)$ can be explicitly constructed such that:* (a) $\rho(L^{(n)}(\boldsymbol{g}/\tilde{N}))\geqslant\rho_0$ *for* *all* $\boldsymbol{g} \in \mathscr{G}_T^{(n)}(\tilde{N}, \rho_0, s)$; *and* (b) *if* $Q_{\mathrm{L}}^{\prime(n)}$ *is the* n^s *copy of an* s-*dimensional rank* 1 *lattice rule* $Q_{\mathrm{L}}^{\prime}$ *of order* $\tilde{N}$ *such that* $\rho(L^{\prime(n)}) \geqslant \rho_0$, *then there exists a* $\boldsymbol{g} \in \mathscr{G}_T^{(n)}(\tilde{N}, \rho_0, s)$ *such that* $Q_{\mathrm{L}}^{\prime(n)}$ *is geometrically equivalent to the* n^s *copy of the rank* 1 *rule generated by* $\boldsymbol{g}/\tilde{N}$.

Proof. By Theorem 4.1, n^s copies of rank 1 rules are geometrically equivalent if and only if the uncopied rank 1 rules are geometrically equivalent. Also,

$$\rho(L^{(n)}(\boldsymbol{g}/\tilde{N})) = \rho_n(L(\boldsymbol{g}/\tilde{N})) = \min\left\{\prod_{j=1}^{s} \max\{1, |nh_j|\}: \boldsymbol{h} \in L^{\perp} - \{\mathbf{0}\}\right\}$$

and so $\mathscr{G}_T^{(n)}(\tilde{N}, \rho_0, s)$ can be constructed by the elimination procedure used in the proof of Theorem 3.1, with the exception that we use ρ_n as our figure of merit for the rank 1 rules in place of ρ, and

$$\begin{aligned}
0 < \quad h_{i_k} \quad &< \frac{\rho_0}{n},\\
0 < |h_{i_{k-1}}| &< \frac{\rho_0}{n^2 h_{i_k}},\\
&\vdots\\
0 < \quad |h_{i_2}| \quad &< \frac{\rho_0}{n^{k-1}|h_{i_3}\cdots h_{i_k}|}\\
|h_1| \quad &< \frac{\rho_0}{n^k|h_{i_2}\cdots h_{i_k}|}
\end{aligned}$$

as the bounds on $h_1, h_{i_2}, \ldots, h_{i_k}$ during the enumeration, where now ρ_0 is the current target value of ρ_n. □

5. Numerical results for rank 1 rules

Preliminary searches were conducted for rank 1 simple rules in dimensions 3–5 terminating at $N = 6066$, 3298 and 1000, respectively. The full results of these searches are presented in the tables of Langtry [10]. All searches were conducted on a Silicon Graphics Datastation 4D/25 workstation running the Unix System V.3 operating system.

Comparing the results with those obtained by previous authors, we note that the omission reported in [2] of the three-dimensional rule $Q_{\mathrm{L}}((1,293,517)/1199)$ from Table 9 of Maisonneuve [18] is not significant, since this rule is geometrically equivalent to $Q_{\mathrm{L}}((1,121,311)/1199)$, which does appear in the table. In $\mathbb{R}^5$ we note that there are two omissions from Table 2 of Bourdeau and Pitre [2] — in particular, there is a second ordered rule $Q_{\mathrm{L}}((1,36,79,84,94)/275)$ of order 275, with ρ value equal to that of the rule reported in [2], and with better P_2 and P_4 values (3.53 and 4.63×10^{-2}, respectively); also, the rule $Q_{\mathrm{L}_L} = Q_{\mathrm{L}}((1,154,170,230,256)/772)$ listed in this table is not, in fact, best ρ, since $\rho(Q_{\mathrm{L}_L}) = 10$ whereas our search produced a rule of lower order ($N = 770$) and the same ρ value and with $P_2 = 8.71 \times 10^{-1}$ and $P_4 = 2.78 \times 10^{-3}$, namely $Q_{\mathrm{L}}((1,72,96,112,332)/770)$. Our search also produced a best ρ five-dimensional rule $Q_{\mathrm{L}}((1,38,194,276,338)/862)$, with $\rho = 12$, $P_2 = 0.76$ and $P_4 = 2.07 \times 10^{-3}$, that has not been previously reported, to the best of our knowledge.

Table 1
Best $\rho\ 2^3$ copies of rank 1 rules over all simplicities

$\tilde{N}$	$N = 2^s\tilde{N}$	ρ	z_s	P_2	P_4	**g**
2	16	4	6.93e−01	2.13e+00	7.43e−02	1 1 1
7	56	8	5.75e−01	3.87e−01	2.68e−03	1 2 3
14	112	12	5.06e−01	1.46e−01	4.46e−04	1 3 5
18	144	16	5.52e−01	9.59e−02	1.58e−04	1 5 7
29	232	20	4.70e−01	4.82e−02	4.61e−05	1 5 13
32	256	24	5.20e−01	4.26e−02	3.60e−05	1 6 9
38	304	28	5.27e−01	3.22e−02	1.93e−05	1 7 11
48	384	32	4.96e−01	2.24e−02	8.44e−06	1 9 14
				2.28e−02	9.69e−06	1 17 21
51	408	36	5.30e−01	1.90e−02	5.63e−06	1 11 16
57	456	40	5.37e−01	1.63e−02	4.54e−06	1 10 25
61	488	48	6.09e−01	1.40e−02	2.68e−06	1 13 19
84	672	56	5.43e−01	9.09e−03	1.29e−06	1 15 26
93	744	60	5.33e−01	7.89e−03	1.03e−06	1 15 25
105	840	64	5.13e−01	6.07e−03	5.86e−07	1 16 38
107	856	72	5.68e−01	5.60e−03	4.26e−07	1 19 47
128	1024	76	5.14e−01	5.06e−03	3.64e−07	1 22 34
134	1072	92	5.99e−01	3.83e−03	1.83e−07	1 23 59
154	1232	96	5.55e−01	3.14e−03	1.35e−07	1 25 69
155	1240	112	6.43e−01	2.93e−03	9.30e−08	1 36 56
181	1448	120	6.03e−01	2.40e−03	7.22e−08	1 31 48
196	1568	144	6.76e−01	2.01e−03	4.53e−08	1 37 57
209	1672	160	7.10e−01	1.81e−03	3.49e−08	1 45 65
287	2296	180	6.07e−01	1.14e−03	1.79e−08	1 45 127
302	2416	200	6.45e−01	9.44e−04	8.49e−09	1 65 94
364	2912	220	6.03e−1	7.95e−04	8.96e−09	1 75 165
392	3136	260	6.67e−01	7.09e−04	4.74e−09	1 74 114
476	3808	264	5.72e−01	4.96e−04	3.20e−09	1 90 125
477	3816	272	5.88e−01	4.90e−04	2.92e−09	1 105 139
494	3952	288	6.04e−01	4.34e−04	2.15e−09	1 88 151
				4.34e−04	2.04e−09	1 107 154
508	4064	304	6.22e−01	4.37e−04	2.39e−09	1 147 235
537	4296	320	6.23e−01	3.82e−04	1.50e−09	1 99 164
566	4528	344	6.40e−01	3.56e−04	1.40e−09	1 109 158
624	4992	352	6.00e−01	3.39e−04	1.22e−09	1 94 166
638	5104	360	6.02e−01	2.89e−04	9.55e−10	1 96 167
645	5160	384	6.36e−01	2.65e−04	6.88e−10	1 119 197
				2.77e−04	8.21e−10	1 148 226
739	5912	400	5.88e−01	2.15e−04	4.84e−10	1 126 196
763	6104	424	6.05e−01	2.04e−04	4.37e−10	1 144 222
776	6208	432	6.08e−01	2.00e−04	4.27e−10	1 201 306
795	6360	440	6.06e−01	1.98e−04	4.20e−10	1 169 366
811	6488	468	6.33e−01	1.92e−04	4.07e−10	1 140 215
862	6896	472	6.05e−01	1.77e−04	3.59e−10	1 165 224
874	6992	480	6.08e−01	1.68e−04	3.22e−10	1 229 338
887	7096	488	6.10e−01	1.64e−04	3.03e−10	1 134 195
906	7248	512	6.28e−01	1.52e−04	2.16e−10	1 208 381

Table 1 (Contd.)

932	7456	560	6.70e−01	1.47e−04	2.17e−10	1 193 431
943	7544	572	6.77e−01	1.38e−04	1.70e−10	1 168 291
1102	8816	576	5.94e−01	1.15e−04	1.39e−10	1 161 265
1126	9008	600	6.07e−01	1.15e−04	1.53e−10	1 164 255
1175	9400	640	6.23e−01	9.70e−05	9.14e−11	1 209 304
1220	9760	864	8.13e−01	8.08e−05	4.36e−11	1 319 501
1703	13 624	880	6.15e−01	5.11e−05	2.49e−11	1 328 474
1735	13 880	896	6.16e−01	5.23e−05	2.81e−11	1 262 381
1742	13 936	920	6.30e−01	5.12e−05	2.66e−11	1 241 412
1758	14 064	936	6.36e−01	5.06e−05	2.59e−11	1 238 539
1793	14 344	944	6.30e−01	4.90e−05	2.54e−11	1 274 463
1840	14 720	952	6.21e−01	4.73e−05	2.30e−11	1 439 578
1855	14 840	984	6.37e−01	4.73e−05	2.30e−11	1 246 836
1879	15 032	1008	6.45e−01	4.33e−05	1.85e−11	1 400 589
1935	15 480	1056	6.58e−01	4.07e−05	1.51e−11	1 268 458

The results of rank 1 searches including non-simple rules in dimensions 3–5 are presented in [10, Appendix B]. These searches were terminated at $N = 4358$, 1169 and 587, respectively, and the results establish that there are nonsimple rank 1 rules which are better with respect to ρ than some of the best ρ rank 1 simple rules listed in [18,9,2]. Those nonsimple rank 1 rules of order exceeding 3916 in $\mathbb{R}^3$ are in fact better with respect to ρ, P_2 and P_4 than any previously published rules of similar orders, although the results of Disney and Sloan [4] and Lyness and Sørevik [17] suggest that higher rank rules may exist that have similar orders and better ρ values. We note, however, that the computational cost of the search procedure is higher in the full rank 1 case than in the case of rank 1 simple rules.

6. Numerical results for 2^s copies of rank 1 rules

Of greater significance is the possibility of conducting efficient searches for n^s copy rules of high order, based on the elimination strategy suggested in the proofs of Theorems 3.1 and 4.4. The results of searches of this type in dimensions three to five for best ρ 2^s copies, with orders up to 16 000, of rank 1 rules are presented in Tables 1–3. These searches reach rules of this order at a fraction of the cost of searches for best ρ rank 1 rules of the same order. Tables extending these results to larger orders and dimensions are available over the Internet in [13].

Comparison of these results with those obtained for rank 1 rules suggests that the best copy rules are generally at least comparable with the best rank 1 rules of similar orders, and often (but not always) better, at least with respect to the criterion ρ. The parameter $z_s = \rho N^{-1}(\log N)^{s-2}$ gives an indication of how ‘good’ a particular value of ρ is, relative to the order N of the rule — the higher the value of z_s, the better the rule is with respect to ρ. One may also compare, for dimensions three to five, the orders and P_2 values for the best 2^s copy rules found in Tables 3 and 4 of Disney and Sloan [4] with the orders and P_2 values for the rules of nearest order in Tables 1–3. The results

Table 2
Best ρ 2^4 copies of rank 1 rules over all simplicities

$\tilde{N}$	$N = 2^s\tilde{N}$	ρ	z_s	P_2	P_4	$\boldsymbol{g}$
2	32	4	1.50e+00	4.58e+00	1.33e−01	1 1 1 1
9	144	6	1.03e+00	7.59e−01	5.52e−03	1 2 3 4
10	160	8	1.29e+00	6.78e−01	4.21e−03	1 2 3 4
16	256	12	1.44e+00	3.41e−01	8.64e−04	1 3 5 7
24	384	16	1.48e+00	2.00e−01	3.35e−04	1 5 7 11
48	768	24	1.38e+00	7.90e−02	4.93e−05	1 7 10 22
58	928	32	1.61e+00	5.76e−02	2.17e−05	1 17 22 26
101	1616	36	1.22e+00	2.80e−02	7.49e−06	1 9 14 40
103	1648	40	1.33e+00	2.71e−02	6.71e−06	1 11 25 30
112	1792	48	1.50e+00	2.40e−02	5.14e−06	1 13 19 29
				2.30e−02	4.46e−06	1 13 23 41
				2.29e−02	3.68e−06	1 34 41 50
135	2160	56	1.53e+00	1.67e−02	1.75e−06	1 16 28 37
145	2320	64	1.66e+00	1.56e−02	1.68e−06	1 17 28 41
193	3088	80	1.67e+00	9.89e−03	6.23e−07	1 21 36 81
237	3792	88	1.58e+00	7.24e−03	3.43e−07	1 29 41 107
243	3888	96	1.69e+00	7.53e−03	3.98e−07	1 24 68 101
318	5088	108	1.55e+00	4.71e−03	1.38e−07	1 35 55 135
336	5376	112	1.54e+00	4.59e−03	1.32e−07	1 41 93 117
353	5648	120	1.59e+00	4.08e−03	1.15e−07	1 34 131 146
369	5904	128	1.63e+00	3.79e−03	8.22e−08	1 39 88 150
432	6912	144	1.63e+00	2.96e−03	5.23e−08	1 49 131 158
449	7184	160	1.76e+00	2.75e−03	4.35e−08	1 67 92 122
525	8400	184	1.79e+00	2.14e−03	2.56e−08	1 118 218 251
549	8784	188	1.76e+00	2.11e−03	2.73e−08	1 47 74 245
562	8992	212	1.95e+00	1.85e−03	1.58e−08	1 53 89 221
709	11 344	216	1.66e+00	1.32e−03	9.90e−09	1 69 96 243
730	11 680	224	1.68e+00	1.32e−03	1.02e−08	1 67 98 345
775	12 400	256	1.83e+00	1.14e−03	6.32e−09	1 89 249 314
952	15 232	336	2.05e+00	8.06e−04	2.99e−09	1 117 257 307

of Disney and Sloan [4] were found by searches over small samples of 2^s copy rules with orders in three 'windows' (approximately 10^3, 10^4 and 10^5 points) for those with good P_2 (rather than ρ) values. Nevertheless, the performances of the two groups of rules are roughly comparable: the P_2 values of the rules from Disney and Sloan [4] are lower in three out of six cases than those from Tables 1–3, equal (in the first two digits) in one case, and higher in two cases, although their orders are higher in five out of six cases.

Lyness and Sørevik [15–17] report good rules of intermediate rank as well as of ranks 1 and s. In dimensions exceeding 3, these rules are predominantly of rank higher than 1. It is important to distinguish between the results reported in [15,16] and those reported in [17]. The former are obtained by searching for best ρ rules over the complete population of lattice rules in a given dimension up to a certain order: in [15] the search is in dimension three over orders up to 3916, and in [16] it is in dimension four over orders up to 562. It is clear that better lattice rules (with

Table 3
Best ρ 2^5 copies of rank 1 rules over all simplicities

$\tilde{N}$	$N = 2^s\tilde{N}$	ρ	z_s	P_2	P_4	$\boldsymbol{g}$
2	64	4	4.50e+00	9.09e+00	2.09e−01	1 1 1 1 1
11	352	8	4.58e+00	1.31e+00	6.52e−03	1 2 3 4 5
22	704	12	4.80e+00	5.68e−01	1.24e−03	1 3 5 7 9
25	800	16	5.97e+00	4.75e−01	7.64e−04	1 4 6 9 11
71	2272	20	4.06e+00	1.39e−01	1.16e−04	1 5 14 17 25
78	2496	24	4.60e+00	1.15e−01	5.77e−05	1 7 10 25 37
85	2720	28	5.09e+00	1.01e−01	4.03e−05	1 7 16 27 40
90	2880	32	5.62e+00	9.38e−02	3.05e−05	2 5 21 38 39
153	4896	34	4.26e+00	5.00e−02	1.15e−05	1 9 14 39 59
160	5120	40	4.87e+00	4.58e−02	8.45e−06	1 11 18 42 56
164	5248	48	5.75e+00	4.32e−02	7.93e−06	1 23 31 37 57
244	7808	56	5.16e+00	2.45e−02	2.51e−06	1 19 26 91 106
252	8064	64	5.78e+00	2.51e−02	2.49e−06	1 16 53 62 88
376	12 032	80	5.51e+00	1.39e−02	7.57e−07	1 21 49 80 155
427	13 664	96	6.07e+00	1.11e−02	4.25e−07	1 37 66 117 172

respect to ρ) than those in these papers cannot be found in these sets. In [17] the results presented are mostly constructed by the process of component scaling described in that paper, and are not necessarily optimal with respect to ρ. We compare firstly the rules presented in [15,16] with those in Tables 1 and 2 that are of the same dimension and of comparable order.

The table in [15] lists 68 rules for 59 distinct orders in the range $16 < N < 3916$, of which 28 are rank 1 rules that appear in earlier publications [18,9]. Table 1 lists 29 maximal rank rules of 28 distinct orders in this range, of which six are equivalent (in the sense of having the same orders and ρ values) to rules which appear in the table of Lyness and Sørevik [15]. In dimension four, Table 2 of Lyness and Sørevik [16] lists 23 best ρ rules of 11 distinct orders in the range $32 < N < 562$, of which three are rank 1 rules that appear in [18]. Table 2 lists five maximal rank rules of distinct orders in this range, of which four are equivalent to rules which appear in [16].

Best ρ results over all ranks are not available for orders exceeding 3916 in dimension three, 562 in dimension four and 2 in dimensions five and above. Consequently, it is possible that searches over restricted classes of rules may give useful results. In particular, the tables of Lyness and Sørevik [17] (particularly Tables 1, 2 and 8) provide many good rules in these ranges — mostly of rank greater than 1. The first two of these tables contain the best rules reported in that paper for dimensions three and four, respectively. Table 8 of Lyness and Sørevik [17] contains the only five-dimensional rules reported in that paper. Rules equivalent to some of those listed in [17] also appear in Tables 1–3. In dimension three, Table 1 contains three rules in the range $3917 < N < 16\,000$ that are equivalent to rules listed in Tables 1 and 5 of Lyness and Sørevik [17]. In dimension four, Table 2 contains three rules in the range $563 < N < 16\,000$) that are equivalent to rules appearing in Tables 2, 6 and 7 of Lyness and Sørevik [17]. In dimension five, Table 8 of Lyness and Sørevik [17] lists 34 rules of 25 distinct orders, of which 8 are rank 1 rules that appear also in [2] and one is of maximal rank and appears also in Table 3.

7. Concluding remarks

As an alternative to using searches to discover good rules, there have been a number of constructions of sequences of rules which are good with respect to some figure of merit, typically z_s or P_α (for example, [1,6,11,26,27,29]. In high dimensions these figures of merit may be preferable to ρ since lists of best ρ rules tend to become increasingly sparse as the dimension increases. The constructions of particular rules of which the author is aware are mostly of rules of rank 1 [1,6,11,27,29] and ranks 2, $s-1$ and s [26]. At least for dimensions exceeding three, these yield rules that do not appear to be competitive (with respect to P_α) with the best higher rank rules discovered by the techniques of Disney and Sloan [4], Joe and Disney [7] and Lyness and Sørevik [17]. Nevertheless, an understanding of the characteristics that are likely to be shared by good rank 1 constructions are of interest, and have been applied in [12] to the construction of good higher rank rules that appear to be comparable with those in the latter works.

The results of this paper demonstrate that good 2^s copies of rank 1 rules may be found by adapting search techniques used in the rank 1 case for $s \geqslant 3$. Related work by Disney [3] considers searches for 2^s copies of rank 1 simple rules in the context of dual lattices, and greatly extends the numerical results presented in this paper.

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References

[1] N.S. Bakhvalov, Approximate computation of multiple integrals, Vestnik Moskov. Univ. Ser. Mat. Meh. Astr. Fiz. Him. 4, (1959) 3–18 (in Russian).
[2] M. Bourdeau, A. Pitre, Tables of good lattices in four and five dimensions, Numer. Math. 47 (1985) 39–43.
[3] S.A.R. Disney, Good lattice integration rules of copy type, Pure Mathematics Preprint, University of New South Wales, Sydney, 1995.
[4] S.A.R. Disney, I.H. Sloan, Lattice integration rules of maximal rank formed by copying rank 1 rules, SIAM J. Numer. Anal. 29 (1992) 566–577.
[5] S. Haber, Parameters for integrating periodic functions of several variables, Math. Comput. 41 (1983) 115–129.
[6] L.K. Hua, Y. Wang, Applications of Number Theory to Numerical Analysis, Springer, and Science Press, Berlin and Beijing, 1981.
[7] S. Joe, S.A.R. Disney, Intermediate rank lattice rules for multidimensional integration, SIAM J. Numer. Anal. 30 (1993) 569–582.
[8] S. Joe, I.H. Sloan, Imbedded lattice rules for multidimensional integration, SIAM J. Numer. Anal. 29 (1992) 1119–1135.
[9] G. Kedem, S.K. Zaremba, A table of good lattice points in three dimensions, Numer. Math. 23 (1974) 175–180.
[10] T.N. Langtry, Algebraic and Diophantine methods in the investigation of lattice quadrature rules, Ph.D. Thesis, University of New South Wales, Kensington NSW, Australia, 1995. Available from the Internet: ⟨URL:http://www.maths.uts.edu.au/staff/tim/tim.html⟩.
[11] T.N. Langtry, An application of Diophantine approximation to the construction of rank 1 lattice quadrature rules, Math. Comput. 65 (1996) 1635–1662.

[12] T.N. Langtry, A generalisation of ratios of Fibonacci numbers with application to numerical quadrature, in: G.E. Bergum, A.N. Philippou, A.F. Horadam (Eds.), Fibonacci Numbers and their Applications, VII, Kluwer, Dordrecht, 1998, pp. 239–253.
[13] T.N. Langtry, Tables of best $\rho\, 2^s$ copies of rank 1 rules, [online], School of Mathematical Sciences, University of Technology, Sydney, 1999. Available from the Internet: ⟨URL:http://www.maths.uts.edu.au/staff/tim/rhosearch.html⟩.
[14] J.N. Lyness, S. Joe, Triangular canonical forms for lattice rules of prime power order, Math. Comput. 65 (1996) 165–178.
[15] J.N. Lyness, T.O. Sørevik, A search program for finding optimal integration lattices, Computing 47 (1991) 103–120.
[16] J.N. Lyness, T.O. Sørevik, An algorithm for finding optimal integration lattices of composite order, BIT 32 (1992) 665–675.
[17] J.N.Lyness, T.O. Sørevik, Lattice rules by component scaling, Math. Comput. 61 (1993) 799–820.
[18] D. Maisonneuve, Recherche et utilisation des 'Bon Treillis'. Programmation et résultats numériques, in: S.K. Zaremba (Eds.), Applications of Number Theory to Numerical Analysis, Academic Press, New York, 1972, pp. 121–201.
[19] H. Niederreiter, Random Number Generation and Quasi-Monte Carlo Methods, SIAM (Society for Industrial and Applied Mathematics), Philadelphia, 1992.
[20] A.J. Pettofrezzo, D.R. Byrkit, Elements of Number Theory, Prentice-Hall, Englewood Cliffs, NJ 1970.
[21] M.V. Reddy, S. Joe, The ultratriangular form for prime-power lattice rules, J. Comput. Appl. Math. 104 (1999) 49–61.
[22] A.I. Saltykov, Tables for computing multiple integrals by the method of optimal coefficients, USSR Comput. Math. Math. Phys. 3 (1963) 235–242.
[23] I.H. Sloan, S. Joe, Lattice Methods for Multiple Integration, Oxford University Press, Oxford 1994.
[24] I.H. Sloan, J.N. Lyness, The representation of lattice quadrature rules as multiple sums, Math. Comput. 52 (1989) 81–94.
[25] I.H. Sloan, L. Walsh, Computer search of rank 2 lattice rules for multidimensional quadrature, Math. Comput. 54 (1990) 281–302.
[26] R.T. Worley, On integration lattices, BIT 31 (1991) 529–539.
[27] S.K. Zaremba, Good lattice points, discrepancy and numerical integration, Ann. Mat. Pura Appl. 73 (1966) 293–317.
[28] S.K. Zaremba, La methóde des "bons treillis" pour le calcul des intégrales multiples, in: S.K. Zaremba (Ed.), Applications of Number Theory to Numerical Analysis, Academic Press, New York, 1972, 31–119.
[29] P. Zinterhof, Gratis lattice points for numerical integration, Computing 38 (1987) 347–353.